

Lattice Boltzmann Modeling of Active Particles

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1 Introduction

The study of active matter systems is gaining interest in recent times from both theoretical and experimental perspectives. These are systems that are capable of consuming energy and converting it into directed motion. Typical examples of active matter range from cultures of bacteria, schools of fish to swarms of birds. Of these, in particular, microswimmers exhibit hydrodynamic coupling with the embedding solvent via flow fields generated by the strokes they make. Therefore, in any computer simulation of such objects, it is essential to introduce hydrodynamic interactions. An obvious way of including solvent interactions is by explicitly simulating fluid molecules. Though such atomistic simulations might yield precise results, the sheer number of entities involved makes it impractical to realize experimentally observed macroscopic properties. For example, note that a mole contains $\sim 10^{23}$ particles. Evidently, handling such large systems is computationally laborious if not impossible. On the other end of the spectrum, there is traditional CFD which solves partial differential equations to simulate hydrodynamics on the macroscopic scale. The main advantage of our topic of discussion, the *Lattice Boltzmann method* (a ‘mesoscopic’ method) over these methods is its parallelizability and ease of implementation.

This handout is aimed to complement the presentation to be delivered. The rest of the handout is organized as follows: First, the Boltzmann transport equation will be discussed. Then, a short review of the central hydrodynamics equations will be given and the equivalence of the Boltzmann equation to Navier-Stokes via the Chapman-Enskog expansion will be discussed. Next, the implementation of the Lattice Boltzmann algorithm will be presented followed by how active particles can be modelled using this method.

2 Boltzmann transport equation

Question: What is the probability of finding a particle around position r with velocity v at time t ?

Let $f(r, v, t)$ be the probability distribution function of particles. This distribution function is the key player in kinetic theory to which Ludwig Boltzmann majorly contributed. He derived an equation that describes the evolution of the probability distribution function in terms of microscopic interactions of particles. To establish this relation, two key assumptions were made:

- Only binary elastic collisions are allowed.
- The position and momentum of a particle is uncorrelated.

For a system of rarified gas, the first assumption is justified given that the density of particles is low. The second assumption, referred to as the ‘Stosszahlansatz’ or the ‘molecular chaos assumption’, helps in simplifying the mathematics of collisions. However, despite the assumption of molecular chaos, we will see that the term representing collisions is quite involved.

In the case where there are no collisions (non-interacting particles), the particle’s position can be updated as $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{v}dt$ where dt is the time interval considered and the velocity can be updated

as $\mathbf{v} \rightarrow \mathbf{v} + \mathbf{F}dt$ (considering unit mass) where \mathbf{F} is the force acting on the particle. Therefore, the probability distribution function can be updated as

$$f(\mathbf{r} + \mathbf{v}dt, \mathbf{v} + \mathbf{F}dt, t + dt)d\mathbf{r}d\mathbf{v} = f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v} \quad (1)$$

The above equation conveys that all particles that arrived at $\mathbf{r} + \mathbf{v}dt$ having velocity $\mathbf{v} + \mathbf{F}dt$ at time $t + dt$ were at \mathbf{r} with velocity \mathbf{v} at time t .

In the presence of rare collisions (interacting particles), not all particles arrive at their new positions. Some of them that were meant to arrive at $\mathbf{r} + \mathbf{v}dt$ at time $t + dt$ do not whereas some that were meant to be at an other position at time time $t + dt$ arrive at $\mathbf{r} + \mathbf{v}dt$ due to collisions. The collision term (Ω) is defined as the rate of change of the difference in populations at position $\mathbf{r} + \mathbf{v}dt$ at time $t + dt$ and that at positions \mathbf{r} at time t . Thus,

$$\Omega[f]d\mathbf{r}d\mathbf{v}dt = f(\mathbf{r} + \mathbf{v}dt, \mathbf{v} + \mathbf{F}dt, t + dt)d\mathbf{r}d\mathbf{v} - f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v} \quad (2)$$

Dividing both sides of 2 by $d\mathbf{r}d\mathbf{v}dt$, we get

$$\Omega[f] = \frac{f(\mathbf{r} + \mathbf{v}dt, \mathbf{v} + \mathbf{F}dt, t + dt) - f(\mathbf{r}, \mathbf{v}, t)}{dt} = \frac{df}{dt} \quad (3)$$

A change in f , i.e. df , can be represented as

$$df = \frac{\partial f}{\partial \mathbf{r}}d\mathbf{r} + \frac{\partial f}{\partial \mathbf{v}}d\mathbf{v} + \frac{\partial f}{\partial t}dt \quad (4)$$

Dividing by dt gives

$$\frac{df}{dt} = \frac{\partial f}{\partial \mathbf{r}} \frac{d\mathbf{r}}{dt} + \frac{\partial f}{\partial \mathbf{v}} \frac{d\mathbf{v}}{dt} + \frac{\partial f}{\partial t} = \frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{\partial f}{\partial \mathbf{v}} \cdot \mathbf{F} + \frac{\partial f}{\partial t} \quad (5)$$

Plugging in the above equation in (3), we get the celebrated Boltzmann transport equation and an answer to the question posed at the beginning of the section.

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{\partial f}{\partial \mathbf{v}} \cdot \mathbf{F} + \frac{\partial f}{\partial t} = \Omega[f] \quad (6)$$

For a system with no forces,

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{\partial f}{\partial t} = \Omega[f] \quad (7)$$

It is important to note that the collision term that appears in 6 is, in general, complex. For example, for the case of binary collisions considered by Boltzmann,

$$\Omega_{12} = \int (f_1' f_2' - f_1 f_2) g \sigma d\Theta dp_2 \quad (8)$$

where the primed and non-primed variables refer respectively to post-collision and pre-collision variables. Here, g is the relative velocity of the colliding particles, σ is the differential cross section and Θ to $\Theta + d\Theta$ is the range of solid angles at which the particles approach each other.

The Lattice Boltzmann method solves a finite-difference version of the Boltzmann transport equation as will be discussed later. Clearly, the above integral makes the Boltzmann equation an integro-differential equation which is cumbersome to solve and this calls for some approximations.

2.1 BGK approximation

First, we recognize that the effect of collisions is to bring the system to equilibrium. Bhatnagar, Gross and Krook [3] introduced a single relaxation time approximation in which the parameter τ indicates the time scale at which the population reaches equilibrium. Under this approximation, the collision operator reads

$$\Omega^{BGK}[f] = -\frac{1}{\tau}(f - f^{eq}) \quad (9)$$

where f_{eq} is the well-known Maxwell Boltzmann equilibrium distribution

$$f^{eq}(\mathbf{r}, \mathbf{v} | \mathbf{u}, t) = \rho(\mathbf{r}, t) \times \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} \exp \left(-\frac{m|\mathbf{v} - \mathbf{u}|^2}{2k_B T} \right) \quad (10)$$

where the symbols have their usual meaning. Now, let us consider the moments of the operator in velocity space. We get,

$$\int \Omega^{BGK}[f] d\mathbf{v} = -\frac{\rho - \rho}{\tau} = 0 \quad (11a)$$

$$\int \Omega^{BGK}[f] \mathbf{v} d\mathbf{v} = -\frac{\rho \mathbf{u} - \rho \mathbf{u}}{\tau} = 0 \quad (11b)$$

$$\int \Omega^{BGK}[f] v^2 d\mathbf{v} = -\frac{\rho u^2 - \rho u^2}{\tau} = 0 \quad (11c)$$

As we will see, the above expressions play a crucial role in deriving continuum hydrodynamics equations.

3 Short review of hydrodynamics

The equations of hydrodynamics are derived from conservation laws. The first equation, known as the *continuity equation* is a statement of mass conservation and is given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (12)$$

The second central equation, known as the *Navier-Stokes equation*, is a statement of momentum conservation and is given by

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot \bar{\boldsymbol{\sigma}} = \rho \mathbf{f} \quad (13)$$

where σ is the stress tensor.

Also, we can use the ideal gas equation of state to relate pressure and density as follow

$$p = \frac{\rho k_B T}{m} \quad (14)$$

To recognize Lattice Boltzmann as a hydrodynamics solver it is important to confirm that the central equations of hydrodynamics that have been established is recovered (at least in some limit).

4 From Boltzmann equation to Navier-Stokes: Chapman-Enskog expansion

In this section, we will take an overview of how the Navier-Stokes equation (equation 13) can be derived from the Boltzmann equation (equation 7) in the limit of slow variations in space and time using the Chapman-Enskog expansion.

To intuitively understand the presence of two scales in a system, consider a fluid in a beaker. The dimensions of the the fluid can be measured using both nanometer ruler and centimeter ruler. In this case, nanometer would correspond to the small scale while the centimeter would correspond to the large scale. Practically, the characteristic small scale parameter is the mean free path of molecules and the large scale parameter would vary according to the system under study (a centimeter ruler is a good instrument to measure the height of fluid in a beaker whereas it is more convenient to measure depth of oceans in kilometers!). The expansion introduces a scaling parameter ϵ that relates the relevant small and large scales. ϵ also corresponds to the Knudsen number that is defined as the ratio of the mean free path to the macroscopic length scale. We will work in the justifiable limit of small Knudsen numbers. Since small scale variables rapidly change they are referred to as the fast variables. Large scale variables are referred to as the slow variables. In the context of hydrodynamics, we are

only interested in the behaviour of slow variables and can thus discard degrees of freedom associated with fast variables.

Let \mathbf{r}_1, t_1 and t_2 be the coarse-grained length, convective time scale and the diffusive time scale respectively. Let \mathbf{r} and t refer to the fast variables. The scaling between slow and fast variables is

$$\begin{aligned} \text{Coarse-grained length: } \quad \mathbf{r}_1 = \epsilon \mathbf{r} &\rightarrow \frac{\partial}{\partial \mathbf{r}} = \epsilon \frac{\partial}{\partial \mathbf{r}_1} \\ \text{Convective time scale: } \quad t_1 = \epsilon t & \\ \text{Diffusive time scale: } \quad t_2 = \epsilon^2 t &\rightarrow \frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} \end{aligned}$$

Using ϵ as perturbation parameter and expanding f

$$f = f^0 + \epsilon f^1 + \epsilon^2 f^2 + \dots$$

$$\Omega[f] = \Omega[f^0] + \epsilon \Omega' f^1 + \dots$$

To get the last equation, $\epsilon f^1 = f - f^0$ has been used.

The modified version of the Lattice Boltzmann equation is

$$f_i(\mathbf{r} + \epsilon \tau \mathbf{c}_i, t_1 + \epsilon \tau, t_2 + \epsilon^2 \tau) - f_i(\mathbf{r}, t_1, t_2) = \Omega_i \quad (15)$$

Performing a multivariable Taylor expansion, we get

$$\epsilon \tau \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \frac{\partial}{\partial \mathbf{r}_1} \right) f_i + \epsilon^2 \tau \left[\frac{\partial}{\partial t_2} + \frac{\tau}{2} \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \frac{\partial}{\partial \mathbf{r}_1} \right)^2 \right] f_i = \Omega_i \quad (16)$$

Now, we can obtain the relevant hydrodynamics equations by performing an order-by-order analysis in terms of ϵ . The equations obtained by comparing the orders are

$$\begin{aligned} \mathcal{O}(\epsilon^0) : \quad \Omega_i^0 &= 0 \\ \mathcal{O}(\epsilon^1) : \quad \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \frac{\partial}{\partial \mathbf{r}_1} \right) f_i^0 &= \frac{1}{\tau} \Omega_i^1 \\ \mathcal{O}(\epsilon^2) : \quad \left[\frac{\partial}{\partial t_2} + \frac{\tau}{2} \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \frac{\partial}{\partial \mathbf{r}_1} \right)^2 \right] f_i^0 &+ \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \frac{\partial}{\partial \mathbf{r}_1} \right) f_i^1 = \frac{1}{\tau} \Omega_i^2 \end{aligned}$$

Conserved quantities need no expansion. Taking moments of the distribution,

$$f_i^0 = f_i^{eq} \quad (17a)$$

$$\rho^0 = \rho = \sum_i f_i^{eq} \quad (17b)$$

$$\mathbf{j}^0 = \mathbf{j} = \sum_i f_i^{eq} \mathbf{c}_i \quad (17c)$$

From the first order equations, we get the continuity equation for incompressible fluids.

$$\frac{\partial \rho}{\partial t_1} + \mathbf{v} \cdot \nabla \rho = 0 \quad (18)$$

From the second order equations and after a lot of algebra, we get the Navier-Stokes equation and

$$\frac{\partial \rho}{\partial t_2} = 0 \quad (19)$$

The above equation explains that there is no net mass transfer due to diffusion. This is expected as diffusion is a random process and no currents are involved. For a detailed, step-by-step derivation of this equivalence, the interested reader is referred to [10].

5 Lattice Boltzmann Algorithm

The Lattice Boltzmann method solves a finite difference discretization of the Boltzmann transport equation (7)

$$\frac{d}{dt}f(\mathbf{r}, \mathbf{v}, t) \approx \frac{f(\mathbf{r}(t) + \mathbf{v}(t)\Delta t, \mathbf{v}(t), t + \Delta t) - f(\mathbf{r}(t), \mathbf{v}(t), t)}{\Delta t} \quad (20)$$

In this algorithm, space, time and velocities are discretized. A regular grid is chosen to discretize space. A finite number of discrete velocities are chosen so that after one time step populations are transferred from one grid point to another. This ensure that the fluid particles are always on the grid. One such example in three dimensions with 19 discrete velocities is the D3Q19 lattice as shown in Figure 1. (Note: $DdQq$ means that there are d spatial dimensions and q discrete velocities).

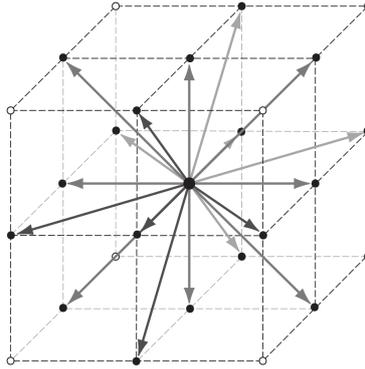


Figure 1: D3Q19 lattice with allowed discrete velocities marked as arrows connecting each node with itself, nearest neighbours and next-nearest neighbours.

The algorithm itself is implemented in two consecutive steps that are iterated over. These are:

- Streaming
- Collision

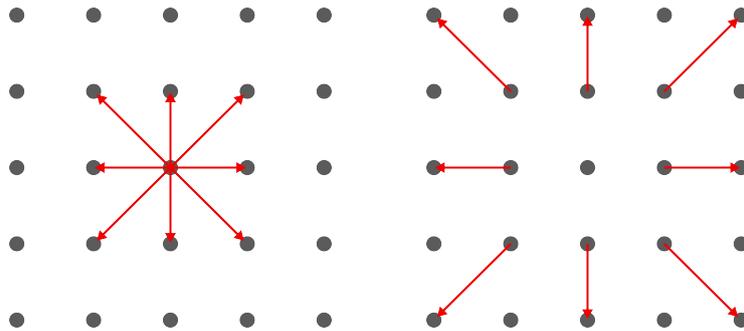


Figure 2: The populations are transported between nodes along the direction of their velocity vectors in the streaming step.

In the *streaming* step (Figure 2), populations are transported between nodes (they might also stay at the same node) along the direction of their velocity vectors. The *collision* step (Figure 3) occurs at a given node. In this step, the velocities are redistributed within the population at the node and made to approach local Maxwell-Boltzmann equilibrium in accordance to the definition of the collision operator that was introduced earlier.

Now that the simulation details of fluid motion in bulk has been discussed, we will now discuss boundary conditions.

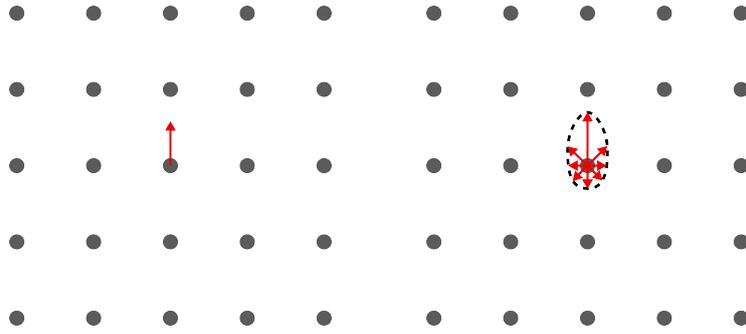


Figure 3: The velocities are re-distributed at a given node in the collision step.

6 Boundary conditions

6.1 Periodic boundary conditions

The first and simplest boundary condition is the periodic boundary condition. This is used when the system can be considered (infinitely) large along the direction in which the boundary condition is applied. The space spanned by periodic boundaries in two dimensions corresponds to a torus. Systems large enough to be approximated by periodic boundaries consist of an infinite number of repeating sub-units. On a computer, this corresponds to the simulation box and its images replicated along all the three dimensions as shown in Figure 4.

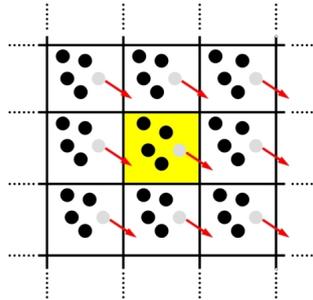


Figure 4: Illustration of periodic boundary conditions. The simulation cell is replicated along all spatial dimensions.

Particles that leave one side of the simulation cell in a direction along which periodic boundary is implemented re-enters the same cell from the other side. In practice, only the events that occur within the simulation cell are monitored.

6.2 No-slip boundary conditions

The no-slip boundary condition is used to represent fluids that have zero velocity at the solid boundary. Physically, this is appropriate when the solid is rugged enough to prevent any net fluid flow at the boundary. In practice, the no-slip boundary condition is implemented using a bounce-back scheme. The principle behind bounce-back scheme is that populations impinging on a rigid wall during streaming are reflected back to where they originally came from. Bounce-back of populations incident on the wall implies that there is no flux across the boundary, i.e., the wall is impermeable to the fluid. Also, the fact that the populations are bounced back rather than bounced forward indicates that there is no relative velocity between the fluid and the boundary, i.e., there is no slip of the fluid on the boundary surface. The implementation of bounce-back boundaries is shown in Figure 5.

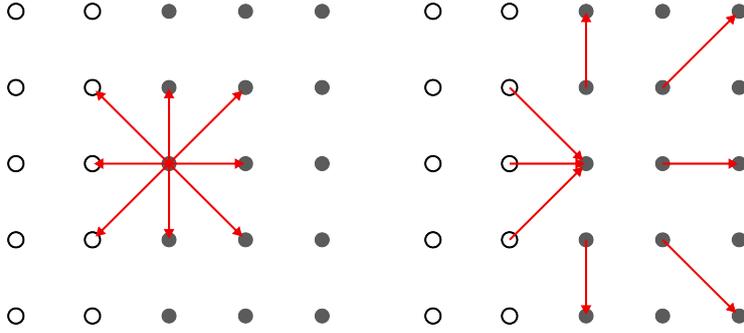


Figure 5: Bounce-back scheme involves reversing the direction of populations impinging the boundary as shown in the pre-streaming and post-streaming stage of the implementation. The filled circles are the fluid nodes and the empty circles are the boundary nodes.

So far, we have considered boundaries that are stationary. In the following section, we will look at how moving boundaries can be handled in lattice Boltzmann.

6.3 Treatment of moving boundaries

6.3.1 Ladd's moving boundary conditions

Here, we will discuss the implementation of moving boundary conditions as presented in Ladd's work [7]. The solid particle is considered to be a boundary that cuts some of the existing links between grid points. The fluid particles that are present on the links that are cut interact with the surface of the solid at the boundary nodes placed midway along the links. At each boundary node, there are two incoming distributions from either side of the boundary. If $\mathbf{v}(t)$ is the velocity of the particle, $\boldsymbol{\omega}(t)$ is the angular velocity of the particle and $\mathbf{r}(t)$ is its center of mass, then the velocity of the boundary $\mathbf{v}_b(\mathbf{r}_b, t)$ at position $\mathbf{r}_b(t)$ is determined using rigid body dynamics as [6]

$$\mathbf{v}_b(\mathbf{r}_b, t) = \mathbf{v}(t) + \boldsymbol{\omega}(t) \times (\mathbf{r}_b(t) - \mathbf{r}(t)) \quad (21)$$

The linear and angular momentum exchanged during bounce-back is transferred to the particle from the grid points (here, D3Q19 lattice is considered) by applying an appropriate force $\mathbf{F}(t)$ and torque $\mathbf{T}(t)$

$$\mathbf{F}(t) = a_{grid}^3 \sum_{\mathbf{r}_b} \sum_{i=1}^{19} \mathbf{c}_i (f_i(\mathbf{r}_b, t) + f_i(\mathbf{r}_f, t)) \quad (22a)$$

$$\mathbf{T}(t) = a_{grid}^3 \sum_{\mathbf{r}_b} \sum_{i=1}^{19} (\mathbf{r}_b - \mathbf{r}) \times \mathbf{c}_i (f_i(\mathbf{r}_b, t) + f_i(\mathbf{r}_f, t)) \quad (22b)$$

where a_{grid} is the distance between the node and its nearest neighbour. The particle is then made to evolve using the updated force and torque using Newtonian dynamics. Note that momentum is locally exchanged between the fluid and the particle keeping the combined momentum of the fluid and particle constant.

This method, though, has its shortcomings. Due to the presence of fluid within the solid particle, forces are exerted on the solid from inside. This is, however, unphysical. Another shortcoming is that the density of the particle must be larger than the density of the fluid.

In the next section, we will discuss the modification by Aidun *et al* [2] that overcomes these shortcomings.

6.3.2 Modification to Ladd's moving boundary condition

Firstly, the unphysical fluid present within the solid particle was removed. This, however, poses its own problem of how cells (equivalent to grid nodes) will be created and destroyed as the solid particle makes its way through the fluid. As the particle moves, the cells that overlap with the particle are simply deleted. The main issue is how the cells that have been revealed by the particle's motion

(the ‘new’ fluid) will be assigned their associated distribution functions. Also, how do we ensure, in this procedure, conservation of momentum and mass? A standard choice is to assign the equilibrium population to these cells with velocity equal to the velocity of the moving particle and a density equal to the average of the densities of the surrounding fluid cells. To conserve momentum, the momentum \mathbf{p}_f of the cells that have been created or destroyed by the moving solid is added to the solid as an additional force [2] [6]

$$\mathbf{F}(t) = \frac{1}{\Delta t} \mathbf{p}_f(\mathbf{r}_f, t) \quad (23)$$

where Δt is the time step. Note that fluid mass is not conserved. Conserving fluid mass would lead to violating the property of incompressibility of the fluid. The average fluid mass fluctuates as the solid moves through the grid.

Now that the moving boundary conditions has been discussed, in the next section we will see how Molecular Dynamics, which governs the evolution of the particle according to the laws of Newtonian dynamics, can be coupled with Lattice Boltzmann method, which governs the flow of the fluid.

7 Coupling Molecular Dynamics and Lattice Boltzmann

Typically to keep the problem simple, the time step of Lattice Boltzmann and Molecular Dynamics is chosen to be identical. Another simplification is made by representing the moving particle as a coupling point rather than an extended object. Ahlrichs and Dünweg [1] introduced a simple dissipative coupling between the particle and the fluid. In analogy to the Stokes formula for a sphere in a viscous fluid, assume that the force on the point particle exerted by the fluid to be proportional to the difference of the velocity of the particle \mathbf{v} and the fluid velocity \mathbf{u} at the position of the particle

$$\mathbf{F} = -\zeta(\mathbf{v} - \mathbf{u}(\mathbf{R}, t)) \quad (24)$$

where $\mathbf{u}(\mathbf{R}, t)$ is the interpolated velocity of the fluid (discussed later) at the center of mass of the particle \mathbf{R} . Here, ζ is a proportionality coefficient referred to as the ‘bare’ frictional coefficient.

Since the fluid velocity is only defined on the grid and the particle has freedom to exist anywhere, it is necessary to interpolate the velocity of the fluid at the particle’s position (see Figure 6).

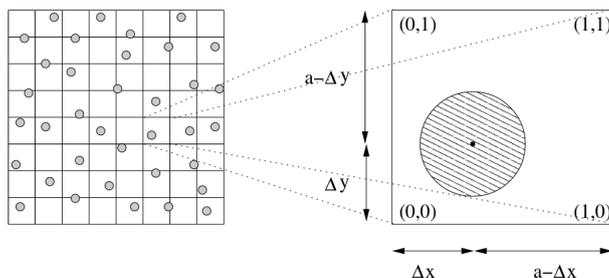


Figure 6: The schematic illustration shows the particle enclosed in the cell defined by four grid points. Here, a is the lattice constant.

The simplest of such an interpolation is the linear interpolation of velocities of grid points containing the particle. The interpolated velocity is then

$$\mathbf{u}(\mathbf{R}, t) = \sum_{\mathbf{r} \in g} \delta_{\mathbf{r}} \mathbf{u}(\mathbf{r}, t) \quad (25)$$

where g denotes the set of points that comprise the cell enclosing the particle. To conserve the combined momentum of the fluid and particle, an opposite force is imparted to the fluid in that cell.

Now that we have discussed how particles and fluid can be coupled, we will now consider a specific example of the motion of swimmers in a fluid.

8 Swimmers in a fluid

In their work, Jana *et al* [5] experimentally observe that *Paramecium* moves along a helical trajectory when confined within a capillary. This section will detail the work of de Graaf *et al* [4] in which this oscillatory motion of swimmers was rationalized using simulations.

The swimmer is modelled as a collection of coupling points by discretizing the surface and the interior. This model is referred to as the ‘raspberry’ model as the discretized surface, when represented by molecular dynamics beads resembles a raspberry.

Consider a ‘raspberry’ swimmer immersed in a Lattice Boltzmann fluid. The fluid domain is confined along one of the three spatial dimensions (say, z). Therefore, periodic boundaries are used along the unconstrained directions and no-slip boundary is implemented along the confined direction via the bounce-back scheme discussed earlier. The swimmer’s evolution is governed by Molecular dynamics while the fluid is simulated using Lattice Boltzmann algorithm. The two are coupled using the mechanism discussed earlier. To prevent the swimmers from penetrating the wall, a short-ranged repulsive Weeks-Chandler-Anderson (WCA) interaction is imposed. Initially, the swimmer is placed off-center and is oriented parallel to the confining boundary.

A force is applied to the center of mass of the rod along its symmetry axis to make the swimmer move and a counter force is applied to the fluid at the front of the rod for a puller and behind the rod for a pusher as shown in the inset of Figure 7.

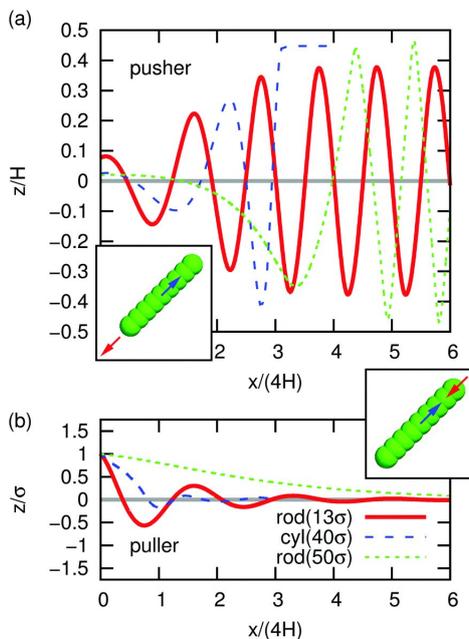


Figure 7: Swimmer’s trajectory when confined between two parallel plates separated by a distance H .

It was observed that all pushers move towards the wall and the pullers move towards the center of the plates. As shown in Figure 7, oscillatory trajectories are observed. The pushers follow a sinusoidal trajectory with increasing amplitude while the pullers’ oscillations are damped towards the center of the confinement.

9 Conclusion

In this overview, we first discussed the Boltzmann transport equation followed by simplification of the collision operator using the BGK approximation. The steps of the Chapman-Enskog expansion, which establishes the commensurateness of the Boltzmann equation and the Navier-Stokes equation, was detailed. Then, we discussed the Lattice Boltzmann algorithm and some examples of commonly used boundary conditions. Finally, we saw how Lattice Boltzmann modeling can be used to understand the behaviour of active particles.

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