Multiphase Flow Laboratory
Aerospace Engineering Group
Shahid Beheshti University

Report 01092017-E2

Title:

A Multiphase Lattice Boltzmann Method based on the Cahn-Hilliard Equation

By:

Eslam Ezzatneshan
Assistant Professor

Summer 2017

Governing Equations

1. Cahn-Hilliard model

In this report, a lattice Boltzmann diffuse interface model [1] is used for simulation of incompressible multicomponent fluids flow with different densities and viscosities. The order parameter C is defined to evaluate the composition of each phase in the domain. If a two-phase fluid flow is considered, say gas as light fluid and liquid as heavy one, C is calculated as the volume fraction of one of the two-phases. This parameter is assumed to be constant in the bulk phases, e.g. $C = 0$ for the gas phase while $C = 1$ for the liquid phase. In the interfacial region however, C changes rapidly but smoothly between 0 to 1. In traditional Navier-Stokes based solvers, the Cohn-Hilliard equation (CHE) efficiently applied to solve the time evaluation of the diffuse interface for such problems:

$$\partial_t C + \mathbf{u}.\nabla C = M\nabla^2\mu \tag{1}$$

where $\mathbf{u}$ is the flow velocity vector and M is the mobility. The chemical potential μ can be derived from the free-energy functional

$$\Psi = \int_V \psi(C, \nabla C)dV = \int_V \left[\beta C^2(C-1)^2 + \frac{\kappa}{2}|\nabla C|^2\right]dV \tag{2}$$

where β is constant and κ is a coefficient related to the surface tension. By minimizing the free energy functional, the chemical potential is given by:

$$\mu = \frac{\partial\psi}{\partial C} = 2\beta C(C-1)(2C-1) - \kappa\nabla^2 C \tag{3}$$

---

definition:

The first term in the right hand side of the equation (3) is known as classical part of the chemical potential μ_0:

$$\mu_0 = \frac{\partial\psi_0}{\partial C} = 2\beta C(C-1)(2C-1)$$

where $\psi_0 = \beta C^2(C-1)^2$ is the bulk energy.

The order parameter C across the interface of a plannar gas-liquid two-phase flow in z −direction can be obtained from Eq. (3) at $\mu = 0$:

$$C(z) = \frac{1}{2} + \frac{1}{2}\tanh(\frac{2z}{D}) \tag{4}$$

where D is the interface thickness and chosen according to accuracy and stability of the numerical solution. Constants β and κ can be computed based on the given surface tension force σ and D with the following equations [2]:

$$\kappa = \frac{\beta D^2}{8} \quad , \quad \sigma = \frac{\sqrt{2\kappa\beta}}{6} \tag{5}$$

With consideration of surface tension, the governing equations of the incompressible fluid flows can be written as:

$$\begin{gathered} \nabla.\mathbf{u} = 0, \\ \rho(\partial_t \mathbf{u} + \mathbf{u}.\boldsymbol{\nabla}\mathbf{u}) = -\nabla p - C\nabla\mu + \nabla.[\eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T)] \end{gathered} \tag{6}$$

where p is pressure, $\rho = C\rho_l + (1 - C)\rho_g$ is the average density and $\eta = C\eta_l + (1 - C)\eta_g$ is the average viscosity. The subscripts l and g denote the liquid phase and gas phase properties, respectively.

2. *Lattice Boltzmann equations*

Herein, the multiphase lattice Boltzmann model developed based on the Cohn-Hilliard equation [2], known as free-energy based model, is used for simulation of multicomponent multiphase flows.

$$\begin{gathered} \frac{\partial g_\alpha}{\partial t} + \mathbf{e}_\alpha.\nabla g_\alpha = -\frac{1}{\lambda}(g_\alpha - g_\alpha^{eq}) + \\ (\mathbf{e}_\alpha - \mathbf{u}).[\nabla\rho c_s^2(\Gamma_\alpha - \Gamma_\alpha(0)) - C\nabla\mu\Gamma_\alpha] \\ g_\alpha^{eq} = t_\alpha\left[p_1 + \rho c_s^2\left(\frac{\mathbf{e}_\alpha.\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha.\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}.\mathbf{u}}{2c_s^2}\right)\right] \end{gathered} \tag{7}$$

$$\begin{gathered} \frac{\partial h_\alpha}{\partial t} + \mathbf{e}_\alpha.\nabla h_\alpha = -\frac{1}{\lambda}(h_\alpha - h_\alpha^{eq}) + \\ (\mathbf{e}_\alpha - \mathbf{u}).\left[\nabla C - \frac{C}{\rho c_s^2}(\nabla p_1 - C\nabla\mu)\right]\Gamma_\alpha + \nabla.(M\nabla\mu)\Gamma_\alpha \\ h_\alpha^{eq} = t_\alpha C\left[1 + \frac{\mathbf{e}_\alpha.\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha.\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}.\mathbf{u}}{2c_s^2}\right] \end{gathered} \tag{8}$$

where, $c_s^2 = 1/3$,

$$\Gamma_\alpha = \Gamma_\alpha(\mathbf{u}) = t_\alpha \left[1 + \frac{\mathbf{e}_\alpha . \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha . \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}.\mathbf{u}}{2c_s^2}\right] \tag{9}$$

and

$$t_\alpha = \begin{cases} \frac{1}{3} & \alpha = 0 \\ \frac{1}{18} & \alpha = 1,\ldots,6 \\ \frac{1}{36} & \alpha = 7,\ldots,18 \end{cases} \tag{10}$$

It should be note that the pressure p in the momentum part of Eq. (6) can be regarded as the sum of the thermodynamic part p_0, hydrodynamic part p_1 and the curvature part:

$$p = p_0 + p_1 - \kappa C \nabla^2 C + \frac{\kappa}{2}|\nabla C|^2 \tag{11}$$

But in the lattice Boltzmann equations used for simulation, only the hydrodynamic part p_1 is appeared. For more details, please see the following note.

Note:

The thermodynamic pressure p_0 is determined by an appropriate equation of state and it appears in the external force term $\mathbf{F}$ which models the non-ideal effects [3]:

$$\mathbf{F} = \nabla \rho c_s^2 - \nabla p_0 + \rho \kappa \nabla \nabla^2 \rho$$

when

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha . \nabla f_\alpha = -\frac{1}{\lambda}(f_\alpha - f_\alpha^{eq}) + (\mathbf{e}_\alpha - \mathbf{u}).\mathbf{F} f_\alpha^{eq}$$

But the discretized form of above lattice Boltzmann equation (DBE) is unstable with such definition for external force term, partly because of parasitic currents which arise from imbalance between the thermodynamic pressure gradient ∇p_0 and the surface tension term $\rho \kappa \nabla \nabla^2 \rho$ due to the truncation error.

It has been shown that the truncation error and the resulting parasitic currents can be eliminated by the potential form of thermodynamic identity, $\nabla p_0 = \rho \nabla \mu_0(\rho)$ [4]. Then, the thermodynamic pressure p_0 defines by:

$$p_0 = C\frac{\partial \psi_0}{\partial C} - \psi_0 = C\mu_0 - \psi_0 = \beta C^2(C-1)(3C-1)$$

Finally, $\mathbf{F}$ for binary fluids is obtained by replacing the order parameter from the density to the phase or composition measure C, and considering the free energy of the system [5]. It includes the hydrodynamic pressure p_1 that enforces incompressibility:

$$\mathbf{F} = \nabla \rho c_s^2 - \nabla p_1 - C\nabla \mu$$

Now, with definition of a new particle distribution function $g_\alpha = f_\alpha c_s^2 + (p_1 - \rho c_s^2)\Gamma_\alpha(0)$, the DBE for the mass and momentum equations transforms into DBE for the pressure evaluation and momentum equations [6], like Eq. (7).

Discretization Procedure

The Navier-Stokes equations and CHE are solved in the multiphase LBM proposed by Lee and Liu [2] by applying the trapezoidal rule along characteristics over time step δt at (x,t) and introducing the nondimensional relaxation time $\tau = \lambda/\delta t$. To ensure the numerical stability in solving high-density ratio problems, the second-order mixed difference (MD) is applied to discretize the derivatives involved in the forcing terms in the pre-streaming collision step, while the standard central difference (CD) in the post-streaming collision step.

$$\begin{aligned}\bar{g}_\alpha(x,t) = \bar{g}_\alpha(x-\mathbf{e}_\alpha\delta t, t-\delta t) - \frac{1}{\tau+0.5}(\bar{g}_\alpha - \bar{g}_\alpha^{eq})\big|_{(x-\mathbf{e}_\alpha\delta t, t-\delta t)} \\ + \delta t(\mathbf{e}_\alpha - \mathbf{u}).[\nabla^{MD}\rho c_s^2(\Gamma_\alpha - \Gamma_\alpha(0)) - C\nabla^{MD}\mu\Gamma_\alpha]_{(x-\mathbf{e}_\alpha\delta t, t-\delta t)}\end{aligned} \quad (12)$$

$$\bar{g}_\alpha^{eq} = g_\alpha^{eq} - \frac{\delta t}{2}(\mathbf{e}_\alpha - \mathbf{u}).[\nabla^{CD}\rho c_s^2(\Gamma_\alpha - \Gamma_\alpha(0)) - C\nabla^{CD}\mu\Gamma_\alpha]$$

and

$$\bar{h}_\alpha(x,t) = \bar{h}_\alpha(x-\mathbf{e}_\alpha\delta t, t-\delta t) - \frac{1}{\tau+0.5}\left(\bar{h}_\alpha - \bar{h}_\alpha^{eq}\right)\Big|_{(x-\mathbf{e}_\alpha\delta t, t-\delta t)}$$
$$+ \delta t(\mathbf{e}_\alpha - \mathbf{u}).\left[\nabla^{MD}\mathrm{C} - \frac{C}{\rho c_s^2}(\nabla^{MD}p_1 - C\nabla^{MD}\mu)\right]\Gamma_\alpha\Big|_{(x-\mathbf{e}_\alpha\delta t, t-\delta t)} \quad (13)$$
$$+ \delta t M(\nabla^2\mu)\Gamma_\alpha|_{(x-\mathbf{e}_\alpha\delta t, t-\delta t)}$$
$$\bar{h}_\alpha^{eq} = h_\alpha^{eq} - \frac{\delta t}{2}(\mathbf{e}_\alpha - \mathbf{u}).\left[\nabla^{CD}\mathrm{C} - \frac{C}{\rho c_s^2}(\nabla^{CD}p_1 - C\nabla^{CD}\mu)\right]\Gamma_\alpha - \frac{\delta t}{2}M(\nabla^2\mu)\Gamma_\alpha$$

1. ***Directional derivatives of macroscopic variable*** ϕ (C, μ or p_1)
   a) First derivative by second-order central difference (CD):
   $$\delta t\mathbf{e}_\alpha.\nabla^{CD}\phi|_{(x)} = \frac{1}{2}[\phi(x+\mathbf{e}_\alpha\delta t) - \phi(x-\mathbf{e}_\alpha\delta t)]$$
   b) First derivative by second-order mixed difference (MD):
   $$\delta t\mathbf{e}_\alpha.\nabla^{MD}\phi|_{(x)} = \frac{1}{2}[\delta t\mathbf{e}_\alpha.\nabla^{BD}\phi + \delta t\mathbf{e}_\alpha.\nabla^{CD}\phi)]_{(x)}$$
   where (BD) is second-order biased-difference, e.g. forward one is:
   $$\delta t\mathbf{e}_\alpha.\nabla^{BD}\phi|_{(x)} = \frac{1}{2}[-\phi(x+\mathbf{2}\mathbf{e}_\alpha\delta t) + 4\phi(x+\mathbf{e}_\alpha\delta t) - 3\phi(x)]$$
   c) Second derivative by second-order central difference:
   $$(\delta t\mathbf{e}_\alpha.\nabla)^2\phi|_{(x)} = [\phi(x+\mathbf{e}_\alpha\delta t) - 2\phi(x) + \phi(x-\mathbf{e}_\alpha\delta t)]$$

2. ***Non-Directional derivatives of macroscopic variable*** ϕ (C, μ or p_1)
   a) First derivative by second-order central difference (CD):
   $$\nabla^{CD}\phi|_{(x)} = \frac{1}{c_s^2\delta t}\sum_{\alpha\neq 0} t_\alpha\mathbf{e}_\alpha(\delta t\mathbf{e}_\alpha.\nabla^{CD}\phi|_{(x)})$$
   b) First derivative by second-order mixed difference (MD):
   $$\nabla^{MD}\phi|_{(x)} = \frac{1}{2}[\nabla^{BD}\phi + \nabla^{CD}\phi]_{(x)}$$
   where
   $$\nabla^{BD}\phi|_{(x)} = \frac{1}{c_s^2\delta t}\sum_{\alpha\neq 0} t_\alpha\mathbf{e}_\alpha(\delta t\mathbf{e}_\alpha.\nabla^{BD}\phi|_{(x)})$$
   c) Laplacian of ϕ

$$\nabla^2\phi|_{(x)} = \frac{1}{c_s^2\delta t^2}\sum_{\alpha\neq 0} t_\alpha\,(\delta t\mathbf{e}_\alpha.\nabla)^2\phi|_{(x)}$$

More details:

In the case of $D3Q19$ model, the first derivative of ϕ in x-direction by non-directional discretization with 2nd-order central difference scheme can be:

$$\begin{aligned}\nabla^{CD}\phi|_{(x)} \quad = \quad & \frac{1}{6}\left(\phi_{i+1,j,k} - \phi_{i-1,j,k}\right) \\ & + \frac{1}{12}\left[\left(\phi_{i+1,j+1,k} - \phi_{i-1,j-1,k}\right) + \left(\phi_{i+1,j-1,k} - \phi_{i-1,j+1,k}\right)\right. \\ & + \left.\left(\phi_{i+1,j,k+1} - \phi_{i-1,j,k-1}\right) + \left(\phi_{i+1,j,k-1} - \phi_{i-1,j,k+1}\right)\right]\end{aligned}$$

The same discretization procedure can be used for the first derivative of ϕ in y- and z-directions.

The Laplacian of ϕ can be calculated using the following finite-difference scheme

$$\begin{aligned}\nabla^2\phi|_{(x)} = & \frac{1}{3}\left[\left(\phi_{i+1,j,k} + \phi_{i-1,j,k}\right) + \left(\phi_{i,j+1,k} + \phi_{i,j-1,k}\right) + \left(\phi_{i,j,k+1} + \phi_{i,j,k-1}\right)\right] \\ & + \frac{1}{6}\left[\left(\phi_{i+1,j+1,k} + \phi_{i-1,j-1,k}\right) + \left(\phi_{i+1,j-1,k} + \phi_{i-1,j+1,k}\right)\right. \\ & + \left(\phi_{i+1,j,k+1} + \phi_{i-1,j,k-1}\right) + \left(\phi_{i+1,j,k-1} + \phi_{i-1,j,k+1}\right) \\ & + \left.\left(\phi_{i,j+1,k+1} + \phi_{i,j-1,k-1}\right) + \left(\phi_{i,j+1,k-1} + \phi_{i,j-1,k+1}\right)\right] - 4\phi_{i,j,k}\end{aligned}$$

Variabels

$$C = \sum_\alpha \bar{h}_\alpha + \frac{\delta t}{2}M\nabla^2\mu$$

$$\rho\mathbf{u} = \frac{1}{c_s^2}\sum_\alpha \mathbf{e}_\alpha\bar{g}_\alpha - \frac{\delta t}{2}C\nabla^{CD}\mu$$

$$p = \sum_\alpha \bar{g}_\alpha - \frac{\delta t}{2}\mathbf{u}.\nabla^{CD}\,\rho c_s^2$$

$$\rho(C) = C\rho_l + (1-C)\rho_g \quad , \quad \rho_{l,g} = \text{const.}$$

$$\tau(C) = C\tau_l + (1 - C)\tau_g \quad , \quad \tau_{l,g} = \frac{\nu_{l,g}}{c_s^2 \delta t} = \text{const.}$$

for the given surface tension force σ and (numerical) interface thickness D,

$$D = \frac{4}{(\rho_l - \rho_g)} \sqrt{\frac{\kappa}{2\beta}}$$

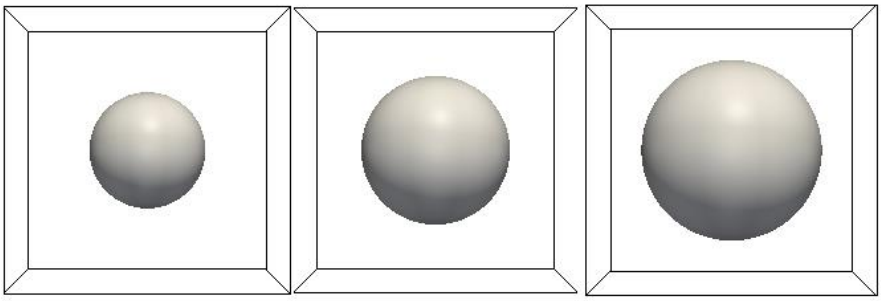
$$\sigma = \frac{(\rho_l - \rho_g)^3}{6} \sqrt{2\kappa\beta}$$

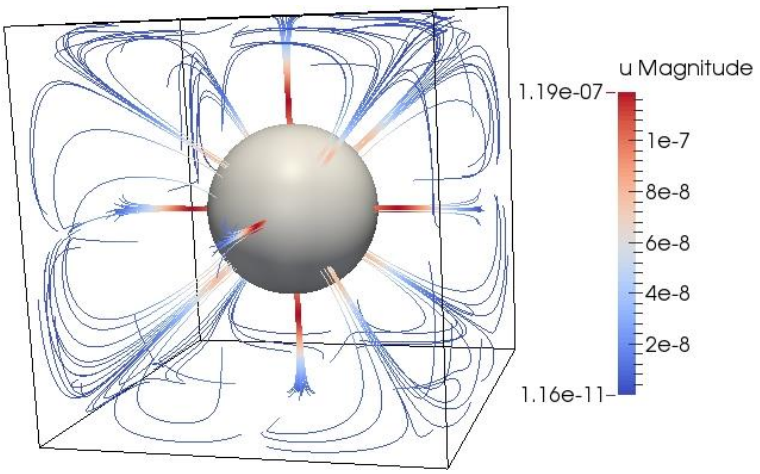
$$\mu = \mu_0 - \kappa \nabla^2 C$$

Results for problems with Periodic B.C.

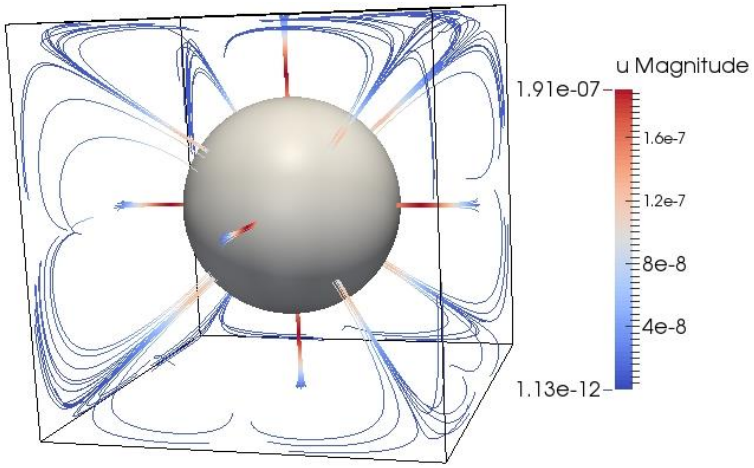
1. One Droplet in Equilibrium State

A droplet in a stationary flow is simulated as a benchmark problem. A computational domain $101 \times 101 \times 101$ is considered and the periodic boundary condition is applied on the all sides of the domain. The interface thickness, density ratio, viscosity ratio, interface tension and relaxation time are $= 5$, $\frac{\rho_l}{\rho_g} = 1000$, $\frac{\eta_l}{\eta_g} = 100$, $\sigma = 10^{-3}$ and $\tau = 1$. To verify the Laplace law of $\Delta p = 2\sigma/R$, three different drop radiuses $R_0 = 25, 30$ and 35 are studied (left to right, respectively).

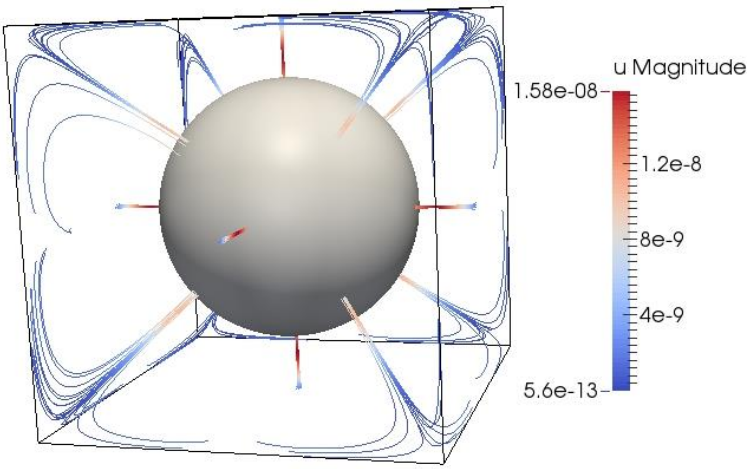




$R_0 = 25$



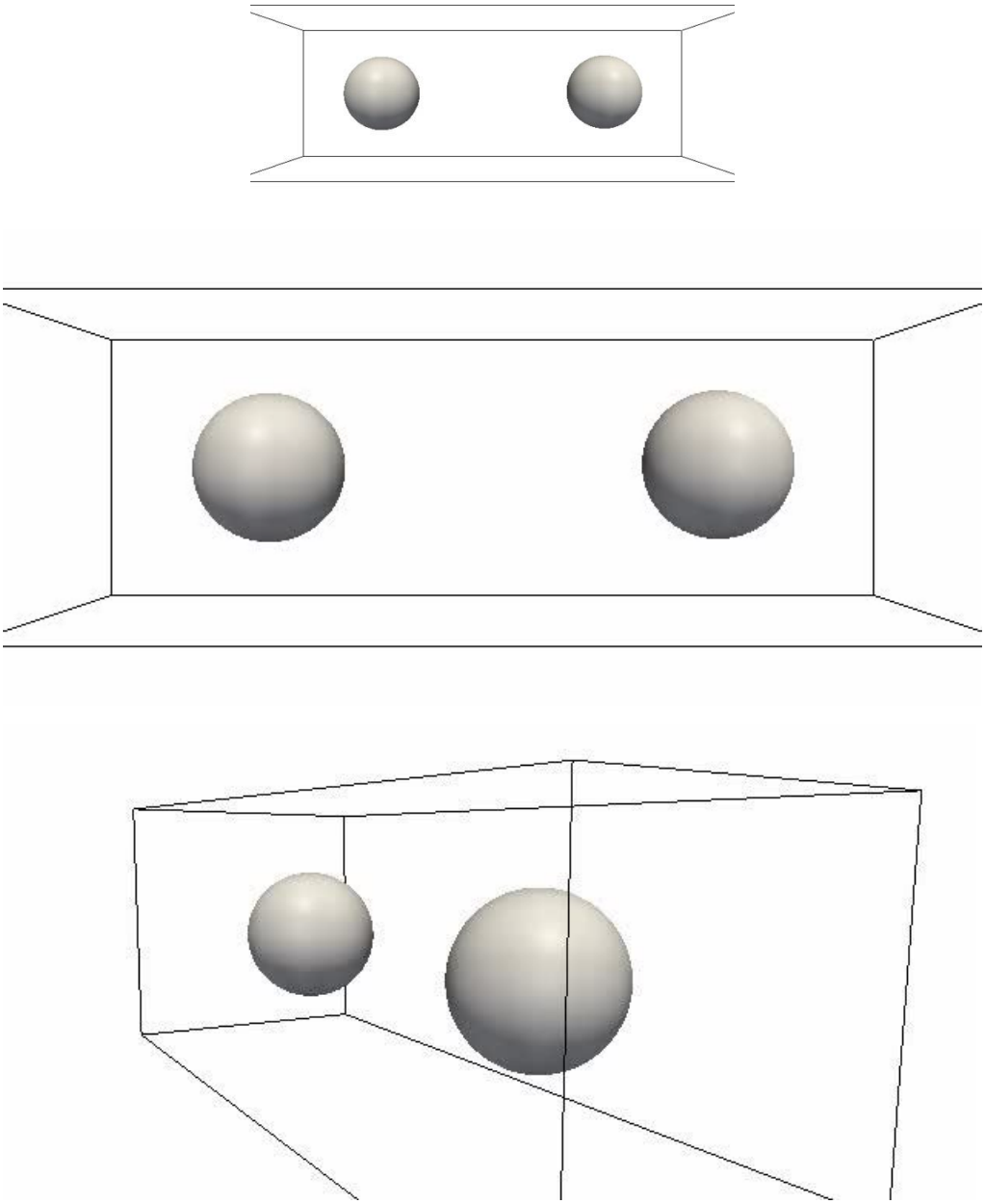
$R_0 = 30$

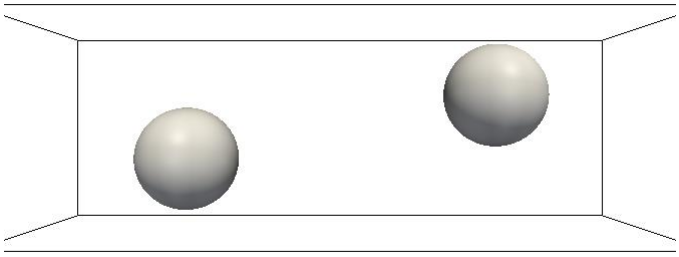


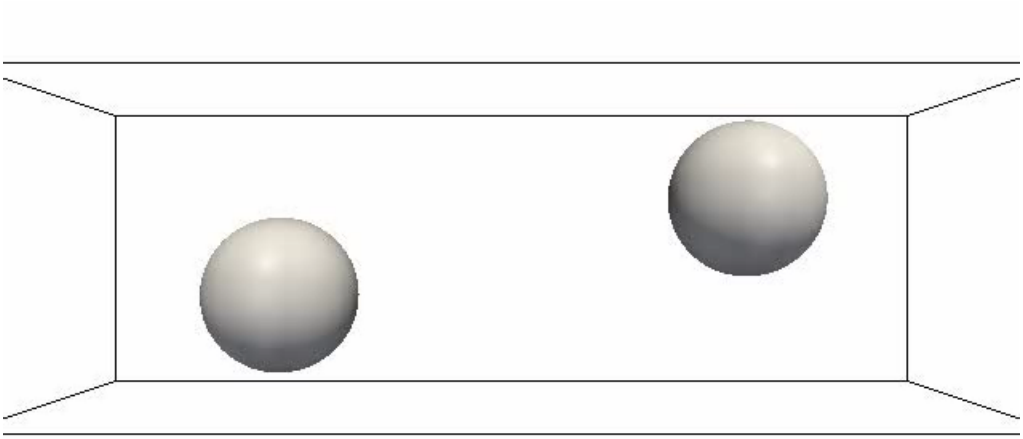
$R_0 = 35$

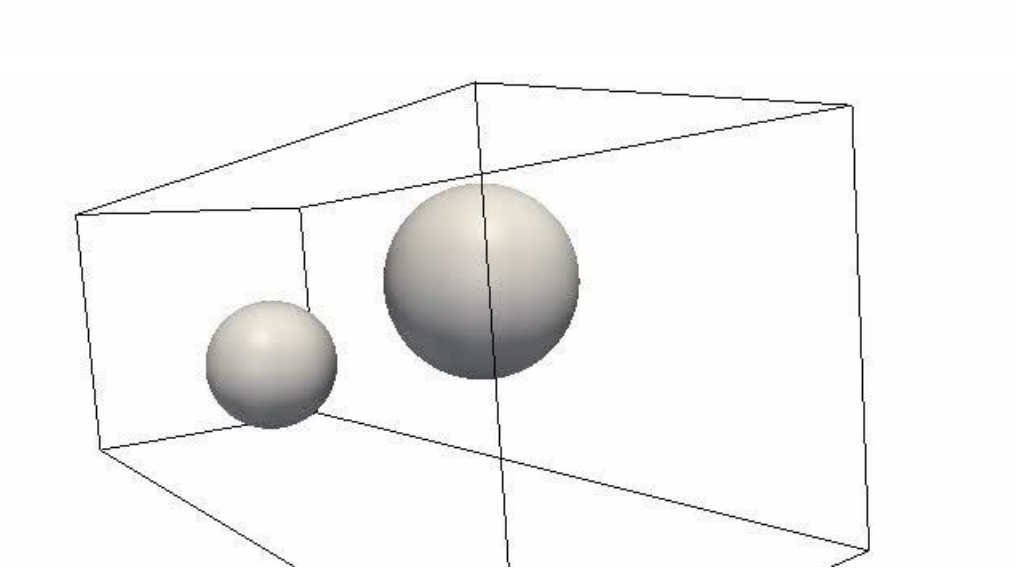
2. *Collision of Two Droplets*

The 3D in-line and off-center droplet collisions are simulated. Two droplets with the same radius $R_0 = 25$ were placed in the flow domain with $301 \times 101 \times 101$ grid points. The periodic boundary condition is applied on the all sides of the domain. The interface thickness, density ratio, viscosity ratio, interface tension and relaxation time are $= 5$, $\frac{\rho_l}{\rho_g} = 1000$, $\frac{\eta_l}{\eta_g} = 100$, $\sigma = 10^{-4}$ and $\tau = 1$. Two dimensionless parameters are Weber number $We = \frac{\rho_l \times 2R \times U^2}{\sigma}$ and Reynolds number $Re = \frac{\rho_l \times 2R \times U}{\eta_l}$, which are calculated based on the droplet diameter and relative impact velocity U. In this study, $We = 800$ and $Re = 60$ are considered.





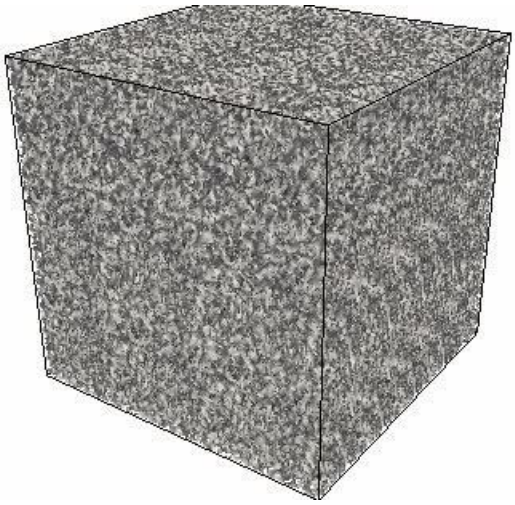


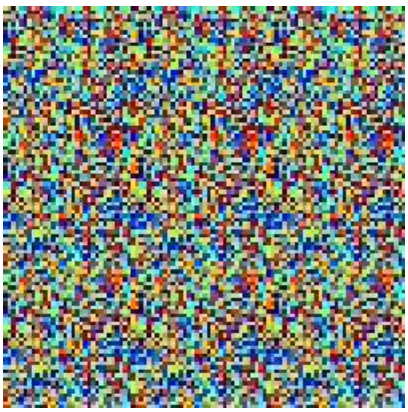


3. Phase Separation

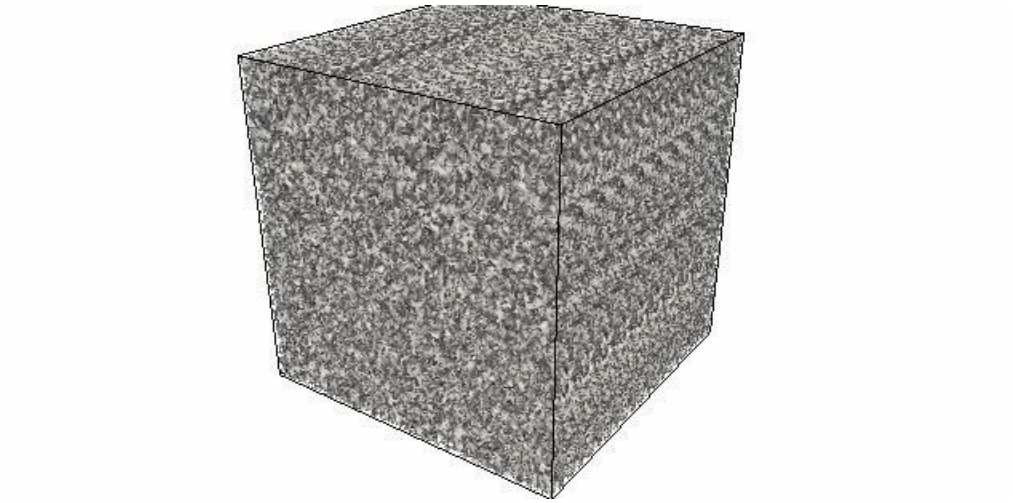
The phase separation from an initial random state is simulated in this section. The numerical simulation is performed in a $101 \times 101 \times 101$ domain. The initial density is taken as $\rho = \rho_{ref} + \tilde{\rho}$, where $\rho_l > \rho_{ref} > \rho_g$ is a reference density and $\tilde{\rho}$ is a small random perturbation. It should be note that, the value of $\tilde{\rho}$ effects on the spinodal decomposition phenomena. Herein, the periodic boundary condition is applied on the all sides of the domain as well. The interface thickness, density ratio, viscosity ratio, and relaxation time are $= 5$, $\frac{\rho_l}{\rho_g} = 10$, $\frac{\eta_l}{\eta_g} = 10$, and $\tau = 1$.

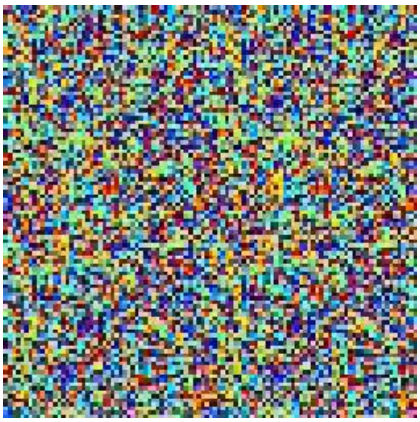
$$\sigma = 10^{-3}, \tilde{\rho} = 0.001$$





$$\sigma = 10^{-4}, \tilde{\rho} = 0.1$$





Implementation of Wall Boundary Conditions:

a) Bounce-back scheme for unknown particle distribution functions g and h at the wall nodes.
b) Two B.C.s related to the C-H equation and contact angle:

$$\mathbf{n}.\nabla\mu|_s = 0,$$

$$\mathbf{n}.\nabla C|_s = \frac{\phi_c}{\kappa}(C_s - C_s^2).$$

where

$$\phi_c = \Omega_c\sqrt{2\kappa\beta}$$
$$\cos\theta^{eq} = -\Omega_c$$

References

1. Lee, T. and L. Liu, *Lattice Boltzmann simulations of micron-scale drop impact on dry surfaces.* Journal of Computational Physics, 2010. **229**(20): p. 8045-8063.
2. Lee, T., *Effects of incompressibility on the elimination of parasitic currents in the lattice Boltzmann equation method for binary fluids.* Computers & Mathematics with Applications, 2009. **58**(5): p. 987-994.
3. He, X., X. Shan, and G.D. Doolen, *Discrete Boltzmann equation model for nonideal gases.* Physical Review E, 1998. **57**(1): p. R13-R16.
4. Lee, T. and P.F. Fischer, *Eliminating parasitic currents in the lattice Boltzmann equation method for nonideal gases.* Physical Review E, 2006. **74**(4).
5. Lee, T. and C.L. Lin, *A stable discretization of the lattice Boltzmann equation for simulation of incompressible two-phase flows at high density ratio.* Journal of Computational Physics, 2005. **206**(1): p. 16-47.
6. Lee, T. and C.L. Lin, *Pressure evolution lattice-Boltzmann-equation method for two-phase flow with phase change.* Phys Rev E Stat Nonlin Soft Matter Phys, 2003. **67**(5 Pt 2): p. 056703.