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Implementation issues and benchmarking of lattice Boltzmann method for moving rigid particle simulations in a viscous flow

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In this work, we revisit implementation issues in the lattice Boltzmann method (LBM) concerning moving rigid solid particles suspended a viscous fluid. Three aspects relevant to the interaction between flow of a viscous fluid and moving solid boundaries are considered. First, the popular interpolated bounce back scheme is examined both theoretically and numerically. It is important to recognize that even though significant efforts had previously been devoted to the performance, especially the accuracy, of different interpolated bounce back schemes for a fixed boundary, there were relatively few studies focusing on moving solid surfaces. In this study, different interpolated bounce back schemes are compared theoretically for a moving boundary. Then, several benchmark cases are presented to show their actual performance in numerical simulations. Second, we examine different implementations of the momentum exchange method to calculate hydrodynamic force and torque acting on a moving surface. The momentum exchange method is well established for fixed solid boundaries, however, for moving solid boundaries there are still open issues such as unphysical force fluctuations and Galilean invariance errors. Recent progress in this direction is discussed, along with our own interpretations and modifications. Several benchmark cases, including a particle-laden turbulent channel flow, are used to demonstrate the effects of different modifications on the accuracy and physical results under different physical configurations. The third aspect is the refilling scheme for constructing the unknown distribution functions for the new fluid nodes that emerge from the previous solid region as a particle moves relative to a fixed lattice grid. We examine and compare the performance of the refilling schemes introduced by Fang et al. (2002), Lallemand and Luo (2003), and Caiazzo (2008). We demonstrate that improvements can be made to suppress force fluctuations resulting from refilling.

1. Introduction

Turbulent flows laden with solid particles are ubiquitous in engineering, biological and environmental applications. Examples include fluidized bed reactors, spray atomization, bubble columns, plankton contact dynamics in ocean water,

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transport of blood corpuscles in the human body, sediment transport, warm rain process, volcanic ash eruptions, dust storms, and sea sprays. In these applications, particles are usually suspended in a turbulent carrier fluid. The interactions between the dispersed and the carrier fluid phases impact the dynamics of suspended particles (e.g., dispersion, deposition rate, collision rate, settling velocity) and the bulk properties of the multiphase flow (e.g., wall or surface drag, turbulence intensity). In some of these applications, the particle size is comparable to or larger than the flow Kolmogorov length [1], which introduces a finite-size effect greatly complicating the description of the flow system. Currently, the only rigorous method is to numerically resolve the disturbance flows around particles, known as the particle-resolved simulation (PRS). This requires an explicit implementation of the no-slip boundary condition on the surface of each moving particle.

PRS of turbulent particle-laden flows requires direct simulation of the turbulent carrier flow and explicit and accurate treatment of many moving fluid–solid interfaces, such that all scales from turbulence integral scale to dissipation scales and particle size are adequately resolved with realistic scale separations that depend on applications. In recent years, several PRS methods based on the Navier–Stokes (N–S) equation have been developed, with the particle–fluid interfaces treated by the immersed boundary method [2,3], direct-forcing [4], local analytical treatment [5], overset grid [1], force-coupling [6], or penalization method [7]. As reviewed in [8,9], these studies have contributed to the understanding of flow modulation by the inertial particles and the dynamic effects due to finite particle size.

As an alternative approach, lattice Boltzmann method (LBM) has also been applied as a PRS method for turbulent particle-laden flows [10,8,9]. The LBM approach features a high-level data locality essential to efficient implementation of PRS. Another advantage is that LBM has the flexibility and simplicity (i.e., via local bounce-back) for implementing interfacial boundary conditions. This offers the potential for the method to be applied to treat turbulent flows laden with non-spherical and deformable particles.

In LBM, a set of mesoscopic distribution functions are solved. The number of microscopic velocities at a give lattice node is usually several times larger than the number of macroscopic hydrodynamic variables in the continuum N–S equation. This feature provides LBM with a much simpler evolution equation and greater flexibilities, but leads to an implementation issue at boundaries or fluid–solid interfaces. Although the macroscopic boundary conditions (i.e., no penetration and no-slip) are clearly established, the method to construct the missing microscopic distribution functions is no unique since the number of unknowns is larger than the number of boundary conditions.

For particle-laden flow simulations, this results in three general issues. First, the unknown distribution functions must be carefully constructed to satisfy the no-penetration and no-slip boundary conditions at the moving fluid–solid interfaces and other considerations of physical consistency and numerical accuracy. Second, to simulate the motion of moving solids in the fluid, hydrodynamic forces need to be accurately calculated from the microscopic distribution functions. Third, for flows with moving fluid–solid interfaces, every time when a previous solid node becomes a fluid node, the information at such a new fluid node needs to be filled.

Over the past 25 years, many efforts have been devoted to these three topics for moving fluid–particle problems. While many different implementations of the velocity boundary condition have been developed for a fixed straight boundary (see the review by Latt et al. [11]), for a moving curved boundary the early efficient implementation may be traced to studies of Ladd and co-workers [12,13]. In those early studies, the standard (or mid-link) bounce back scheme was used, causing a curved boundary to be effectively approximated by a zigzag staircase. Later on, different interpolated (and sometime extrapolated) bounce back schemes are proposed to capture more precisely the real fluid–solid interface [14–21]. Even though each boundary treatment scheme has been separately tested and applied to different physical problems, to our knowledge, they are yet to be systematically compared and benchmarked under same conditions. For the users of LBM, it is still not clear which boundary-condition implementation scheme to choose, especially when the solid boundaries are moving in a nonuniform flow.

Regarding hydrodynamic force evaluation in LBM, the most popular and efficient approach is the momentum exchange method (MEM), whose general concept has been introduced in the early studies [12,18,22]. Recently, the Galilean variance property of MEM has been questioned and remedies are proposed in several studies [23–26]. This problem was largely ignored in early works because of three reasons. First, benchmark cases used to test a force evaluation model were mostly limited to fixed solid boundaries where the Galilean invariance is not an issue. Second, while the Galilean invariance errors resulting from MEM may be present at every boundary node, for simple cases with symmetric solid particle shapes, it is usually thought that the local errors can cancel with each other such that the calculated net hydrodynamic force acting on a moving particle remains accurate. Third, because the local Galilean invariance error typically has a magnitude of $\mathcal{O}\left(Ma^2\right)$, where Ma is the Mach number, it is normally thought to be negligible. In light of the very recent developments [24,25], we will point out some incorrect suggestions made in the literature in attempt to restore Galilean invariance, as well as the subtle difference in the recent correct treatments by Wen et al. [25] and Chen et al. [26]. We will demonstrate that a lack of Galilean invariance could lead to unphysical results in more general situations (*e.g.*, particle-laden turbulent flows). Therefore, careful and thorough tests are still required to re-examine previous MEM models when applied to complex flow configurations. The recent studies [25,26] have demonstrated the deficiencies of previous MEM implementations, using simple to moderately complex moving-particle problems.

The refilling scheme for a new fluid node has been considered in several previous studies [27–31]. Lallemand and Luo [27] suggested a scheme based on quadratic extrapolation along the solid local outer normal direction. Fang et al. [28] averaged