Physical symmetry and lattice symmetry in the lattice Boltzmann method

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The lattice Boltzmann method (LBM) is regarded as a specific finite difference discretization for the kinetic equation of the discrete velocity distribution function. We argue that for finite sets of discrete velocity models, such as LBM, the physical symmetry is necessary for obtaining the correct macroscopic Navier-Stokes equations. In contrast, the lattice symmetry and the Lagrangian nature of the scheme, which is often used in the lattice gas automaton method and the existing lattice Boltzmann methods and directly associated with the property of particle dynamics, is not necessary for recovering the correct macroscopic dynamics. By relaxing the lattice symmetry constraint and introducing other numerical discretization, one can also obtain correct hydrodynamics. In addition, numerical simulations for applications, such as nonuniform meshes and thermohydrodynamics can be easily carried out and numerical stability can be ensured by the Courant-Friedricks-Lewey condition and using the semi-implicit collision scheme. [S1063-651X(97)50501-0]

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In recent years, the lattice Boltzmann method (LBM) has attracted attention as an alternative numerical scheme for simulation of fluid flows [1]. Unlike traditional numerical methods which solve for macroscopic variables, LBM is based on the mesoscopic kinetic equation for the particle distribution function. The macroscopic quantities, such as density and velocity, are then obtained through moment integrations of the distribution function. The kinetic nature of LBM introduces a number of advantages, such as linearity of the convection operator (the nonlinear macroscopic term is obtained through a multiscale expansion, avoiding solving the nonlinear Riemann problem) and the recovery of the Navier-Stokes (NS) equations in the nearly incompressible limit, thus avoiding solving difficult Poisson equations for the pressure. In addition, since LBM seeks the minimum set of velocities in phase space, only one or two speeds and a few moving directions are used in LBM, and the numerical solution of the kinetic equation is very simple.

The lattice Boltzmann method starts from the following Boltzmann equation for the discrete velocity distribution in two and three dimensions [2]:

$$\frac{\partial f_i}{\partial t}+\mathbf{e}_i\cdot\nabla f_i=\Omega_i \quad (i=1,2,\ldots,N), \tag{1}$$

where f_i is the particle velocity distribution function, $\mathbf{e}_i$ is the velocity along the ith direction, N is the number of different velocities in the model, and Ω_i is the collision operator. It should be pointed out that in the phase space, the space variable $\mathbf{x}$ and the velocity variable $\mathbf{e}_i$ are independent. While only a small set of discrete velocities are used in LBM to approximate the Boltzmann kinetics of the continuum velocity, the Boltzmann equation is valid for continuum variables x and t.

For the single time relaxation approximation or the lattice BGK [3], $\Omega_i=-(1/\varepsilon\tau)(f_i-f_i^{\mathrm{eq}})$, where f_i^{eq} is the local equilibrium distribution, τ is the relaxation time, and ε is a small parameter, proportional to the Knudsen number [4]. Density and momentum are defined as velocity moments of the distribution function, f_i, $\rho=\Sigma_i f_i$, and $\rho\mathbf{u}=\Sigma_i f_i\mathbf{e}_i$. For thermal problems, an internal energy E can be defined as $\frac{1}{2}\Sigma_i f_i\mathbf{e}_i^2=\rho E+(\rho/2)|\mathbf{u}|^2$. The equilibrium distribution function f_i^{eq} depends on density, momentum, energy, and the specific lattice used. Its functional form can be tuned so that the appropriate macroscopic equations are obtained. The macroscopic equations are derived from Eq. (1) by means of a multiscale Chapman-Enskog expansion [4].

A commonly used lattice Boltzmann method, the so-called lattice BGK model [3], is a specific discretization of Eq. (1). If we replace the time derivative by a first order time difference, use a first order upwind space discretization for the convective term $\mathbf{e}_i\cdot\nabla f_i$, and use a downwind collision term $\Omega(\mathbf{x}-\mathbf{e}_i,t)$ for $\Omega(\mathbf{x},t)$, we have a finite difference equation for f_i:

$$f_i(\mathbf{x},t+\Delta t)=f_i(\mathbf{x},t)-\alpha[f_i(\mathbf{x},t)-f_i(\mathbf{x}-\mathbf{e}_i\Delta x,t)] -\frac{\beta}{\tau}[f_i(\mathbf{x}-\mathbf{e}_i\Delta x,t)-f_i^{\mathrm{eq}}(\mathbf{x}-\mathbf{e}_i\Delta x,t)], \tag{2}$$

where $\alpha=\Delta t/\Delta x$, $\beta=\Delta t/\varepsilon$, and Δt and Δx are the time step and the grid step, respectively. Choosing $\Delta t=\Delta x=\Delta y=\varepsilon$ we then obtain the following standard LBM equation [3]:

$$f_i(\mathbf{x}+\mathbf{e}_i,t+1)-f_i(\mathbf{x},t)=-\frac{f_i(\mathbf{x},t)-f_i^{\mathrm{eq}}(\mathbf{x},t)}{\tau}. \tag{3}$$

The above discretization to Eq. (1) only has first order convergence in space and time. However, it has been shown [4] that since Eq. (3) has a Lagrangian nature in space discretization, the discretization error has a special form which can be included in viscous terms, resulting in second order accuracy both in space and time. For the seven-speed hexagonal LBM model [3], the kinematic viscosity for Eq. (2)

can be obtained analytically: $\nu=|\mathbf{e}|^2\varepsilon\tau/4-|\mathbf{e}|^2\Delta t/8$. For Eq. (3), we have $\nu=\tau/4-1/8$. The first part in ν is the physical viscosity and the negative part of the viscosity is the consequence of taking account of discretization error and replacing Ω by the downwind operator [5].

It should be pointed out, however, that this particular discretization and the condition $\Delta t=\Delta x$ are not necessary. Actually, any standard finite difference (FD) scheme [4,6–8] will serve the purpose of solving Eq. (1) as well. The use of Eq. (3) reflects the historical fact that LBM came about as a refinement, or a by-product of the lattice gas automaton method (LGA) [9]. In the latter, ''Boolean'' particles reside in a discrete lattice, subject to the automaton dynamics of streaming and collision. One of the main ideas driving the initial LGA efforts was to produce the *simplest* microdynamics that would yield hydrodynamics behavior. Recovering rotational invariant macroscopic equations from a discrete finite velocity microscopic dynamics imposes constraints on the symmetry of the lattice used, unlike the continuum Boltzmann equation with infinite velocities, for which rotational invariance is automatically recovered. For LBM this is obtained from physical symmetry and lattice symmetry. By the physical symmetry we mean the symmetry attached to the velocity space and the equilibrium distribution for velocities, including the combination of specific weights in equilibrium distribution functions for different speeds, the choice of parameters in the equilibrium distribution function, and a sufficient number of moving velocity directions N. The lattice symmetry requirements are that the number of lattice directions (in **x** space) and the number of lattice links are the same as those for the particle distribution functions [10]. One of the fundamental differences between LGA and LBM is that while in LGA individual particles are followed, in LBM the ''molecular chaos'' assumption is used, leading to the loss of particle-particle correlations. At this point it is important to distinguish between the symmetry needed to recover the correct macroscopic equations (*physical symmetry*), and the symmetry that is required from the lattice (*lattice symmetry*). Because of the ''streaming'' step (particle or distribution functions hopping between neighboring cells) the two symmetries go together. While the streaming of particles is an essential part of LGA dynamics, it is not crucial for LBM. Any discretization of Eq. (1), such as FD or finite element method will suffice to get the Navier-Stokes equations. In this way, what we termed the *physical* symmetry can be separated from the lattice symmetry.

Once this is recognized, a variety of options become available for the method. For example, introducing nonuniform meshes (or any non-Cartesian coordinates, such as cylindrical or spherical) would be as easy as in other conventional schemes, such as FD. All existing LBM models could be extended to this approach. This could be accomplished with the present approach by simply discretizing the gradient operator in the convection term in the appropriate coordinates. One possible way to release the constraint of the lattice symmetry is to use the finite difference scheme for the lattice Boltzmann equation (FDLBE). For example, the central difference scheme for smooth solutions can be utilized to calculate the spatial gradient in Eq. (1), $\partial f_i/\partial x=D_x f_i=[f_i(x+\Delta x,y)-f_i(x-\Delta x,y)]/(2\Delta x)$, $\partial f_i/\partial y=D_y f_i=[f_i(x,y+\Delta y)-f_i(x,y-\Delta y)]/(2\Delta y)$.

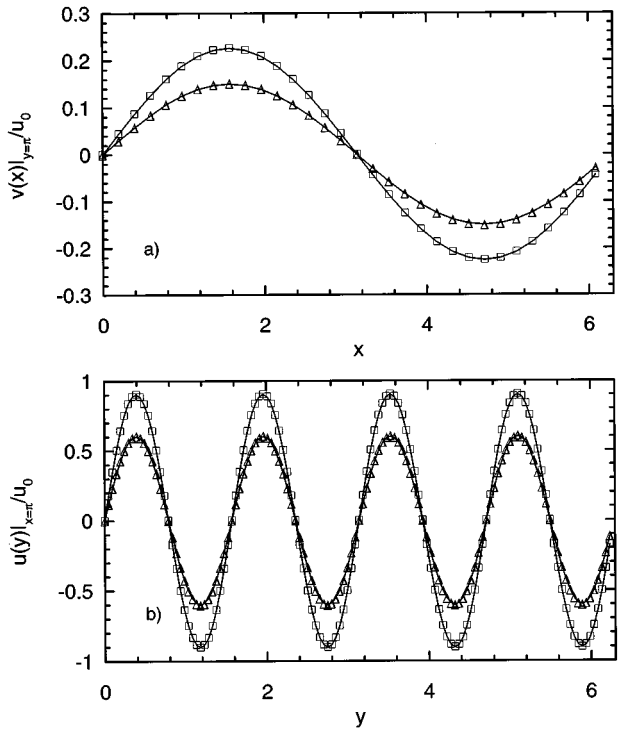

FIG. 1. Simulation of 2D Taylor vortex with FDLBE at $t=10$ (□) and 50 (△). The analytical solution (solid lines) for the velocity is $u(x,y,t)=-u_0\exp[-\nu t(k_1^2+k_2^2)]\cos(k_1x)\sin(k_2y)$ and $v(x,y,t)=u_0(k_1/k_2)\exp[-\nu t(k_1^2+k_2^2)]\sin(k_1x)\cos(k_2y)$, where $u_0=0.01$, and $k_1=1$ and $k_2=4$ are the wave numbers in the x and y directions, respectively. (a) $v(x)|_{y=\pi}/u_0$ vs x; (b) $u(y)|_{x=\pi}$ vs y. The relaxation time $\varepsilon\tau$ is 0.0018.

The temporal discretization is obtained using second order Runge-Kutta (modified Euler) method. The time evolution of particle distribution functions is then derived by $f_i^{[n+(1/2)]}=f_i^{(n)}-\Delta t/2R_i^{(n)}$ and $f_i^{(n+1)}=f_i^{(n)}-\Delta tR_i^{[n+(1/2)]}$, where $R_i=-(e_{ix}D_x+e_{iy}D_y)f_i-(f_i-f_i^{\mathrm{eq}})/\varepsilon\tau$. Thus, combination of these specific space and time discretizations results in a second order in both time and space. Only the physical viscosity will survive in this approach.

As the first example, we apply the FDLBE scheme to simulate the evolution of the two-dimensional Taylor vortex flow in a square periodic domain using a nonuniform mesh. Eight moving velocities and one rest velocity ($N=9$) are used [3,11], but the diagonal spatial links are not needed. For this system, the kinematic viscosity, ν, is $\varepsilon\tau/3$. 32×128 grid points are used, i.e., $\Delta x=4\Delta y$. Numerical and analytical solutions for this decaying flow are presented in Fig. 1, showing excellent agreement.

To demonstrate the flexibility of LBE with the lattice symmetry released, we present an example of a LBE application in cylindrical coordinates. Consider the fluid flow between two coaxial cylinders. The fluid is at rest initially. The outer cylinder suddenly starts to rotate with a constant velocity V, while the inner cylinder is kept still all the time. For this classic problem, an analytical solution can be derived based on the Fourier-Bessel expansion [12]. It is convenient to describe this problem in cylindrical coordinates, in which the only nonzero angular component of velocity v_θ depends on the radial coordinate r. Here, the origin of the

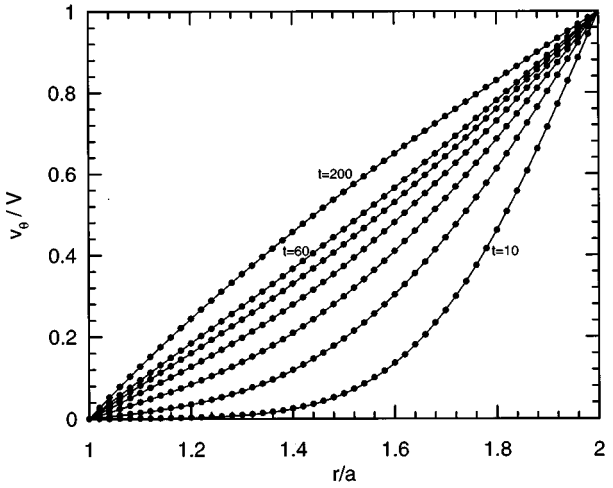

FIG. 2. Normalized numerical velocity profiles (solid lines) as functions of r for $t=10$, 20, 30, 40, 50, 60, and 200, compared with those of analytical solution (dots). The radius ratio $b/a=2$. The relaxation time $\varepsilon\tau$ equals 0.001. 53×1000 grid points in radial and angular directions have been used in the numerical simulation.

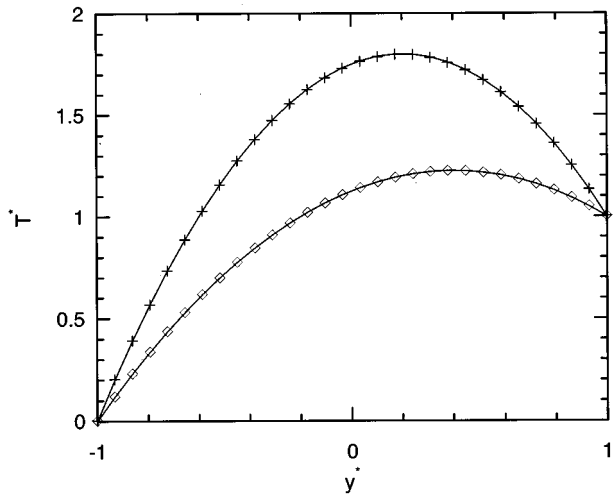

FIG. 3. Normalized temperature $T^\star=(T-T_0)/(T_1-T_0)$ for Couette flow with heat transfer for Brinkman numbers $B_r=5$ ($\diamond$) and $B_r=10$ ($+$). Solid line is the analytical solution as given in the text. The top wall moves with speed $u_0=0.1$, and the bottom wall is at rest.

coordinate $r=0$ coincides with the center of the geometry. $r=a$ and $r=b$ correspond to the inner and outer cylinder, respectively. The time-dependent velocity, $v_\theta(r,t)$, can be written as $v_\theta(r,t)=A(r/a-a/r)+A\Sigma_{n=1}^{\infty}A_nZ_n(r/a)\exp(-\nu\lambda_n^2t)$, where $A=abV/(b^2-a^2)$ is a constant, $Z_n(r/a)=J_1(\lambda_nr/a)-[J_1(\lambda_n)/Y_1(\lambda_n)]Y_1(\lambda_nr/a)$ are eigenfunctions, and eigenvalues λ_n with $n=1,2,\ldots$ are roots of equation $J_1(\lambda_nb/a)-J_1(\lambda_n)/Y_1(\lambda_n)Y_1(\lambda_nb/a)=0$. A_n's are constant coefficients determined by $A_n=\int_a^b r(r/a-a/r)Z_n(r/a)dr/\int_a^b r[Z_n(r/a)]^2dr$.

LBE simulation is performed in the domain $a\leqslant r\leqslant b$, and $0\leqslant\theta\leqslant2\pi$. The numerical grid is defined on the cylindrical coordinates (r_m,θ_n), where $r_m=a+(m-1)(b-a)/(M-1)$ and $\theta_n=2\pi(n-1)/N$, with M and N being numbers of grid points in radial and angular directions, respectively. The particle distribution function $f_i(r_m,\theta_n)$ is defined along nine directions $\mathbf{e}_i$ as those of regular square lattice in Cartesian space in the velocity space, but on *cylindrical grid points* in physical coordinate space. The collision operator can be easily processed using velocity components v_x, v_y in the Cartesian coordinates as intermediate quantities. The cylindrical velocity components v_r and v_θ can be obtained by projecting v_x and v_y onto radial and angular unit vectors $\mathbf{e}_r$ and $\mathbf{e}_\theta$. Nevertheless, the convection term is now calculated in cylindrical coordinates, i.e., $\mathbf{e}_i\cdot\nabla f_i=\mathbf{e}_i\cdot\mathbf{e}_r\partial f_i/\partial r+\mathbf{e}_i\cdot\mathbf{e}_\theta\partial f_i/r\partial\theta$. Again, using the central difference scheme for the spatial discretization and the second order Runge-Kutta scheme for time advance results in a second order scheme in both space and time. The extrapolation method [13] has been adopted to treat the wall-boundary on the cylinders to achieve second order accuracy for the boundary conditions. In the angular direction, the periodic boundary condition is naturally applied. In Fig. 2 we present the angular velocity as a function of r at different time steps, compared with those from the analytical solution. The agreement is excellent. It should be mentioned that the unidirectional feature of the rotating cylinder problem is not preassumed in our numerical method. Therefore, the LBE in cylindrical coordinates presented here is applicable to more general problems.

The standard lattice Boltzmann discretization in Eq. (3) often encounters numerical instability for high Reynolds number flows [4] and for thermal problems. In general, numerical stability requires that the time step and spatial step satisfy the Courant-Friedricks-Lewey (CFL) condition [14,4]: $|\mathbf{e}_i|\Delta t/\Delta x\leqslant1$. The standard LBE assumes $\Delta t=\Delta x$, leading to $|\mathbf{e}_i|\leqslant1$. For the seven-velocity hexagonal model, this condition is marginally satisfied. That is the reason why the scheme is often unstable when viscosity gets small ($\tau\rightarrow1/2$). For the 13-velocity thermal model [15], the standard LBM does not satisfy this CFL condition for the velocity distribution function with speed 2. For this system, only a very narrow temperature range can be simulated. With FDLBE, the stability can be ensured by relaxing the Lagrangian particle convection and by adjusting $\Delta t(\leqslant\Delta x/|\mathbf{e}_i|)$. To demonstrate this idea, we simulate the thermal conduction in a channel with the top wall moving at a constant speed U_0 [15]. The analytical solution for the temperature distribution can be written as $T^\star=(T-T_0)/(T_1-T_0)=\frac{1}{2}(1+y^\star)+(B_r/8)(1-y^{\star2})$, where $y^\star=y/L$, B_r is the Brinkman number, $U_0^2/(T_1-T_0)^2$, L is the channel width, and T_0 and T_1 are temperatures at the top and the bottom wall, respectively. The FDLBE method has been used to discretize the 13-velocity thermal model equation as proposed in Ref. [15]. The agreement between theory and simulation shown in Fig. 3. We emphasize that the results are obtained on a *rectangular* mesh using the 13-velocity model (three speeds). In addition, since the CFL condition is satisfied ($\alpha=0.2$), we did not encounter any numerical stability problem here, as often occurred in previous numerical simulations [15]. In fact, using the FDLBE the range of the particle speed can be extended, which helps in simulating problems with a broad range of temperature.

The use of semi-implicit schemes may be another solution

for improving numerical stability without much additional computational work. Actually Eq. (2) can be solved by the following scheme: $f_i(\mathbf{x},t+\Delta t)=f_i(\mathbf{x},t)-\alpha[f_i(\mathbf{x},t)-f_i(\mathbf{x}-\mathbf{e}_i\Delta x,t)]-\beta/\tau[f_i(\mathbf{x},t+\Delta t)-f_i^{\mathrm{eq}}(\mathbf{x},t+\Delta t)]$. In this equation, the unknown density and momentum in $f_i^{\mathrm{eq}}(\mathbf{x},t+\Delta t)$ can easily be obtained through moment equations, preventing one from solving a tridiagonal matrix. The implicit method will allow a larger time step ($\Delta t \gg \varepsilon\tau$) in the integration of Eq. (2) for simulating flows at high Reynolds numbers, where $\varepsilon\tau$ is small.

We point out that for interface problems, such as shock waves and two-phase flows, an upwind finite difference for Eq. (1) might have some advantages. This is so because an upwind scheme is more capable of capturing steep gradients than the second order central-difference discretization. This is also one of reasons why the LBM is a good scheme for two-phase fluid flows. Accordingly, a possible extension is to combine a second-order upwind method with a slope limiter [16] that will make the discretization become first order where the gradient is greater than a certain threshold, thus allowing for a better capture of the interface. We are presently exploring this possibility.

Other similar kinetic approaches to the NS equations exist. For example, the gas-kinetic finite volume method [17] is a kinetic method that uses a relaxation operator as an approximation to the collision term in the Boltzmann equation. The scheme, however, also makes use of an infinite velocity space, unlike LBM and FDLBE, which are characterized by using only a small set of velocities. The kinetic-type relaxation method for solving the hyperbolic conservation system has been proposed by Jin and Xin [16]. This approach uses the relaxation approach to model the nonlinear terms, and thus, it is free of nonlinear Riemann solvers. Both of these models were developed mainly for shock capture in Euler systems, whereas the lattice Boltzmann method is more focused on viscous complex flows in the nearly incompressible limit [1,11].

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[1] *Lattice Gas Methods for PDE: Theory, Applications and Hardware*, Physica D Vol. **47**, edited by G. D. Doolan (Elsevier Science, Amsterdam, 1991).
[2] The Broadwell model, J. E. Broadwell, Phys. Fluids **7**, 1013 (1964), can be regarded as a one-dimensional lattice Boltzmann model.
[3] S. Chen, H. Chen, D. O. Martínez, and W. H. Matthaeus, Phys. Rev. Lett. **67**, 3776 (1991); H. Chen, S. Chen, and W. H. Matthaeus, Phys. Rev. A **45**, 5339 (1992); Y. H. Qian, D. d'Humieres, and P. Lallemand, Europhys. Lett. **17**, 479 (1992).
[4] J. D. Sterling and S. Chen, J. Comput. Phys. **123**, 196 (1996).
[5] The effect of the downwind collision on viscosity has been overlooked in previous studies [1,3,4].
[6] F. Nannelli and S. Succi, J. Stat. Phys. **68**, 3 (1992).
[7] M. B. Reider and J. D. Sterling, Comput. Fluids **24**, 459 (1995).
[8] G. R. McNamara, A. L. Garcia, and B. J. Alder, J. Stat. Phys. **81**, 395 (1995).
[9] U. Frisch, B. Hasslacher, and Y. Pomeau, Phys. Rev. Lett. **56**, 1505 (1986).
[10] J. M. V. A. Koelman, Europhys. Lett. **15**, 603 (1991).
[11] D. O. Martínez, W. H. Matthaeus, S. Chen, and D. C. Montegomery, Phys. Fluids **6**, 1285 (1994).
[12] G. K. Batchlor, *An Introduction to Fluid Dynamics* (Cambridge University Press, Cambridge, 1992).
[13] S. Chen, D. Martinez, and R. Mei, Phys. Fluids **8**, 2527 (1996).
[14] R. Peyret and T. D. Taylor, *Computational Methods for Fluid Flow* (Springer-Verlag, Berlin, 1983).
[15] F.J. Alexander, S. Chen, and J.D. Sterling, Phys. Rev. E **47**, R2249 (1993).
[16] S. Jin and Z. P. Xin, Commun. Pure Appl. Math. **48**, 235 (1995); R. E. Caflisch, S. Jin, and G. Russo, SIAM J. Num. Anal. (to be published).
[17] K. Xu, L. Martinelli, and A. Jameson, J. Comput. Phys. **120**, 48 (1995).