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On the basis of single phase lattice Boltzmann model(LBM), we construct a new LBM, which is more physical and computationally efficient, by introducing an effective attraction between particles with the same color in the equilibrium function to simulate immiscible two-phase flow. The separating simulation of two fluids illustrates its value.

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Conventional methods for simulating two-phase flow consist of numerical integration of the Navier-Stokes equations and molecular dynamics simulations.[1] These techniques are extremely computationally intensive and particularly difficult to implement in random geometry. In recent years, the lattice Boltzmann method(LBM) has been proved competitive.[2]

Several authors have set up lattice Boltzmann schemes for two-phase systems. Gunstensen *et al.*[3] developed the multiphase LBM in 1991. It was based on the two-phase lattice gas model proposed by Rothman and Keller[4] in 1988. Later, Grunan *et al.*[5] extended this model to allow variations of density and viscosity. However, as pointed by Chen *et al.*, [6] the multiphase LBM by Gunstensen *et al.* has two drawbacks: first, the procedure of redistribution of the colored density at each site requires time-consuming calculations of local maxima; second, the perturbation step with the redistribution of colored distribution functions causes an anisotropy surface tension that induces unphysical vortices near interfaces.

We think the second point above is crucial, since the procedure they adopt is more or less artificial. We here present a new lattice Boltzmann model for two-phase fluid flows:

Denote $f_a(\boldsymbol{x},t)$, $f_a^{\rm r}(\boldsymbol{x},t)$, and $f_a^{\rm b}(\boldsymbol{x},t)$ as the particle distribution functions at space $\boldsymbol{x}$ and time t for total, red and blue fluids, respectively. Here $a = 0, 1, \cdots, n$, $n = 6$ means FHP-7bit model,[7] a hexagonal lattice with rest particles at every site and $f_a(\boldsymbol{x},t) = f_a^{\rm r}(\boldsymbol{x},t)+f_a^{\rm b}(\boldsymbol{x},t)$. The lattice Boltzmann equation for both red and blue fluids can be written as follows:

$$f_a^k(\boldsymbol{x}+\boldsymbol{e}_a, t+1) = f_a^k(\boldsymbol{x},t) + \Omega_a^k(\boldsymbol{x},t) \qquad (1)$$

where k denotes either the red or blue fluid.

$\Omega_a^k(\boldsymbol{x},t)$ is the collision operator to describe the process of relaxation to local equilibrium. For simplicity, we use a linearized collision operator with a single time relaxation parameter τ^k (Ref. 2)

$$\Omega_a^k = -\frac{1}{\tau^k}(f_a^k - f_a^{k\rm eq}). \qquad (2)$$

where $f_a^{k\rm eq}$ is the local equilibrium state depending on the local density and velocity. The local equilibrium state can be arbitrarily chosen [8] with the exception that it must satisfy the conservation of mass and momentum:

$$\rho^{\rm r} = \sum_a f_a^{\rm r} = \sum_a f_a^{\rm req} \qquad (3a)$$

$$\rho^{\rm b} = \sum_a f_a^{\rm b} = \sum_a f_a^{\rm beq}, \qquad (3b)$$

and

$$\rho\boldsymbol{v} = \sum_{a,k} f_a^k \boldsymbol{e}_a = \sum_{a,k} f_a^{k\rm eq}\boldsymbol{e}_a \qquad (4)$$

with $\rho^{\rm r}$ and $\rho^{\rm b}$ density of the red and blue fluid respectively, $\rho = \rho^{\rm r} + \rho^{\rm b}$ the total density and $\boldsymbol{v}$ the local velocity.

Define the local color gradient as

$$\boldsymbol{F} = c_s^2 \sum_a \boldsymbol{e}_a[\rho^{\rm r}(\boldsymbol{x}+\boldsymbol{e}_a) - \rho^{\rm b}(\boldsymbol{x}+\boldsymbol{e}_a)]. \qquad (5)$$

To begin and maintain attractions between the particles with the same color, we choose the equilibrium distribution for both red and blue fluids as follows:

$$f_a^{k\rm eq} = \frac{1}{3}\left[\rho^k c_s^2 + \boldsymbol{e}_a\cdot\rho^k\boldsymbol{v}^k + \frac{2}{\rho^k}(\boldsymbol{e}_a\cdot\rho^k\boldsymbol{v}^k)^2 - \frac{1}{2\rho^k}(\rho^k v^k)^2\right], \qquad (6a)$$

$$f_0^{k\rm eq} = \rho^k(1-2c_s^2) - \frac{1}{\rho^k}(\rho^k v^k)^2, \qquad (6b)$$

where

$$\rho^{\rm r}\boldsymbol{v}^{\rm r} = b_f(\boldsymbol{F}) + \rho^{\rm r}\boldsymbol{v}, \qquad (7a)$$

$$\rho^{\rm b}\boldsymbol{v}^{\rm b} = -b_f(\boldsymbol{F}) + \rho^{\rm b}\boldsymbol{v}, \qquad (7b)$$

with b_f a parameter to adjust the intention of attraction.

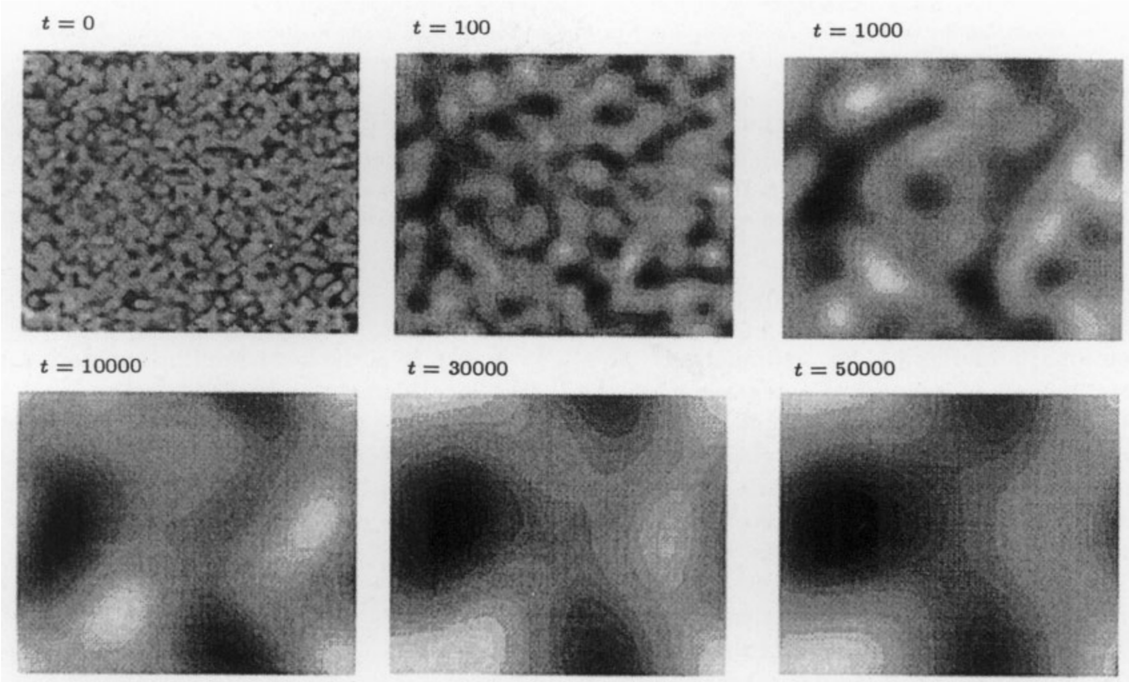

Fig. 1. Decomposition simulation of two-phase, illustrated at representative time steps. The initial configuration is a random mixture with a 3.5:6.5 mass ratio.

To demonstrate the application of the presented LBM, we show the separating simulation of two immiscible fluids below.

Figure 1 illustrates the non-equilibrium behavior of the two-fluid automation. The initial density of red phase at every site is randomly produced between 0.65 and 0.75. The blue particle density is determined by the condition: $\rho^r + \rho^b = 1$. Boundaries are periodic, both horizontally and vertically. Each particle distribution of six directions equals to one-nineth of the density and the rest particle distribution accounts for one-third of the density. In the plot, we show the density ratio of the red to the total and no averaging has been performed. The parameters are chosen as $\tau = 1.15$, $b_f = 0.107$.

Our aim in this paper is to present a more physical lattice Boltzmann approach to modeling phase separation. In our model, the recoloring skill of Gunstensen's LBM is replaced by an effective attraction between particles with the same color. Our simulation result illustrated that our model is physical and computationally efficient as well. We anticipate this model will be applicable to more complex two-phase fluid problems.

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