Immersed Boundary-Finite Difference Lattice Boltzmann Method for Liquid-Solid Two-Phase Flows*

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Abstract

An immersed boundary method based on a finite difference lattice Boltzmann method (IB-FDLBM) is presented. The FDLBM solves the discrete Boltzmann equation including an additional collision term by using finite difference schemes. The additional term works as a negative viscosity in the macroscopic level and allows us to alter the fluid viscosity while keeping the other relevant parameters of the simulation fixed. The immersed boundary method employs a direct-forcing method, which utilizes external forces at Lagrangian points embedded on immersed boundaries to impose the no-slip boundary condition. Several benchmark simulations are carried out to validate the developed method, i.e., flows past a circular cylinder, a falling particle, and interaction between two falling particles. Couette flows between a stationary and a rotating cylinder are also simulated at various values of the relaxation time for collision. The main conclusions obtained are as follows: (1) steady flows past a stationary circular cylinder are well predicted, (2) the motions of particles falling through liquids predicted using IB-FDLBM quantitatively agree well with those obtained using immersed boundary methods based on the lattice Boltzmann equation (IB-LBM), (3) the developed method well predicts the interaction between two particles falling through a liquid, e.g., the drafting-kissing-tumbling motion, and (4) distortion of velocity fields in circular Couette flows at high relaxation times is removed by the additional collision term.

Key words: Immersed Boundary, Finite Difference Lattice Boltzmann Method, Falling Particles, Circular Couette Flow

1. Introduction

The lattice Boltzmann method (LBM)\(^{(1)}\) has come into use for predicting and modeling fluid flows. The basis of LBM is the lattice Boltzmann equation (LBE), which describes the time evolution of the discrete particle velocity distribution function. The macroscopic variables such as the density and momentum are defined as particle velocity moments of the distribution function. LBM employs a purely explicit time integration for LBE and the discrete particle collision operator in LBE has a local nature. Consequently the computation in LBM is much simpler than those in traditional Navier-Stokes solvers and is suitable for parallel computing. This advantage promotes rapid advancement of LBM and it has been widely used for predicting various flows such as flows in porous medium\(^{(2)}\), turbulent...
flows\(^{(3)}\), and two-phase flows\(^{(4)-(6)}\). LBM however has some restrictions, e.g., (1) when the relaxation time is decreased while keeping the relevant dimensionless numbers constant, the spatial resolution needs to be increased, and (2) the Lagrangian nature of LBE requires that a discrete particle moves from a lattice point to its neighbor during one time step, and therefore, the lattice spacing and the time step size cannot be altered independently.

Various methods combining LBM and an immersed boundary method (Immersed Boundary LBM: IB-LBM) have been recently developed for predicting liquid-solid two-phase flows\(^{(7)-(12)}\), and various particulate flows have been simulated such as a drafting-kissing-tumbling (DKT) motion of two particles or sedimentation of thousands of particles. However IB-LBM simulations of planar and circular Couette flows show a remarkable increase in errors in velocity near the immersed boundary with increasing the relaxation time\(^{(13)}\), that is, a high viscosity causes non-negligible errors in velocity since the viscosity increases with the relaxation time. This error narrows the range of the relaxation time to be used in IB-LBM. In addition, IB-LBM is not free from the above-mentioned restrictions of LBM.

In this study, an immersed boundary method is, therefore, proposed to mitigate these restrictions. The discrete Boltzmann equation\(^{(14)}\) is utilized instead of LBE and is solved using an ordinary finite difference scheme to assign the lattice spacing and the time step size independently. This class of LBM is referred to as finite difference lattice Boltzmann method (FDLBM). An additional collision term proposed by Tsutahara et al.\(^{(15)}\) is, then, implemented into the proposed IB-FDLBM. It works as a negative viscosity in the macroscopic level, with which we can control the viscosity without changing the spatial resolution. Several benchmark simulations are carried out for the validation of the proposed method: (1) flows past a stationary circular cylinder, (2) a single particle falling in a liquid, and (3) a DKT motion of two particles. Simulations of a circular Couette flow are also carried out to examine whether or not the proposed method gives accurate predictions by tuning the parameter of additional collision even at high relaxation times.

2. Immersed Boundary-Finite Difference Lattice Boltzmann Method

The discrete Boltzmann equation based on the single-relaxation time approximation for single phase flows is given by\(^{(14)}\)

\[
\frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = -\frac{1}{\phi} (f_i - f_i^{eq}),
\]

where \(f_i\) is the particle velocity distribution function in the \(i\)th direction, \(f_i^{eq}\) the equilibrium distribution function, \(t\) the time, \(c_i\) the particle velocity, and \(\phi\) the relaxation time. Tsutahara et al.\(^{(15)}\) replaced the distribution function in the advection term with the following distribution function including the additional collision term for numerical stability:

\[
g_i = f_i - \frac{A}{\phi} (f_i - f_i^{eq}),
\]

where \(A\) is a parameter, which works as a negative viscosity in the macroscopic level. This modification enables us to control the viscosity without changing the spatial resolution and to use a large time step even at a low \(\phi\) by increasing \(A\). The external forcing term, \(F_i\), is introduced to satisfy the boundary conditions at immersed boundaries:

\[
\frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = -\frac{1}{\phi} (f_i - f_i^{eq}) + F_i.
\]
The macroscopic fluid density, $\rho$, and velocity, $\mathbf{u}$, are given by

$$\rho = \sum_{i=0}^{Q-1} f_i, \quad (4)$$

$$\rho \mathbf{u} = \sum_{i=0}^{Q-1} c_i f_i, \quad (5)$$

where $Q$ is the number of discrete velocities. In this study, the two-dimensional nine-velocity (D2Q9) model is used for the discrete velocity. The equilibrium distribution function is, therefore, given by

$$f_i^{eq} = W_i \rho \left[ 1 + \frac{3(c_i \cdot u)}{c^2} + \frac{9(c_i \cdot u)^2}{2c^4} - \frac{3u \cdot u}{2c^2} \right], \quad (6)$$

where $W_i$ is the weighting function and $c$ the lattice velocity ($c = 1$). The values of $c_i$ and $W_i$ are summarized in Table 1. Applying the Chapman-Enskog expansion to Eq. (3) recovers the macroscopic conservation equations for incompressible Newtonian fluids:

$$\nabla \cdot \mathbf{u} = 0, \quad (7)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} + \frac{F}{\rho}, \quad (8)$$

where the superscript $T$ denotes the transpose, $F$ is the external force acting on the fluid at immersed boundaries to satisfy the boundary condition and $p$ the pressure given by $p = \rho c_s^2/3$, which gives the speed of sound, $C_s = c/\sqrt{3}$. The kinematic viscosity, $\nu$, is given by

$$\nu = \frac{1}{3}(\phi - A). \quad (9)$$

The fluid motion is computed by solving Eq. (3) on Eulerian grids, whereas moving bodies immersed in a flow field are represented using Lagrangian points and their motions are calculated by solving an equation of motion (Fig. 1). The Eulerian coordinates at the grid point $I$ and the coordinates of the $L$th Lagrangian point are $x_L = (x_L, y_L)$ and $X_L = (X_L, Y_L)$, respectively. The method proposed by Dupuis et al.$^{(16)}$ is utilized to impose the boundary conditions at immersed boundaries. Thus, the external force, $F(X_L, t)$, acting on the fluid to impose the no-slip boundary condition is given by

$$F(X_L, t) = \rho \frac{u_L(X_L, t) - u(X_L, t)}{\Delta t}, \quad (10)$$

<table>
<thead>
<tr>
<th>Table 1 Discrete particle velocity and weighting coefficients in the D2Q9 model</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
</tr>
<tr>
<td>$c_x$</td>
</tr>
<tr>
<td>$c_y$</td>
</tr>
<tr>
<td>$W_i$</td>
</tr>
</tbody>
</table>
Fig. 1 Immersed boundary method. The intersections of mesh lines define Eulerian points \((x_{IJ})\) while the solid points on the body surface represent Lagrangian points \((X_L)\).

where \(\Delta t\) is the time step, \(u_P(X_L, t)\) the velocity at the \(L\)th Lagrangian point of the solid particle \(P\), and \(u(X_L, t)\) the fluid velocity interpolated onto \(X_L\). The fluid velocity is interpolated using

\[
u(X_L, t) = \sum_{x_{IJ}\in\Omega} u(x_{IJ}, t) \delta(x_{IJ} - X_L) \Delta V,
\]

where \(\delta\) is the smoothed delta function, \(\Delta V\) the computational cell volume and \(\Omega\) the domain in which \(\delta \neq 0\). The delta function is given by

\[
\delta(x_{IJ} - X_L) = \delta_x \delta_y \left( \frac{x_{IJ} - X_L}{\Delta x} \right) \left( \frac{y_{IJ} - Y_L}{\Delta y} \right),
\]

where \(\Delta x\) and \(\Delta y\) are the lattice spacings in the \(x\) and \(y\) directions, respectively. The one-dimensional delta function, \(\delta_h\), is given by

\[
\delta_h(r) = \begin{cases} 
\frac{1}{4} \left[ 1 + \cos \left( \frac{\pi r}{2} \right) \right] & \text{for } |r| \leq 2 \\
0 & \text{for } |r| > 2
\end{cases}
\]

The force calculated by using Eq. (10) is then distributed onto Eulerian grid points:

\[
F(x_{IJ}, t) = \sum_{L=1}^{N_m} F(X_L, t) \delta(x_{IJ} - X_L) \Delta S \Delta x
\]

where \(N_m\) is the number of Lagrangian points and \(\Delta S\) the area segment of a solid body, e.g., \(\Delta S = 2\pi R/N_m\) for a circular cylinder of radius \(R\) and unit length. The external forcing term \(F_i(x_{IJ}, t)\) is, then, given by

\[
F_i(x_{IJ}, t) = 3W_i c_i \cdot F(x_{IJ}, t),
\]

whose moments satisfy \(\Sigma_i F_i = 0\) and \(\Sigma_i c_i F_i = F\).

The motions of solid particles are calculated by solving the following equations:

\[
M_p \frac{dU_p}{dt} = F_p
\]
\[ I_P \frac{d\omega_P}{dt} = T_P \]  

(17)

where \( M_P \) is the mass of the particle \( P \), \( U_P \) the translational particle velocity, \( I_P \) the tensor for moment of inertia, \( \omega_P \) the angular velocity, \( T_P \) the torque, and \( F_P \) the force acting on \( P \), which consists of drag force, lift force, gravity, particle-particle and particle-wall interaction forces and so on. The velocity \( u_P \) is given by \( u_P = U_P + \omega \times (X_L - X_P) \), where \( X_P \) is the position vector for the center of gravity of the particle \( P \).

The second-order Runge-Kutta scheme is used for the time integration of Eq. (3):

\[
\begin{align*}
 f_i^{n+1/2} &= f_i^n + \frac{\Delta t}{2} \left[ -c_i \cdot \nabla g_i - \frac{1}{\phi} (f_i - f_i^{eq}) + F_i \right] \\
 f_i^{n+1} &= f_i^n + \Delta t \left[ -c_i \cdot \nabla g_i - \frac{1}{\phi} (f_i - f_i^{eq}) + F_i \right]^{n+1/2} 
\end{align*}
\]

(18)  

(19)

where the superscript \( n \) is the discrete time, i.e. \( t = n\Delta t \). The advection term is discretized using a third-order upwind scheme.

The equation of motion is discretized as

\[
 U_P^{n+1} = U_P^n + (U_P^n - U_P^{n-1}) \frac{\rho_p \Delta t}{M_P} + F_P \Delta t 
\]

(20)

where \( \rho_p \) is the particle density. The second term in the R.H.S. is introduced by Feng and Michaelides(9) to stably simulate particles of \( \rho_P \approx \rho \). The particle position is updated using

\[
 X_P^{n+1} = X_P^n + \frac{\Delta t}{2} (U_P^{n+1} + U_P^n) 
\]

(21)

Equation (17) is discretized similarly.

An extrapolation method proposed by Watari & Tsutahara(18) is used for the boundary condition of a computational domain. This method gives distribution functions at the domain boundary through extrapolation using the distribution functions at adjacent lattice points.

3. Validation

3.1 Flow past a stationary circular cylinder

Flows past a stationary circular cylinder are used for validation since many experimental and numerical results are available for comparison. The flow depends on the Reynolds number:

\[
 Re = \frac{U_0 D}{v} 
\]

(22)

where \( U_0 \) is the free stream velocity and \( D \) the diameter of the cylinder. Flows at \( Re = 20 \) and 40 are tested. The computational domain is shown in Fig. 2. The dimensions of the domain are \( 40D \) and \( 40D \) in the \( x \) and \( y \) directions. The cylinder is located at \((20D, 20D)\) and the ratio, \( D/\Delta x \), is 40. The number of Lagrangian points is 360 and these points are evenly distributed at the cylinder surface. The uniform flow along the \( x \)-axis at \( U_0 \) comes from the left boundary. The right boundary is continuous outflow. The top and bottom
boundaries are slip walls.

The drag force, $F_D$, is calculated by summing up $F(X_L, t)$ for all the Lagrangian points:

$$ F_D = -\sum_{L=1}^{N_L} F_s(X_L, t) \Delta S \Delta x, $$

where $F(X_L, t) = (F_x(X_L, t), F_y(X_L, t))$. The drag coefficient, $C_D$, is defined by

$$ C_D = \frac{F_D}{\frac{1}{2} \rho U_0^2 D}, $$

Fig. 2 Computational domain for flows past a circular cylinder.

Fig. 3 Streamlines and velocity fields of steady flows past a circular cylinder.
Figures 3(a) and (b) show the streamlines about the cylinder at Re = 20 and 40. A pair of steady symmetric vortices is formed behind the cylinder in each case. The length of the vortex increases with Re. These results are in good agreement with experimental observations\(^{(19)}\). Table 2 shows a comparison of the drag coefficient with numerical results in literature. The results obtained with the proposed IB-FDLBM agree well with those obtained using the other methods. In Figs. 3(a) and (b), some streamlines penetrate into the cylinder surface. As pointed out by Wu & Shu\(^{(10)}\), it is difficult for the immersed boundary method based on a direct-forcing method to perfectly satisfy the no-slip boundary condition, and the non-physical penetration is apt to take place. However, as shown in Figs. 3(c) and (d), the error in velocity at the cylinder surface is very small and good predictions of the vortex shape and drag coefficient are obtained.

### Table 2 Comparison of drag coefficient for steady flow past a circular cylinder

<table>
<thead>
<tr>
<th>Method</th>
<th>Re = 20</th>
<th>Re = 40</th>
</tr>
</thead>
<tbody>
<tr>
<td>IB-LBM(^{(12)})</td>
<td>2.090</td>
<td>1.572</td>
</tr>
<tr>
<td>IB-LBM(^{(10)})</td>
<td>2.091</td>
<td>1.565</td>
</tr>
<tr>
<td>FDM(^{(20)})</td>
<td>2.01</td>
<td>1.51</td>
</tr>
<tr>
<td>IB-FDLBM Present</td>
<td>2.135</td>
<td>1.58</td>
</tr>
</tbody>
</table>

*FDM: finite difference method*
3.2 Single Particle Falling Through Liquid

A falling particle in a liquid-filled container is one of the typical benchmark tests of moving boundary problem for validating immersed boundary based methods\(^8\)(\(^{11}\)). Figure 4(a) shows the computational domain. All the walls are no-slip walls. The initial particle location is (1 cm, 4 cm), and the particle is initially at rest. The fluid and particle densities are \(1.0\times 10^3\) kg/m\(^3\) and \(1.25\times 10^3\) kg/m\(^3\), respectively. The acceleration of gravity, \(g\), is 9.81 m/s\(^2\). The particle diameter is 0.25 cm. The numbers of lattice points in the \(x\) and \(y\) directions are 201 and 601, respectively. The parameters for collision are \(\phi = 0.65\) and \(A = 0.5\). The time step size is \(5\times 10^{-6}\) s. The number of Lagrangian points on the surface is 360. The particle falls rectilinearly as shown in Figs. 4(b)-(d). The vorticity contour shows that the symmetric wake structure is formed behind the particle due to the rectilinear motion. The time evolutions of the \(y\) coordinate, \(\text{YP}\), of the particle and \(\text{Re}\) using the falling velocity are shown in Fig. 5. The particle accelerates and reaches its terminal condition. Then the velocity is suddenly retarded just before reaching the bottom wall. The present method gives the same prediction as that obtained by a finite element method\(^{21}\) and that obtained by using an IB-LBM proposed by Dupuis\(^{16}\).

3.3 Drafting-Kissing-Tumbling Motion of Two Particles

A problem of two particles with DKT has been used as a benchmark problem for validating IB-LBMs\(^7\)(\(^{11}\))(\(^{22}\)). Figure 6(a) shows the computational domain. All the walls are no-slip walls. The particles, P1 and P2, are initially located at (1 cm, 6.8 cm) and (0.999 cm, 7.2 cm), respectively, and the initial velocities are zero. The other input parameters are as follows: \(\rho = 1.0\times 10^3\) kg/m\(^3\), \(\rho_p = 1.01\times 10^3\) kg/m\(^3\), \(\mu = 1.0\times 10^{-3}\) Pa\(\cdot\)s, \(g = 9.81\) m/s\(^2\), \(D = 0.20\) cm, \(\phi = 0.65\), \(A = 0.5\) and \(\Delta t = 5\times 10^{-5}\) s. The numbers of lattice points in the \(x\) and \(y\) directions are 201 and 801, respectively. For particle-particle and particle-wall collisions, the models proposed by Glowinski et al.\(^{23}\) are adopted. For particle-particle collision, the repulsive force, \(F_{pp'}\), between the particles \(P\) and \(P'\) is given by

\[
F_{pp'} = \begin{cases} 
\frac{\zeta_{pp'}}{\varepsilon_p} \left[ \frac{|x_p - x_{p'}| - R_p - R_{p'} - \zeta_p}{\zeta_p} \right] \frac{x_p - x_{p'}}{|x_p - x_{p'}|} & \text{for } |x_p - x_{p'}| < R_p + R_{p'} + \zeta_p \\
0 & \text{otherwise}, 
\end{cases}
\]  

(25)

where \(R_p\) and \(R_{p'}\) are the radii of the particles \(P\) and \(P'\), respectively. For particle-wall collision, the repulsive force, \(F_{pw}\), acting on the particle \(P\) is given by

\[
F_{pw} = \begin{cases} 
\frac{\zeta_{pw}}{\varepsilon_w} \left[ \frac{|x_p - x_w| - 2R_p - \zeta_w}{\zeta_w} \right] \frac{x_p - x_w}{|x_p - x_w|} & \text{for } |x_p - x_w| < 2R_p + \zeta_w \\
0 & \text{otherwise}, 
\end{cases}
\]  

(26)

where \(\varepsilon_p = \varepsilon_w = 2.0\), \(\zeta_p = \zeta_w = 3\) and \(c_{pp'} = c_{pw} = (\rho_p - \rho)\pi R^2 g\).

Successive images of the predicted particles and vorticity contour are shown in Figs. 6(b)-(e). The particles show drafting \((t = 1.5\) s\), kissing \((t = 2\) s\) and tumbling motions \((t = 3\) s\). The particle paths in the \(x\) and \(y\) directions are compared with those predicted using IB-LBMs\(^{16}\)(\(^{22}\)). As shown in Fig. 7, good agreement is obtained, and therefore, the proposed method is applicable to problems involving multiple particles interacting with each other.
Fig. 4 Computational domain and vorticity contour of flow about single falling particle.

Fig. 5 Particle position and Reynolds number.

Fig. 6 DKT motion of two particles.
4. Simulations of Circular Couette Flows

Le & Zhang (13) reported a large distortion of velocity field for several simple flows, e.g., a circular Couette flow, by using the IB-LBM proposed by Dupuis et al. (16). They showed that a large velocity slip at the immersed boundaries occurs when using high relaxation times. In this section, the circular Couette flow is simulated using the present method in order to prove its feasibility of using a high relaxation time. Figure 8 shows the numerical setup. The dimensions of the computational domain are 200 and 200 in the $x$ and $y$ directions, respectively, and $\Delta x = \Delta y = 1$. The inner circular ring is rotating at velocity $U_0 = 0.01$, while the outer circular ring is at rest. They are located at the center of the domain, and their radii are 45 and 70, respectively. The number of Lagrangian points is 720 for both rings. Periodic boundary conditions are adopted for all the domain boundaries.

Figure 9 shows the predicted velocity component in the azimuthal direction in the steady state. In these simulations, $A$ is fixed at 0.5. Hence the viscosity increases with $\phi$, i.e., from left to right figures. The fluid rotation is induced by rotation of the inner cylinder. With the direct-forcing method, both particle velocity distributions in the fluid and in the solid are solved. This causes pseudo-fluid velocities inside the inner and outer cylinders. At $\phi = 1$, the flow is axisymmetric, whereas the axisymmetry breaks at $\phi = 5$ and 10. The velocity profile in the horizontal cross-section at $I = 101$ for the half of domain is shown in Fig. 10. The solid line in the fluid region is the analytical solution given by
Although the velocities inside the cylinder predicted by the simulation have no physical meaning, they are compared with the velocity profile for rigid body rotation. The developed method with $\phi = 1$ gives good predictions. However, the discrepancy in velocity near the cylinder surfaces becomes larger with increasing $\phi$. The error in the velocity near the surface also causes the distortion of the velocity profile inside the cylinder. Then simulations are carried out with different values of $A$. The velocity profiles for various $A$ at $\phi = 5$ and 10 are shown in Figs. 11 and 12. The error decreases with increasing $A$ and good agreements between the prediction and theory are obtained when $\phi - A = 1$. The additional collision term reduces the viscosity without increasing spatial resolution, i.e., $\nu = (\phi - A)/3$, and therefore, a relatively large $\phi$ can be used compared with LBE based immersed boundary methods.
Fig. 10 Velocity profile along the horizontal line at different relaxation times.

Fig. 11 Velocity profile of circular Couette flow at $\phi = 5$.

Fig. 12 Velocity profile of circular Couette flow at $\phi = 10$. 
5. Conclusion

A lattice Boltzmann method (LBM) for predicting fluid-solid flows was proposed. The method is a combination of a finite difference lattice Boltzmann method (FDLBM) based on a discrete Boltzmann equation and an immersed boundary method (IBM). The FDLBM allows us to determine the lattice spacing and the time step independently. An additional collision term, which works as a negative viscosity in the macroscopic scale, is added for enhancing the numerical stability. IBM is based on the direct-forcing method, in which an external forcing term to impose the boundary condition at the immersed boundaries is added to the discrete Boltzmann equation. The force is calculated at Lagrangian points at the immersed boundary and is distributed onto Eulerian grids. The proposed method was validated through the following benchmark tests: (1) flows past a stationary circular cylinder, (2) a single particle falling in a liquid, and (3) interaction of two falling particles. According to Le & Zhang\(^{(13)}\), an IB-LBM causes large errors in velocity near moving boundaries when the relaxation time is large. Circular Couette flows between a rotating cylinder and a stationary cylinder were, therefore, simulated to examine whether or not IB-FDLBM gives accurate predictions even with a large relaxation time. As a result, the following conclusions are obtained:

(1) Steady flows past a stationary circular cylinder are well predicted.
(2) The motions of particles falling through liquids predicted using IB-FDLBM quantitatively agree with those obtained using IB-LBMs.
(3) The proposed method well predicts the interaction between two falling particles, e.g., the drafting-kissing-tumbling motion.
(4) Increasing the parameter in the additional collision term reduces the viscosity without increasing spatial resolution, and therefore, relatively larger relaxation times can be used compared with IB-LBMs.

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References


