Discrete effects on boundary conditions for the lattice Boltzmann equation in simulating microscale gas flows

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The lattice Boltzmann equation (LBE) has shown its promise in the simulation of microscale gas flows. One of the critical issues with this advanced method is to specify suitable slip boundary conditions to ensure simulation accuracy. In this paper we study two widely used kinetic boundary conditions in the LBE: the combination of the bounce-back and specular-reflection scheme and the discrete Maxwell's scheme. We show that (i) both schemes are virtually equivalent in principle, and (ii) there exist discrete effects in both schemes. A strategy is then proposed to adjust the parameters in the two kinetic boundary conditions such that an accurate slip boundary condition can be implemented. The numerical results demonstrate that the corrected boundary conditions are robust and reliable.

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With the rapid development in microelectromechanical systems (MEMS), gas flows associated with microdevices have received particular attention over the last decade [1,2]. One of the most important features of microscale gas flows is that gases usually possess a relatively large Knudsen number, $\mathrm{Kn}=\lambda/H$, where λ represents the mean-free path of the gas and H is the smallest characteristic length of the device. As Kn is above a critical value, the continuum assumption will break down and the classical Navier-Stokes equations cannot directly be applied to this type of high-Knudsen number flows. In contrast, since the Boltzmann equation was derived without invoking the continuum assumption, it can be used to model rarefied gas flows ranging from the continuum regime ($\mathrm{Kn}<0.001$) to free molecular regime ($\mathrm{Kn}>10$) [3]. Therefore, the Boltzmann equation is a good starting point for developing reasonable numerical methods for microscale gas flows. Accordingly, a variety of Boltzmann-equation-based methods, such as the finite-difference method [4], the discrete-velocity method [6], the gas-kinetic scheme [5], and the lattice Boltzmann equation (LBE) method [7], have been proposed for simulating microscale gas flows from different viewpoints.

The LBE, which is a discrete approximation to the continuous Boltzmann equation, has recently been recognized as one of the most promising approaches for simulation of microscale flows [8–21]. It should be recognized, however, that most previous LBE models virtually correspond to the Navier-Stokes equations in the macroscopic scale. When these models are applied to near-continuum flows ($\mathrm{Kn}<0.1$), in which the bulk flow remains continuous, suitable slip boundary conditions must be specified to capture possible boundary effects on the flow behavior. Therefore, the development of slip-boundary conditions is a critical issue for the simulation of near-continuum gas flows with the LBE method.

Two basis types of kinetic boundary condition have been proposed for LBE in simulation of microscale gas flow: one is the discrete Maxwellian boundary condition (DMBC) [22], which is a straightforward discretization of Maxwell's diffuse-reflection boundary condition in kinetic theory; the other is the combination boundary condition (CBC) [23], which combines the no-slip bounce-back and the free-slip specular-reflection schemes. Some improved version of the two basic boundary conditions were also proposed recently. For instance, Tang *et al.* generalized the original fully diffusive DMBC by introducing a numerical accommodation coefficient to adjust the degree of slip [13], while Sofonea and Sekerka proposed several versions of the DMBC for some finite-difference LBE models [14]. The CBC scheme was also generalized and analyzed by Sbragaglia and Succi [17] recently, and was extended to a straight wall located at arbitrary location between lattice nodes by Szalmás [24].

Recently, it was shown that the CBC and DMBC schemes both correspond to a second-order slip-boundary condition [17,25]. However, the relationship between the DMBC and CBC is still unknown. There is also another important question about the DMBC and CBC: It is understood that there exist so-called discrete effects in the LBE, which must be minimized to capture correct fluid dynamics behavior. For example, the relaxation time in the LBE must be modified to account for the numerical viscosity [26], and the forcing term must include a factor dependent on the relaxation time [27]. Therefore, it is natural to ask whether such discrete effects also exist in the DMBC and CBC, and if any, how the effects can be minimized. The objective of this work is twofold: to identify the inherent relationship between the DMBC and CBC; and to examine whether there exist discrete effects in these two types of kinetic boundary condition.

We start our analysis with the extension of LBE from continuum flows to near-continuum flow. Without loss of generality, we consider the isothermal D2Q9 BGK-LBE (two-dimensional nine-velocity) model [26],

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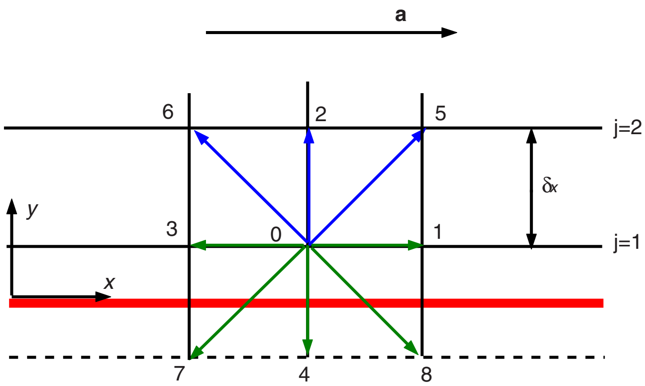

FIG. 1. (Color online) Lattice and boundary arrangement in the D2Q9 model. The solid wall is placed at $j=1/2$. The discrete velocities of D2Q9 are $\boldsymbol{c}_0=(0,0)$, $\boldsymbol{c}_1=-\boldsymbol{c}_3=c(1,0)$, $\boldsymbol{c}_2=-\boldsymbol{c}_4=c(0,1)$, $\boldsymbol{c}_5=-\boldsymbol{c}_7=c(1,1)$, and $\boldsymbol{c}_6=-\boldsymbol{c}_8=c(-1,1)$.

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta_t,t+\delta_t)-f_i(\boldsymbol{x},t)=-\frac{1}{\tau}[f_i-f_i^{(eq)}]+\delta_t\boldsymbol{F}_i, \quad (1)$$

where $\{f_i(\boldsymbol{x},t):i=0,1,\ldots,8\}$ are the discrete distribution function associated with the gas molecules moving with the discrete velocities $\{\boldsymbol{c}_i:i=0,1,\ldots,8\}$ at position $\boldsymbol{x}\in\mathcal{L}$ and time t [$\mathcal{L}$ being a regular square lattice with spacing δ_x (see Fig. 1)]; δ_t is the evolution time increment, $\boldsymbol{F}_i=w_i(1-\frac{1}{2\tau})[\frac{\boldsymbol{c}_i-\boldsymbol{u}}{c_s^2}+\frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})\boldsymbol{c}_i}{c_s^4}]\cdot\boldsymbol{a}$ is a forcing term accounting for the body force $\boldsymbol{a}$ [27]; $f_i^{(eq)}=w_i\rho[1+\frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2}+\frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4}-\frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}]$ is the discrete equilibrium distribution function that depends on the density $\rho=\Sigma_i f_i$ and velocity $\rho\boldsymbol{u}=\Sigma_i\boldsymbol{c}_i f_i+0.5\delta_t\boldsymbol{a}$. Here, w_i's are given by $w_0=4/9$, $w_1=w_2=w_3=w_4=1/9$, and $w_5=w_6=w_7=w_8=1/36$; the parameter c_s relates to the lattice speed $c=\delta_x/\delta_t$ and the temperature T as $c_s^2=RT=c^2/3$, with R the gas constant.

The discrete velocity set and the discrete equilibrium distribution functions given above can ensure that the D2Q9 is accurate for solving the Navier-Stokes equations. However, this LBE model cannot be directly applied to flows beyond the slip region. Even for near-continuum flows, the LBE should also be modified to account for the rarefaction effects. First, it is noted that in simulation of continuum flows, the relaxation time is determined by the Reynolds number. In contrast, in microscale gas flows the characteristic dimensionless number is the Knudsen number Kn. Therefore, the relation between the relaxation time in the LBE and the Knudsen number must be given appropriately first.

The relaxation time τ in the BGK LBE model can be related to the mean-free path λ of the gas as [28] $(\tau-0.5)\delta_t=\lambda/c^*$, where c^* is a certain microscopic velocity to be determined. The choice of c^* is rather diverse in the literature. The most widely used choice is the lattice speed c [9,11,13–17,25], and the mean molecular velocity $(8RT/\pi)^{1/2}$ is also used by some researchers [13,18]. Whenever c^* is used, it must satisfy the "consistent requirement" [28]: in the continuum limit, the relation $(\tau-0.5)\delta_t=\mu/p$ must be fulfilled, where μ and p are the viscosity and pressure of the gas, respectively. Guo *et al.* have shown that in order to match such a requirement one must choose $c^*=(\pi RT/2)^{1/2}$ [28]. With this choice, we can obtain the relationship between τ and Kn as

$$\tau=0.5+\sqrt{\frac{2\chi}{\pi}}\frac{\mathrm{Kn}}{\Delta}, \quad (2)$$

where Δ is the ratio of the lattice spacing to the characteristic length $\Delta=\delta_x/H$, χ is a model-dependent constant defined as $c=\sqrt{\chi RT}$ ($\chi=3$ for D2Q9).

The second important issue in the extension of LBE to near-continuum flows is how to specify kinetic boundary conditions. In the DMBC, a numerical accommodation coefficient σ can be introduced to control the degree of slip [13]. The accommodation coefficient is similar to that used in gas kinetic theory, and in most of the existing applications it indeed takes the physical values used for the Boltzmann equation. However, as will be shown later, such a choice is questionable due to discrete effects. Unlike the DMBC, the CBC slip-boundary condition is realized by adjusting the fraction of the bounce-back part.

We now examine the CBC and DMBC. To simplify the analysis, we consider a unidirectional gas flowing over a flat surface (Fig. 1) in which ρ is a constant, $v=0$, and $\partial_x\phi=0$ for any variable ϕ. After collision at time t, the unknown distribution functions, f_2, f_5, and f_6, can be determined from the boundary conditions: $f_2=f_4^*+2r\rho w_2\boldsymbol{c}_2\cdot\boldsymbol{u}_w/c_s^2$, $f_5=rf_7^*+(1-r)f_8^*+2r\rho w_5\boldsymbol{c}_5\cdot\boldsymbol{u}_w/c_s^2$, and $f_6=rf_8^*+(1-r)f_7^*+2r\rho w_6\boldsymbol{c}_6\cdot\boldsymbol{u}_w/c_s^2$ for CBC (r being the bounce-back fraction); and $f_2=\sigma f_2^{(eq)}(\boldsymbol{u}_w)+(1-\sigma)f_4^*$, $f_5=\sigma f_5^{(eq)}(\boldsymbol{u}_w)+(1-\sigma)f_8^*$, and $f_6=\sigma f_6^{(eq)}(\boldsymbol{u}_w)+(1-\sigma)f_7^*$ for DMBC (σ being the accommodation coefficient). Here $\boldsymbol{u}_w$ is the wall velocity, $f_i^*=f_i+\frac{1}{\tau}[f_i-f_i^{(eq)}]+\delta_t F_i$ is the postcollision distribution function. With these conditions, we can obtain that

$$u_2=\frac{1-2\tau+2r(\tau-2)}{1-2\tau+2r(\tau-1)}u_1+\frac{6(2\tau-1)+r(8\tau^2-20\tau+11)}{(2\tau-1)[1-2\tau+2r(\tau-1)]}\delta_t a \quad (3)$$

for the CBC, and

$$u_2=\frac{1-2\tau+\sigma(\tau-2)}{1-2\tau+\sigma(\tau-1)}u_1+\frac{6(2\tau-1)+\sigma(4\tau^2-10\tau+11/2)}{(2\tau-1)[1-2\tau+\sigma(\tau-1)]}\delta_t\boldsymbol{a} \quad (4)$$

for the DMBC. It is interesting to note that if we set $r=\sigma/2$, Eqs. (3) and (4) become identical, meaning that under this condition, the CBC and DMBC are *equivalent*.

From the LBE (1), we can obtain that the streamwise velocity u satisfies $\nu(u_{j+1}-2u_j+u_{j-1})=-a\delta_x^2$, where $\nu=c_s^2(\tau-0.5)\delta_t$. It is clear this is nothing but a central finite-difference discretization of the Navier-Stokes equation $\nu\partial_y u+a=0$. Again, this demonstrates that the D2Q9 LBE is only a solver for the Navier-Stokes equations. For Poiseuille flow, the finite-difference equation gives that

$u_j=4u_0y_j'(1-y_j')+u_s$, where $y_j'=(j-0.5)\delta_x/H$, $u_0=aH^2/8\nu$, and u_s is slip velocity at the wall. Substituting u_1 and u_2 into Eq. (3), we can obtain

$$U_s := \frac{u_s}{u_0} = \frac{2(1-r)(2\tau-1)}{r}\Delta + \frac{4(2\tau-1)^2-3}{3}\Delta^2, \quad (5)$$

which indicates that the pure bounce-back scheme ($r=1$) also generates a nonzero slip velocity proportional to Δ^2, which is consistent with the result of previous studies [8]. Based on Eq. (2), we can also rewrite Eq. (5) as

$$U_s = \frac{4(1-r)}{r}\sqrt{\frac{6}{\pi}}\mathrm{Kn} + \frac{32}{\pi}\mathrm{Kn}^2 - \Delta^2 \quad (6)$$

$$= \frac{4(2-\sigma)}{\sigma}\sqrt{\frac{6}{\pi}}\mathrm{Kn} + \frac{32}{\pi}\mathrm{Kn}^2 - \Delta^2. \quad (7)$$

Equations (6) and (7) show that the slip velocity includes three parts: a first-order slip proportional to Kn, a second-order slip proportional to Kn^2, and a numerical part depending on the number of grid numbers (recall that $\Delta=\delta_x/H$).

Equation (7) shows that for a fully diffusive boundary ($\sigma=1$), the nondimensional slip velocity is $U_s=5.528\mathrm{Kn}+10.186\mathrm{Kn}^2-\Delta^2$. On the other hand, gas kinetic theory gives that for a fully diffusive boundary the slip velocity is [3] $U_s=4.586\mathrm{Kn}+7.804\mathrm{Kn}^2$. This means that contrary to the intuition implied in previous studies [13,14,22], the DMBC, which is a straightforward discretization of the continuous Maxwell's boundary condition, does not lead to the same result as that of the continuous one even with the same accommodation coefficient. Such a difference is due to the discrete effects: the additional Δ^2 term comes from the finite size of the lattice, and the inconsistencies in the terms proportional to Kn and Kn^2 originate from the discretization of the molecular velocity space. It can be speculated that such effects can be reduced by refining the lattice and increasing the symmetry of the discrete velocity set. It is also noted that even as $\Delta\to 0$, the slip velocity predicted by the LBE with the discrete boundary conditions is over 20% for all $\mathrm{Kn}>0$ in comparison with that of the kinetic theory due to the discrete effects.

Let us now focus on how to correct the discrete effects to implement an exact slip-boundary condition in LBE. A usually adopted boundary condition for near-continuum flows is the second-order slip boundary condition, $u_s=A_1\lambda\left(\frac{\partial u}{\partial \boldsymbol{n}}\right)_{wall}-A_2\lambda^2\left(\frac{\partial^2 u}{\partial^2 \boldsymbol{n}}\right)_{wall}$, where $\boldsymbol{n}$ is the unit normal vector of the boundary pointing into the flow, and A_1 and A_2 are two parameters relating to the gas-wall interactions. It can be shown that for Poiseuille flow the Navier-Stokes equations with this boundary condition yield a slip velocity $U_s=4A_1\mathrm{Kn}+8A_2\mathrm{Kn}^2$. Therefore, in order to realize the above second-order boundary condition in LBE, we should choose the bounce-back fraction r in the CBC (or $\sigma/2$ in the DMBC) as

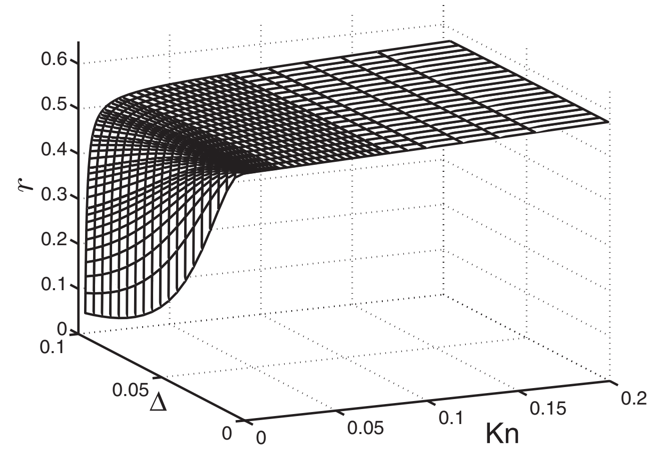

FIG. 2. Dependence of r on Kn and Δ for the fully diffuse walls.

$$r = \left\{1 + \sqrt{\frac{\pi}{6}}\left[\frac{\Delta^2}{4\mathrm{Kn}} + A_1 + \left(2A_2 - \frac{8}{\pi}\right)\mathrm{Kn}\right]\right\}^{-1}. \quad (8)$$

It is clear that r or σ depends on not only the given boundary condition, but also on the lattice size and the Knudsen number. It is also noted that the relaxation time τ influences on the correctness of the boundary conditions implicitly. Actually, with Eq. (2) we can rewrite the first term $\Delta^2/4\mathrm{Kn}$ in the square brackets of Eq. (8) as $6\mathrm{Kn}/\pi(2\tau-1)^2$. Therefore, for a given Kn, different choices of τ (depending on the lattice size used) results in different values of $\boldsymbol{r}$ or σ. In fact, the influence of τ on the boundary condition was already observed in the study of the purely bounce-back scheme (i.e., $r=1$) for the no-slip boundary condition ($A_1=A_2=0$) about ten years ago [29]. In this case, there is always a nonzero slip unless $\tau=0.5+\sqrt{3}/4\approx 0.933$. Such an unphysical slip has also been reported in the study of gaseous microscale flows [10].

Figure 2 shows the dependence of r on Kn and Δ for the fully diffusive case [$A_1=2\zeta/\sqrt{\pi}$, $A_2=(1+2\zeta^2)/\pi$, with $\zeta=1.016$]. It is seen that r changes in a wide range in order to realize the same fully diffusive boundary condition, depending on both the lattice and the Knudsen number. It is noted that for a given Δ, there exists a critical Knudsen number, Kn_c, above which the rapid change in r with Kn becomes gradual. It is also observed that $r>0.5$ for relative large values of Kn, implying that more molecules should be bounced back than specular reflected. On the other hand, $r<0.5$ for small values of Kn, i.e., more molecules are specular reflected. Such adjustments are reasonable: it is seen from Eq. (6) that $U_s(r=0.5)$ will be larger than that of the theoretical one if Kn is large enough, and therefore in order to minimize the fictitious slip, one should increase the nonslip or bounce-back portion in CBC. On the other hand, for small values of Kn $U_s(r=0.5)$ could also be smaller than the theoretical one because the term proportional to Δ^2 always has a negative contribution, and therefore the slip or specular-reflection portion should be enhanced. The above analysis also indicates that the CBC has a wider parameter range than that of the DMBC: In the case that r or $\sigma/2$ should be greater than 0.5,

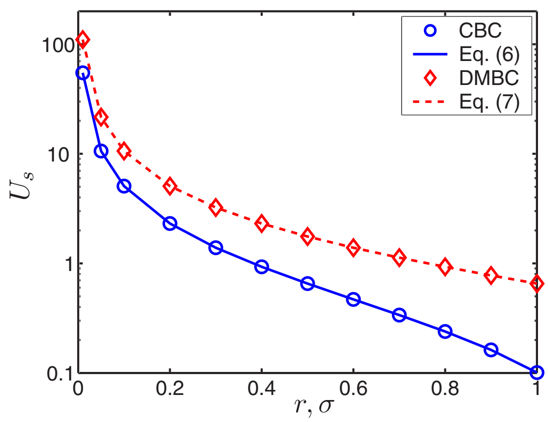

FIG. 3. (Color online) Slip velocity as functions of r and σ (Kn=0.1).

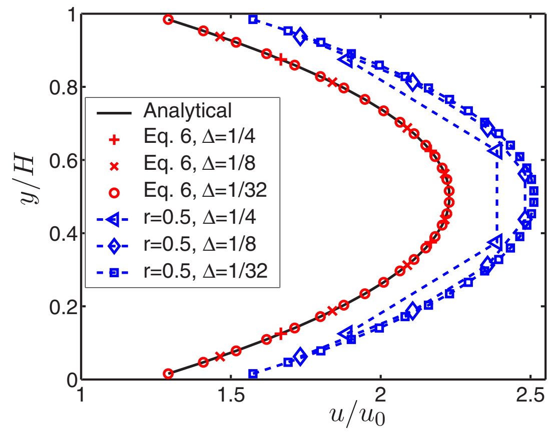

FIG. 4. (Color online) Velocity profiles with different lattice sizes for a purely diffusive wall (Kn=0.2).

the CBC is still reasonable but the DMBC is unphysical since σ should always be smaller than 1.

We now examine the above theoretical results by applying the D2Q9 LBE to the Poiseuille flow in a channel with height H. The flow is driven by a constant body force $a=10^{-5}$. First, the dependence of U_s against r (or σ) and Kn in the CBC (or DMBC). Simulations are performed on a lattice with $\Delta=1/32$, and periodic boundary conditions are applied at the inlet and outlet of the channel. The simulated slip velocities as a function of r and σ for Kn=0.1 are shown in Fig. 3. It is seen that the numerical predictions are in excellent agreement with the theoretical results given by Eqs. (6) and (7).

The discrete effects in the CBC are also examined. Simulations are carried out with Kn=0.2 and on three lattices with $\Delta=\frac{1}{4}$, $\frac{1}{8}$, and $\frac{1}{32}$, respectively. The channel walls are assumed to be fully diffusive, and the bounce-back fraction r is determined from Eq. (8) for each Δ. The simulated velocities are shown in Fig. 4. Clearly, the LBE results are in excellent agreement with the analytical solution in all cases, even with only four grid points. For comparison, the results with $r=0.5$ are also shown. Some apparent grid-dependent deviations from the exact velocity profiles are observed. These results demonstrate that it is necessary to correct r to make the realization of the boundary condition more accurate.

In summary, we have shown that like in the LBE, discrete effects also exist in the two widely used kinetic boundary conditions CBC and DMBC, which lead to significant deviations in predicting the flow behavior with the LBE from the exact solution. We have also shown that the discrete effects can be minimized by adjusting the bounce-back fraction in the CBC and the numerical accommodation coefficient in the DMBC, depending on the Knudsen number, the specified boundary condition, and the lattice used. Numerical results demonstrate that these corrections are essential to ensure accurate simulation of microscale gas flow behavior. Although the results present in this work are for the BGK-LBE, the analysis method employed here can also be applied to other LBE models. Actually, during the review process of this paper, we have made a similar analysis about the CBC and DMBC for the generalized LBE with multiple relaxation times (MRT) [30]. It is again found that some discrete effects still exist in the boundary conditions in that case. However, due to the use of multiple relaxation times, the correction method to minimize the discrete effects is quite different from the present one given by Eq. (8): in the MRT-LBE, the bounce-back portion r only depends on A_1 appearing in the second-order boundary condition, and is irrelevant to Kn, A_2 and Δ; on the other hand, one of the relaxation times must be chosen according to Kn, A_2 and Δ in order to realize the exact boundary condition. This fact indicates that discrete effects in boundary condition may be a general problem in LBE models, but the correction methods may be different for different models.

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