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Improved coupling of time integration and hydrodynamic interaction in particle suspensions using the lattice Boltzmann and discrete element methods

Duo Wang [a,*], Christopher R. Leonardi [a,b], Saiied M. Aminossadati [a]

[a] School of Mechanical and Mining Engineering, The University of Queensland, Brisbane, QLD 4067, Australia
[b] Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

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ABSTRACT

This paper introduces improvements to the simulation of particle suspensions using the lattice Boltzmann method (LBM) and the discrete element method (DEM). First, the benefit of using a two-relaxation-time (TRT) collision operator, instead of the popular Bhatnagar–Gross–Krook (BGK) collision operator, is demonstrated. Second, a modified solid weighting function for the partially saturated method (PSM) for fluid–solid interaction is defined and tested. Results are presented for a range of flow configurations, including sphere packs, duct flows, and settling spheres, with good accuracy and convergence observed. Past research has shown that the drag, and consequently permeability, predictions of the LBM exhibit viscosity-dependence when used with certain boundary conditions such as bounce-back or interpolated bounce-back, and this is most pronounced when the BGK collision operator is employed. The improvements presented here result in a range of computational viscosities, and therefore relaxation parameters, within which drag and permeability predictions remain invariant. This allows for greater flexibility in using the relaxation parameter to adjust the LBM timestep, which can subsequently improve synchronisation with the time integration of the DEM. This has significant implications for the simulation of large-scale suspension phenomena, where the limits of computational hardware persistently constrain the resolution of the LBM lattice.

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has emerged as a powerful numerical method for the simulation of fluid flow problems. Applications of the LBM include laminar flows in porous media [1–4], fluid–particle interactions [5–10], non-Newtonian fluid flows [11–16], and much more. The mesoscopic construction of the LBM, and its facilitation of bounce-back boundary conditions, means that it is an ideal candidate for the simulation of fluid flows in complex geometries [9]. For similar reasons, the LBM is also well-suited to solving particle suspension problems [17]. However, the efficient and accurate coupling of the LBM with particle-based methods is non-trivial.

A range of collision operators (see Section 2.1) and boundary conditions are now available for the formulation of an LBM model. Within the context of simulating particle suspensions, the single-relaxation-time (SRT) Bhatnagar–Gross–Krook (BGK) collision operator [18] along with a simple bounce-back scheme (SBB) remains the most popular combination.

* Corresponding author.
E-mail addresses: d.wang3@uq.edu.au (D. Wang), c.leonardi@uq.edu.au (C.R. Leonardi), s.aminossadati@uq.edu.au (S.M. Aminossadati).

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However, several shortcomings of BGK-LBM formulations have been widely reported in the literature, including poor stability and accuracy, particularly at low viscosities or high Reynolds number. Although increasing the grid resolution can help mitigate these problems, this is not computationally efficient, especially for large-scale simulations involving millions of nodes, or more. When also using SBB for hydrodynamic boundaries, the exact location of the no-slip interface becomes a function of the relaxation parameter [19] (i.e. computational viscosity), and as such cannot be interpreted as halfway between a fluid and boundary node.

The use of a multiple-relaxation-time (MRT) collision operator [20] can overcome some of the deficiencies of BGK-LBM formulations. However, the exact location of the no-slip boundary still depends on the computational viscosity [21]. This issue was well documented by Pan et al. [3], who found that when simulating fluid flow through a porous medium, the calculated permeability, which is a physical property of the medium itself, changed with the computational viscosity. This represents a significant issue for a range of LBM applications, beyond porous media and suspension flows. Although it was found that viscosity-dependence was reduced by using an MRT formulation, the accuracy of the permeability predictions was dependent on the use of higher-order boundary conditions such as quadratically-interpolated (QIBB) or multi-reflection bounce-back (MRBB). Other improvements [2,4,22] have been made to better describe fluid–solid boundaries on the underlying lattice but, like the QIBB and MRBB conditions, many of the improved boundary conditions require non-local computations. Conversely, the use of a partially saturated method (PSM) for fluid–solid boundaries, such as that proposed by Noble and Torczynski [23], is attractive. The introduction to the lattice Boltzmann equation (LBE) of the solid volume fraction in a cell improves the precision with which the no-slip boundary is represented. Validation in the literature [7,8,24] has shown that the technique is also capable of accurately computing the momentum exchange between fluids and solids using only local computations.

It is worthwhile to note that Prestininzi et al. [25] recently presented an alternate interpretation of the viscosity-dependence of boundary conditions in BGK-LBM formulations. In this work, the authors show that the issue can be overcome when the Knudsen number, Kn, is kept small and constant. However, to keep Kn constant at varying relaxation parameter requires adjustment of the grid resolution, which is impractical in most engineering simulations (e.g. fully resolving the flow through small and tortuous pore networks, or around a suspended particle) due to limitations on memory and processor time. Further, the LBM is most often employed to mimic the Navier–Stokes equations, where the Knudsen number should have no effect on the results. To account for it in such simulations would be paradoxical.

In some early LBM models of particle suspensions, the interactions among the solid particles were either ignored or treated in a simplified fashion. However, to simulate an industry case where particles are densely packed or in frequent contact, the particle interactions must be appropriately characterised. To address this, the discrete element method (DEM) has been employed to model the kinematics and mechanical interaction of solid particles. The discrete system in the DEM is solved by an explicit, central-difference time integration scheme, which is to some degree consistent with the LBM [26]. The explicit construction of both methods allows for the development of a coupled LBM–DEM framework to resolve fluid–particle systems. Such an approach was first proposed by Cook et al. [27], and soon became one of the most popular for the modelling of particle suspensions [9,10,28,29], providing fundamental insights on the complex physical phenomena that they contain.

A number of practical computational issues must be taken into consideration when coupling the LBM and the DEM. Of primary importance is the synchronisation of their respective timesteps, Δt_{LBM} and Δt_{DEM}, which is complicated by the manner in which they are defined. The LBM timestep (in physical units) is calculated exactly from the lattice spacing, Δx, the relaxation parameter, τ, and the fluid viscosity, ν (see Section 2.1). Meanwhile, the DEM timestep is determined using a Courant–Friedrichs–Levy (CFL) criterion based on the physical properties (e.g. density, stiffness) of the solid, meaning that it can assume any value below a critical threshold. In some cases the LBM and DEM computations can be performed using equivalent timesteps, however it is often the case that the DEM timestep must be less than the LBM timestep [9,10,30]. In such circumstances, sub-cycling can be employed to allow a number of DEM timesteps to be performed within one LBM timestep. However, the number of sub-cycles should be kept to a minimum (e.g. not allow a boundary to move across more than one lattice spacing) as the hydrodynamic load applied to the moving boundary will remain constant in that time.

It would be beneficial to the construction of LBM–DEM models if the relaxation parameter, τ, could be used (within other constraints) as a free parameter that allows the optimal choice of the LBM timestep from the perspective of coupling to the DEM. This is not possible, however, as the choice of τ and the associated computational viscosity has implications for the precision of hydrodynamic coupling, as already discussed. Instead, τ is often prescribed a value of one when using BGK-LBM formulations with boundary conditions based on bounce-back, which minimises error but renders timestep coupling awkward. Therefore, the aim of this work is to define a choice of LBM collision operator and boundary conditions which reduces the dependence of hydrodynamic coupling on computational viscosity, and maintains the locality of operations offered by boundary conditions based on the bounce-back principle. This will allow greater flexibility in the choice of relaxation parameter and LBM timestep, and result in more efficient coupling of time integration with the DEM. The TRT-LBM formulation and the PSM boundary condition are used as the basis of this research.

The contents of this paper are organised as follows. In Section 2 the LBM, DEM, and PSM boundary condition are introduced in detail, along with a brief discussion of a selection of other fluid–solid boundary conditions. The computational issues related to the coupling of the LBM and DEM are then discussed in Section 3. Testing and validation results are presented in Section 4, with Section 4.1 comparing various formulations of the LBM–DEM framework, and the remainder of the section demonstrating the improved performance of the formulation defined herein. Finally, a brief summary and discussion of the results is included in Section 5.

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