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Review

# Multi-flexible fiber flows: A direct-forcing immersed boundary lattice-Boltzmann lattice-spring approach

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ABSTRACT

We demonstrate that a lattice-Boltzmann lattice-spring method can be used to simulate a dynamic behavior of a suspension of a large number of flexible fibers in finite Reynolds number flows. In the method, lattice-Boltzmann equation is adopted to simulate fluid velocity and vorticity while lattice-spring model with three-body forces can be employed to model the bending deformation of solid bodies. In order to realize the non-slip boundary condition, a forcing term is simply calculated by using the Newtonian second law and imposed with an immersed boundary scheme. The method is validated by comparing the present results with experiments and existing theories and methods. Subsequently, the method is applied to simulate a dynamic process of flexible fibers settling on a static or moving screen/wire net while a fiber mat is simultaneously built over the screen and resists fluid flowing. The number of fibers, fiber density and flexibility, and ratio of the relative velocity of the screen/wire to fluid can be systematically varied at different levels. Their influences on drainage rate are computed and evaluated.



## 1. Introduction

There are extensive applications of particulate flows in chemical engineering (fluidized bed in reactor, particle separation, screening, filtration) and sciences (biological particle coagulation and dispersion, blood flows and cell adhesion, sands sedimentation in rivers), and in various industries (pharmaceutical, petroleum, food process, paper industry etc.). Due to the importance, engineers and scientists have paid a great attention to the subject of the particulate flows in both experimental and theoretical studies. Most investigations currently focus on the rigid particle-fluid problems. Very few studies are reported on deformable particle-flow problems. Some direct simulation methods are developed to model the solid particle motion in fluids. Among the traditional finite element method, the most popular one is an arbitrary Lagrangian Eulerian scheme (Hu, 1996) based on Galerkin finite element approach. In this method, the meshes are moving with solid particles and the meshes need to be re-meshed when unacceptable element deformation is detected. It is obvious that the re-meshing process largely increases computational load and limits to a system with a small number of particles. This method is recently extended to treat deformable particles (Gao et al., 2011, 2013), only two dimensional cases at a very low Reynolds number were reported. Later, Glowinski et al. (1999) with others (Glowinski et al., 2001; Patankar et al., 2000; Wan. and Turek., 2006) presented a Lagrange-multiplier-based fictitious-domain method for the motion of large numbers of rigid particles in a Newtonian fluid. Their finite element formulation allows use of a fixed structured grid and avoids re-mesh process. However, their reports are limited to rigid solid particles.

Peskin (1977) was the first to propose an immersed boundary method (IBM) to treat deformable bodies associated with blood flow. Later, the IBM had been applied to particulate flows (Fogelson and Peskin, 1988). In Peskin's method, regular Eulerian grids are operated for fluid domain and the Lagrangian grids of deformable particles move over the fixed fluid grids. A forcing term is added on the interface between the fluid and solid to force the solid boundary velocity equal to the fluid velocity (non-slip boundary condition) through Dirac delta function. For fluid field, the Navier–Stokes equations can be solved either by traditional computational fluid dynamics (CFD) or by a lattice-Boltzmann method (LBM) (Succi, 2001). The solid particles can be either rigid or deformable.

Ladd (1994) had firstly proposed a moving boundary condition in the LBM and applied it to particulate flows. Later, Koch and

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others (Aidun and Clausen, 2010; Aidun et al., 1998; Benzi et al., 1992; Duenweg and Ladd, 2009; Feng and Michaelides, 2004, 2005; Koch and Ladd, 1997; Luo et al., 2017; Qi, 1999; Qi and Gordnier, 2015; Qi et al., 2014a, 2014b, 2010; Whittington, 1998) had demonstrated that the LBM is the most simple and efficient method to simulate particle suspensions. Unlike traditional CFD, one of features of the lattice-Boltzmann method (LBM) is that micro-kinetic nature of fluid particle collision and streaming, similar to convection-diffusion of fluid momentum, is presented through the lattice-Boltzmann equation at every time step. The method allows ones to simulate flows efficiently in complex geometrical solid boundaries. The main features and advantages as well as disadvantages of LBM are briefly summarized in a recent article by Succi (2015). Feng and Michaelides (2004) were the first to combine the advantage of LBM with IBM to deal with rigid particles. For deformable particles, a lattice-spring model was proposed to handle the deformation of a flexible body by Buxton et al. (2005). In their method, the deformable solid body is discretized as individual particles located in a regular lattice and connected by a two-body spring force between two neighboring particles as a bond. The two-body force can deal with extension and compression but cannot accurately handle the bending deformation, because the two-body central force is a function of distance between two neighboring solid particles and does not provide any bonding angle information between two adjacent bonds or springs. Wu and Aidun (2010a, 2010b, 2010c) took Buxton's spring model in their LB simulation. Subsequently, a three-body force with angular information between two adjunct bonds was added into the lattice-spring model to handle bending deformation by Wu et al. (2014). Other authors such as Duenweg and Ladd (2009) and Basagaoglu et al. (2013, 2008) also utilized LBM and bead-spring model to simulate the soft materials in flows.

Unfortunately, both Wu and Aidun (2010a, 2010b, 2010c) and Wu et al. (2014) used the same forcing term as those by He et al. (1998) and Feng and Michaelides (2004) to take account of the interactions between fluids and solid particles. Guo et al. (2002) proved that this type forcing (body force) term cannot be operated for an unsteady body force case because the Navier–Stokes equations cannot be entirely recovered due to extra-terms caused by the spatial and temporal variation of the body force and they proposed a new forcing term, which enables the LB equation to recover the Navier–Stokes equations with a second-order accuracy for unsteady, non-uniform body forces. This new force term is called split-force and used by Kang and Hassan (2011) and Delouei et al. (2014) for rigid particle cases. We will adopt the direct split-forcing term by Guo et al. (2002) in this work.

Among all particulate flows, a slender fiber system is difficult to cope with due to a large aspect ratio and deformability, which may complicates the fluid-solid interaction, although a numerical method based on a slender body theory has been extensively applied to simulate multi fibers by Butler and others (Butler and Shaqfeh, 2002; Saintillan et al., 2006; Shin et al., 2006, 2009). Their reports were limited either to very low Reynolds number or to rigid fibers. To consider inertial effect, some numerical methods for finite Reynolds flows were also developed (Dahlkild, 2011; Kuusela et al., 2001; Zhang et al., 2013) for rigid fibers. Lindstrom and Uesaka reported a flexible fiber model in fluid (Lindström and Uesaka, 2007, 2008). They used vorticity-vector potential form of the Navier–Stokes equations for fluid while fibers were modeled as a chain of segments interacting with themselves through a contact force. They also considered short and long-range hydrodynamic interactions. Their semi-dilute regime results for rheological properties showed deviations from hydrodynamic interaction theories. Salahuddin et al. (2012, 2013) used a lattice-Boltzmann equation to simulate fluid and fibers were modeled as a chain of rods where 4 nodes were distributed on the circumference of each cross section of the fiber. The interaction between fluid and fiber was treated by an external boundary force. However, the direct relationship between the fiber rigidity and structure of the fiber and the effects of rigidity on motion were not reported.

In order to effectively investigate effects of fiber rigidity on motion, we present a direct-forcing immersed boundary lattice-Boltzmann lattice-spring approach to simulate a suspension with a large number of flexible fibers. The approach is comprised of the following portions, and its advantage is briefly summarized as follows:

1. The LBM will be employed to simulate fluid flow behavior and structure on fixed Eulerian nodes. Most importantly, the Boltzmann equilibrium distribution function physically represents a natural distribution of fluid particles and is presented at every time step so that the error is controlled. In contrary, the traditional CFD is a sole numeric approximation and lacks such the equilibrium function. The algorithm of the LB method for fluid domain is extremely simple and consists of only two operations, collision and streaming. This simplicity essentially comes from two major reasons. First, when one derives the Navier–Stokes equation from the LB equation, the fluid distribution function is expanded to the second order of the small Knudsen number (the ratio of the mean free length to the characteristic spatial scale of the whole fluid system), called the Chapman–Enskog expansion or multi-scale analysis, so that collision, convection, and diffusion time scales are separated. This greatly simplifies the algorithm. Second, the fluid collision matrix of the LB equation is also linearized by either the Bhatnagar–Groos–Krook (BGK) approximation or multi relaxation time models.
2. The distinct feature of the LB method is well known that the computation efficiency in the LB method is much higher than that in the traditional finite element and differential methods, due to the parallel nature of the LB algorithm itself, where only local information at one grid needs to be transferred to its neighboring grids, and the same simple operations are repeated on all grids. The code is easy to be parallelized in a GPU based CUDA code (Wu and Qi, 2017; Wu et al., 2017). Also, the fluid grids are fixed so that the method is easy to handle moving and flexible solid boundaries.
3. The lattice-spring model with three-body forces is utilized to mimic motion of discretized flexible fibers where moving Lagrangian solid particles are connected by elastic harmonic springs and angular bonds. This fiber model can consider not only extension, compression, but also bending deformation. It is noted that two body central force cannot treat bending deformation. The deformation and motion of a flexible fiber are treated with an elastic model without resorting to a nonlinear Euler Bernoulli beam equation, which is a 4th order differential equation. The present approach allows us to accurately simulate a large number of fibers in a finite Reynolds number flow. In addition, the lattice-spring model can be used to construct solid particles in any shape, such as rectangular, plate-like, non-spherical, spherical, cylindrical, etc., to treat deformation easier due to the use of elastic springs, and to accurately handle fibers with a large aspect ratio.
4. The split-force term proposed by Guo et al. (2002) will be adopted to correctly address interactions between solids and flows. This algorithm takes into account the nonlinear effects of lattice discrete and unsteady interaction forces on the solid-fluid interfaces, and the Navier–Stokes equations are exactly recovered.
5. The fluid force or the force on solid nodes for non-slip boundary condition is simply calculated from the difference be-