Electronic Supplementary Materials

For https://doi.org/10.1631/jzus.A2200047

Influence of wettability in immiscible displacements with lattice Boltzmann method

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Abstract This supplementary material for "Influence of wettability in immiscible displacements with Lattice Boltzmann method" contains fundamental theory of lattice Boltzmann method in Section S1 and the transformation matrix in Section S2.

S1 Fundamental theory

The discrete Boltzmann equation can be expressed as (Shan et al., 2006):

$$\frac{\partial f}{\partial t}+\xi_\alpha\frac{\partial f}{\partial x_\alpha}+\frac{F_\alpha}{\rho}\frac{\partial f}{\partial \xi_\alpha}=\Omega(f)\#(\mathrm{S1})$$

where f denotes distribution function, which satisfies:

$$\int f\mathrm{d}^D\xi=\rho\#(\mathrm{S2})$$
$$\int f\xi_\alpha\mathrm{d}^D\xi=\rho u_\alpha\#(\mathrm{S3})$$
$$\int\frac{1}{2}f|\boldsymbol{\xi}-\boldsymbol{u}|^2\mathrm{d}^D\xi=\rho\epsilon\#(\mathrm{S4})$$

where t denotes time, ξ_α and $\boldsymbol{\xi}$ denotes particle velocity, x_α denotes spatial location, F_α denotes unit volume force ($\alpha\in\{x,y,z\}$, which satisfies Einstein convention in 3D problems), ρ denotes density, D denotes number of spatial dimensions, $\Omega(f)$ denotes collision operator, u_α and $\boldsymbol{u}$ denote macroscopic velocity, and ϵ denotes internal energy density.

To simplify the calculations, the commonly used linear Bhatnagar-Gross-Krook (BGK) form is applied:

$$\Omega(f)=\frac{1}{\tau}(f-f^{eq})\#(\mathrm{S5})$$

where τ denotes dimensionless relax time, and f^{eq} denotes Maxwell-Boltzmann equilibrium distribution function. The BGK operator guarantees mass, momentum and energy conservation during collisions.

Compared with the empirical discretization developed from the early lattice gas cellular automaton (LGCA), Guass-Hermite quadrature can be naturally used to discretize the velocity based on the Hermite expansion of equilibrium distribution function (Chen and Doolen, 1998). D1Q3, D2Q9 and D3Q27 are three velocity discrete lattices derived from this discrete approach, where D means dimensions, and Q represents the number of discrete velocities. In cases where the effects of higher-order terms are not considered, the diffusion problem uses D2Q5 or D3Q15 models, while a simplified D3Q19 model is used for general 3D fluid flow problems.

Considering the computational efficiency, the D2Q9 lattice model is adopted in this article, and the lattice velocity vector $\boldsymbol{c}_i$ is:

$$\boldsymbol{c}_i = \begin{cases} (0,0), & i = 0 \\ (\cos[\pi(i-1)/2], \quad \sin[\pi(i-1)/2])c, & i = 1,2,3,4 \\ \sqrt{2}(\cos[\pi(i-5)/2+\pi/4], \quad \sin[\pi(i-5)/2+\pi/4])c, & i = 5,6,7,8 \end{cases} \#(S6)$$

where $c = \delta x/\delta t$, δx denotes lattice spacing, and δt denotes time step.

The distribution function still satisfies the conservation after the velocity discretization:

$$\sum_i f_i = \rho \#(S7)$$

$$\sum_i f_i \, c_{i\alpha} = \rho u_\alpha \#(S8)$$

$$\sum_i f_i \, c_{i\alpha} c_{i\beta} = \rho u_\alpha u_\beta + \sigma_{\alpha\beta} \#(S9)$$

where $\sigma_{\alpha\beta}$ denotes stress tensor ($\sigma_{\alpha\beta} = -\rho c_s^2 \delta_{\alpha\beta}$ if $f = f^{eq}$ where the lattice sound speed c_s equals $c/\sqrt{3}$). Under isothermal condition, the equation of state is $p = \rho c_s^2$, where p denotes pressure.

With the characteristic method to discrete time and space, the final discrete form becomes:

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \delta t, t + \delta t) = f_i(\boldsymbol{x},t) + \Omega_i\big(f_i(\boldsymbol{x},t)\big) \#(S10)$$

During the simulation process, the above equations are divided into two steps:

(1) collision:

$$f_i^{\dagger}(\boldsymbol{x}, t) = f_i(\boldsymbol{x}, t) + \Omega_i\big(f_i(\boldsymbol{x},t)\big) \#(S11)$$

(2) streaming:

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \delta t, t + \delta t) = f_i^{\dagger}(\boldsymbol{x}, t) \#(S12)$$

where

$$\Omega_i = \frac{1}{\tau}\big(f_i - f_i^{eq}\big) \#(S13)$$

$$f_i^{eq} = w_i \rho \left(1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2}\right) \#(S14)$$

and w_i denotes weight related to the lattice model. The kinetics viscosity $\nu = c_s^2\left(\tau - \frac{\Delta t}{2}\right)$ can be achieved with Chapman-Enskog expansion, which establishes the connection of the Lattice Boltzmann equations to the Navier-Stokes equations.

S2 Transformation matrix $\boldsymbol{M}$

The transformation matrix $\boldsymbol{M}$ can be explicitly given by (Lallemand and Luo, 2000):

$$\boldsymbol{M} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{bmatrix} \#(\mathrm{S15})$$

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