Lattice Boltzmann model with nearly constant density

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An improved lattice Boltzmann model is developed to simulate fluid flow with nearly constant fluid density. The ingredient is to incorporate an extra relaxation for fluid density, which is realized by introducing a feedback equation in the equilibrium distribution functions. The pressure is dominated by the moving particles at a node, while the fluid density is kept nearly constant and explicit mass conservation is retained as well. Numerical simulation based on the present model for the (steady) plane Poiseuille flow and the (unsteady) two-dimensional Womersley flow shows a great improvement in simulation results over the previous models. In particular, the density fluctuation has been reduced effectively while achieving a relatively large pressure gradient.

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The simulation of the incompressible fluid flow is an important area of practical interest. The most important issue on such simulation is the robustness and accuracy of the numerical scheme. In the past decade, the lattice Boltzmann (LB) method [1,2] and its recent modification, the lattice-BGK (LBGK) method [3,4] have become a promising scheme towards this direction. Although the LBGK method was initially proposed to simulate the incompressible Navier-Stokes equations, the latter can be derived from the LBGK equation, through the Chapman-Enskog procedure, only if the density fluctuation is *assumed* negligible. Unfortunately, this assumption is usually violated for most practical cases. In fact, the equation of state $p=c_s^2\rho$, with constant c_s^2, from the conventional LBGK models implies that any pressure gradient should lead to density variation. There have been efforts to eliminate or reduce the so-called compressible effect [5–9] by redefining the velocity. However, explicit mass conservation has fallen into neglect in these models.

Consider, e.g., the LBGK simulation for the flow in an equiwidth tube. Macroscopically, the flow is driven by pressure gradient. By the viewpoint of LB, the flow is due to the difference of the moving distribution functions (DF's), rather than the rest ones, between two ends of the tube. More specifically, the fluid flows usually from the end with greater moving DF's to the end with smaller moving DF's. As the ratio between the rest and moving parts of DF's is mainly determined through the equilibrium distribution functions(EDF's) assumed [3,4], it follows that the greater the moving DF's, the greater the rest ones, and thus the larger the total DF's, or, the fluid density, if the velocity of the node is fixed. In this sense, the flow is driven by the density gradient in the LB model. Large density gradient is required in order to simulate large pressure gradient. On the other hand, to achieve incompressibility, it is necessary to keep the density, namely, the total DF's, (at least nearly) constant. One natural approach to attack this difficulty is to directly incorporate the equation of state for the real fluid with the LB model, based on the free energy approach presented by Yeomans and co-workers (see, e.g., [10]), by which a small density gradient may result in large pressure gradient. However, for nearly incompressible fluid, as the coefficient of compressibility is exceedingly small, namely, quite small change of density will result in enormous changes of the pressure and the direct incorporation of the equation of state with LB model will likely ruin the numerical stability [11].

In this paper, a simple but effective LB model is presented to simulate incompressible fluid flow by incorporating an extra density relaxation, which is realized by introducing a feedback equation [12] for the ratio between the rest and moving parts of EDF's. When the total density at a node is greater (smaller) than the prespecified value ρ_0, a very small amount of the rest (moving) particles are changed into the moving (rest) particles in the EDF's, so that in the following streaming step, more (less) particles will leave the node. The density at the node will decrease (increase) to approach ρ_0. This extra relaxation keeps the density at any fluid node evolve into a (nearly) prespecified constant, achieving the incompressibility of the system, while the pressure p in this model is dominated by the total moving particles at a node. To demonstrate the accuracy of the present model, numerical simulations based on the present model have been performed for the (steady) plane Poiseuille flow and the (unsteady) two-dimension (2D) Womersley flow. The results show a considerable improvement over the conventional LBGK model, and the typical incompressible model as proposed by He and Lou [9] at higher frequencies. In particular, the density fluctuation has been reduced effectively while relatively large pressure gradient is established.

We choose to work on a square lattice in two dimensions, generalization to higher dimensions and other underlying lattice or nonuniform grid is straightforward. Let $f_i(\mathbf{x},t)$ be a nonnegative real number describing the DF of the fluid density at site $\mathbf{x}$ at time t moving in direction $\mathbf{e}_i$. Here $\mathbf{e}_0=(0,0)$, $\mathbf{e}_i=(\cos\pi(i-1)/2, \sin\pi(i-1)/2), i=1,2,3,4$, and $\mathbf{e}_i=(\cos\pi(2i-1)/4), \sin\pi(2i-1)/4)$, for $i=5,6,7,8$ are the nine possible velocity vectors. The DF's evolve according to a Boltzmann equation that is discrete in both space and time [3,4]

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

where τ is the dimensionless collision relaxation time. The density ρ and macroscopic velocity $\mathbf{u}$ are defined by

$$\rho=\sum_{i=0}^{8} f_i, \qquad \rho\mathbf{u}=\sum_{i=0}^{8} f_i\mathbf{e}_i. \tag{2}$$

The EDF's f_i^{eq} are usually supposed to be dependent only on the local density ρ and flow velocity $\mathbf{u}$. In this paper the EDF's are chosen as

$$f_0^{eq}=A_0\rho-\frac{2}{3}\rho u^2.$$

$$f_i^{eq}=A_1\rho+\frac{1}{9}\rho\left[3(\vec{e}_i\cdot\vec{u})+\frac{9}{2}(\vec{e}_i\cdot\vec{u})^2-\frac{3}{2}u^2\right], \quad i=1,2,3,4,$$

$$f_i^{eq}=\frac{A_1}{4}\rho+\frac{1}{36}\rho\left[3(\vec{e}_i\cdot\vec{u})+\frac{9}{2}(\vec{e}_i\cdot\vec{u})^2-\frac{3}{2}u^2\right], \quad i=5,6,7,8, \tag{3}$$

with

$$A_0+5A_1=1, \tag{4}$$

to guarantee the mass conservation $\Sigma_{i=0}^{8} f_i^{eq}=\Sigma_{i=0}^{8} f_i$. Unlike that in the conventional LBGK model [3], the ratio of A_0 and A_1 are not fixed but perturbed to control the density at the considered nodes. Initially, A_1 is determined by

$$\sum_{i=1}^{8} f_i^{eq}=\sum_{i=1}^{8} f_i. \tag{5}$$

Denoting by A_1^0 the solution of A_1 from Eq. (5), before each collision step, we change the value of A_1 slightly from A_1^0 to some other value [12],

$$A_1=A_1^0+s(\rho,\tau), \tag{6}$$

where s is a function of ρ and τ. The simplest feedback is the linear response function, given by

$$s(\rho,\tau)=-b(\tau)\left(1-\frac{\rho}{\rho_0}\right). \tag{7}$$

Here b is a constant for given τ, and ρ_0 is the expected, or prespecified, value of density for all the nodes in the fluid domain. Equations (6) and (7) represent an effort to turn some rest (moving) particles into the moving (rest) ones in the EDF's when $\rho>\rho_0$ ($\rho<\rho_0$). Therefore, in the next streaming step, more (less) particles will leave the node with $\rho>\rho_0$ ($\rho<\rho_0$), resulting in a decrease (an increase) of ρ towards ρ_0.

The technique of feedback can also be understood as an extra relaxation that relaxes the system towards a state with prespecified constant density at any fluid node, while still keeps the conventional stress relaxation by Eq. (1) to achieve arbitrary viscosity. The parameter b in Eq. (7) characterizes the density relaxation speed. Larger value of b helps to reduce the fluctuation of density. However, the scheme will lose stability for the parameter b above a critical value b_c. Figure 1 shows the result for b_c determined numerically for the unsteady Womersley flow for the period $T=2000$. In practical simulation, the value of b is usually chosen to be a little smaller than b_c in case of instability caused by boundary. The contribution of feedback to A_1 is small (usually less than 0.1%) and there is no problem of numerical instability provided that an appropriate of b is chosen..

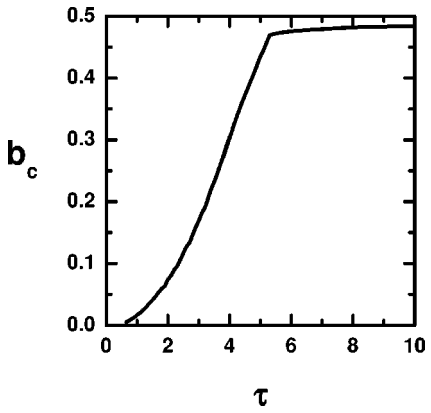

FIG. 1. The critical value b_c determined numerically.

By using Chapman-Enskog procedure, from Eqs. (1) and (3), the macroscopic equations can be worked out as following,

$$\partial_t\rho+\partial_\alpha(\rho u_\alpha)=0,$$

$$\begin{aligned}\partial_t(\rho u_\alpha)+\partial_\beta(\rho u_\alpha u_\beta)&=-\partial_\alpha p+\left(\tau-\frac{1}{2}\right)\partial_\alpha\left[\left(\frac{1}{3}-3A_1\right)\partial_\gamma(\rho u_\gamma)\right]\\&+\partial_\beta\left(\tau-\frac{1}{2}\right)\left[\frac{1}{3}\rho(\partial_\alpha u_\beta+\partial_\beta u_\alpha)\right.\\&\left.+\left(\frac{1}{3}-3A_1\right)(u_\alpha\partial_\beta\rho+u_\beta\partial_\alpha\rho)-\partial_\gamma(\rho u_\alpha u_\beta u_\gamma)\right],\end{aligned} \tag{8}$$

where the pressure $p=3A_1\rho$. If $\rho=\rho_0=$constant we obtain the following equations for the incompressible fluid flow,

$$\partial_\alpha u_\alpha=0,$$

$$\partial_t u_\alpha+\partial_\beta(u_\alpha u_\beta)=-\frac{1}{\rho_0}\partial_\alpha p+\nu\partial_\beta\partial_\beta u_\alpha, \tag{9}$$

where the viscosity $\nu=2\tau-1/6$. In the following we will find that the density variation $\delta\rho=\rho-\rho_0$ is small as compared with the pressure variation.

To demonstrate the accuracy of the present scheme, the plane Poiseuille flow and the 2D Womersley flow are simulated with the pressure and wall boundary condition proposed by Zou and He [13]. We find that the velocities for $0.75\leqslant\tau\leqslant 60$ agree with the analytical solution to a very high accuracy. Consider, e.g., a system with size $N_x\times N_y=21\times 21$. The maximal values of the relative error $\mathrm{err}(\mathbf{x}_i,t)$ are 5.0×10^{-3}, 1.0×10^{-4}, 1.0×10^{-5} for the maximal velocities 0.1, 0.01, and 0.001, respectively. Here $\mathrm{err}(\mathbf{x}_i,t)$ is defined at any node $\mathbf{x}_i$ and time t in the fluid domain as follows:

$$err(\mathbf{x}_i,t)=\frac{|\mathbf{u}(\mathbf{x}_i,t)-\mathbf{u}_0(\mathbf{x}_i,t)|}{|\mathbf{u}_0(\mathbf{x}_i,t)|}, \tag{10}$$

where $\mathbf{u}_0$ is the analytical solution. The density deviation $\delta\rho$ is found to decrease exponentially with time t after the first few steps. For $\tau=0.75$ and $b=0.001$, e.g., $\delta\rho\propto\exp(-\epsilon t)$ with $\epsilon\approx0.0022$ after first 100 steps for any node. We briefly compare our simulation results with those from conventional LBGK simulation. In the conventional LBGK model, $p=\rho/3$ so that the velocity at the centerline u_c increases linearly along the tube. The density is fixed to be ρ_0 in the present scheme so that the compressibility error is effectively reduced. Take the case for $\tau=6.5$ and $u_0\approx0.01$ for example, u_c changes about 5% from the inlet to the outlet in the conventional LBM while u_c varies less than 0.01% through the tube in our simulation.

The geometric configuration of the 2D Womersley flow (pulsatile flow in the 2D channel) [14] is identical to that of the plane Poiseuille flow, except that the flow is driven by a periodic pressure gradient at the entrance to the channel. The incompressible Navier-Stokes equation for the laminar flow is:

$$\frac{\partial u_x}{\partial t}=-\frac{\partial P}{\partial x}+\nu\frac{\partial^2 u_x}{\partial y^2}, \tag{11}$$

where the pressure gradient driving the flow is given by

$$\frac{\partial P}{\partial x}=\mathrm{Re}[Ae^{i\omega t}] \tag{12}$$

with an amplitude A and frequency ω. The solution of the above equation is

$$u_x(y,t)=\mathrm{Re}\left[i\frac{A}{\omega}\left(1-\frac{\cos[\lambda(2y/L_y-1)]}{\cos\lambda}\right)e^{i\omega t}\right], \tag{13}$$

where λ is given in terms of the Womersley number κ, as follows:

$$\lambda^2=-i\kappa^2,\quad \kappa^2=\frac{L_y^2\omega}{4\nu}. \tag{14}$$

In the simulation, the system size and the boundary conditions are the same as those used in the previous simulation for the Poiseuille flow. The period of the driving pressure is T ($\omega=2\pi/T$) and the magnitude of the total pressure drop along the channel is ΔP ($A=\Delta P/L_x$). The initial state of the velocity field is set to be zero everywhere in the system. The calculation of the velocity field always began with $10T$ initial steps to attain sufficient convergence.

In Fig. 2(a), the relative global error L^2 is plotted vs the maximal velocity in the system V_{max} for $\tau=0.75$ and $\tau=6.5$. Here L^2 is defined by

$$L^2=||\delta\mathbf{u}||^2=\frac{||\sum_i \mathbf{u}(\mathbf{x}_i,t)-\mathbf{u}_0(\mathbf{x}_i,t)||^2}{||\sum_i \mathbf{u}_0(\mathbf{x}_i,t)||^2}. \tag{15}$$

The summation is over the entire system; $\mathbf{u}_0$ is the analytical solution given by Eq. (13). In the simulation, $b=0.08$ and 0.20 for $\tau=0.75$ and $\tau=6.5$, respectively. It is clearly seen

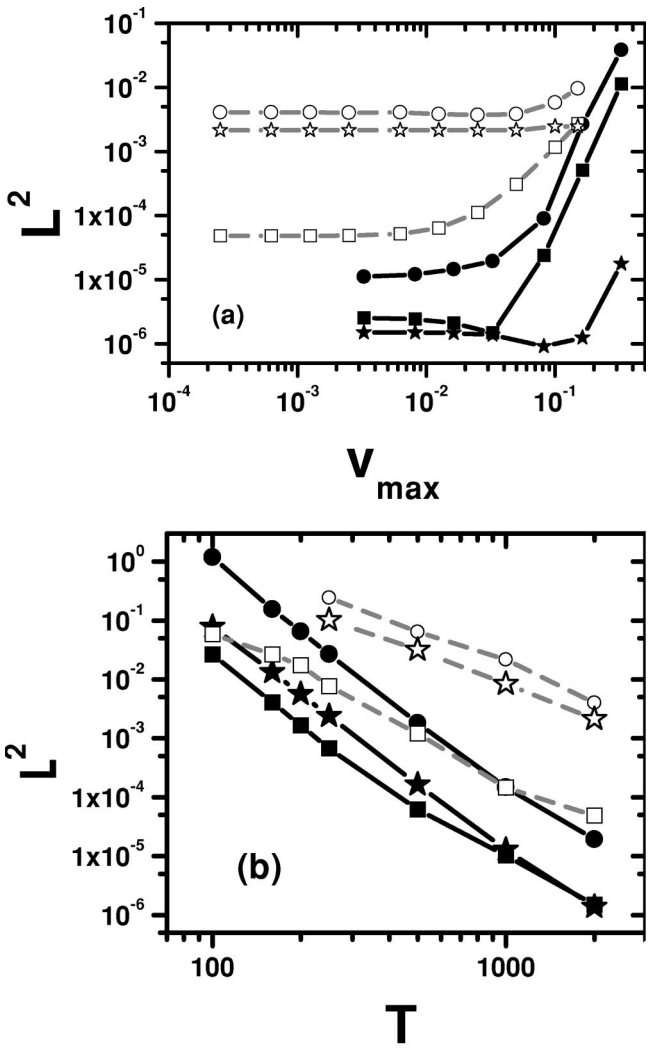

FIG. 2. Relative global error of velocity field L^2 in 2D Womersley flow for the LBGK model (circles), the He-Lou model (stars), and the present model (squares) with $\tau=0.75$ (filled symbols) and $\tau=6.5$ (open symbols). (a) Log-log plot of L^2 vs V_{max} for $T=2000$, where V_{max} is the maximal velocity in fluid domain. (b) Log-log plot of L^2 vs T for $A=0.0001$, where A is the amplitude of the driving pressure gradient.

that the present scheme improves the simulation results over those of the LBGK model greatly. In particular, L^2 is considerably reduced in the present model in comparison with He-Lou model for the case with $\tau=6.5$ and $V_{max}<0.1$.

We next consider the accuracy for the unsteady flow with various periods. Typical results are shown in Fig. 2(b) for $\tau=0.75$ and $\tau=6.5$. It is interesting to find the approximate power-law scaling $L^2\sim T^{-\zeta}$. The exponent ζ is dependent on τ, with $\zeta\approx3.5$ for $\tau=0.75$ and $\zeta\approx2.2$ for $\tau=6.5$, for all three models. More important, it is noted that the present model gives the smallest global errors. We emphasize that *the present scheme gives the best results at higher frequencies*, which is very important for the practical application of the lattice Boltzmann methods.

In the unsteady flow, the density at any node in the fluid domain does fluctuate around the expected density ρ_0 even

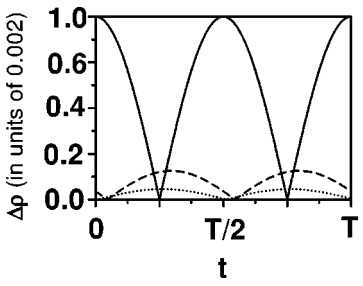

FIG. 3. The density difference $\Delta\rho$ between the inlet and outlet as a function of time t in a period for the case with $T=2000$ and $A=0.0001/3$, based on the conventional LBGK model and the present model with $\tau=0.75$ (dashed line) and $\tau=6.5$ (dotted line).

in the present model. The density deviation is, however, very small compared to the model by Qian [3] for the same driven pressure gradient. Figure 3 shows the density difference $\Delta\rho$ between the inlet and outlet as a function of time t in a period, for the case with $T=2000$ and $A=0.0001/3$, based on the conventional LBGK model and the present model with $\tau=0.75$ and $\tau=6.5$. It is seen that the density deviation in the present model is only a small fraction of that in the conventional LBGK model, suggesting that our scheme provides a good approach to incompressible fluid flow.

Finally, it is noted that as the DF's in the present model denote the fluid particle distributions, the conservation of the total DF's in the entire system, d_s, naturally results in an explicit mass conservation for closed system. In the previous incompressible models that are based on the redefinition of the velocity (see, e.g. [9]), the total DF's at a node, d_n, represents the pressure, rather than the density, the mass conservation for the system is established, only implicitly, by keeping the number of fluid nodes, N_n, unchanged during simulation. This lack of explicit mass conservation may lead to serious problems especially for closed systems. Let us consider for example, the fluid that fills a balloon. If the pressure outside the balloon increases during the simulation, then, d_n, which represents the pressure in fluid domain, should increase to balance the outside pressure. The total distribution functions in the balloon increase accordingly since the mass conservation demands that N_n stays constant. As a result, one has to put an extra global constraint on the boundary condition to add some more DF's to the system. This difficulty also arises in the system with a bubble of ''blue'' fluid inside an immiscible ''red'' fluid. The case is, however, much simpler if simulated using the present model. The mass conservation is naturally guaranteed, and the system will evolve into a state with greater A_1, while keeping the density almost unchanged.

To summarize, we have developed an LB model for incompressible fluid flow by introducing an extra relaxation for fluid density, or explicitly, by making only *very small* time-dependent perturbation to the ratio of the rest and moving parts of the EDF's. In our model, the density deviation $\delta\rho$ has been reduced effectively. Most of the compressible effect in the previous LB models has been eliminated. Moreover, we find that the numerical results can be further improved if a more complex feedback function is chosen [16]. The present model will be applied to study the pulsatile flow in the blood vessel [15]. We believe that the method can be extended to *target* the density, which may be related to the temperature, pressure, etc., in other LB models [17,18].

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