5. Multiphase flow & the lattice-Boltzmann method

5.1 Introduction

The lattice-Boltzmann method finds significant application in multiphase flow. It has been used for simulating gas bubbles or liquid drops moving through a continuous phase liquid (emulsions), for solid particles dispersed in a gas or a liquid (suspensions), and for liquid drops in a gas − as in sprays. Simulation of multiphase flow – with the lattice-Boltzmann method or with any other numerical scheme – can be done at various levels of detail.

In *interface-resolved* methods, the interfaces between the phases (solid-fluid interfaces in suspensions, fluid-fluid interfaces with interfacial tension in emulsions) are captured explicitly in the simulation (see Figure 5.1). In *particle-unresolved* simulations, the "particles" (that – next to solid particles – can also be drops or bubbles) are typically smaller than the lattice spacing and are thus not explicitly resolved (see Figure 5.2). However, the effect of the particles on the continuous fluid phase – and vice versa – needs to be accounted for as accurately as possible.
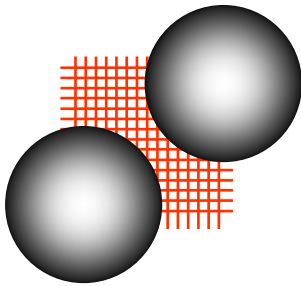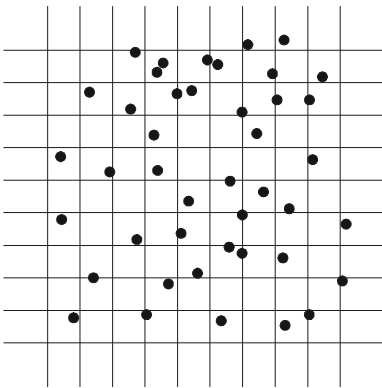

Figure 5.1 Interface-resolved: $d>\Delta$.

Figure 5.2 Particle-unresolved: $d<\Delta$.

In the current lecture notes we will be discussing two types of multiphase flow simulations involving the lattice-Boltzmann method. In the first type, these are interface-resolved simulations of a system of two immiscible fluids with interfacial tension. For this we will be exploring the *diffuse interface free energy lattice-Boltzmann method*. In the second type, these are particle-unresolved simulations of solid-fluid systems that require a procedure for solving the *volume-averaged Navier-Stokes equation* by means of the LB method.

As an aside: particle-resolved simulations of suspension (solid-fluid systems) can be done with the lattice-Boltzmann method as well. One option for this is the immersed boundary

method as discussed in LN04. Extending the 2D example of a cylinder immersed in a fluid to 3D will give you the opportunity to simulate – in principle – arbitrarily shaped particles moving through fluid by representing the particle by a set of closely spaced marker points on its surface.

5.2 Free energy lattice-Boltzmann method

We are dealing with a system of two immiscible fluids, one being the continuous phase, the other the dispersed phase that is in the form of droplets (e.g. oil droplets in water with water the continuous phase and oil the dispersed phase). The two fluids in general have different viscosities (symbols ν_c and ν_d) and densities (ρ_c and ρ_d). The interface between the liquids is associated with an interfacial tension (symbol γ). Interfacial tension has SI unit N/m which is the same as J/m^2. It can thus be associated with the energy per interfacial surface area; in terms of the Young-Laplace equation it can be associated with a pressure difference over a curved surface ($\Delta p \propto \gamma/R$ with R the radius of curvature).

The *free energy lattice-Boltzmann* method is a *diffuse interface* method. It works by solving a single Navier-Stokes equation and a single continuity equation. The density and viscosity in these equations varies in space and time. Density and viscosity are equal to ρ_c and ν_c in the continuous phase fluid, to ρ_d and ν_d in the dispersed phase fluid and change sharply but continuously in the interface between the two fluids. The interface thus has finite thickness – i.e. it is *diffuse*. The method uses an order parameter (symbol ϕ) to keep track of which fluid is where (order *parameter* is a bit misleading terminology as the order parameter is a continuous function in space and time $\phi(\mathbf{x},t)$). In one of the two fluids (say the continuous fluid) $\phi = -1$, in the other $\phi = 1$, and ϕ transits between these two values over the interface. In this way the local density and viscosity are directly related to the order parameter; e.g. for the viscosity $\nu = \nu_c \frac{1}{2}(1-\phi) + \nu_d \frac{1}{2}(1+\phi)$.

Governing equations

The governing equations of this fluid-fluid system are written in the following form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial x_\alpha} = 0 \tag{5.1}$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} = -\frac{\partial P_{\alpha\beta}^{th}}{\partial x_\beta} + \frac{\partial}{\partial x_\beta}\left[\nu\left(\frac{\partial \rho u_\alpha}{\partial x_\beta} + \frac{\partial \rho u_\beta}{\partial x_\alpha}\right)\right] \tag{5.2}$$

$$\frac{\partial \phi}{\partial t} + \frac{\partial \phi u_\beta}{\partial x_\beta} = M \frac{\partial^2 \mu}{\partial x_\beta^2} \tag{5.3}$$

Next to (fluid) mechanics, this set of equations contains the thermodynamics related to fluid-fluid interfaces. Equation 5.1 is the familiar continuity equation; Eq. 5.2 is the Navier-Stokes equation (without forcing) with a new pressure term $P_{\alpha\beta}^{th}$ which is called the thermodynamic pressure tensor. Equation 5.3 is a transport equation in the order parameter ϕ. The term on the right-hand side contains a constant *M* called mobility; the function μ is the chemical potential that depends on ϕ according to

$$\mu = A\phi - A\phi^3 - \kappa \frac{\partial^2 \phi}{\partial x_\beta^2} \tag{5.4}$$

with $A < 0$ and κ two constants. In (chemical) thermodynamics, the chemical potential is the derivative of free energy: $\mu = \dfrac{DF}{D\phi}$. This assists interpretation of Eq. 5.4. It implies that F has two minima, at $\phi = \pm 1$ that are responsible for the phase separation between the two fluids. In addition, there is an energy penalty for having a curved interface (see the last term of Eq. 5.4) so that the parameter κ relates to interfacial tension.

Also the thermodynamic pressure tensor includes interfacial tension effects:

$$P_{\alpha\beta}^{th} = \left[\tfrac{1}{3} c_s^2 \rho + A \left(\tfrac{1}{2}\phi^2 - \tfrac{3}{4}\phi^4 \right) - \kappa\phi \frac{\partial^2 \phi}{\partial x_\gamma^2} - \tfrac{1}{2} \left(\frac{\partial \phi}{\partial x_\gamma} \right)^2 \right] \delta_{\alpha\beta} + \kappa \frac{\partial \phi}{\partial x_\alpha} \frac{\partial \phi}{\partial x_\beta} \tag{5.5}$$

We recognize the very first term as the ideal gas contribution. The rest of the terms have to do with multiphase (immiscible fluids) and interface effects.

Lattice-Boltzmann based numerical procedure
The thermodynamics contained in the set of equations 5.1 – 5.5 is known as Cahn-Hilliard thermodynamics. The set of equations can be numerically solved with a lattice-Boltzmann scheme (as well as with any other method for solving partial differential equations) along the following lines. Start by defining two distribution functions f_i and g_i where f_i takes care of the hydrodynamics, and g_i of the order parameter. For now, the distributions evolve according to a BGK collision operator with relaxation times τ_f and τ_g respectively

$$f_i\left(\mathbf{x}+\mathbf{c_i}, t+1\right) - f_i\left(\mathbf{x},t\right) = -\frac{1}{\tau_f}\left[f_i\left(\mathbf{x},t\right) - f_i^{eq}\left(\mathbf{x},t\right)\right] \tag{5.6}$$

$$g_i\left(\mathbf{x}+\mathbf{c_i}, t+1\right) - g_i\left(\mathbf{x},t\right) = -\frac{1}{\tau_g}\left[g_i\left(\mathbf{x},t\right) - g_i^{eq}\left(\mathbf{x},t\right)\right] \tag{5.7}$$

Free-energy LBM has also been performed with the multiple relaxation time (MRT) collision operator with results favourable over BGK collisions at the expense of increased complexity. For the latter reason we – for now – stick to the lattice-BGK procedure.

Some macroscopic properties are

$$\rho = \sum_i f_i \quad \rho\mathbf{u} = \sum_i \mathbf{c_i} f_i \quad \phi = \sum_i g_i \tag{5.8}$$

The expressions for the equilibrium distributions are very complicated; we include them here to show how the LBM time stepping procedure would work and to show which parameters are involved in the time stepping process.

$$f_i^{eq} = w_i \rho \left[1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta \left(c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta} \right)}{2c_s^4} \right] + \frac{w_i}{c_s^2} \left(p_b - c_s^2 \rho - \kappa \phi \frac{\partial^2 \phi}{\partial x_\alpha^2} \right) + \kappa w_i^{\alpha\beta} \frac{\partial \phi}{\partial x_\alpha} \frac{\partial \phi}{\partial x_\beta} \quad (5.9)$$

$$i \neq 0, \quad f_0^{eq} = \rho - \sum_{i\neq 0} f_i^{eq}$$

$$g_i^{eq} = w_i \left[\frac{\Gamma \mu}{c_s^2} + \frac{\phi u_\alpha c_{i\alpha}}{c_s^2} + \frac{\phi u_\alpha u_\beta \left(c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta} \right)}{2c_s^4} \right] i \neq 0, \quad g_0^{eq} = \phi - \sum_{i\neq 0} g_i^{eq} \qquad (5.10)$$

A number of new symbols show up in Eqs. 5.9 and 5.10. The bulk pressure p_b in Eq. 5.9 is part of the diagonal terms in the thermodynamic pressure tensor (Eq. 5.5)

$$p_b = c_s^2 \rho + A \left(\tfrac{1}{2} \phi^2 - \tfrac{3}{4} \phi^4 \right) \qquad (5.11)$$

The weighing factors $w_i^{\alpha\beta}$ in Eq. 5.9 depend on the velocity set that is used. For the D2Q9 set we have been using mostly

$$w_{1,2}^{xx} = w_{3,4}^{yy} = \tfrac{1}{3} \quad w_{3,4}^{xx} = w_{1,2}^{yy} = -\tfrac{1}{6} \quad w_{5-8}^{xx} = w_{5-8}^{yy} = -\tfrac{1}{24} \quad w_{1-4}^{xy} = 0 \quad w_{5-8}^{xy} = \tfrac{1}{4} \qquad (5.12)$$

(note that $w_0^{\alpha\beta}$ are not needed given Eq. 5.9). In Eq. 5.10 a new parameter Γ appears. This is a tuneable numerical parameter and will be discussed below.

Starting from known distribution functions f_i and g_i on a lattice, a time step would proceed as follows: determine ρ, $\mathbf{u}$ and ϕ through Eq. 5.8. This provides us with the ingredients to determine the equilibrium distribution functions f_i^{eq} and g_i^{eq} through Eqs. 5.9 and 5.10. Tricky issues are the spatial gradients of ϕ that require finite difference approximations, the chemical potential μ that is a function of ϕ as well as its gradients (Eq. 5.4), and the bulk pressure that depends on ρ and ϕ. Once f_i^{eq} and g_i^{eq} have been determined, we can perform a collision and determine the post-collision distributions f_i^* and g_i^*, and then we stream: $f_i(\mathbf{x}+\mathbf{c_i}, t+1) = f_i^*(\mathbf{x}, t)$ and $g_i(\mathbf{x}+\mathbf{c_i}, t+1) = g_i^*(\mathbf{x}, t)$.

Choice of parameters
The list of parameters in the above is extensive; some are physical and some are numerical, some are both. Choosing and tuning these parameters proofs to be a delicate process. As explained in LN03, the translation between physical units and lattice units goes via dimensionless numbers. For flows with interfaces these are, next to the Reynolds number, the capillary number $\mathrm{Ca} = \rho \nu U / \gamma$ with U a characteristic velocity and/or the Weber number $\mathrm{We} = \rho U^2 d / \gamma$ with d a characteristic length scale such as a drop diameter. The capillary number equates viscous forces with interface-related forces; the Weber number inertial forces with interface forces.

As an example, let us consider a system of two immiscible liquids having (roughly) the same density $\rho_c \approx \rho_d = \rho$, kinematic viscosities ν_c and ν_d, and interfacial tension γ, all are in lattice units (i.e. we already went through the dimensional analysis process of translating SI to

lattice units). The relaxation time τ_f of the f_i distribution determines the kinematic viscosity according to $\nu = \dfrac{2\tau_f - 1}{6}$. It should be realized, however, that viscosity and therefore τ_f are not constant. Instead they are part of the solution process since viscosity depends on the order parameter according to $\nu = \nu_c \frac{1}{2}(1-\phi) + \nu_d \frac{1}{2}(1+\phi)$.

The interfacial tension depends on the parameters A and κ as they show up in Cahn-Hilliard thermodynamics:

$$\gamma = \tfrac{2}{3}\sqrt{2\kappa A} \tag{5.13}$$

An important physical/numerical choice to be made is the thickness of the interface (symbol ξ). The way it relates to Cahn-Hilliard coefficients is

$$\xi = \sqrt{2\kappa/A} \tag{5.14}$$

If κ and A are in lattice units, ξ is the interface thickness in lattice units, i.e. it is the number of lattice spacings over which the order parameter changes from 1 to −1 and vice versa. The interface thickness is – of course – also a physical property. In liquid-liquid systems it is of the order of a few nanometer. From a numerical point of view, however, the interface needs to be resolved such that ξ is 2 – 3 lattice units. This implies that if we want to simulate a real, physical interface, the lattice spacing needs to be of the order of 1 nm, and a droplet with a size of 1 μm would require a thousand lattice nodes over its diameter. This is unpractical for most applications. For this reason, ξ is mostly chosen as a numerical parameter, based on stability and computational affordability of simulations. Once we have made our choice for γ and ξ, the parameters A and κ are fixed.

There are three more parameters to consider in a free-energy LBM simulation: M (Eq. 5.3), τ_g (Eq. 5.7) and Γ (Eq. 5.10). These are not independent:

$$M = \Gamma\left(\tau_g - \tfrac{1}{2}\right) \tag{5.15}$$

It is common practice to set $\tau_g = 1$ which means that each time step g_i will relax to equilibrium. This leaves Γ as a free parameter for which literature suggests values in the range $\Gamma = 10^{-1} - 10$ in lattice units. For an interpretation in non-dimensional terms, a numerical Peclet number is defined as $\text{Pe} = \dfrac{U\xi}{MA}$. The Peclet number is the ratio between convection and diffusion. It contains Γ via M. Long story short: there is no solid theory that guides choosing the M, τ_g, Γ combination and people use reference data (e.g. experimental data on droplet breakup) for tuning purposes and then apply the same set of parameters to make predictions for cases for which no reference data are available.

One last word of advice relates to the way in which spatial derivatives of ϕ are determined. In Eqs. 5.5 and 5.9 terms such as $\dfrac{\partial^2 \phi}{\partial x_\gamma^2}, \dfrac{\partial \phi}{\partial x_\alpha}$ appear. The choice of stencil for estimating these derivatives from finite difference approximations also is a delicate one.

5.3 Volume-averaged Navier-Stokes equation for solid-fluid systems

Quite a change of topic here: We are now dealing with a Newtonian fluid (gas or liquid) loaded with solid particles. For the sake of simplicity, all particles are spherical and all have the same diameter d. We want to perform a numerical simulation of this system but cannot afford to use a grid with a spacing much smaller than d. This means that we cannot explicitly impose a no-slip condition at the surface of the particles and thus cannot resolve the flow around each particle. Instead we have a grid on which we intend to solve the fluid flow with a spacing $\Delta > d$ as in Figure 5.2, or $\Delta \approx d$. This grid acts as a filter: it erases / smears out / averages the details that are finer than the grid spacing.

Therefore instead of being suitable for solving the Navier-Stokes equation, the grid is suitable for solving the *volume-averaged* Navier-Stokes equation.

Volume-averaged Navier-Stokes equation

The volume-averaged mass balance (continuity equation) and the volume-averaged momentum balance (in the form of the Cauchy equation Eq. 1.16) read

$$\frac{\partial \rho \phi^c}{\partial t} + \frac{\partial}{\partial x_\alpha}\left(\rho \phi^c u_\alpha\right) = 0 \tag{5.16}$$

$$\frac{\partial \rho \phi^c u_\alpha}{\partial t} + \frac{\partial \rho \phi^c u_\alpha u_\beta}{\partial x_\beta} = \phi^c \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} + F_{s\alpha} \tag{5.17}$$

The symbol ϕ^c is the local continuous phase (fluid) volume fraction. The local solids volume fraction is $\phi^d = 1 - \phi^c$. In terms of Figure 5.2, it is the volume fraction per cell occupied by solids and fluid. The forcing term $F_{s\alpha}$ in Eq. 5.17 is the force per unit volume exerted by the particles on the fluid. The fluid velocity u_α is the volume-averaged *interstitial* fluid velocity, i.e. the velocity averaged over that part of the volume only occupied by fluid.

In order to understand how to solve Eqs. 5.16 and 5.17 with the lattice-Boltzmann method, they are rewritten in the following form

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha}\left(\rho u_\alpha\right) = -\frac{\rho}{\phi^c}\left[\frac{\partial \phi^c}{\partial t} + u_\alpha \frac{\partial \phi^c}{\partial x_\alpha}\right] \tag{5.18}$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} - \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} - \frac{F_{s\alpha}}{\phi^c} = -\frac{\rho}{\phi^c}\left[u_\alpha \frac{\partial \phi^c}{\partial t} + u_\alpha u_\beta \nabla \frac{\partial \phi^c}{\partial x_\beta}\right] \tag{5.19}$$

If we would set the right-hand side of Eqs. 5.18 and 5.19 to zero, they form a set of equations that can be solved with any single-phase LB method (the Navier-Stokes equation has a forcing term $F_{s\alpha}/\phi^c$ but we know how to deal with that). Extending the single-phase LB method with *source terms* representing the right-hand sides allows us the solve Eqs. 5.18 and

5.19. A source term in the momentum balance is a body force so that the term on the right-hand side of Eq. 5.19 is an additional forcing term

$$F_\alpha^\phi = -\frac{\rho}{\phi^c}\left[u_\alpha\frac{\partial\phi^c}{\partial t}+u_\alpha u_\beta\nabla\frac{\partial\phi^c}{\partial x_\beta}\right] \tag{5.20}$$

A source term in the mass balance (continuity equation) is mass source. One option for this to be incorporated is via the collision operator such that $\sum_i\Omega_i = S^\phi$ with

$$S^\phi = -\frac{\rho}{\phi^c}\left[\frac{\partial\phi^c}{\partial t}+u_\alpha\frac{\partial\phi^c}{\partial x_\alpha}\right] \tag{5.21}$$

The mass source term. It can be distributed over the velocity directions using the weighing factors w_i of the velocity set: $S_i^\phi = w_i S^\phi$.

Determination of the source terms requires knowledge of ϕ^c and its spatial and temporal derivatives (as well as of ρ and u_α that are directly available from the distribution function f_i). This knowledge is available if we know where all the solid particles are. We then determine how much solids volume is present in each cell (see Figure 5.1). This requires a *mapping* operation: Lagrangian (solid particles) information needs to be mapped on the Eulerian grid. Once we know how the solids volume fraction ϕ^d is distributed, we know how $\phi^c = 1 - \phi^d$ is distributed. The way we perform the mapping operation, and the way keep track of the solid particles in the flow field are very interesting topics but beyond the scope of these lecture notes.

5.4 An overall summary & some closing remarks
Starting from the molecular concept of matter, kinetic theory and the notion of distribution functions in physical and velocity space a discrete system was postulated. It has three levels of discretization: space, time and velocity. This discrete system – the lattice-Boltzmann equation (Eq. 2.3) – was hypothesized to represent the Navier-Stokes equations. This was substantiated through a Chapman-Enskog analysis. The main reason for including this analysis in the lecture notes was mainly to provide you with the assumptions underlying the analysis, not so much with the mathematical details. It is – in my mind – perfectly legitimate to work with the LB equation without a complete understanding of its theoretical underpinning.

Working with the LB method has many practical issues to deal with, coding, boundary conditions and scaling / dimensional analysis. It also is important to understand some of the (severe) limitations of the method: time step constraints due to compressibility effects, and the use of uniform square or cubic grids. Local grid refinement – not discussed in these notes – is an option in LB but is definitely more complicated than in mainstream CFD.

Extensions make the LB method attractive in many applications: the immersed boundary method makes it "easy" to deal with complex geometrical features and moving boundaries, the direct availability of the viscous stresses in the solution is useful when doing large-eddy simulations of turbulence. Multiphase flow also is an important application. A diffuse

interface method (free-energy LB method) was discussed in quite some detail. A main issue here is the choice of parameters. This mainly is an issue of Cahn-Hilliard thermodynamics, not so much of (LB) numerics.

I hope these notes and the lectures have been useful. Will be more than happy to discuss further about your specific applications and see if the LB method can be of any use.

Aberdeen, UK, August 2018.