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Simulation of finite-size particles in turbulent flows using the lattice Boltzmann method

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Abstract. Particle laden turbulent flows occur in a variety of industrial applications. While the numerical simulation of such flows has seen significant advances in recent years, it still remains a challenging problem. Many studies investigated the rheology of dense suspensions in laminar flows as well as the dynamics of point-particles in turbulence. Here we will present results on the development of numerical algorithms, based on the lattice Boltzmann method, suitable for the study of suspensions of finite-size particles under turbulent flow conditions. The turbulent flow is modeled by the lattice Boltzmann method, and the interaction between particles and carrier fluid is modeled using the bounce-back rule. Direct contact and lubrication force models for particle-particle interactions and particle-wall interaction are taken into account to allow for a full four-way coupled interaction. The accuracy and robustness of the method is discussed by validating the velocity profile in turbulent pipe flow, the sedimentation velocity of spheres in duct flow and the resistance functions of approaching particles. Preliminary results from the turbulent pipe flow simulations with particles show that the angular and axial velocities of the particles are scattered around values of mean axial velocity and shear rate obtained from the Eulerian velocity field.

AMS subject classifications: 76F10, 76F25, 76F65, 74F10

Key words: lattice Boltzmann method, moving bounce-back, turbulent pipe flow, particles in turbulence, finite-size particles, stresslet

1 Introduction

Turbulent suspension flows are relevant in many engineering applications and natural processes. Some prominent examples involving turbulent suspension flows include

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aerosol and pollutant transport, dust storms, sediment transport in river basins, flow of microalgae in photo-bioreactors, avalanches, slurries, and several other industrial processes. In many of these examples, particles in turbulence are non-living objects, eg. sand particles in dust storms. However, there are examples like the flow in tubular photo-bioreactors or the transport of plankton in lakes, estuaries and in the ocean where the particles are actually living cells. In the latter cases, apart from studying the dynamics of particles, it is also important to study the effect of hydrodynamic stresses on the cells which might have detrimental effects and can even destroy cells. For example in photo-bioreactors, cell damage due to shear is one of the key problems in upscaling photo-bioreactors for micro-algae culture. All devices include walls and thus particle-fluid coupling in the near wall region is also more crucial for the understanding of flow physics as well as cell transport and damage.

Pioneering theoretical work to understand the rheology of dilute suspension flows was done by Einstein [1], Batchelor [2], and Batchelor et al. [3]. However, the rheology of suspensions or turbulent flows laden with particles still remain a subject of investigation as the constitutive equations relating stress to rate of strain are not generally known for such complex flows. Over the past decades, advanced computational and experimental methods have been developed and utilized to study the particle laden turbulent flows. However, most studies have either investigated the rheology of dense suspensions in laminar flows [4–7] or the dynamics of point-particles in turbulence [8–14]. The validity of the point-particle approach is questionable when particle mass loading is significant or there exists a strong coupling between the particles and the fluid phase. The finiteness of the particle size and Reynolds number becomes important for larger particles and explicit models would require solving the full non-linear Navier-Stokes equation with the proper boundary conditions at the particle surface. The simulation of these finite-size particles exhibit additional complexities due to the multi-scale nature of the problem and local flow around the particle at finite Reynolds number. Consequently, adequate description of dynamics of the finite-size particles and their coupling with the surrounding fluid has emerged as one of the major open question for the fluid dynamics community.

A significant amount of effort has been invested in the development of efficient numerical schemes for the direct numerical simulation of suspensions of solid spheres in flows at varying Reynolds number. A variety of different schemes are being developed based on finite difference or finite volume solution methods for the Navier-Stokes equations combined with efficient schemes for the implementation of the solid particle boundary conditions. Pan et al. [15] were among the first to simulate finite-size particles in turbulent channel flow to study the effect of particle size relative to the dissipative length scale on turbulence intensities and Reynolds stress. A DNS study of dilute particle laden turbulent flow in a vertical channel with large number of fully resolved finite-size rigid particles was conducted by Uhlmann [16, 17], where they observed the formation of large-scale elongated streaklike structures and discussed the effect of particles on the Eulerian flow field. Kidanemariam et al. [18] investigated heavier particles in an open-channel and looked into the preferential accumulation of particles and their relation with flow
structures. Shao et al. [19] used fictitious domain method to study effects of large particles on the turbulence statistics in channel flow.

There has been some significant work recently on the suspension of finite-size particles in turbulent channel using immersed boundary method for volume fractions varying up to 20%, where researchers looked into the modification of the Eulerian flow field by the carrier phase and the dynamics of the particles and their migration [20–22], as well as the modified scaling laws in presence of the particles [23]. Several researchers [24–27] also studied the effect of particles on transition to turbulence in wall-bounded flows. Bäbler et al. [28] have looked into the breakup of solid aggregates suspended in a turbulent flow where the aggregates are assumed to be small with respect to the Kolmogorov length scale and it is assumed that breakup is caused by hydrodynamic stresses. The key aspect that is missing is an approach where we can capture the small-scale fluctuations on the surface of the finite-size particles and use them to derive a quantity which can be used to quantify the effect of straining flow on the finite-size particles.

An alternative method for the direct simulation of suspensions is based on the lattice-Boltzmann method (LBM). The lattice Boltzmann method has been an effective tool for the simulation of particle suspensions with applications in many industrial and biological problems. Simulation of arterial flows [7, 29] and finite-size fibers in turbulent channel flow [30] are some prominent examples showcasing the versatility of the method. Ten Cate et al. [31] simulated finite-size particles in isotropic turbulence using lattice Boltzmann method and presented results on turbulence spectra and particle collisions. Gao et al. [32] and Wang et al. [33] used lattice Boltzmann method with bounce-back scheme to study turbulence modification by finite-size particles in channel flow.

However, DNS of particle laden turbulent pipe flow using LBM has never been reported previously, perhaps due to the fact that standard LBM is restricted to cubic grid in Cartesian coordinates that does not conform with the cylindrical pipe surface. In order to establish LBM as a viable tool for turbulent flow simulations, it is important to be able to perform DNS of particle laden turbulent pipe flow with LBM.

The objective of this work is to demonstrate the use LBM as a tool for simulation of turbulent pipe flows with finite-size particles. In the past, the symmetric component of first moment of the traction (force per unit area) at the particle surface i.e. stresslet has been used by researchers [34, 35] as a quantity which shows the contribution of individual particle to the suspension rheology. In this work, we aim to present stresslet also as a quantitative measure to study the influence of the small-scale fluctuations of the local straining flow field on the finite-size particles, a field which has been unexplored previously. As anticipated, we will use LBM to simulate the turbulent suspension flow. The connection of LBM to molecular mechanics makes it possible to derive simple local rules for the interactions between the fluid and the suspended solid particles.

The remaining part of this paper is organized as follows. In section 2, the method used to simulate suspensions including fluid-particle interaction is outlined. Here we also discuss the computation of the properties which can be used to quantify the straining effect of the flow-field on the particles. A series of comparisons of particle-fluid flow problems
with known solutions is presented in section 3 to demonstrate the accuracy and robustness of the approach and implementation. In section 4, we simulate turbulent pipe flow without particles and compare our results with DNS results from the literature. In section 5, we give example of the computation of stresslet for a simple shear flow. Finally, we present some preliminary results for particles in turbulent pipe flow in section 6.

2 Methodology

The simulation algorithm consists of three major components: the fluid solver, the model to simulate the particulate phase and the particle-particle interaction. The description of the lattice Boltzmann method as a flow solver has been discussed in numerous texts in the past and the reader is encouraged to consult [36] or [37] for more details on the method. We used the D3Q27 Bhatnagar-Gross-Krook (BGK) lattice Boltzmann method to simulate the fluid flow. The specific reason for choosing the D3Q27 lattice model will be discussed later in section 4.

In this section, we focus on modeling of the finite-size particles, their coupling with the fluid and the interaction among them.

To simulate the hydrodynamic interactions between the solid particles in the suspension, the lattice Boltzmann model must be modified to incorporate the boundary conditions imposed on the fluid by the solid particles. Pioneering work for simulation of finite-size particles in fluids using LBM involves the work done by Ladd [38]. He proposed the solid bounce back (SBB) scheme which couples the particles with the fluid while keeping the momentum conserved. The basic methodology to model the particle-fluid interaction is illustrated in figure 1.

The solid particles are defined by a boundary surface, which can be of any size or shape. When placed on the lattice, the boundary surface cuts some of the links between lattice nodes. The fluid particles moving along these links interact with the solid surface at boundary nodes placed halfway along the links. Thus, the particle boundary is approximated by a staircase which becomes more and more accurate as the particle size becomes larger. Ten Cate et al. [39] demonstrated that an accurate representation of the sphere’s motion and the associated flow field could be obtained at a resolution of approximately 8 gridpoints per particle diameter. The method proposed by Ladd [38] combines the Newtonian dynamics of the solid particles with a discretized Boltzmann equation for the fluid phase. In this method, nodes on either side of the boundary surface are treated in an identical fashion, so that fluid fills the whole volume of space, both inside and outside the solid particles. The interior fluid was kept for computational convenience only, since it avoids the necessity of creating and destroying fluid as the particle moves. In this formulation, where particles are treated as shells of mass containing fluid, the fluid inside the particles has the potential to affect particle dynamics. In order to run simulations with neutrally buoyant particles, the mass of the shell containing the interior fluid must approach zero. This creates instabilities in the particle update procedure. Consequently, this
method was limited to solid particles with density larger than the fluid density. Aidun et al. [40] overcome this problem by proposing a model in which there is no fluid to occupy the solid particle volume, fluid nodes appear and disappear as the solid particle moves through the domain. Therefore, the computational algorithm is somewhat more involved than that of Ladd’s model [38]. However, it was argued that if the number of solid particles in the system is not very large, the computational time for these two methods will be about the same. Several other variations and applications of the method were also discussed, eg. by Behrend [41] and Aidun and Lu [42]. Mid-point bounce back proposed by Aidun et al. [40] for the analysis of solid particles with inertia suspended in a fluid was used for particle-fluid coupling in this work. The main features of this implementation are:

1. Bounce back: the mid point bounce back was implemented for the fluid outside of the particle. Hence, the fluid inside is neither updated by the bounce back nor it is
used for the momentum update of the particle.

2. Newly covered nodes: momentum of the newly covered node is transferred to the particle.

3. Newly uncovered nodes: density at newly uncovered nodes is computed as average density of neighboring fluid nodes. The velocity of the boundary node \( u_b \) is determined by the solid particle velocity, \( U \), angular velocity, \( \omega \) and center of mass position, \( R \): \( u_b(r) = U + \omega \times (r - R) \). These density and velocity values are used to initialize the equilibrium populations at the node. The computed momentum at the node is subtracted from the particle momentum.

As for any discrete computational method, LBM is limited to a gap width between solid particles larger than one lattice unit. As the solid particles approach each other, leaving no fluid node between the solid surfaces, the method cannot accurately calculate the hydrodynamic interaction between the solid particles. In order to resolve the hydrodynamic force between solid particles near contact, relatively large numbers of lattice nodes need to be used in the computational domain. One approach to resolve this difficulty is to amend the solid-fluid interaction calculation with a model of lubrication force based on theoretical lubrication approximation for a small gap between regular shaped objects. Ladd and Nguyen [43] suggested a lubrication correction for the normal forces between two spheres (denoted i and j in subscripts) according to eq. (2.1). The lubrication force diverges as the gap, \( h = r_{ij} - 2R \) between the two particles approach zero and are therefore clipped at a specific value to avoid numerical instabilities.

\[
\begin{align*}
    f_{ij} &= -f_{ji} = -\frac{3}{2} \pi R^2 \mu \hat{r}_{ij} \cdot (v_i - v_j) \left( \frac{1}{h} - \frac{1}{\Delta_c} \right) \\
    \text{with } \Delta_c &= \frac{2}{3} \text{ for } \tau = 1
\end{align*}
\]  

(2.1)

In the above equation, \( f_{ij} \) is the normal lubrication force on sphere i due to another sphere j, \( \hat{r}_{ij} = (r_i - r_j) / |r_i - r_j| \) represents the unit vector along the direction joining the center of mass of two particles, \( v_i \) and \( v_j \) are the velocities of the two particles, \( R \) is the radius of the particle(s) and \( \mu \) is the dynamic viscosity of the suspending medium. The cut-off parameter, \( \Delta_c \), represents the separation below which the lubrication force becomes active and the value of \( \Delta_c \) depends on relaxation parameter, \( \tau \) with \( \Delta_c = 2/3 \) for \( \tau = 1 \). Ladd et al. [43] determined the value of \( \Delta_c \) for different values of \( \tau \) by computing the drag force on a spherical particle and their results are used as reference for our simulations.

On top of the lubrication force, a short-range repulsive force is added to prevent overlapping of particles. For \( h \leq h_c \) a Hookean repulsive force is given by eq. (2.2)

\[
F_r(h) = \epsilon \begin{cases} 
    (h_c - h), & \text{if } 0 \leq h \leq h_c \\
    h_c, & \text{if } h \leq 0
\end{cases}
\]  

(2.2)

where \( \epsilon \) is a stiffness parameter and the force is applied along the direction connecting the center of mass of the two particles. The force is cut-off in magnitude achieved at \( h = 0 \).
The above treatment introduces two additional parameters, $h_c$ and $\epsilon$. In this case, care must be taken to ensure that the influence of the non-hydrodynamic repulsion modeling is sufficiently small to be neglected. However, the repulsion force should also be strong enough to avoid overlap of the particles. We have used $h_c = 0.2$ and $\epsilon = 20$ for our simulations (all values are in appropriate lattice units) as a compromise between the requirements. Further investigation is needed to obtain the optimum values of $h_c$ and $\epsilon$ for different flow configurations.

With the net force and the torque calculated from the above equations, the motion of the solid particle is simply determined by solving Newton’s equations for the linear and angular momentum. In the simulations discussed here, these equations are solved using a leap-frog integration scheme to obtain the complete motion of the suspended particles in the fluid. The angular dynamics was integrated by the method of quaternions, as discussed in [44], for representing orientations and rotations of finite-size particles.

In order to quantify the effect of a straining flow-field on particles, we look into the first moment of force, $M_{ij}$, on the surface of the particles:

$$M_{ij} = \int_{S_p} \sigma_{ik} n_k x_j ds$$

where $x_j$ is the vector connecting surface element to center of mass of the particle, $n_k$ is the outward unit normal from the particle surface, $\sigma_{ik}$ is the fluid stress tensor and the integration takes place over the surface of the particle $S_p$. The isotropic part of $M_{ij}$, shown and subtracted below, is of no dynamic significance since its divergence goes to zero. The traceless matrix can be decomposed into its symmetric and antisymmetric components, $M_{ij} - \frac{1}{3} M_{ij} \delta_{jk} = S_{ij} + T_{ij}$, where torque constitutes the antisymmetric component. It is important to notice that the torque is only a part of the first moment of the force distribution,

$$T_{ij} = \int_{S_p} [\sigma_{ik} x_j - \sigma_{jk} x_i] n_k ds$$

and that here we are also interested in the stresslet,

$$S_{ij} = \int_{S_p} [\sigma_{ik} x_j + \sigma_{jk} x_i] n_k ds - \frac{1}{3} \int_{S_p} \sigma_{ik} x_j \delta_{jk} n_k ds$$

From a physical perspective, the stresslet is the result of the resistance of the rigid particle to a straining motion. Unlike the hydrodynamic force and torque, which have direct relation to the momentum of a particle, the stresslet is not needed in the equations of motion for a particle. Still, it has a very important role in suspension mechanics, as it describes the added stress associated with the particles in a suspension, and is thus essential for understanding of the rheology of suspensions at the single particle level. The computation of forces locally on the surface of the particle using the bounce back scheme enables us to compute the stresslet matrix directly.

Clausen et al. [45] studied the Galilean invariance in LBM and its effect on the calculation of rheological properties of suspension. They find a link-wise error term and
this term was shown to scale with the square of the velocity. In the majority of cases, the effect of this Galilean error was found to be negligible for the particle dynamics and stresslet calculations. However, in quantities dependent on external traction vectors such as normal stress differences in suspensions, magnitudes are exceedingly small, and these Galilean errors may be significant. They proposed that the Galilean error can be canceled by creating an internal boundary node (IBN) with distributions set to \( f_{i}^{eq}(\rho, u_{b}) \) (equilibrium distribution computed using fluid density \( \rho \) and boundary velocity \( u_{b} \)) at every link inside the particle. The equilibrium distribution from these internal boundary nodes undergo the normal bounce back operation with the particle, thus exactly canceling the error terms. We implemented the correction suggested by Clausen et al. [45] in our code on top of the mid-point bounce back scheme proposed by Aidun et al. [40].

From a computational point of view, the lattice Boltzmann method is highly attractive since the local nature of the algorithm makes it optimal for parallel computing. In principle, communications are required only once per time step as the population distributions advected directly across sub-domain boundaries. Although, additional communication steps are involved in practical simulation codes, for instance related to data reduction and output, these do not dominate the computational cost. However, the particle-particle interaction and parallelization of particle treatment can significantly affect the efficiency. The particle treatment is fully parallelized in our code and we are currently working on its optimization to achieve good scaling. The flow solver has been implemented on parallelized code and run on multiple processors showing good scaling results (see figure 2).

3 Dynamics of particles at low Reynolds number

In this section, the method is examined and validated by application to three canonical test cases involving particles for which solutions are well known.

3.1 Spheroid in a shear flow

The motion of a solid spheroid in a simple shear flow is analyzed in this section to validate our results for the rotational dynamics of particles at small Reynolds number. Jeffrey [46] studied the motion of an spheroid at vanishing Reynolds number and obtained analytical solutions. In particular, his solution shows that the motion of a spheroid, is periodic with a period given by eq. (3.1):

\[
T = \frac{2\pi(a^2 + b^2)}{abG}
\]

(3.1)

where \( G \) is the shear rate, \( a \) and \( b \) are the radii of the spheroid. In a period of time \( T \), the particle completes one full rotation. The Reynolds number is \( Re = Gd^2/\nu \), where \( d = 2a \) (\( a \) being the major radius).
In our simulation, a spheroid with semi-major radius \((a)\) and semi-minor radius \((b)\) is placed at the center of cubic domain of side \(H\). The two walls are separated by a distance \(H\) in vertical direction and move in opposite direction with velocity \(U\) (see schematic in figure 3). Periodic boundary conditions are used in axial and span-wise direction. The spheroid is free to rotate but its translational motion is negligible due to the symmetry of the set-up. The confinement ratio \(a/H\) for all the simulations was kept equal to 0.3125 while the Reynolds number was varied by changing the wall velocity. For different Reynolds number, the computational results agree well with Jeffery’s analytical solution and the numerical results of F. Janoschek (personal communication), as shown in figure 3. The deviation of our results from the analytical results can most probably be attributed to the high confinement ratio. For the large confinement ratio, the effect of the viscous shear stress on the spheroid due to the presence of the boundary walls becomes significant resulting in the deviation from the analytical solution for an unbounded domain obtained by Jeffrey [46]. However, the large confinement ratio also overshadows the effect of (small) finite Reynolds number. Consequently, our results show almost no
Figure 3: Non-dimensional angular velocity ($\omega / G$) for a spheroid with normalized time ($tG$) at different Reynolds number compared with Jeffery's solution for $Re = 0$ and the numerical results of F. Janoschek (personal communication).

Reynolds number dependence.

3.2 Particle settling under gravity

The sedimentation of a single spherical particle in a box is considered in this section in order to validate the particle dynamics under linear motion. In this simulation, a spherical particle of diameter $D$ is released in a vertical square channel of width $L$ which then settles under gravity. The sphere is initially released at the center of the cross-section of the channel with zero velocity in a fluid and settles along the axis of the channel finally reaching its terminal velocity.

Since the walls are at a finite distance from the particle, the terminal velocity will be less than the terminal velocity of an unconfined particle. Here results from analysis of the three-dimensional problem are presented and compared with the experiments of Miyamura et al. [47] and the numerical results of Aidun et al. [40]. Miyamura et al. [47] conducted a series of experiments to study the wall effects on the steady settling velocities of single solid spheres in square cylinders filled with highly viscous jelly solutions. The lattice Boltzmann simulation has been carried out for a three-dimensional sedimentation in the same conditions as the experiments. In the present analysis, the channel is divided
into $512 \times 32 \times 32$ lattice units. In this simulation, the range of particle Reynolds numbers is from 0.0012 to 0.0746, and the solid-to-fluid density ratio is two. The wall effect is quantified with the ratio

$$\zeta = \frac{u_t}{u_0} \quad (3.2)$$

where $u_t$ is the terminal velocity with nearby boundary walls, and $u_0$ is the unconfined terminal velocity from Stokes equation. Figure 4 shows a comparison of the results from our computational analysis with the best curve fit to the experimental data of Miyamura et al. [47]. As shown in this figure, there is good agreement between the experiments and our computational results.

3.3 Interaction of approaching spheres

The accuracy of the present method with lubrication forces is studied using the interaction of two identical spheres approaching each other. The results are compared with analytical results of Jeffrey and Onishi [48] and the numerical results of Janoschek et al. [49]. In the numerical set-up, one particle with radius $R$ is placed at a small (less than 1 lattice unit) random offset with respect to the center of a cubic box. Periodic boundary conditions are applied in the three directions on the cubic box. The size of the box
was chosen to be $15R$ as suggested by [49] in order to compromise between the computational cost and the undesirable effect of boundaries. Another particle is placed at a random angular position with respect to the first particle but a fixed surface separation $h$. The first particle near the center of the lattice is held fixed while the other translate towards the first with a velocity $v$ such that it gives a fixed particle based Reynolds number $Re = |v| R / v = 6 \times 10^{-8}$. The relaxation time was kept equal to one giving $v = 1/6$ for all simulations.

The simulations are allowed to run 1000 time steps (in lattice units) until a steady state is reached. The motion of the particle during this time is negligible as the Reynolds number was very small. Hence, no changes in the discretization are observed and the forces on the particles are due to bounce-back and lubrication only. For each $R$, the magnitude of the force is averaged over 15 random configurations with the same value of $h$ and normalised by the drag force on a sphere obtained from Stokes law. Figure 5 displays the force on the sphere related to the particle motions explained above at resolutions $R = 2, 4$ and 8 and agrees well with previous analytical and numerical results.
4 Turbulent pipe flow

Now, we consider the flow in a cylindrical pipe without particles. The Reynolds number based on the friction velocity and the diameter of the pipe \((Re_\tau = u_\tau D/\nu = 360)\) is used in the subsequent discussion. The friction velocity can be related to the wall shear stress as \(\rho u_\tau^2 = \tau_w\). When the force field is conservative, such as gravity, it can be expressed as a pressure gradient and vice-versa. A constant pressure gradient is included here as a force term. It is possible to find a relation between the external source term and the wall shear stress by considering the momentum balance between pressure and the viscous forces as \(2\pi R dx \tau_w = \pi R^2 dP\), which can be rearranged to \(\tau_w = \frac{1}{2} R \frac{dp}{dz}\). In the simulations, the pipe-length is set equal to twice the diameter. Periodic boundary conditions are used in the stream-wise (axial) direction. We used mid-point bounce back boundary condition for the solid boundaries to impose no-slip on the cylindrical wall [37]. The domain is discretized by a cubic mesh of \(256 \times 128 \times 128\) with 256 lattice points in the stream-wise and 128 in the lateral directions.

The simulation starts from the laminar flow and with a random positioning of the particles. Transition naturally occurs at fixed Reynolds number because of the fluctuations added by the presence of the particles. This turbulent flow field created using the finite-size spherical particles is then used to restart another simulation without the particles. The duration of the full simulation without particles was 2 million (in lattice units). Statistics for the analysis are collected after the initial transient phase when the flow adjusts to the absence of particles and reaches a pseudo-steady state. The integral time scale is computed using the diameter and friction velocity \(t^+ = D/u_\tau\). Turbulence statistics (figure 6) are obtained from averaging over the full length of the pipe and over at least \(50t^+\). The difference between the radial profiles in horizontal and vertical direction obtained from the contour plots is taken as an estimate of the error. The DNS data of Eggels et al. [50] was used as the reference data. In the presentation of the results, \(y^+\) is defined as \(y^+ = \frac{D^+}{r^+} - r^+\), where \(r\) is the radial coordinate in the cylindrical coordinate system with a pipe center as an origin, \(D\) is the diameter of the pipe and the + sign denotes the normalization with wall length, \(\nu/u_\tau\). The axial and the root-mean-square (RMS) velocity are normalized by the friction velocity, \(u_\tau\). As shown in figure 7a and 7b, the mean fluid velocity profile and turbulent intensities match well with the DNS data.

We also observed the effect of lattice models (D3Q19 versus D3Q27) on the rotational invariance of turbulent pipe flow [51]. Only the D3Q27 lattice model could achieve the rotational invariance, in terms of long-time-averaged turbulence statistics, and generate results comparable to DNS data (figure 7a and 7b), while the D3Q19 lattice model exhibit strong angular dependency. Hence, the D3Q27 lattice was used in all our pipe flow simulations.
Figure 6: Plots of the axial and RMS velocities normalized by the friction velocity for turbulent pipe flow without particles, at $Re_{f} = 360$ and obtained by averaging over 50 integral time scales and over the length of the pipe.
Figure 7: Radial velocity profiles normalized by friction velocity, \( u_\tau \), and wall length, \( \nu / u_\tau \) for turbulent pipe flow without particles at \( Re_\tau = 360 \) and the comparison with the simulations of Eggels et al. [50].

5 Stresslet on a sphere in shear flow

We now discuss the computation of stresslet on a spherical particle in a shear flow and compare the results with the analytical values of Faxén laws. The Faxén laws are the relations between the motion (of the particle and fluid) to the forces, torque, stresslet and flow it experiences under low Reynolds number conditions in dilute regime. The derivation of these results uses the reciprocal theorem (Kim and Karrila, 1989, Chapter 3 [52]). Here we simply give the results for the stresslet applied to a sphere:

\[
S = \frac{20}{3} \pi \mu r^3 \left( 1 + \frac{r^2}{10} \nabla^2 \right) E(x=0)
\]

where \( r \) is the radius of the particle and \( E \) is the rate of strain in ambient flow. The \( x=0 \) implies that the ambient fields are evaluated at the position occupied by the center of particle when the particle is not present.

In the simulation, a spherical particle of diameter \( d \) is placed at the center of a cubic domain of side \( H \). The two walls are separated by a distance \( H \) and move in opposite direction with velocity \( U \) (see schematic in figure 8). Periodic boundary conditions are used in axial, \( x \) and span-wise direction, \( z \). In such a situation, the only non-zero velocity derivative is \( \partial u / \partial y \). Consequently, the only non-zero components of stresslet are \( S_{xy} \) and \( S_{yx} \) and are equal. The particle based Reynolds number (Re=\( Gd^2/\nu \)) varies from 0.03 to 0.4267.

The simulations are allowed to run 2000 time steps (in lattice units) until a steady state is reached. The translational motion of the particle during this time is negligible due to the symmetry of the problem. We computed the ratio \( S_{xy}^*/S_{xy} \) of the value of \( S_{xy} \) from the
simulation (in steady state) using the momentum exchange along each link node with the value obtained from Faxén laws. The diameter of the particle is gradually decreased to eliminate wall effects, and the $S_{xy}$ component of the stresslet normalized by the analytic result is shown in figure 8 for four different channel height.

The deviation from the analytical results depends on several parameters, i.e. flow resolution (system size), particle resolution (particle diameter), Reynolds number and the confinement ratio ($H/d$). The slight increase in error for higher $H/d$ for $H=55$ can be due the discretization of particle surface at small diameters. Nevertheless, it was observed that the error remains below 5% for a confinement ratio ($H/d$) higher than 4. for different resolutions.

Figure 8: $S_{xy}$ component of stresslet tensor on a sphere in a shear flow, normalized by the solution obtained from Faxén laws, for different domain sizes and particle discretizations. The results approach the analytical solution for $H/d \geq 4$. Schematic of the set-up is shown in the inset.
6 Particles in turbulent pipe flow

The presence of finite-size particles can have both enhancing or diminishing effect on the turbulence intensity in the pipe flow. On one hand, the motion of inertial particle in turbulent flow costs energy and increase the effective viscosity and therefore the turbulence intensity should decrease. One can also argue that the presence of finite-size particles in the flow generates additional vortices at the length scale of the particles and hence the turbulence levels should increase. In order to make a quantitative comparison between the flow with and without particles, we decided to keep the energy input in the flow as constant. This is achieved by varying the volume force \( f \) at each time step in order to obtain fixed energy input \( \langle f \cdot v \rangle_{1-\phi} \), where \( v \) is the velocity of fluid in axial direction, \( \phi \) is the volume fraction of the particles and \( \langle \cdot \rangle_{1-\phi} \) represents phase averaged dot product.

The domain for simulation with particles was discretized at a slightly higher resolution of \( 480 \times 240 \times 240 \) and 64 neutrally buoyant particles, each with a radius of 6 lattice units, were randomly initialized at \( t = 0 \). The Reynolds number based on the friction velocity and on the diameter of the pipe (\( Re_{\tau} = u_{\tau}D/\nu \)) for the simulation was 250. A slightly lower Reynolds number and higher resolution was chosen compared to the previous section to keep the flow field fully resolved in presence of the particles. The particle based Reynolds number (\( Re_p = u_p d/\nu \)), where \( u_p \) is the particle velocity and \( d \) is the particle diameter varies from 30, near the wall, to 250, near the center of the pipe. The rest of the details remain the same as discussed in the previous section. Figure 9 shows the results for the joint probability distribution function of axial and angular velocity with radial position of the center of mass of particles obtained from the simulation. It can be observed that the particles stay close to the wall as also observed by Picano et al. [9] for inertial point-particles in turbulent pipe flow at comparable Reynolds and Stokes number. The finite size of the particles results in the excluded region near the wall. Axial velocity is normalized by the friction velocity of the corresponding simulation, the angular velocity is normalized by the ratio of friction velocity to lattice resolution (\( \Delta_x = 1 \)) and the radial positions are normalized with the radius of the pipe.

The particle axial velocity is compared with the mean Eulerian velocity obtained from another simulation without particles but with the same energy input. It was observed that the axial velocity of particles is scattered around the mean velocity obtained from the Eulerian field. The angular velocity of a sphere in a shear flow with shear rate \( G \), is given by \( G/2 \). For this reason, the magnitude of angular velocities of the particles is compared with the half of shear rate (\( G/2 \)), again obtained from another simulation with the same energy input. The angular velocities of the particles increases towards the wall due to the high-shear region and scattered around the values of shear rate obtained from the Eulerian field.

The results discussed in the present work corresponds to a low volume fraction of about 0.27%. In principle, the method proposed by Aidun et al. [40] and discussed in the present manuscript is capable of simulating very dense suspension as demonstrated by Janoschek et al. [53], where they simulated volume fractions close to 50% for laminar
Figure 9: Joint PDF of axial velocity (left) and magnitude of angular velocity (right) with radial position of the particles. Color bar indicates $\log_{10}$ of probability. Blue lines indicate mean axial velocity (left) and half of mean shear rate (right) obtained from Eulerian field of another turbulent pipe simulation without particles and with same energy input as the one with particles.

flow in blood vessels. However, it becomes challenging to have sustained turbulent flow with increasing volume fraction due to increase in effective viscosity. The situation becomes more challenging if one wants to keep the energy input constant with increasing volume fraction because the forcing needs to be increased to compensate for the decrease in eulerian velocity. The parameters and the resolution for the simulation have to be carefully adjusted to run simulations with sustained turbulence at higher volume fractions and this will be discussed in subsequent works.

7 Concluding remarks

In this study, we demonstrated the applicability of the method based on the solution of discrete Boltzmann equation coupled with moving bounce back scheme to study wide variety of problems involving rotation of a spheroid in shear flow, settling of sphere in channels and interaction of approaching spheres. More precisely, a simulation approach has been developed for the study of turbulent flows with suspended finite-size particles in complex geometries, where besides the dynamics of particles and Eulerian properties of fluid, it is also possible to compute additional stresses due the the presence of particles. It was shown that the lattice Boltzmann method with D3Q27 lattice model could produce turbulent statistics comparable to DNS data. Besides looking into the dynamics of particles and statistics of velocity field, we also provided a validation where we directly computed the stresslet from the momentum exchange on the surface of the particle
in shear flow.

The shortcoming of the method is that the momentum exchange operation with moving boundary nodes is not completely mass conserving. This is because when the fluid node is uncovered, the density at the node is assumed to be the average of neighboring fluid nodes. However, the effect is usually negligible and the total mass of the system remains conserved at a macroscopic level. Overall, the method provides a versatile and numerically efficient tool for the study of suspension of particles in turbulent flows.

We also discussed some initial DNS results obtained using the code to study the particle dynamics in turbulent pipe flow. It was observed that the mean axial and angular velocity of particles was scattered around the values obtained from the Eulerian field of another simulation with the same energy input. This will be studied further to have a probabilistic estimate of the velocities of particles in turbulent flows from the Eulerian velocity field.

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References


