SIMULATION OF WETTING PHENOMENA USING THE REAL-CODED LATTICE GAS METHOD

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Abstract

With the introduction of color particles and a color-separating algorithm to the real-coded lattice gas method, some wetting related phenomena were simulated. A fluid-fluid wetting showed various patterns of dissipative phases according to the wettability between immiscible fluids, and a solid-fluid wetting showed that the contact angle of a droplet on a solid-surface changes by the geometric- and chemical-condition of the surface.

1. Introduction

There are great academic and practical interests in wetting related phenomena, where the interfacial energy plays an important role. As to the interfacial energy on a solid-fluid interface, it is difficult to be measured directly, and we usually introduce the value named contact angle to estimate it. The contact angle is a simple and intuitive value for estimating the interfacial energy, but in which there are some physical obscurities. The contact angle is influenced by geometric roughness and contamination of a surface, so that it does not give the interfacial energy itself directly. Furthermore, the contact angle is determined by the balance of the interfacial energy in an equilibrium state, and there is poor universality in investigating the non-equilibrium dynamics of a wetting. It is important to light on the relationship between the interfacial energy and surface condition.

The real-coded lattice gas method\[1\], we call it RLG, is a kind of a particle-based fluid model like Molecular Dynamics (MD). Instead of real molecules, RLG uses hypothetical particles, which have no volume and whose motion transports non-dimensional mass, momenta and kinetic energy. This reduction of physics makes RLG possible to simulate macroscopic flow phenomena, which have not been practicable by MD. Furthermore, we can describe boundary conditions as interactions among particles, and can easily define the framework for analyzing the dynamics of a surface-fluid interaction included in wetting phenomena. From these viewpoints, RLG is expected to be a versatile tool for complex hydrodynamics.

We developed the RLG method into an immiscible multi-phase fluid model by introducing color particles and a color-separating algorithm\[2-4\]. The color-separating algorithm, including a control parameter of wettability, allows us to simulate an immiscible multi-phase flow under the various wetting conditions. Using this novel fluid model, some wetting related dynamics, like a pattern formation of dissipative phases and a droplet wetting on a solid surface, were investigated.
2. The model

In this section, first the algorithm of the RLG method is explained, and subsequently, it is developed into an immiscible multi-phase fluid model, which can control the wettability between different phases.

2.1. Real-coded lattice gas

RLG consists of two sequential procedures, which describe the streaming and the collision of hypothetical particles. The particle has continuous values for their position and velocity. In the streaming process, they renew their positions according to their velocities. Subsequently in the collision process, they renewal their velocities by colliding with other particles, which occupy the same position. These two processes are executed for all particles simultaneously, and a successive calculation of the streaming and the collision brings the evolution of a whole system.

The streaming process is described in a standard way as

$$\mathbf{x}_i^s = \mathbf{x}_i + \mathbf{v}_i \Delta t,$$

(2.1)

where $\mathbf{x}_i$, $\mathbf{x}_i^s$ and $\mathbf{v}_i$ denote a pre-, post-streaming position and present velocity of particle $i$ respectively. $\Delta t$ is a discrete time step and equals to 1 in the following simulation. The velocity of a particle doesn’t change during the streaming process. In the collision process, space is discretized by the Wigner-Seitz cell centered on the nodes of a regular lattice, and particles in the same cell undergo collision. The collision is defined as a rotation of velocity deviations of every particle from the local mean velocity for each cell,

$$\mathbf{v}_i^c = \mathbf{V}_{\phi_i} + \Omega_{\phi_i} (\mathbf{v}_i - \mathbf{V}_{\phi_i}),$$

(2.2)

where $\mathbf{v}_i$ and $\mathbf{v}_i^c$ are pre- and post-collision velocities, $\mathbf{V}$ and $\Omega$ are the local mean velocity and a rotation matrix at cell $\hat{\mathbf{x}}_i$, which particle $i$ belongs in. The size of a spatial cell is 1 for each side, and these cells define the collision volume. For the particles in the same cell, the same rotation $\Omega$ is applied, but $\Omega$ may differ from cell to cell. The way to choose the rotation angle is related to the characteristic transport coefficients of the RLG fluid. The total mass, momenta and kinetic energy of particles are conserved locally in each cell under multi-particle collision dynamics, and it has been derived that these streaming and collision dynamics are lead to be hydrodynamic equations via the Boltzmann approximation and the Chapman-Enskog analysis[1].

2.2. The 2-phase model

Next, we introduce color particles and a color-separating algorithm into the RLG framework, in order to reproduce the flow phenomena including an immiscible binary-fluid wetting. First, we consider two colors, such as black and white for each particle, and the number of particles with color $\phi$ at cell $\hat{\mathbf{x}}$ is described as

$$N^{\phi}_{\hat{\mathbf{x}}} = \sum_i \delta(\hat{\mathbf{x}} - \hat{\mathbf{x}}_i) \delta(\phi - \phi_i),$$

(2.3)

where $\phi_i$ is a color of particle $i$, and $\delta$ is the Dirac’s delta function. In the same way, the sum of the relative velocities of particles with color $\phi$ to the local mean velocity at cell $\hat{\mathbf{x}}$ in the post-collision state is described as

$$Q^{\phi}_{\hat{\mathbf{x}}} = \sum_i \Omega_{\phi_i} (\mathbf{v}_i - \mathbf{V}_{\phi_i}) \delta(\hat{\mathbf{x}} - \hat{\mathbf{x}}_i) \delta(\phi - \phi_i),$$

(2.4)
Fig.1: Phase separation of binary fluids.
There are 256$^2$ cells; boundaries are periodic, both horizontally and vertically. The initial configuration ($t=0$) is a random mixture of black and white particles, and the snapshots show the time evolution. Black and white (light gray) areas in the figures denote the fluids of each color respectively. The last figure ($t=75000$) shows the equilibrium state of the phase separation, characteristic in the periodic boundary system, where not a circular, but a flat interface crossing the boundary makes the interface length minimum.

and we call it “color flux”. The color flux means a local deviation of color momentum after collision. On the other hand, the vector named “color field” is defined as following

$$F^{\phi}_{\vec{x}} = \sum_{n} \frac{N_{n}^{\phi}}{r_{n}} e_{n}, \quad (2.5)$$

where $\vec{x}_{n}$ is a neighboring cell of $\vec{x}$, $r_{n} = \vec{x}_{n} - \vec{x}$, $r_{n} = |r_{n}|$ and $e_{n} = r_{n}/r_{n}$. The color field is the direction-weighted sum of the numbers of particles, that means a local color gradient around the cell. In the following, neighboring cells within the distance of 2 cells are considered; there are 12 neighboring cells in 2-dimensional space. Using the color flux and the color field, “color work” is defined as

$$W_{\vec{x}} = Q_{\vec{x}}^{\phi} \cdot F_{\vec{x}}^{\varphi} + Q_{\vec{x}}^{\varphi} \cdot F_{\vec{x}}^{\phi}, \quad (2.6)$$

which means the work performed by the flux against the field between different colors $\phi$ and $\varphi$. By choosing the rotation matrix in eq. (2.4) as to minimize the color work (2.6), a separating tendency between different colors can be implemented into the collision process. The result of 2-dimensional simulation of spontaneous phase separation using the color-separating algorithm is shown in Fig.1. The snapshots show the time evolution of a mixture system. The far right figure corresponds to the equilibrium state after the phase separation. When the amount of two fluids is nearly in the periodic boundary system, not a circular interface, but a flat interface crossing boundaries makes the length of the interfacie minimum.

2.3. The multi-phase model

The color-separating algorithm can be extended easily to that for more than three-phase fluid by redefining the color work as the following,

$$W_{\vec{x}} = \sum_{\phi, \varphi, \rho} \chi_{\phi\varphi} (Q_{\vec{x}}^{\phi} \cdot F_{\vec{x}}^{\varphi}), \quad (2.7)$$

where $\chi_{\phi\varphi}$ ($= \chi_{\varphi\phi}$) is a weight coefficient for the pair of colors $\phi$ and $\varphi$, and call it “interfacial energy parameter” or $\chi$-parameter. The interfacial energy parameter is defined
Fig.2: A fluid-fluid wetting with different wettability.

There are $256^2$ cells; boundaries are periodic, both horizontally and vertically, and the figures show two periods of the system toward each direction. The initial configuration is a random mixture of black, gray and white colored particles. All figures show the snapshot in the equilibrium state at time step 30000. The wettability between a white (light gray) fluid and others (black and gray) has been changed.

as the relative strength of a separation tendency of a specific color pair to other pairs. For instance, when there are three colors of fluid, black(b), gray(g) and white(w), three $\chi$-parameters can be defined as $\chi_{bg}$, $\chi_{gw}$ and $\chi_{bw}$. If $\chi_{bg}$ is smaller than others, the color pair black and gray is easier to wet relatively to other pairs. Mixtures of more than three fluids yield different phenomena than those observed in a binary-fluid system, and the interfacial energy parameter allows us to simulate various situations of wetting.

3. Simulations

In this section, we apply the multi-phase fluid model formulated above to the simulations of some wetting related phenomena. They are categorized roughly into a fluid-fluid and solid-fluid wetting, and all simulations were carried out in 2-dimensional space.

3.1. A fluid-fluid wetting

First, we deal with a wetting between fluids. Fig.2 shows the results of phase separation for a mixture of three immiscible fluids represented by black, gray and white (light gray). $\chi_{bg}$ is 1.0 for all cases, and other combinations of $\chi$-parameters, which are related to white, have been changed. They are indicated below the figure for each case.

We can see that the difference of a wetting property determines the characteristic structure of dissipative phases, and also there is a critical point in a dissipative pattern at $\chi_{bw} = \chi_{gw} = 0.5$. This is simply explained with the balance of the interfacial energy at the contact point of three fluids (Fig.3). When the interfacial energy is in balance at the triple point, there exists a specific contact angle. But when it is larger than a resultant of the others, the triple point can no longer stay, and the contact angle changes dramatically. The balance breaks when $\chi_{bw}$ and $\chi_{gw}$ are less than 0.5, and the variation of dissipative patterns comes to arise there.

Fig.3: Balance at the triple point.
The sketch shows a balance of the interfacial energy at the triple point of three fluids of black, gray and white. $\chi_{\phi\psi}$ are the interfacial energy parameters. When $\chi_{bg}$ is larger than a resultant of the other pairs, the contact point moves to the left, and the contact angle changes dramatically.
There are $256 \times 128$ cells; Vertical boundaries are periodic, and horizontal ones are solid walls. In the initial condition, a block with $64 \times 32$ cells, consists of gray particles, is placed on a bottom surface, and an atmosphere region is filled by white particles. The bottom wall is colored by black. Each case except for the far left figure in Fig.4 is in the equilibrium state at $t = 12000$. In Fig.5 and Fig.6, $\chi_{bg}$, $\chi_{gw}$ and $\chi_{bw}$ are fixed at 1.0. In Fig.6, a 4th color corresponding to a contaminant is introduced (denoted by "c"). A contaminant is a small amount, and hard to distinguish in the figure, however, it is adhering on the solid surface (a bottom of the figure). $\chi_{bc}$ and $\chi_{sc}$ are fixed at 0.0 and 1.0 respectively, that is, a contaminant is wetting with a solid surface and non-wetting with an atmosphere fluid.

3.2. A solid-fluid wetting

Next, the color-algorithm was modified to simulate a solid-fluid wetting. A solid surface is implemented as a bounce-back wall, which reverses the velocity of a particle invading into the wall. The wall is also colored, and this effect appears in calculating the color field near the wall. A colored wall behaves as a colored cell, and $N_{\phi}$ in eq. (2.5) for the wall is counted by using the mean density of particles. In the following, a droplet wetting on a solid surface without gravity is simulated.

3.2.1. A smooth surface

Fig.4 shows a droplet wetting on an atomically smooth solid surface with different wettability. The far left figure is a snapshot at the initial condition, and others from (a) to (d) are in the equilibrium state after 12000 time steps running. A droplet consists of gray particles, and an atmosphere region is filled by white particles. The bottom boundary is a solid wall colored by black. $\chi_{bw}$ and $\chi_{gw}$ are fixed at 1.0 in all cases, and $\chi_{bg}$, which determines the wettability between a droplet and a wall, has been changed in each case. In the case of (c), three $\chi$-parameters are all 1.0, and a droplet contacts with a solid surface perpendicularly. Small $\chi_{bg}$ means that the wettability between a droplet and a wall is large, and in the case of (a), a droplet shows a total wetting on a surface. On the contrary,
large $x_{bg}$ in (d) makes the wall repel a droplet strongly. These are well-known geometric forms of a droplet wetting.

3.2.2. A rough surface

Fig.5 shows a droplet wetting on a rough solid surface. The rough surface is represented by a sine curve, and the wave number, corresponding to the roughness of the surface, has been changed. The amplitude of a wave was fixed at 8.0. The cases of (a) and (b) show that the contact angle for an inclined surface also follows the angle for a smooth surface locally. In addition, the results of (c), (d) and (e) predict that when the roughness is enough minute, the contact point is stable at the peak of ridges, and there will be a discrete transition of a wetting front.

3.2.3. A contaminated surface

The last simulation of a droplet wetting is on a contaminated surface shown in Fig.6. There exist four colors, which represent a droplet (gray), an atmosphere (white), a wall (black: bottom of the figure) and a contaminant; the contaminant is adhering on a solid surface, and a very small amount relatively to other fluids, so it can not be seen clearly. The wettability between a contaminant and a droplet has been changed. In the case of high wettability, a wetting front of a droplet rises gently, and in the case of low wettability, a contaminant repels a droplet.

4. Conclusions

We introduced a general algorithm for describing the immiscible multi-fluid hydrodynamics into the RLG method. Phase separations of three-phase fluid mixtures and droplet's behavior on a solid surface have been demonstrated under the various wetting conditions. In the latter case, it was observed that a droplet could have a discrete transition of a wetting front between the ridges on a rough surface. These results show that the RLG method, which can describe hydrodynamics and surface dynamics equivalently from a constructive approach, has a great potential for the investigation of wetting phenomena from the mesoscopic viewpoint.

References


