

ME615: Microfluidics
Project Report:
Modeling of Droplet Dynamics Using Multi-phase Lattice Boltzmann Method

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(Dated: January 4, 2023)

In this project, we used the Shan-Chen model that is a widely used for predicting the behavior of multi-phase fluids to simulate the relaxation, collision, coalescence and separation of droplets within the context of three case studies. Simulation developed provided valuable insights into the mechanisms of droplet collision and coalescence in microfluidic channels and can be used to design and optimize microfluidic systems for droplet-based applications.

INTRODUCTION

Microfluidic devices have attracted significant attention recently due to their potential for a wide range of applications, including drug delivery, chemical synthesis, and lab-on-a-chip systems [1]. One key aspect of microfluidic devices is the presence of droplets, which can be formed and manipulated in various ways to perform specific tasks. Accurate simulation of droplet flow and breakup in microfluidic devices is therefore crucial for designing and optimizing these systems [2].

The Lattice Boltzmann method (LBM) is a computational fluid dynamics (CFD) approach widely used to simulate fluid flow in microfluidic devices. It is particularly well-suited to model complex geometries and boundary conditions and is relatively fast and efficient compared to other CFD methods [3]. However, the LBM is limited to single-phase flow and is not well-suited for simulating multi-phase flows involving droplets and dispersed phases.

To address this limitation, the Shan-Chen model was developed as a two-fluid model based on the LBM and designed explicitly for simulating multi-phase flows [4]. The Shan-Chen model can accurately capture the interaction between the different phases, including the transfer of momentum, energy, and mass, which is crucial for accurately predicting the behavior of droplets in microfluidic devices.

Overall, the Shan-Chen model is an essential tool for understanding and predicting the behavior of droplets in microfluidic systems and has been widely used in various applications. This project report will review some applications of the Shan-Chen model in droplet microfluidics, including its use in simulating droplet shape relaxation, coalescence, and transport within microfluidic channels.

METHODS AND IMPLEMENTATION

The Navier-Stokes equations are a set of differential equations describing fluids' motion. They can be used to predict the velocity and pressure of a fluid as it flows

through a given domain. The equations are given by:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

where ρ is the density, \mathbf{u} is the velocity, p is the pressure, μ is the viscosity, and \mathbf{f} is any external force acting on the fluid [3].

The Lattice Boltzmann Method (LBM) is a computational fluid dynamics (CFD) approach to model fluid flow without relying on finite-difference or finite-element discretization of the Navier-Stokes equation but with a different formulation that reduces to Navier-Stokes in continuum limit [5]. It is based on the Boltzmann transport equation, which describes the behavior of a gas or fluid at the microscopic level. This equation is derived using statistical mechanics and the kinetic theory of gases, in which isotropy of velocity distribution and point particles is assumed, meaning there is no directional preference. Hence, the flow is modeled not using the continuum description of fluid mechanics but rather the mesoscopic description of the dynamics of an ensemble of microscopic particles. In lattice form with no external forces, the Boltzmann equation can be written as:

$$f_i(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{r}, t) + \Omega_i (f^{eq}(\mathbf{r}, t) - f_i(\mathbf{r}, t)) \quad (3)$$

where f_i is the probability of finding a particle at position \mathbf{r} and time t velocity with velocity \mathbf{c}_i , f^{eq} is the equilibrium distribution function, Ω_i is the collision (scattering) integral controlling the relaxation process to the local equilibrium state, i denotes the directions of the discrete number of velocities (0, ..., # of connected nodes). Although the collision integral $\Omega_i = \frac{\partial f_i}{\partial t}|_{\mathbf{c}_i}$ is a complicated momentum-space integral over the product of particle distribution functions, Bhatnagar-Gross-Krook (BGK) approximation for Ω_i at low Mach numbers yields $\Omega_i = \frac{1}{\tau}$ where τ is the relaxation factor [?]. With a proper assumption that low Mach numbers are the case in microfluidics, the discretized form of the Boltzmann

equation can be written as:

$$f_i(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{r}, t) + \frac{\Delta t}{\tau} (f_i^{eq}(\mathbf{r}, t) - f_i(\mathbf{r}, t)) \quad (4)$$

Using BGK approximation together with the Maxwellian distribution of particle velocities from kinetic theory, local Maxwellian and local equilibrium distributions can be written as follows, respectively:

$$f = \frac{3\rho}{2\pi} e^{-\frac{3}{2}(\mathbf{c}-\mathbf{u})^2} \approx \frac{3\rho}{2\pi} e^{-\frac{3}{2}c^2} \left[1 + 3(\mathbf{c} \cdot \mathbf{u}) - \frac{3}{2}u^2 \right] \quad (5)$$

$$f^{eq} = w_i \rho \left(1 + \frac{u_a c_{ia}}{c_s^2} + \frac{u_a u_b (c_{ia} c_{ib} - c_s^2 \delta_{ab})}{2c_s^4} \right) \quad (6)$$

where a and b denote the coordinates on the lattice grid, w_i are the weighting factors given for the lattice and $c_s^2 = \sum_i w_i c_i^2$ is the square of the lattice speed of sound [3].

The aforementioned lattices must be created to satisfy isotropy in velocity distribution, which yields the following set of equations relating to directions and weight factors:

$$\begin{aligned} \sum_i w_i &= 1 \\ \sum_i w_i e_{i\alpha} e_{i\beta} &= \frac{1}{3} c^2 \delta_{\alpha,\beta} \\ \sum_i w_i e_{i\alpha} e_{i\beta} e_{i\gamma} e_{i\delta} &= \frac{1}{9} c^4 (\delta_{\alpha,\beta} \delta_{\gamma,\delta} + \delta_{\alpha,\gamma} \delta_{\beta,\delta} + \delta_{\alpha,\delta} \delta_{\beta,\gamma}) \end{aligned} \quad (7)$$

The D2Q9 is considered an adequate method to model fluid flows in 2D, therefore we employ the following set of directions shown in (Fig. 1) and weight factors associated with D2Q9.

$$\begin{aligned} \mathbf{e}_i &= \begin{cases} (0,0) & (i=0) \\ (\pm 1, 0)c, (0, \pm 1)c & (i=1, 2, 3, 4) \\ (\pm 1, \pm 1)c & (i=5, 6, 7, 8) \end{cases} \\ w_i &= \begin{cases} 4/9 & (i=0) \\ 1/9 & (i=1, 2, 3, 4) \\ 1/36 & (i=5, 6, 7, 8) \end{cases} \end{aligned} \quad (8)$$

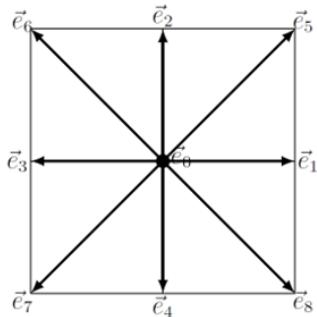


FIG. 1. 2D lattice configuration for D2Q9 method [3].

The equations provided so far only supports single-phase flow simulations. The Shan-Chen model can be further introduced to include multi-phase flows commonly appearing in microfluidics. The model represents each phase as a separate distribution function and therefore consists of additional terms in the equilibrium distribution function to account for surface tension and interface curvature [4]. These terms allow the model to capture droplets' behavior in microfluidic systems accurately. For two-phase flow involving a continuous fluid phase and dispersed droplets, the distribution functions for the fluid and droplets can be written as:

$$f_i^f(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i^f(\mathbf{r}, t) = -\frac{1}{\tau} [f_i^f(\mathbf{r}, t) - f_i^{eq,f}(\mathbf{r}, t)] \quad (9)$$

$$f_i^d(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i^d(\mathbf{r}, t) = -\frac{1}{\tau} [f_i^d(\mathbf{r}, t) - f_i^{eq,d}(\mathbf{r}, t)] \quad (10)$$

where f_i^f and f_i^d are the distribution functions for the fluid and droplets, respectively, and $f_i^{eq,f}$ and $f_i^{eq,d}$ are the corresponding equilibrium distribution functions. Both f_i^f and f_i^d include the potential contributions from each other with scaling parameters controlling the amplitude of the molecular interaction force in between, denoted by G . While $G < 0$ denotes a repulsive force between the phases forming an interface, $G > 0$ denotes an attractive force resulting in the mixing of two phases [?].

Lastly, the density and velocity of the lattices are determined by following relations at each timestep and substituted back to local distributions given in Eqn. (5, 6) and (9, 10).

$$\rho(\mathbf{r}, t) = \sum_{i=1}^n f_i(\mathbf{r}, t) \quad (11)$$

$$\mathbf{u}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \sum_{i=1}^n f_i(\mathbf{r}, t) \mathbf{c}_i \quad (12)$$

where n is the number of velocity directions on the lattice, f_i is the distribution function for particle velocity \mathbf{c}_i at position \mathbf{r} and time t , ρ is the fluid density, and \mathbf{u} is the fluid velocity.

SIMULATIONS AND RESULTS

By using the equation introduced in the previous section, a simulation was developed in MATLAB environment, which consisted of three case studies:

- Droplet Shape Relaxation
- Collision of Droplets in Free-Space
- Coalescence and Splitting in a Microfluidic Channel

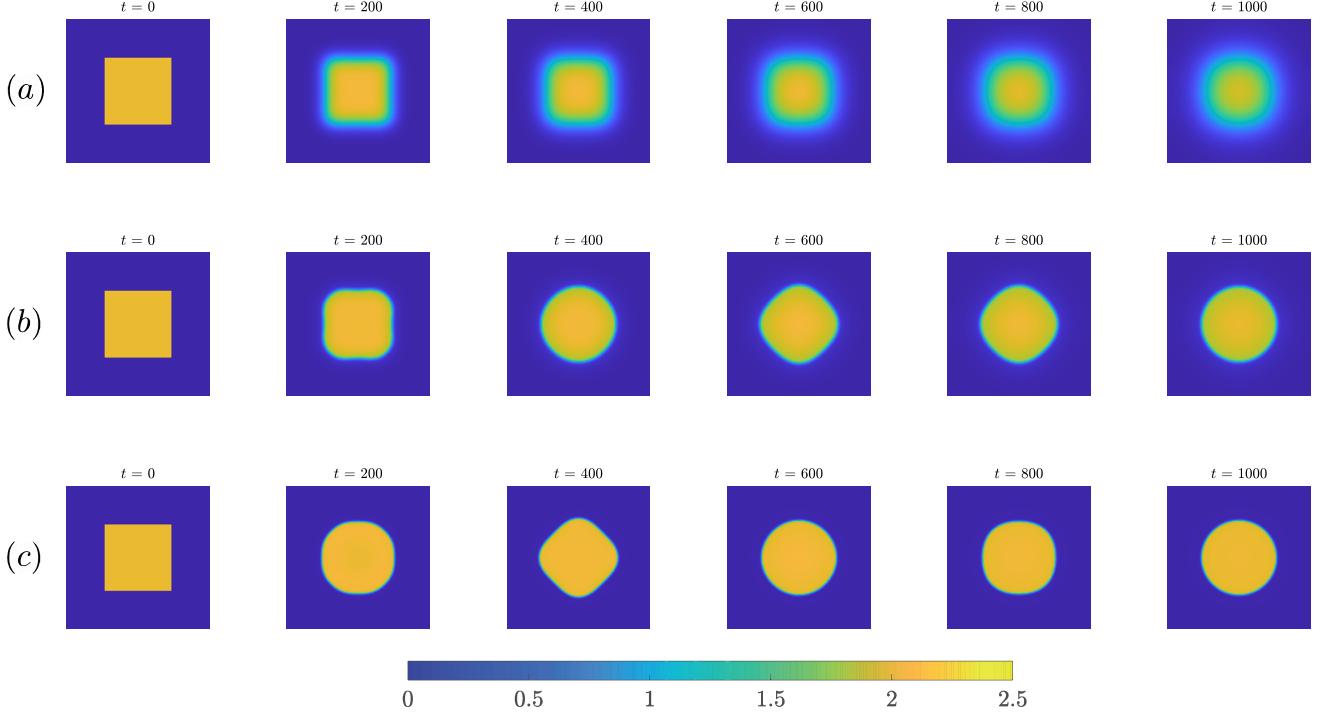


FIG. 2. Rectangular droplet relaxation: $G = -0.4$ (a), $G = -0.8$ (b), $G = -1.2$ (c); color bar denotes density difference $\Delta\rho = \rho(x, y) - \rho_{fluid}$. As the intermolecular interaction force increase from (a) to (c), the interface between the two phases becomes more evident.

Droplet Shape Relaxation

In a microfluidic droplet system, the shape of the droplets can change due to various factors such as surface tension, viscous forces, and external flow. This process is known as the droplet shape relaxation [1]. If the droplet is moving through a viscous fluid, the fluid will exert a drag force on the droplet, which can cause the droplet to deform and change shape.

Primarily, the relaxation of the droplet shape can be described using the Laplace pressure equation, which relates the surface tension at the droplet interface to the curvature of the droplet [2]. If the curvature of the droplet changes, the surface tension will adjust to maintain the balance of forces at the interface. This can lead to a change in the shape of the droplet.

In this case study, we simulated the relaxation of the rectangular droplet, shown in Fig. 3, immersed in a static fluid. At the initial time $t = 0$, the rectangular membrane separating the fluids is removed.

The relaxation of the droplet shape will be purely driven by the surface tension at the droplet interface, which is directly related to the amplitude of the molecular interaction force G .

If the amplitude of the molecular interaction force is high, the rectangular droplet will tend to become more

spherical relatively quickly over time due to the increased surface tension since high surface tension will cause the droplet to minimize its surface area, which is eventually achieved by forming a spherical shape [4]. On the other hand, if the amplitude of the molecular interaction force is low, the droplet will have relatively lower surface tension and weaker cohesive forces between the molecules, allowing the droplet to have a larger surface area and a diffusive interface between two fluids at the same instant.

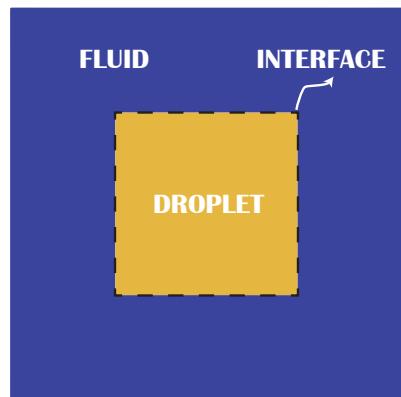


FIG. 3. Droplet suspended in the bulk fluid by a rectangular membrane. To achieve the droplet shape relaxation, the membrane is removed after $t = 0$.

Collision of Droplets in Free-Space

In this study, we aimed to perform a transient collision simulation of droplets by introducing momentum to droplets to move them into the center of the domain. This stage was designed as an intermediate step to move the droplets as we desire within the domain before we introduce walls to the microfluidic system.

As a first step, we initialized four stationary droplets axis-symmetrically placed over the domain. These droplets of the same size were then given initial velocities towards to center for a predetermined amount of time $t < 200$, as shown in Fig. 4.

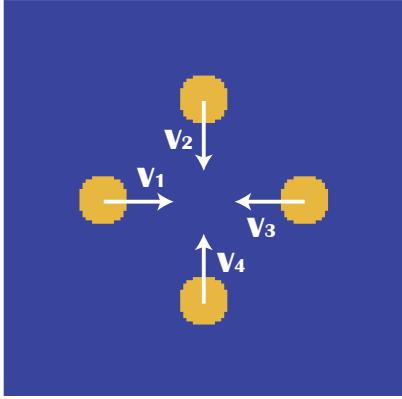


FIG. 4. At $t = 0$, four identical droplets start moving towards each other under the influence of initially induced momentum to undergo collision.

As we assigned the initial velocities, we considered both perfectly symmetric and slightly perturbed velocity vectors. For the perfectly symmetric case shown in Fig. 5 (a), we observed that the droplets formed a larger ring-shaped droplet as they merged. Due to the symmetry, the fluid trapped inside the larger droplet cannot find an exit during the collision. Due to the repulsive inter-molecular forces, we observe a circular shape for both the droplet and the trapped fluid to minimize the surface area. On the other hand, when we perturb the velocities by small amounts (20% of the original value) as shown in Fig. 5 (b), we observe that some of the droplets reach the center slightly quicker than the others, resulting in the sequential merging of the droplets, providing enough time and space for bulk fluid at the center to escape. This eventually leads to a perfect coalescence of the droplets having the expected circular shape without any fluid trapped inside.

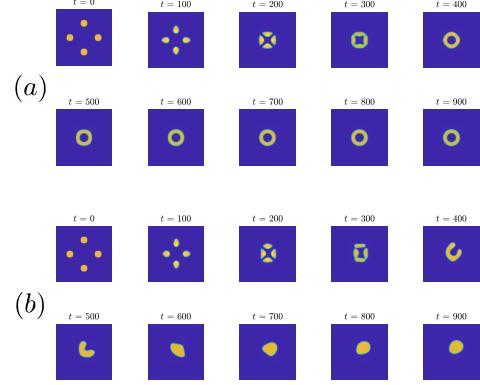


FIG. 5. Droplets moving towards the center axis-symmetric velocities (a), slightly perturbed axis-symmetric velocities (b).

Coalescence and Splitting in Microfluidic Channel

As the final goal of our project, we examine an exemplary microfluidic channel that can transport droplets together with coalescence and splitting dynamics. For this reason, we introduce stationary boundaries to the system maintained by the bounce-back boundary condition [5].

Following Fig. 6, the lattice can avoid collision with the boundary if f_7, f_4, f_8 are determined to hit the wall. At any time-step and spatial part of the domain, if the bounce-back condition is required by determining f_7, f_4, f_8 will hit the wall, the middle lattice is set to $f_2 = f_4$, the left lattice is set to $f_5 = f_7$, and the right lattice is set to $f_6 = f_8$ for the next time-step [5].

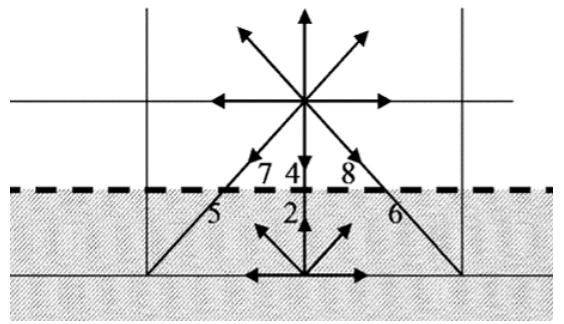


FIG. 6. Illustration of bounce-back boundary condition for D2Q9 method [5].

Although there are many other boundary conditions, such as immersed boundaries for curved structures, Boundary Element Method (BEM), or Discrete-Element Method (DEM) based conditions for moving boundaries, we only consider rigid and stationary walls with the bounce-back boundary condition [5].

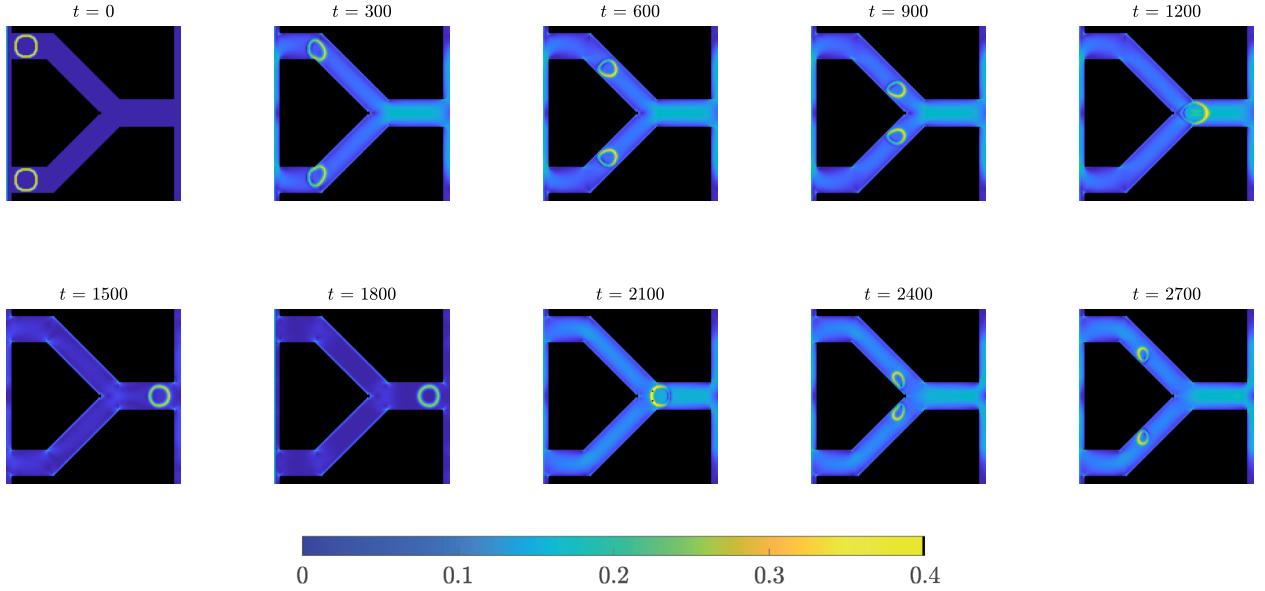


FIG. 7. Transport of the droplets inside the microfluidic channel to perform the first coalescence and then splitting of droplets; color bar denotes velocity of the fluid v_{fluid} , and therefore maximum value is present at the interface. Complete animation is provided as a supplementary file.

For the simulation depicted in Fig. 7, we introduce two droplets at the beginning of the channels. For a predetermined amount of time $t < 1300$, we introduce a flow to the fluid at the entrances of two channels to allow the droplets to meet at the junction. As we observe coalescence, we stop the introduced flow and let the larger droplet undergo relaxation, again for a predetermined amount of time $1300 < t < 1800$. After $t > 1800$, we introduce a flow in the opposite direction to demonstrate splitting the larger droplet into two parts.

DISCUSSION

In this project, we successfully applied the stationary boundary condition in the Shan-Chen model to study multi-phase flows in microfluidic channels. While this is an important step toward simulating and optimizing droplet-based microfluidic systems, the practical limits of the simulations constrained us from studying droplet-based logic gates, which was the ultimate goal of this study. While the method was successful for small lattice structures, and the developed method to simulate multi-phase systems within confined channels was novel, we faced computational challenges when analyzing larger

and more complex channel geometries for logic gates presented in the literature. To sum up, we were able to properly model some of the droplet-based microfluidic examples that were introduced to us in our course.

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