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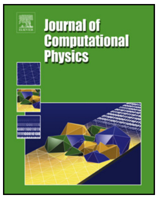

An immersed boundary-lattice Boltzmann method for single- and multi-component fluid flows

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ABSTRACT

The paper presents a numerical method to simulate single- and multi-component fluid flows around moving/deformable solid boundaries, based on the coupling of Immersed Boundary (IB) and Lattice Boltzmann (LB) methods. The fluid domain is simulated with LB method using the single relaxation time BGK model, in which an interparticle potential model is applied for multi-component fluid flows. The IB-related force is directly calculated with the interpolated definition of the fluid macroscopic velocity on the Lagrangian points that define the immersed solid boundary. The present IB–LB method can better ensure the no-slip solid boundary condition, thanks to an improved spreading operator. The proposed method is validated through several 2D/3D single- and multi-component fluid test cases with a particular emphasis on wetting conditions on solid wall. Finally, a 3D two-fluid application case is given to show the feasibility of modeling the fluid transport via a cluster of beating cilia.

1. Introduction

The numerical simulation of phenomena involving moving/deformable boundaries in multi-component flows is attracting more and more the interest of physicists and engineers, especially in recent biofluidic applications. In this context, the scope of this work is to develop a numerical tool to simulate the beating of epithelial cilia to transport the mucus in airways [1]. Epithelial cells have whip-like appendages extending from their surface, designed to move the surrounding fluid. The numerical challenges thus include the simulation of slender flexible structures in large deformations, in a two-component fluid flow environment: the periciliary fluid whose properties are close to those of water and the mucus [2]. Note that although this work mainly aims at simulating the transport of mucus by ciliary motion, a wide spectrum of applications can be found in biomechanics (inner ear, sperm cells), aerodynamics (control of boundary layers around airfoils [3]), or animal propulsion studies [4].

In the present work, the numerical simulation involving mucus and periciliary fluid is tackled via an interparticle potential Multi-Component Multi-Phase (MCMP) Lattice Boltzmann (LB) model [5]. Based on the original Shan–Chen's model [6,7], this MCMP scheme applies an Explicit-Forcing (EF) scheme [8] in order to take into account external force effects, instead of modifying the equilibrium velocity as in [6,7]. As shown in the work of Porter et al. [5], the EF interparticle potential LB model adopted in the present paper can allow one to reduce the magnitude of spurious currents near the fluid–fluid

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interface, as well as to increase the density or viscosity ratio, compared to the original SC model. More details about the thermodynamic consistency of different forcing schemes can be found in the works of Huang et al. [9] and Li et al. [10].

As an alternative to conventional numerical methods, LB method has been widely applied for simulating fluid flow problems with diverse physical phenomena, because of its inherent advantages, such as the microkinetic level for dealing with the fluid properties and the simplicity for parallel implementation, etc. Besides, one important feature of LB method is that it can fully recover the Navier–Stokes (NS) equations at the macroscopic scale [11,12].

To incorporate moving solid boundaries in the fluid domain, we choose to couple the LB method with an Immersed Boundary (IB) method. Originally introduced by Peskin [13] for simulating blood flow in the heart, IB method is now widely used and several variants have been proposed within the framework of NS solvers [4,14–16]. Using IB method allows one to easily introduce moving solid boundaries in fluid flows simulated on a fixed Cartesian grid, which is the case for the present LB solver.

When considering body force term in the fluid domain, one should redefine or correct the macroscopic velocity in the framework of LB method for both single- and multi-component fluid cases in order to fully recover NS equations [7,17]. In such case, the macroscopic fluid velocity is calculated as the sum of two terms: one is related to the distribution functions of LB model, and the other is the body force-related term. The main idea of IB method is to calculate an appropriate body force-related term so that the fluid can have a desired macroscopic velocity on the Lagrangian points defining the solid wall. Hence, a straightforward method is to first calculate the IB-related force at these Lagrangian points, based on the definition of the macroscopic fluid velocity, and then distribute it onto the neighboring Eulerian nodes with the spreading operator, following Peskin [13,18]. Such kind of IB–LB method, like the one of Chen et al. [19], can be categorized as explicit IB–LB algorithm, which is now known to have issues in ensuring the no-slip solid boundary condition [20]. To overcome this drawback, Wu and Shu [20] proposed an implicit velocity-correction IB–LB method, which relies on resolving a system of equations at each time-step in order to calculate the IB-related force that ensures the no-slip boundary condition.

In the present paper, an IB–LB method is proposed to simulate single- and multi-component fluid flows in the presence of fixed or moving solid boundaries. The macroscopic fluid velocity is split into two parts, and the IB-related force is directly obtained from the definition of the macroscopic fluid velocity at the Lagrangian points. However, we follow the method proposed by Pinelli et al. [16] to amend the spreading operator in order to improve the reciprocity of interpolation-spreading operations. As a consequence, with such spreading operator, the no-slip solid boundary condition can be better ensured, comparing to the ordinary explicit IB–LB coupling approach. Similar to the method proposed by Wu and Shu [20], the resolution of a linear system of equations is also required, but only when the positions of the Lagrangian points change with time. It means that in the case of static solid boundary cases the resolution of the system will be carried out only once at the beginning of the simulation, which turns out to be an advantage of the present method. In addition, it may be worth noting that the present IB–LB method appears to be formally faster than the one proposed by Favier et al. [21], since only one LB calculation is required within one time-step, avoiding the need of an extra prediction step.

Besides, another novelty of the present work lies in the extension of the proposed IB–LB method to multi-component fluid cases. The key point is to calculate the IB-related force by means of the definition of the macroscopic velocity for each fluid component. Once these forces are obtained, the spreading procedure is the same as in the single-component fluid case. Furthermore, with the proposed IB–LB coupling method one can take into account different wetting properties of solid wall, by adding the IB-related force after considering the fluid–solid adhesion force model proposed by Martys and Chen [22]. For the sake of clarity, we summarize the advantages of the proposed IB–LB coupling method as follows:

- Moving and curved solid boundary condition can be easily incorporated into the fluid simulation. The extension to multi-component cases is straightforward and different wetting conditions can be imposed on curved walls, which is relatively difficult to handle using the classical bounce-back method
- IB-related force is incorporated by means of the definition of macroscopic velocity, in such a way that no extra prediction sub-step is required at each time-step
- The no-slip solid boundary condition can be enhanced with an improved spreading operator. For static IB condition, the resolution of a linear system of equations is required only once at the beginning of numerical simulation, because of the explicit feature of the proposed method

To our knowledge, the only attempt to combine multi-phase flow and immersed boundary was done by Shao et al. [23]. One of the interest of this article is the development of a method to implement Neumann boundary condition in the frame of immersed boundary method. Then they apply this boundary condition to the contact line of a droplet on a wall. We successfully reproduce the contact line dynamics, as Shao et al. [23] did, but using a different interparticle potential MCMP model, a different IB method implementation, and more importantly, Dirichlet boundary conditions appear to be sufficient in our numerical framework.

The article is organized as follows. Section 2 first gives the basic equations of the LB method for single- and multi-component models. Then the main idea of the proposed IB–LB method is shown in the second part of this section, followed by a brief introduction of the approach to define the spreading operator. In Section 3, several 2D/3D numerical test cases are shown to validate the proposed IB–LB method. A 3D two-fluid case on the fluid transport by a cluster of beating cilia is presented in Section 4 in order to show the feasibility of simulating mucus flows in airways. Finally, the conclusions are drawn in Section 5.