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Finite-Difference Lattice Boltzmann Methods for Binary Fluids

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In this proceeding we summarize our recent studies on two-fluid lattice Boltzmann methods for binary fluids. We first clearify Sirovich's kinetic theory, then based on which three multispeed discrete velocity models are formulated, which are for the Euler equations, isothermal Navier-Stokes equations and the complete Navier-Stokes equations, respectively. Each formulated discrete velocity model, together with an appropriate finite-difference scheme, composes a finite-difference lattice Boltzmann method. The validity of the methods is verified by investigating (i) the Couette flow and (ii) the uniform relaxation process of the two components.
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I. INTRODUCTION

Lattice Boltzmann Method (LBM) is a numerical scheme to simulate kinetic systems. The LBM recovers the hydrodynamic descriptions in the small Knudsen number limit. It has become a viable and promising numerical scheme for simulating fluid flows. There are several options to discretize the Boltzmann equation: (i) Standard LBM (SLBM)[1]; (ii) Finite-Difference LBM (FDLBM)[1–3]; (iii) Finite-Volume LBM[1, 4]; (iv) Finite-Element LBM[1, 5]; etc. These kinds of schemes are expected to be complementary in the LBM studies.

Even though various LBMs for multicomponent fluids[6, 8–20] have been proposed and developed , (i) most existing methods belong to the SLBM[6, 8–17], and/or based on the single-fluid theory[8–15, 17, 18, 21]; (ii) in Refs. [6, 7] two SLBMs are proposed, but these two models are not convenient (if not impossible) to simulate thermal and compressible systems, even isothermal and incompressible systems only if the two components have different particle masses. In this study we develop two-fluid FDLBMs for thermal and compressible binary fluids.

II. FORMULATION AND VERIFICATION OF THE FDLBMS

The formulation of a FDLBM consists of three steps: (i) select or design an appropriate discrete velocity model (DVM), (ii) formulate the discrete local equilibrium distribution function, (iii) choose a finite-difference scheme. The continuous Boltzmann equation has infinite velocities, so the rotational invariance is automatically satisfied. Recovering rotational invariant macroscopic equations from a discrete finite velocity microscopic dynamics imposes constraints on the isotropy of DVM used. In our studies, the proposed FDLBMs are based on the two DVMs described below.

$$\mathtt{DVM1}: \mathtt{v}_0 = 0,\ \mathtt{v}_{ki} = \mathtt{v}_k \left[\cos\left(\frac{i\pi}{6}\right), \sin\left(\frac{i\pi}{6}\right)\right], i = 1,2,\cdots,12, \tag{1}$$

where k indicates the k-th group of particle velocities and i indicates the direction of the particle speed. It is easy find that (i) its odd rank tensors are zero, and (ii) its initial four even rank tensors satisfy

$$\begin{aligned} &\textstyle\sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta} = 6v_k^2\delta_{\alpha\beta},\ \sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta}v_{ki\gamma}v_{ki\delta} = \frac{3}{2}v_k^4\Delta_{\alpha\beta\gamma\delta}, \\ &\textstyle\sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta}v_{ki\gamma}v_{ki\delta}v_{ki\mu}v_{ki\nu} = \frac{1}{4}v_k^6\Delta_{\alpha\beta\gamma\delta\mu\nu}, \\ &\textstyle\sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta}v_{ki\gamma}v_{ki\delta}v_{ki\mu}v_{ki\nu}v_{ki\lambda}v_{ki\pi} = \frac{1}{32}v_k^8\Delta_{\alpha\beta\gamma\delta\mu\nu\lambda\pi}, \end{aligned} \tag{2}$$

where α, β, $\cdots$ indicate x or y component and

$$\Delta_{\alpha\beta\gamma\delta} = \delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}, \tag{3}$$

$$\Delta_{\alpha\beta\gamma\delta\mu\nu} = \delta_{\alpha\beta}\Delta_{\gamma\delta\mu\nu} + \delta_{\alpha\gamma}\Delta_{\beta\delta\mu\nu} + \delta_{\alpha\delta}\Delta_{\beta\gamma\mu\nu} + \delta_{\alpha\mu}\Delta_{\beta\gamma\delta\nu} + \delta_{\alpha\nu}\Delta_{\beta\gamma\delta\mu}, \tag{4}$$

$$\begin{aligned}\Delta_{\alpha\beta\gamma\delta\mu\nu\lambda\pi} &= \delta_{\alpha\beta}\Delta_{\gamma\delta\mu\nu\lambda\pi} + \delta_{\alpha\gamma}\Delta_{\beta\delta\mu\nu\lambda\pi} + \delta_{\alpha\delta}\Delta_{\beta\gamma\mu\nu\lambda\pi} + \delta_{\alpha\mu}\Delta_{\beta\gamma\delta\nu\lambda\pi} \\ &\quad + \delta_{\alpha\nu}\Delta_{\beta\gamma\delta\mu\lambda\pi} + \delta_{\alpha\lambda}\Delta_{\beta\gamma\delta\mu\nu\pi} + \delta_{\alpha\pi}\Delta_{\beta\gamma\delta\mu\nu\lambda}.\end{aligned} \tag{5}$$

It is clear that this DVM is isotropic up to, at least, its 9th rank tensor.

$$\text{DVM2}: \mathbf{v}_0 = 0,\ \mathbf{v}_{ki} = \mathrm{v}_k\left[\cos\left(\frac{i\pi}{4}\right), \sin\left(\frac{i\pi}{4}\right)\right], i = 1, 2, \cdots, 8. \tag{6}$$

Similarly, (i) its odd rank tensors are zero, and (ii) its initial three even rank tensors satisfy

$$\begin{aligned}&\textstyle\sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta} = 4v_k^2\delta_{\alpha\beta},\ \sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta}v_{ki\gamma}v_{ki\delta} = v_k^4\Delta_{\alpha\beta\gamma\delta}, \\ &\textstyle\sum_{i=1}^{12} v_{ki\alpha}v_{ki\beta}v_{ki\gamma}v_{ki\delta}v_{ki\mu}v_{ki\nu} = \frac{1}{6}v_k^6\Delta_{\alpha\beta\gamma\delta\mu\nu}.\end{aligned} \tag{7}$$

DVM 2 is isotropic up to its 7th rank tensor.

We consider a binary mixture with two components, A and B, where the masses and temperatures of the two components are not significantly different. The interparticle collisions can be divided into two kinds: collisions within the same species (self-collision) and collisions among different species (cross-collision)[22]. Based on the DVM (1), the 2-dimensional BGK[23] kinetic equation for species A reads,

$$\partial_t f_{ki}^A + \mathbf{v}_{ki}^A \cdot \frac{\partial}{\partial \mathbf{r}} f_{ki}^A - \mathbf{a}^A \cdot \frac{(\mathbf{v}_{ki}^A - \mathbf{u}^A)}{\Theta^A} f_{ki}^{A(0)} = J_{ki}^{AA} + J_{ki}^{AB} \tag{8}$$

where

$$J_{ki}^{AA} = -\left[f_{ki}^A - f_{ki}^{A(0)}\right]/\tau^{AA},\ J_{ki}^{AB} = -\left[f_{ki}^A - f_{ki}^{AB(0)}\right]/\tau^{AB} \tag{9}$$

$$f_{ki}^{A(0)} = \frac{n^A}{2\pi\Theta^A}\exp\left[-\frac{(\mathbf{v}_{ki}^A - \mathbf{u}^A)^2}{2\Theta^A}\right],\ f_{ki}^{AB(0)} = \frac{n^A}{2\pi\Theta^{AB}}\exp\left[-\frac{(\mathbf{v}_{ki}^A - \mathbf{u}^{AB})^2}{2\Theta^{AB}}\right] \tag{10}$$

$$\Theta^A = k_B T^A/m^A,\ \Theta^{AB} = k_B T^{AB}/m^A \tag{11}$$

$f^{A(0)}$ and $f^{AB(0)}$ are the corresponding Maxwellian distribution functions. n^A, $\mathbf{u}^A$, T^A are the local density, hydrodynamic velocity and temperature of species A. $\mathbf{u}^{AB}$, T^{AB} are the hydrodynamic velocity and temperature of the mixture after equilibration process. $\mathbf{a}^A$ is the acceleration of species A due to the effective external field.

For species A, we have

$$n^A = \sum_{ki} f_{ki}^A,\ n^A\mathbf{u}^A = \sum_{ki} \mathbf{v}_{ki}^A f_{ki}^A,\ P^A(e_{\text{int}}^A = n^A k_B T^A) = \sum_{ki} \frac{1}{2} m^A (\mathbf{v}_{ki}^A - \mathbf{u}^A)^2 f_{ki}^A \tag{12}$$

where P^A (e_{int}^A) is the local pressure (internal energy). For species B, we have similar relations. For the mixture, we have

$$\mathbf{u}^{AB} = \left(\rho^A\mathbf{u}^A + \rho^B\mathbf{u}^B\right)/\rho,\ nk_BT^{AB} = \sum_{ki}\frac{1}{2}\left[(\mathbf{v}_{ki}^A - \mathbf{u}^{AB})^2 m^A f_{ki}^A + (\mathbf{v}_{ki}^B - \mathbf{u}^{BA})^2 m^B f_{ki}^B\right] \tag{13}$$

where $\rho^A = n^A m^A$, $n = n^A + n^B$ and $\rho = \rho^A + \rho^B$. Three sets of hydrodynamic quantities (for the two components A, B and for the mixture) are involved, but only two sets of them are independent. So this is a two-fluid model. Without lossing generality, we focus on hydrodynamics of the two individual species. By expanding the local equilibrium distribution function $f^{AB(0)}$ around $f^{A(0)}$ to the first order in flow velocity and temperature, the BGK model (8-11) becomes

$$\partial_t f_{ki}^A + \mathbf{v}_{ki}^A \cdot \frac{\partial}{\partial \mathbf{r}} f_{ki}^A - \mathbf{a}^A \cdot \frac{(\mathbf{v}_{ki}^A - \mathbf{u}^A)}{\Theta^A} f_{ki}^{A(0)} = Q_{ki}^{AA} + Q_{ki}^{AB} \tag{14}$$

$$Q_{ki}^{AA} = -\left(\frac{1}{\tau^{AA}} + \frac{1}{\tau^{AB}}\right)\left[f_{ki}^A - f_{ki}^{A(0)}\right] \tag{15}$$

$$\begin{aligned} Q_{ki}^{AB} &= -\frac{f_{ki}^{A(0)}}{\rho^A\Theta^A}\{\mu_D^A (\mathbf{v}_{ki}^A - \mathbf{u}^A)\cdot(\mathbf{u}^A - \mathbf{u}^B) \\ &\quad +\mu_T^A\left[\frac{(\mathbf{v}_{ki}^A - \mathbf{u}^A)^2}{2\Theta^A} - 1\right](T^A - T^B) - M^A\left[\frac{(\mathbf{v}_{ki}^A - \mathbf{u}^A)^2}{2\Theta^A} - 1\right](\mathbf{u}^A - \mathbf{u}^B)^2\} \end{aligned} \tag{16}$$

where $\mu_D^A = \rho^A\rho^B/(\tau^{AB}\rho)$, $\mu_T^A = k_B n^A n^B/(\tau^{AB}n)$, $M^A = n^A\rho^A\rho^B/(2\tau^{AB}n\rho)$.

Now, we go to the second step: formulate $f_{ki}^{A(0)}$. The continuous Maxwellian $f^{A(0)}$ possesses an infinite sequence of moment properties. The Chapman-Enskog analysis[24] shows that, requiring the discrete $f_{ki}^{A(0)}$ to follow the initial eight ones is sufficient to describe the same Navier-Stokes equations,

$$\frac{\partial \rho^A}{\partial t} + \frac{\partial}{\partial r_\alpha}(\rho^A u_\alpha^A) = 0, \tag{17}$$

$$\begin{aligned} &\tfrac{\partial}{\partial t}(\rho^A u_\alpha^A) + \tfrac{\partial}{\partial r_\beta}\left(\rho^A u_\alpha^A u_\beta^A\right) + \tfrac{\partial P^A}{\partial r_\alpha} - \rho^A a_\alpha^A - \tfrac{\partial}{\partial r_\beta}\left[\eta^A\left(\tfrac{\partial u_\alpha^A}{\partial r_\beta} + \tfrac{\partial u_\beta^A}{\partial r_\alpha} - \tfrac{\partial u_\gamma^A}{\partial r_\gamma}\delta_{\alpha\beta}\right)\right] \\ &\quad + \tfrac{\rho^A\rho^B}{\tau^{AB}\rho}(u_\alpha^A - u_\alpha^B) = 0, \end{aligned} \tag{18}$$

$$\begin{aligned} &\tfrac{\partial e^A}{\partial t} + \tfrac{\partial}{\partial r_\alpha}\left[(e^A + P^A)u_\alpha^A\right] - \rho^A\mathbf{a}^A\cdot\mathbf{u}^A - \tfrac{\partial}{\partial r_\alpha}\left[k^A\tfrac{\partial(k_B T^A)}{\partial r_\alpha} + \eta^A u_\beta^A\left(\tfrac{\partial u_\alpha^A}{\partial r_\beta} + \tfrac{\partial u_\beta^A}{\partial r_\alpha} - \tfrac{\partial u_\gamma^A}{\partial r_\gamma}\delta_{\alpha\beta}\right)\right] \\ &\quad + \tfrac{\rho^A\rho^B}{\tau^{AB}\rho}\left[(u^A)^2 - \mathbf{u}^A\cdot\mathbf{u}^B\right] + \tfrac{n^A n^B}{\tau^{AB}n}k_B(T^A - T^B) - n^A\tfrac{\rho^A\rho^B}{2\tau^{AB}n\rho}(\mathbf{u}^A - \mathbf{u}^B)^2 = 0, \end{aligned} \tag{19}$$

where

$$e^A = e_{\mathrm{int}}^A + \frac{1}{2}\rho^A(u^A)^2,\ \eta^A = P^A\tau^{AA}\tau^{AB}/(\tau^{AA} + \tau^{AB}),\ k^A = 2n^A\Theta^A\tau^{AA}\tau^{AB}/(\tau^{AA} + \tau^{AB}). \tag{20}$$

Recall that $\mathbf{u}^A$ ($\mathbf{u}^B$) is a small quantity. By using Eq. (17), $P^A = n^A k_B T^A$, and neglecting the second and higher order terms in $\mathbf{u}^A$, Eq. (18) shows that the diffusion velocity, $u_\alpha^B - u_\alpha^A$, is related to the gradients of n^A and T^A.

The first three requirements on $f_{ki}^{A(0)}$ are referred to Eq. (12) with f_{ki}^A replaced by $f_{ki}^{A(0)}$, and the remaining five are

$$\sum_{ki} m^A v_{ki\alpha}^A v_{ki\beta}^A f_{ki}^{A(0)} = P^A\delta_{\alpha\beta} + \rho^A u_\alpha^A u_\beta^A \tag{21}$$

$$\sum_{ki} m^A v_{ki\alpha}^A v_{ki\beta}^A v_{ki\gamma}^A f_{ki}^{A(0)} = P^A\left(u_\gamma^A\delta_{\alpha\beta} + u_\alpha^A\delta_{\beta\gamma} + u_\beta^A\delta_{\gamma\alpha}\right) + \rho^A u_\alpha^A u_\beta^A u_\gamma^A \tag{22}$$

$$\sum_{ki}\frac{1}{2}m^A\left(v_{ki}^A\right)^2 v_{ki\alpha}^A f_{ki}^{A(0)}=2n^A k_B T^A u_\alpha^A+\frac{1}{2}\rho^A\left(u^A\right)^2 u_\alpha^A \tag{23}$$

$$\sum_{ki}\frac{1}{2}m^A\left(v_{ki}^A\right)^2 v_{ki\alpha}^A v_{ki\beta}^A f_{ki}^{A(0)}=2P^A\Theta^A\delta_{\alpha\beta}+\frac{1}{2}P^A\left(u^A\right)^2\delta_{\alpha\beta}$$
$$+3P^A u_\alpha^A u_\beta^A+\frac{1}{2}\rho^A\left(u^A\right)^2 u_\alpha^A u_\beta^A \tag{24}$$

$$\sum_{ki}\frac{1}{2}m^A\left(v_{ki}^A\right)^4 v_{ki\alpha}^A f_{ki}^{A(0)}=\left[12P^A\Theta^A+6P^A\left(u^A\right)^2+\frac{1}{2}\rho^A\left(u^A\right)^4\right]u_\alpha^A \tag{25}$$

The requirement equation (25) contains the fifth order of the flow velocity $\mathbf{u}^A$. So it is sufficient to expand $f_{ki}^{A(0)}$ in polynomial up to the fifth order of $\mathbf{u}^A$:

$$\begin{aligned}
f_{ki}^{A(0)} &= n^A F_k^A\left\{\left[1-\frac{(u^A)^2}{2\Theta^A}+\frac{(u^A)^4}{8\left(\Theta^A\right)^2}\right]+\frac{v_{ki\xi}^A u_\xi^A}{\Theta^A}\left[1-\frac{(u^A)^2}{2\Theta^A}+\frac{(u^A)^4}{8\left(\Theta^A\right)^2}\right]\right.\\
&+\frac{v_{ki\xi}^A v_{ki\pi}^A u_\xi^A u_\pi^A}{2\left(\Theta^A\right)^2}\left[1-\frac{(u^A)^2}{2\Theta^A}\right]+\frac{v_{ki\xi}^A v_{ki\pi}^A v_{ki\eta}^A u_\xi^A u_\pi^A u_\eta^A}{6\left(\Theta^A\right)^3}\left[1-\frac{(u^A)^2}{2\Theta^A}\right]\\
&\left.+\frac{v_{ki\xi}^A v_{ki\pi}^A v_{ki\eta}^A v_{ki\lambda}^A u_\xi^A u_\pi^A u_\eta^A u_\lambda^A}{24\left(\Theta^A\right)^4}+\frac{v_{ki\xi}^A v_{ki\pi}^A v_{ki\eta}^A v_{ki\lambda}^A v_{ki\delta}^A u_\xi^A u_\pi^A u_\eta^A u_\lambda^A u_\delta^A}{120\left(\Theta^A\right)^5}\right\}\\
&+\cdots
\end{aligned} \tag{26}$$

where

$$F_k^A=\frac{1}{2\pi\Theta^A}\exp\left[-\frac{(v_k^A)^2}{2\Theta^A}\right]. \tag{27}$$

The truncated equilibrium distribution function $f_{ki}^{A(0)}$ (26) contains the fifth rank tensor of the particle velocity $\mathbf{v}^A$ and the requirement (22) contains its third rank tensor. Thus, a DVM being isotropic up to its 8th rank tensors is enough to recover the physical isotropy of the continuous Boltzmann equations to the Navier-Stokes level. So DVM (1) is an appropriate choice. To calculate the discrete $f_{ki}^{A(0)}$, one first needs calculate the factor F_k^A. F_k^A is determined by the eight requirements on $f_{ki}^{A(0)}$ and the isotropic properties of the DVM (1). We finally obtain

$$\begin{aligned}
\sum_{ki}F_k^A &= 1,\ \sum_k F_k^A\left(v_k^A\right)^2=\frac{\Theta^A}{6},\ \sum_k F_k^A\left(v_k^A\right)^4=\frac{2}{3}\left(\Theta^A\right)^2,\\
\sum_k F_k^A\left(v_k^A\right)^6 &= 4\left(\Theta^A\right)^3,\ \sum_k F_k^A\left(v_k^A\right)^8=32\left(\Theta^A\right)^4,\ \sum_k F_k^A\left(v_k^A\right)^{10}=320\left(\Theta^A\right)^5
\end{aligned} \tag{28}$$

Once a zero speed, $v_0^A=0$, and other five nonzero ones, v_k^A ($k=1,\ 2,\ 3,\ 4,\ 5$) are chosen, F_k^A ($k=0,\ 1,\ 2,\ 3,\ 4,\ 5$) will be fixed.

We come to the third step: finite-difference implementation of the discrete kinetic method. There are more than one choices[2, 18] available. One possibility is shown below,

$$f_{ki}^{A,(n+1)}=f_{ki}^{A,(n)}+\left[\mathbf{a}^A\cdot\frac{\left(\mathbf{v}_{ki}^A-\mathbf{u}^A\right)}{\Theta^A}f_{ki}^{A(0)}+Q_{ki}^{AA,(n)}+Q_{ki}^{AB,(n)}-\mathbf{v}_{ki}^A\cdot\frac{\partial f_{ki}^{A,(n)}}{\partial\mathbf{r}}\right]\Delta t, \tag{29}$$

where the second superscripts n, $n+1$ indicate the consecutive two iteration steps, Δt the time step; the spatial derivatives are calculated as

$$\frac{\partial f_{ki}^{A,(n)}}{\partial\alpha}=\begin{cases}(3f_{ki,I}^{A,(n)}-4f_{ki,I-1}^{A,(n)}+f_{ki,I-2}^{A,(n)})/(2\Delta\alpha) & \text{if } v_{ki\alpha}^A\geq 0\\ (3f_{ki,I}^{A,(n)}-4f_{ki,I+1}^{A,(n)}+f_{ki,I+2}^{A,(n)})/(-2\Delta\alpha) & \text{if } v_{ki\alpha}^A<0\end{cases}, \tag{30}$$

where $\alpha = x, y$, the third subscripts $I-2$, $I-1$, I, $I+1$, $I+2$ indicate consecutive mesh nodes in the α direction.

If the kinetic numerical scheme is required to recover the hydrodynamics only up to the isothermal Navier-Stokes level, Eqs. (17)-(18) or the Euler level, Eqs.(17)-(19) with $\eta^A = k^A = 0$, following the same procedures, it is easy to find that DVM 2 is enough. For the isothermal Navier-Stokes equation, Eq. (28) is replaced by

$$\sum_{ki} F_k^A = 1,\ \sum_k F_k^A \left(v_k^A\right)^2 = \tfrac{\Theta^A}{4},\ \sum_k F_k^A \left(v_k^A\right)^4 = \left(\Theta^A\right)^2, \\ \sum_k F_k^A \left(v_k^A\right)^6 = 6\left(\Theta^A\right)^3. \tag{31}$$

For the complete Euler equation, Eq. (28) is replaced by

$$\sum_{ki} F_k^A = 1,\ \sum_k F_k^A \left(v_k^A\right)^2 = \tfrac{\Theta^A}{4},\ \sum_k F_k^A \left(v_k^A\right)^4 = \left(\Theta^A\right)^2, \\ \sum_k F_k^A \left(v_k^A\right)^6 = 6\left(\Theta^A\right)^3,\ \sum_k F_k^A \left(v_k^A\right)^8 = 48\left(\Theta^A\right)^4. \tag{32}$$

In summary, to recover the two-dimensional complete Navier-Stokes equations, a 2-dimensional 61-velocity (D2V61) model is needed; a D2V33 model is sufficient to recover the two-dimensional Euler equations; recovering the two-dimensional isothermal Navier-Stokes equations can resort on a simpler D2V25 model. In principle, a DVM with lower isotropy can be replaced by one with higher isotropy. But in practical simulations, one generally needs choose the simplest one.

The validity of the formulated the FDLBMs is verified through two test examples. (The Boltzmann constant $k_B = 1$.) The first one is the isothermal and incompressible Couette flow with a single component. In this case, $A = B$. The initial state of the fluid is static. The distance between the two walls is D. At time $t = 0$ they start to move at velocities U, $-U$, respectively. It is clear that all the three models (D2V25, D2V33, D2V61) work for such a system. The horizontal velocity profiles of species A or B along a vertical line agree with the following analytical solution,

$$u = \gamma y - \sum_j (-1)^{j+1}\frac{\gamma D}{j\pi}\exp\left(-\frac{4j^2\pi^2\eta}{\rho D^2}t\right)\sin\left(\frac{2j\pi}{D}y\right), \tag{33}$$

where $\gamma = 2U/D$ is the imposed the shear rate, j is an integer, the two walls locate at $y = \pm D/2$. (For example, see Fig. 1.)

The second one is the uniform relaxation process, which is an ideal process to indicate the equilibration behavior of the mixture. By neglecting the force terms and terms in spatial derivatives, the Navier-Stokes equations (17)-(19) give

$$\frac{\partial}{\partial t}\rho^A = 0, \tag{34}$$

$$\frac{\partial}{\partial t}\left(\mathbf{u}^B - \mathbf{u}^A\right) = -\frac{1}{\rho}\left(\frac{\rho^A}{\tau^{BA}} + \frac{\rho^B}{\tau^{AB}}\right)\left(\mathbf{u}^B - \mathbf{u}^A\right), \tag{35}$$

$$\frac{\partial\left(T^B - T^A\right)}{\partial t} = -\frac{1}{n}\left(\frac{n^A}{\tau^{BA}} + \frac{n^B}{\tau^{AB}}\right)\left(T^B - T^A\right) + \frac{\rho^A\rho^B}{2k_B n\rho}\left(\frac{1}{\tau^{AB}} - \frac{1}{\tau^{BA}}\right)\left(\mathbf{u}^B - \mathbf{u}^A\right)^2. \tag{36}$$

(The Euler equations play the same role as the Navier-Stokes equations in this case. Both the D2V61 and D2V33 works.) The flow velocities of the two components equilibrate exponentially with time. (For example, see Fig. 2(a).) The equilibration of flow velocities also affects that of the temperatures. When the flow velocity difference is zero, the temperatures equilibrate exponentially with time. (For example, see Fig. 2(b).) The simulation results agree well with Eqs. (35) and (36).

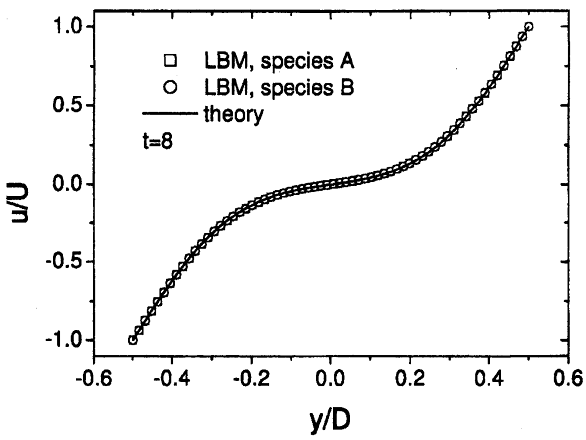

FIG. 1: Horizontal velocity profiles along a vertical line for the two species, A and B, at time $t = 8$. The symbols are for simulation results. The solid line corresponds to the theoretical result, Eq. (33). Parameters used in the two-fluid FDLBM are $m^A = m^B = 1$, $T = 1$, $n^A = n^B = 1$, $\gamma = 0.001$, $\tau^{AA} = \tau^{BB} = \tau^{AB} = \tau^{BA} = 0.2$. Parameters used in Eq. (33) are $\eta = \eta^A = 0.1$, $\rho = \rho^A = 1$.

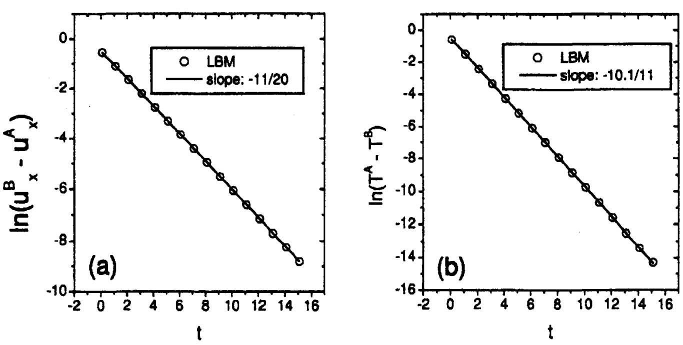

FIG. 2: Uniform relaxation processes. (a) Equilibration of velocities; (b) Equilibration of temperatures. The symbols are for simulation results. The solid lines possess the theoretical slopes. Common parameters for the simulations in (a) and (b) are $n^A = 10$, $n^B = 1$, $m^A = 1$, $m^B = 10$, $\tau^{AA} = \tau^{BB} = 1$, $\tau^{AB} = 10$, $\tau^{BA} = 1$. In (a) the initial conditions are $u_x^{A(0)} = -u_x^{B(0)} = -0.3$, $u_y^{A(0)} = u_y^{B(0)} = 0$, and $T^{A(0)} = 1.3$, $T^{B(0)} = 0.7$. The slope of the solid line in (a) is $-11/20$, which is consistent with Eq. (35). In (b) the initial conditions are $\mathbf{u}^{A(0)} = \mathbf{u}^{B(0)} = 0$, and $T^{A(0)} = 1.3$, $T^{B(0)} = 0.7$. The slope of the solid line in (b) is $-10.1/11$, which is consistent with the first term of right-hand side of Eq.(36). The second superscript "(0)" denotes the corresponding initial value. This figure shows an example where the particle masses of the two species are significantly different.

III. CONCLUSIONS AND REMARKS

The Chapman-Enskog analysis shows what properties the discrete Maxwellian distribution function $f_{ki}^{A(0)}$ should follow. Those requirements tell the lowest order of the flow velocity $\mathbf{u}^A$ in the Taylor expansion of $f_{ki}^{A(0)}$. The highest rank of tensors of the particle velocity $\mathbf{v}^A$ in the requirements on the truncated $f_{ki}^{A(0)}$ determines the needed isotropy of the DVM. The incorporation of the force terms makes no additional requirement on the isotropy of the DVM. The present approach works for binary neutral fluid mixtures. One possibility to introduce interfacial tension is to modify the pressure tensors[14], which is implemented by changing the force terms[3]. The specific force terms or pressure tensors depend on the system under consideration, which are out of the scope of this Letter, but can be resolved under the same two-dimensional 61-velocity model (D2V61). For binary fluids with disparate-mass components, say $m^A \ll m^B$, only if the total masses and temperatures of the two species are not significantly different, Sirovich's kinetic theory works, so do the corresponding FDLBMs. (See Fig. 2 for an example.) When the masses and/or the temperatures of the two components are greatly different, the two-fluid kinetic theory should be modified. In those cases, the Navier-Stokes equations and the FDLBMs are not symmetric about the two components, but the FDLBMs can still be resolved under the D2V61 model. The formulation procedure is straightforward. A more detailed description is referred to [25, 26]. We finally emphasize that the numerical errors from the finite-difference schemes result in artificial viscosities in the simulation. The comparison of various finite-difference schemes, discussion on numerical accuracy and stability are referred to Refs. [2, 3, 18].

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