Kinetic boundary conditions in the lattice Boltzmann method

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Derivation of the lattice Boltzmann method from the continuous kinetic theory [X. He and L. S. Luo, Phys. Rev. E **55**, R6333 (1997); X. Shan and X. He, Phys. Rev. Lett. **80**, 65 (1998)] is extended in order to obtain boundary conditions for the method. For the model of a diffusively reflecting moving solid wall, the boundary condition for the discrete set of velocities is derived, and the error of the discretization is estimated. Numerical results are presented which demonstrate convergence to the hydrodynamic limit. In particular, the Knudsen layer in the Kramers' problem is reproduced correctly for small Knudsen numbers.

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I. INTRODUCTION

In recent years, the lattice Boltzmann method (LBM) has emerged as an alternative tool for the computational fluid dynamics [1]. Originally, the LBM was developed as a modification of the lattice gas model [2]. Later derivations [3,4] revealed that the method is a special discretization of the continuous Boltzmann equation. The derivation of the LBM [4] from the Boltzmann equation is essentially based on Grad's moment method [5], together with the Gauss-Hermite quadrature in the velocity space.

Another important issue was to retain positivity of discrete velocities populations in the bulk. Recently, a progress has been achieved in incorporating the H theorem into the method [6–8], and thus retaining positivity of the populations in the bulk. On the contrary, despite of several attempts [9–16] a fully consistent theory of the boundary condition for the method is still lacking. It appears that the concerns about positivity of the population, and the connection with the continuous case, are somewhat ignored while introducing the boundary condition. The way the no-slip condition for the moving wall is incorporated in the method [10–12] is especially prone to danger of loss of positivity of the populations at the boundary. A clear understanding of the boundary condition becomes demanding for the case of moving boundary, complicated geometries, chemically reactive, or porous walls.

The theory of boundary conditions for the continuous Boltzmann equation is sufficiently well developed to incorporate the information about the structure and the chemical processes on the wall [17]. The realization that the LBM is a special discretization of the Boltzmann equation allows us to derive the boundary conditions for the LBM from continuous kinetic theory. In this work we demonstrate how this can be done in a systematic way.

The outline of the paper is as follows: In Sec. II we give a brief description of the LBM. In Sec. III we briefly describe how boundary condition is formulated for the continuous kinetic theory. In Sec. IV we derive the boundary condition for the LBM and in Sec. V we demonstrate some numerical simulation to validate the result.

II. OVERVIEW OF THE METHOD

In the LBM setup, one considers populations f_i of discrete velocities $\mathbf{c}_i$, where $i=1,\ldots,b$, at discrete time t. It is convenient to introduce b-dimensional population vectors $\boldsymbol{f}$.

In the isothermal case considered below, local hydrodynamic variables are given as

$$\rho=\sum_{i=1}^{b} f_i(\mathbf{r},t), \tag{1}$$

$$\rho\mathbf{u}=\sum_{i=1}^{b} \mathbf{c}_i f_i(\mathbf{r},t).$$

The basic equation to be solved is

$$f_i(\mathbf{r}+\mathbf{c}_i,t+1)-f_i(\mathbf{r},t)=-\beta\alpha[\boldsymbol{f}(\mathbf{r},t)]\boldsymbol{\Delta}_i[\boldsymbol{f}(\mathbf{r},t)], \tag{2}$$

where β is a fixed parameter in the interval [0,1] and is related to the viscosity. A scalar function of the population vector α is the nontrivial root of the nonlinear equation

$$H(\boldsymbol{f})=H(\boldsymbol{f}+\alpha\boldsymbol{\Delta}[\boldsymbol{f}]). \tag{3}$$

The function α ensures the discrete-time H theorem. In the previous derivations [3,4] of the LBM from the Boltzmann equation, a quadratic form for the equilibrium distribution function f^{eq}, was obtained by evaluating the Taylor series expansion of the absolute Maxwellian equilibrium on the nodes of a properly selected quadrature. This was done to ensure that the Navier-Stokes equation is reproduced up to the order $O(M^2)$, where M is the Mach number. However, the disadvantage of expanding equilibrium distribution function is that the condition of monotonicity of the entropy production is not guaranteed. In order to avoid this problem, in the entropic formulation [6–8], the Boltzmann H function, rather than the equilibrium distribution, is evaluated at the nodes of the given quadrature, to get the discrete version of the H function as

$$H=\sum_{i=1}^{b} f_i\ln\left(\frac{f_i}{w_i}\right), \tag{4}$$

where w_i denotes the weight associated with the corresponding quadrature node $\mathbf{c}_i$. In the Appendix the derivation of the H function is presented. Afterwards, the collision term is constructed from the knowledge of the H function [Eq. (4)]. The collision term $\boldsymbol{\Delta}$ is constructed in such a way that it satisfies a set of admissibility conditions needed to have a proper H theorem and conservation laws (see Ref. [8] for details).

The LBM model with the Bhatnagar-Gross-Krook (BGK) collision form [4,18], can be considered as a limiting case of the entropic formulation. To obtain the lattice BGK equation, the function α in the Eq. (2) is set equal to 2, and for the collision term $\mathbf{\Delta}$ BGK form is chosen. The equilibrium function used in the BGK form is obtained as the minimizer of the H function [Eq. (4)] subjected to the hydrodynamic constrains [Eq. (1)], evaluated up to the order M^2 [6]. Derivation of the boundary conditions done in the subsequent section applies to both the forms of the LBM.

III. BOUNDARY CONDITION FOR THE BOLTZMANN EQUATION

Following Ref. [17], we briefly outline how boundary condition is formulated in the continuous kinetic theory. We shall restrict our discussion to the case where the mass flux through the wall is zero. For the present purpose, a wall ∂R is completely specified at any point $(\mathbf{r}\in\partial R)$ by the knowledge of the inward unit normal $\mathbf{n}$, the wall temperature T_{w}, and the wall velocity $\mathbf{U}_{\mathrm{w}}$. Hereafter, we shall denote the distribution function in a frame of reference moving with the wall velocity as $g(\boldsymbol{\xi})$, with $\boldsymbol{\xi}=\mathbf{c}-\mathbf{U}_{\mathrm{w}}$. The distribution function reflected from the nonadsorbing wall can be written explicitly, if the scattering probability is known. In explicit form

$$|\boldsymbol{\xi}\cdot\mathbf{n}|g(\boldsymbol{\xi},t)=\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|g(\boldsymbol{\xi}',t)B(\boldsymbol{\xi}'\rightarrow\boldsymbol{\xi})d\boldsymbol{\xi}'\,(\boldsymbol{\xi}\cdot\mathbf{n}>0), \tag{5}$$

where the non-negative function $B(\boldsymbol{\xi}'\rightarrow\boldsymbol{\xi})$ denotes the scattering probability from the direction $\boldsymbol{\xi}'$ to the direction $\boldsymbol{\xi}$. If the wall is nonporous and nonadsorbing, the total probability for an impinging particle to be reemitted is unity

$$\int_{\boldsymbol{\xi}\cdot\mathbf{n}>0}B(\boldsymbol{\xi}'\rightarrow\boldsymbol{\xi})d\boldsymbol{\xi}=1. \tag{6}$$

Equations (5) and (6) ensure that the reflected distribution functions are positive and the normal flux through the wall is zero. A further restriction on the form of function B is dictated by the condition of detailed balance [17],

$$\begin{aligned}|\boldsymbol{\xi}'\cdot\mathbf{n}|&g^{\mathrm{eq}}(\boldsymbol{\xi}',\rho_{\mathrm{w}},0,T_{\mathrm{w}})B(\boldsymbol{\xi}'\rightarrow\boldsymbol{\xi})\\&=|\boldsymbol{\xi}\cdot\mathbf{n}|g^{\mathrm{eq}}(-\boldsymbol{\xi},\rho_{\mathrm{w}},0,T_{\mathrm{w}})B(-\boldsymbol{\xi}\rightarrow-\boldsymbol{\xi}').\end{aligned} \tag{7}$$

A consequence of this property is that, if the impinging distributions are wall Maxwellian, then the reflected distributions are also wall Maxwellian. Thus,

$$\begin{aligned}|\boldsymbol{\xi}\cdot\mathbf{n}|&g^{\mathrm{eq}}(-\boldsymbol{\xi},\rho_{\mathrm{w}},0,T_{\mathrm{w}})\\&=\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|g^{\mathrm{eq}}(\boldsymbol{\xi}',\rho_{\mathrm{w}},0,T_{\mathrm{w}})B(\boldsymbol{\xi}'\rightarrow\boldsymbol{\xi})d\boldsymbol{\xi}'.\end{aligned} \tag{8}$$

This equation can also be understood as a weaker statement of the detailed balance condition [17]. This form of the detailed balance is very attractive for our present purpose because of its integral nature, so that a discretization can be done in a natural way.

In this paper, we only consider the diffusive boundary conditions because the steps associated with the discretization are easier to appreciate due to the mathematical simplicity in this case. In this model of the wall it is assumed that the outgoing stream has completely lost its memory about the incoming stream. Thus, the scattering probability B is independent of the impinging directions, and is equal to

$$B(\boldsymbol{\xi}'\rightarrow\boldsymbol{\xi})=\frac{|\boldsymbol{\xi}\cdot\mathbf{n}|g^{\mathrm{eq}}(-\boldsymbol{\xi},\rho_{\mathrm{w}},0,T_{\mathrm{w}})}{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|g^{\mathrm{eq}}(\boldsymbol{\xi}',\rho_{\mathrm{w}},0,T_{\mathrm{w}})d\boldsymbol{\xi}'}\equiv B(\boldsymbol{\xi}). \tag{9}$$

Thus, the explicit expression for the reflected distribution function is

$$\begin{aligned}g(\boldsymbol{\xi},t)=&\frac{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|g(\boldsymbol{\xi}',t)d\boldsymbol{\xi}'}{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|g^{\mathrm{eq}}(\boldsymbol{\xi}',\rho_{\mathrm{w}},0,T_{\mathrm{w}})d\boldsymbol{\xi}'}\\&\times g^{\mathrm{eq}}(-\boldsymbol{\xi},\rho_{\mathrm{w}},0,T_{\mathrm{w}})\quad(\boldsymbol{\xi}\cdot\mathbf{n}>0).\end{aligned} \tag{10}$$

We need to transform this equation into the stationary coordinate system. As the equilibrium distribution depends only on the difference between the particle velocity and the local velocity, we have

$$\begin{aligned}f(\mathbf{c},t)=&\frac{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f(\mathbf{c}',t)d\mathbf{c}'}{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f^{\mathrm{eq}}(\mathbf{c}',\rho_{\mathrm{w}},U_{\mathrm{w}},T_{\mathrm{w}})d\boldsymbol{\xi}'}\\&\times f^{\mathrm{eq}}(\mathbf{c},\rho_{\mathrm{w}},U_{\mathrm{w}},T_{\mathrm{w}})\quad(\mathbf{c}-\mathbf{U}_{\mathrm{w}})\cdot\mathbf{n}>0.\end{aligned} \tag{11}$$

In the following section, we will show how the discretization of the Eq. (11) can be performed.

IV. DISCRETIZATION OF THE BOUNDARY CONDITION

In the derivation of the lattice Boltzmann equation for the bulk various integrals, which are evaluated at the nodes of a Gauss-Hermite quadrature [3], are of the form

$$I=\int_{\boldsymbol{\xi}\in R^D}\exp(-\boldsymbol{\xi}^2)\,\phi(\boldsymbol{\xi})d\boldsymbol{\xi}, \tag{12}$$

where D is the spatial dimension. This form of the integral is well approximated by the Gauss-Hermite quadrature. However, the situation is different on the boundary because integrals appearing in Eq. (11) are over half-space. The choice of the quadrature in the bulk was based on the properties of integrals in the R^D. If we would evaluate the integrals in Eq. (11) using a quadrature defined in the half-space, this may introduce an undesirable mismatch of the nodes of the quadrature used on the boundary and that in the bulk. Thus, we here apply the quadrature used in the bulk even for the boundary nodes. Next, we shall estimate the extra error introduced by this procedure in comparison to the discretization error present in the bulk.

The discrete distribution function used in the LBM is the projection of the continuous distribution function in a finite-dimensional orthonormal Hermite basis [4]. The equilibrium also need to be projected in this basis to have correct conservation laws. This solution has a major drawback that the positivity of the distribution function is lost in the truncation. This problem is circumvented, if we evaluate the Boltzmann H function, rather than its minimizer under the constrains of conservation of the hydrodynamic variables, for the discrete case. Indeed, the local equilibrium can also be written as

$$f^{\mathrm{eq}}(\mathbf{c},\rho_{\mathrm{w}},U_{\mathrm{w}},T_{\mathrm{w}})=\exp(\alpha+\boldsymbol{\zeta}\cdot\mathbf{c}+\gamma\mathbf{c}^2), \tag{13}$$

where α, $\boldsymbol{\zeta}$, and γ are the Lagrange multipliers needed for the minimization of the Boltzmann H function under the constraints of conservation of the hydrodynamic variables. These Lagrange multipliers are calculated from the requirement that the moments of the equilibrium distribution f^{eq} are known hydrodynamic quantities. Now, once we have evaluated the projection of the Boltzmann H function on a finite-dimensional Hermite basis, we calculate the equilibrium from the knowledge of the discrete H function. It turns out that the equilibrium corresponding to the discrete H function also has the same functional form as Eq. (13). Only difference is that the Lagrange multipliers has to be calculated from the discrete conservation laws. One example of explicit form of such equilibrium distribution function is given in Ref. [7].

First projecting the distribution functions in the Hermite basis and then evaluating the integrals appearing in Eq. (11) by quadrature, we have

$$\tilde{f}(\mathbf{c}_i,t)=\frac{\sum_{\boldsymbol{\xi}_i'\cdot\mathbf{n}<0}|(\boldsymbol{\xi}_i'\cdot\mathbf{n})|\tilde{f}(\mathbf{c}_i',t)}{\sum_{\boldsymbol{\xi}_i'\cdot\mathbf{n}<0}|(\boldsymbol{\xi}_i'\cdot\mathbf{n})|\tilde{f}^{\mathrm{eq}}(\mathbf{c}_i',U_{\mathrm{w}},\rho_{\mathrm{w}})}\tilde{f}^{\mathrm{eq}}(\mathbf{c}_i,U_{\mathrm{w}},\rho_{\mathrm{w}}),$$

$$(\mathbf{c}_i-\mathbf{U}_{\mathrm{w}})\cdot\mathbf{n}>0, \tag{14}$$

where

$$\tilde{f}(\mathbf{c}_i,t)=w_i\rho\frac{f(\mathbf{c}_i,t)}{f^{\mathrm{eq}}(\mathbf{c}_i,0,\rho)} \tag{15}$$

denotes the rescaled distribution function evaluated at nodes of the quadrature. This rescaled distribution function is the distribution function used in the LBM [3,4]. The discrete equilibrium distribution function $\tilde{f}^{\mathrm{eq}}$ is the projection of the equilibrium distribution on the finite-dimensional Hermite basis and calculated by the procedure discussed above. Before estimating error associated with this formula, a few remarks about the preceding equation is in order. First, in the isothermal case the wall temperature is a redundant quantity and is dropped from the argument of equilibrium distribution. To get a boundary condition for the lattice BGK equation, the true discrete equilibrium appearing in the Eq. (14) can be replaced by the equilibrium used in the BGK model [18]. This substitution is justified because up to order $O(M^2)$ the true equilibrium can be replaced by the BGK equilibrium. However, positivity of the reflected distributions may be lost in this truncation in the same way it happens in the bulk for lattice BGK model. A similar expression for the boundary conditions was earlier postulated by Gatingnol in the context of discrete velocity models of the kinetic theory [21].

In order to estimate the extra error introduced on the boundary in comparison to the bulk, we write the ratio of two integrals appearing in the Eq. (11) as

$$I=\frac{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f(\mathbf{c}',t)d\mathbf{c}'}{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f^{\mathrm{eq}}(\mathbf{c}',\rho_{\mathrm{w}},U_{\mathrm{w}},T_{\mathrm{w}})d\boldsymbol{\xi}'}$$

$$=1+\frac{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f^{\mathrm{neq}}(\mathbf{c}',t)d\mathbf{c}'}{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f^{\mathrm{eq}}(\mathbf{c}',\rho_{\mathrm{w}},U_{\mathrm{w}},T_{\mathrm{w}})d\boldsymbol{\xi}'}, \tag{16}$$

where $\boldsymbol{f}^{\mathrm{neq}}=\boldsymbol{f}-\boldsymbol{f}^{\mathrm{eq}}$. As discussed above, the evaluation of the integral appearing in the denominator is straightforward in the sense that the order of accuracy of this evaluation is same as that of moments evaluation in the bulk. In order to evaluate the integral appearing in the numerator, we perform Hermite expansion of the nonequilibrium part of the distribution function around the zero velocity equilibrium. The result is

$$f^{\mathrm{neq}}(\mathbf{c},t)=f^{\mathrm{eq}}(\mathbf{c},\rho_{\mathrm{w}},0,T_{\mathrm{w}})\sum_{i=0}^{N}\frac{a^{(i)}}{i!}\mathcal{H}^{(i)}(\mathbf{c}). \tag{17}$$

The first two expansion coefficients of the nonequilibrium part of the population are $(a^{(0)}=0,a_i^{(1)}=0)$. In case of the isothermal hydrodynamics, only nonzero Hermite coefficient needs to be kept is $a_{ij}^{(2)}$. This is a symmetric tensor and is independent of the particle velocity $\mathbf{c}$. After using the symmetry of the second-order Hermite polynomials,

$$I=1+\frac{1}{2}\frac{a_{\alpha\beta}^{(2)}\int|\boldsymbol{\xi}_i'\cdot\mathbf{n}|f^{\mathrm{eq}}(\mathbf{c}',\rho_{\mathrm{w}},0,T_{\mathrm{w}})\mathcal{H}_{\alpha\beta}^{(2)}(\mathbf{c}')d\mathbf{c}'}{\int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0}|\boldsymbol{\xi}'\cdot\mathbf{n}|f^{\mathrm{eq}}(\mathbf{c}',\rho_{\mathrm{w}},U_{\mathrm{w}},T_{\mathrm{w}})d\mathbf{c}'}. \tag{18}$$

This expression can be evaluated using the Gauss-Hermite quadrature. The result is

$$I = 1 + \frac{\sum_{\xi_i' \cdot \mathbf{n} < 0} a^{(2)}_{\alpha\beta} w_i |\boldsymbol{\xi}_i' \cdot \mathbf{n}| \mathcal{H}^{(2)}_{\alpha\beta}(\mathbf{c}_i')}{\sum_{\xi_i' \cdot \mathbf{n} < 0} |\boldsymbol{\xi}_i' \cdot \mathbf{n}| \tilde{f}^{\mathrm{eq}}(\mathbf{c}', \rho_{\mathrm{w}}, U_{\mathrm{w}})}. \tag{19}$$

This expression gives an estimate of the order of the accuracy of the Eq. (14). In evaluation of the moments (up to the second-order moment) of the distribution function, no extra error is introduced as compared to the bulk. This happened because first odd order Hermite coefficient appearing in the expansion is zero. Due to the expansion around global equilibrium, used in the derivation, the boundary condition is valid only up to the order $O(M^2)$.

Now, for purely diffusive scattering, we have a closed form expression for the reflected populations with the same order of accuracy as the bulk node. However, we have said nothing about the grazing directions. Unlike continuous kinetic theory, here we need to specify the conditions in the grazing directions. Only information we have about the grazing populations is their positivity. A simple way to fix the grazing population is to let them evolve according to the lattice Boltzmann equation like nodes in the bulk region. This condition is implemented in the simulations presented in the following section.

V. NUMERICAL TESTS

The boundary condition derived in the preceding Section [Eq. (14)], retains one important feature of original Boltzmann equation, the Knudsen number dependent slip at the wall. To show this, we have performed a numerical simulation of the Kramers' problem [17]. This is one of the few problems where solution of the continuous Boltzmann equation is known analytically. This problem is a limiting case of the plane Couette flow, where one of the plate is moved to infinity, while keeping a fixed shear rate. We compare the analytical solution for the slip velocity at the wall calculated for the linearized BGK collision model with the numerical solution in the Fig. 1. We have performed the numerical computation for the D2Q9 lattice with the entropic formulation of the LBM [7,8] with the expression of the H function given by Eq. (A5). The agreement between the two results for Knudsen number going to zero is very good. This is indeed an important result as it shows that with the proper implementation of the boundary condition, the solution of the LBM converge to the hydrodynamic limit (Knudsen number going to zero) in the same way as the Boltzmann equation.

By simulating the Kramer's problem, we have shown that the present boundary condition can be used for stationary wall. To validate the boundary condition for the moving wall, we have performed simulation of the lid-driven cavity flow. The plot of stream function is given in Fig. 2 for Reynolds number Re = 1000. The location of the primary and secondary vortex and the magnitude of the stream functions agrees well with the previous simulations [20].

Once we have shown that the diffusive boundary condition used for the continuous Boltzmann equation can be reformulated for the discrete case, the question arises that, can this procedure be applied for a more sophisticated scattering kernels used in the continuous kinetic theory (see, for examples Ref. [17]). The answer is in affirmative for any condition written in the integral form, while in general it cannot be done for a pointwise condition like purely specular reflection. For example, a very general form of scattering probability, written in the integral form and can be easily modified for nonzero mass flux, is given in the Ref. [17] [see Eq. (6.26) of the Chap. 3]. This form of the scattering probability can be discretized using the present method.

It is instructive to compare the "bounce-back" condition used in the literature with the present boundary condition. It

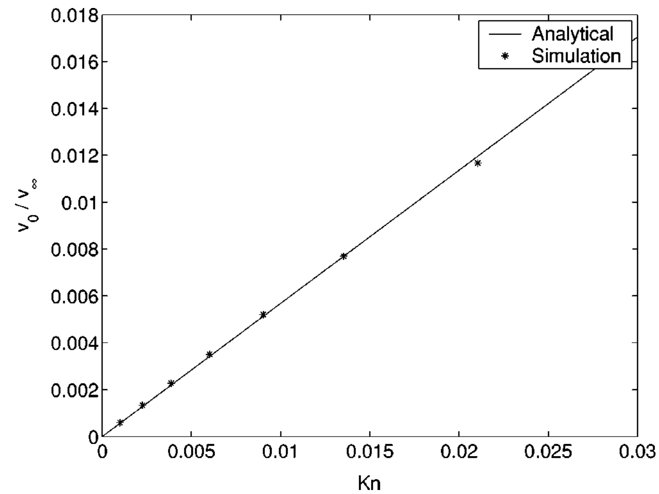

FIG. 1. Relative slip observed at the wall in the simulation of the Kramers' problem for shear rate $a = 0.001$, box length $L = 32$, $v_\infty = a \times L = 0.032$. All the quantities are given in the dimensionless lattice unit.

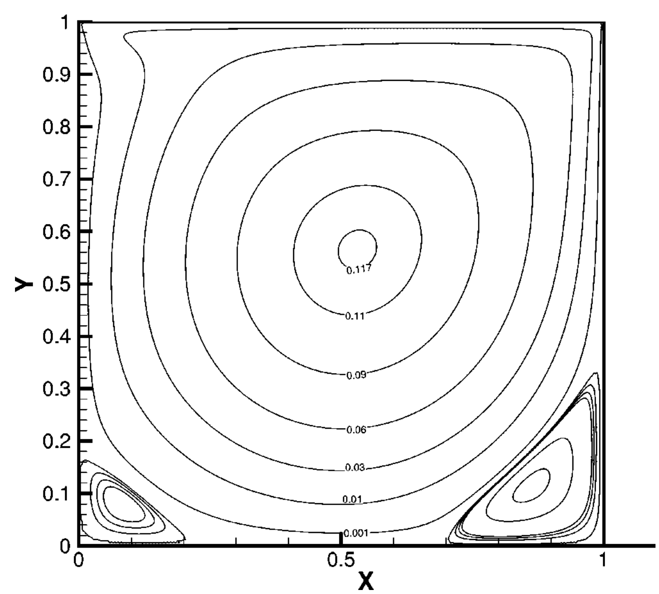

FIG. 2. Stream function for Re = 1000 in a simulation of lid driven cavity flow. Parameters used are grid size 320×320, and lid velocity $V = 0.075$. All the quantities are given in the dimensionless lattice unit.

can be seen easily that the present boundary condition reduces to the bounce-back condition for the three velocity model used in the one-dimensional case. However, there is no correspondence between the two condition in the higher dimensions.

The present boundary condition retains the positivity at the boundary nodes. This is a major advantage in comparison to other proposed boundary conditions for the purpose of the numerical stability. The Knudsen number dependent wall slip is a manifestation of the kinetic nature of the lattice Boltzmann equation. This nature of the scheme can be a burden if one is interested in solving the macroscopic creeping flow problems with very small grid size. This will put some restriction on the simulation of creeping flow in very small grids (lattice Knudsen number $=\nu/Lc_s$). However, the restriction is not severe because of the fact that we still have the freedom to choose velocity very small to attain zero Reynolds number situation. In fact, the same condition is required for the validity of the LBM simulation of the hydrodynamics in the bulk. To conclude, we have proposed boundary conditions based on the kinetic theory considerations. A systematic way of dealing with the conditions at the boundary is developed for the lattice Boltzmann method. The present work opens the way to the future development for the cases of reactive, porous or adsorbing walls.

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APPENDIX: DERIVATION OF THE *H* FUNCTION

The Boltzmann H function is

$$H=\int f\ln f\,d\boldsymbol{\xi}. \tag{A1}$$

This expression written in terms of the logarithm of the distribution function ($\mu=\ln f$) is

$$H=\int \mu\exp(\mu)\,d\boldsymbol{\xi}. \tag{A2}$$

We have chosen to work with the variable μ because the projection of it on to the Hermite basis preserves positivity of the distribution function f. The expansion of the function μ is

$$\mu=A^{(0)}\mathcal{H}^{(0)}(\mathbf{c})+A^{(1)}_{\alpha}\mathcal{H}^{(i)}(\mathbf{c})+A^{(2)}_{\alpha\beta}\mathcal{H}^{(i)}_{\alpha\beta}(\mathbf{c}). \tag{A3}$$

This expression can also be written as

$$\mu=A^{(0)}\mathcal{H}^{(0)}(\mathbf{c})+A^{(1)}_{\alpha}\mathcal{H}^{(i)}(\mathbf{c})+B^{(2)}_{\alpha\beta}\mathcal{H}^{(i)}_{\alpha\beta}(\mathbf{c})-\frac{\mathbf{c}^2}{2}. \tag{A4}$$

The expansion coefficient A is calculated by the requirement that the moments of $\exp(\mu)$ are hydrodynamic variables. The expansion used here is a slightly different form of the Grad's moment expansion [19] and is known as the maximum entropy approximation [22–24]. Now, the Boltzmann H function is in an integral form suited for the evaluation in the Gauss-Hermite quadrature [see Eq. (12)]. This evaluation gives the discrete form of the H function as

$$H=\sum_{i=1}^{b}\tilde{f}_i\ln\left(\frac{\tilde{f}_i}{w_i}\right), \tag{A5}$$

where

$$\tilde{f}(\mathbf{c}_i,t)=w_i(2\pi k_B T_0)^{D/2}\exp\left(\frac{\mathbf{c}_i^2}{2}\right)f(\mathbf{c}_i,t), \tag{A6}$$

where T_0 is the reference temperature. In two dimension, the nodes of the quadrature and the corresponding weights are

$$\mathbf{c}_i=\begin{cases}\{0,0\} & \text{if } i=0\\ c\left\{\left(\cos\left(\frac{\pi(i-1)}{2}\right),\sin\left(\frac{\pi(i-1)}{2}\right)\right)\right\} & \text{if } i=1,2,3,4\\ c\sqrt{2}\left\{\left(\cos\left(\frac{\pi(2i-9)}{4}\right),\sin\left(\frac{\pi(2i-9)}{4}\right)\right)\right\} & \text{if } i=5,6,7,8,\end{cases} \tag{A7}$$

and

$$w_i=\begin{cases}\frac{4}{9} & \text{if } i=0\\ \frac{1}{9} & \text{if } i=1,2,3,4\\ \frac{1}{36} & \text{if } i=5,6,7,8.\end{cases} \tag{A8}$$

Here the magnitude of the discrete velocity c is related to the reference temperature by the relation $c=\sqrt{(3k_BT_0)}$. With this, the entropy expression derived here coincide with the expression derived in Ref. [6], by a different argument.

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