Periodic Boundary Conditions of Discrete Element Method-Lattice Boltzmann Method for Fluid-Particle Coupling

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Abstract

This paper presents a periodic boundary condition for the coupled discrete element and lattice Boltzmann method for simulating fluid-particle systems. Detailed implementation of this special boundary condition is given. Besides, the detailed procedure of immersed moving boundary scheme for fluid-solid coupling is proposed. The accuracy and applicability of the proposed periodic boundary condition are well demonstrated by two benchmark tests, i.e. single particle transport and multiple particle migration in an infinite tube filled with water. It is found that the novel periodic boundary condition proposed for discrete element and lattice Boltzmann method can greatly improve the computational efficiency of the later which is computationally expensive when thousands of particles are involved.

Keywords

Periodic boundary condition; Discrete element method; Lattice Boltzmann method; Fluid-particle coupling; Multi-phase flow

1 Introduction

The fluid-particle coupling has a wide range of applications in Geotechnical Engineering, Petroleum Engineering and Chemical Engineering. The challenging is to efficiently and accurately approach the microscopic fluid-solid interaction at the pore level in fluid-particle systems. Much work has been done on the numerical modelling of the fluid-particle coupling problems [1-4]. Since the coupled Discrete Element Method and Computational Fluid Dynamics (DEMCFD) technique was proposed in the 1990s [5], it has attracted extensive interest of researchers. The DEMCFD promotes the development of the numerical research of fluid-particle systems and becomes the dominant research tool in this research area soon [2,3,6,7].

In 2004, a fully particle-based Discrete Element Method and Lattice Boltzmann Method (DEMLBM) was proposed for resolving the fluid-particle interactions at the grain level [8]. In this method, the fluid flow is simulated using the mesoscopic lattice Boltzmann equation rather than the macroscopic Navier-Stokes equations in DEMCFD. In addition, the fluid-particle interactions are directly implemented by solving the collision of fluid and solid nodes near the particle surface [9]. No empirical equations or averaging technique for the calculation of hydrodynamic forces, which are used in CFD, are required. Although the state of the art technique has been proven promising for the fluid-particle systems, its computing cost is rather expensive when a great many particles are involved. One of the effective ways for greatly reducing its computational cost is to parallelize the coupled DEMLBM approach; An alternative is to implement the Periodic Boundary Condition (PBC) in the DEMLBM framework.

In numerical methods, the PBC are often used for approximating a large (infinite) system by using a small part called a unit cell. It can not only improve the computing efficiency by reducing the number of particles required, but also eliminate the undesired effects of wall boundaries. There has been much research on the applications of PBC in either DEM or LBM.

The application of PBC to the two-dimensional liquefaction simulations using DEM was reported by Thornton [10]. The general liquefaction characteristics of saturated soils under cyclic loading is well simulated and complete liquefaction can be captured in the loose assembly. One year later, a 3D quasi-static shear deformation of granular media was examined by performing numerical simulations on polydisperse systems of elastic spheres using PBC [11]. Zeghal & Shamy [12] used the DEMCFD technique, built in the commercial software ABAQUS, to investigate the liquefaction behaviours of a saturated granular assembly. As said by the authors the PBC code used in this paper was provided by other researchers. A radial PBC for the axi-symmetric DEM simulations was proposed by Cui et al. [13]. Detailed implementation of this special PBC was illustrated and validations were made through numerical tests. In 2011, Radjai & Dubois [14] gave the implementation of general PBC for DEM in more detail. Three aspects, i.e. position, force and velocity of the particle, are considered. Recently, the implementation of radial PBC for DEM simulation of particle flow in cylindrical vessels was also reported by Yang et al. [15]. More applications of PBC for DEM can be seen elsewhere [16,17].

The early application of PBC to LBM was reported by Skordos [18] for the two-dimensional decaying shear flow. The introduction of PBC for LBM was given through a simple problem that involves parallel walls of infinite length. Periodic conditions were implemented in the streamwise X direction by treating nodes on the inflow and outflow faces as nearest neighbours if they share common Y and Z coordinates [19]. More detailed implementation of PBC can be seen in the first LBM book [20]. A few years later, Kim & Pitsch [21] proposed a generalized periodic boundary condition for lattice Boltzmann method simulation of a pressure driven flow in a periodic geometry. The accuracy of the generalized periodic boundary condition is analysed for both incompressible and compressible flows. Subsequently, an adaptive generalized periodic boundary condition for lattice Boltzmann simulations of pressure-driven flows through confined repetitive geometries is reported by Gräser & Grimm [22].

To the best of the authors' knowledge, the implementation of PBC for DEMLBM has not been reported anywhere. In order to greatly improve the computational efficiency of DEMLBM, a PBC for LBM with Immersed Moving Boundary (IMB) scheme is proposed in this paper. The accuracy and applicability of this PBC procedure are demonstrated through two benchmark tests.

2 Numerical Methods

For the sake of consistency, a brief description of DEM, LBM and IMB will be given in this section. Detailed introduction of these methods and their coupling can be seen in the references [8,9].

2.1 Discrete element method

In DEM, the Newton's second law is utilised to determine the translation and rotation of each particle arising from the contact forces, whilst the force-displacement law is used to update the contact force that keeps changing due to the relative motion of particles at each contact. The dynamic behaviour is represented numerically by a time-stepping algorithm in which the velocities and accelerations are assumed to be constant within each time step. Because the propagation speed of disturbances is a function of the physical properties of the discrete medium, a sufficiently small time step should be chosen so that, at each time step, disturbances cannot propagate from a particle farther than its neighbouring particles. Therefore, at all times the resultant forces on any particle are determined exclusively by the neighbouring particles in contact.

The Newton's second law governing the motion of a particle is given by

$$m\boldsymbol{a} + c\boldsymbol{v} = \boldsymbol{F}_c + \boldsymbol{F}_f + m\boldsymbol{g} \tag{1}$$

$$I\ddot{\theta} = T_c + T_f \tag{2}$$

where m and I are respectively the mass and the moment of inertia of particles, c is a damping coefficient, $\boldsymbol{a}$ and $\ddot{\theta}$ are acceleration and angular acceleration, $\boldsymbol{F}_c$ and T_c are, respectively, contact forces and corresponding torques, $\boldsymbol{F}_f$ and T_f are hydrodynamic forces and corresponding torques.

2.2 Lattice Boltzmann method

The lattice Boltzmann method is a modern numerical approach in computational fluid dynamics. In conventional CFD, the fluid phase is treated as continuum governed by the Navier-Stokes equations. The primary variables are pressure, velocity and density. In LBM the fluid domain is divided into regular lattices and the fluid phase is treated as a group of (imaginary) particle packages resided at the lattice nodes. Each particle package includes several particles, such as 9 particles in the commonly used D2Q9 model. The flow of fluid can be achieved through resolving the particle collision and streaming processes, and the lattice Boltzmann equation is used to solve the streaming and collision process of fluid particles. The primary variables of LBM are the so-called fluid density distribution functions associated with the fluid particles. Both mass and momentum of fluid particles are characterised by the fluid density distribution functions.

The lattice Boltzmann equation is described by

$$f_i(\boldsymbol{x} + \boldsymbol{e}_i\Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = \Omega \tag{3}$$

where f_i are the fluid density distribution functions; x and e_i are the coordinate and velocity vectors at the current lattice node; t and Ω are, respectively, the current time and the collision operator.

In the BGK Model [23], Ω is characterised by a relaxation time τ and the equilibrium distribution functions $f_i^{eq}(x,t)$.

$$\Omega = -\frac{\Delta t}{\tau}\left[f_i(x,t) - f_i^{eq}(x,t)\right] \tag{4}$$

2.3 Immersed moving boundary

The immersed moving boundary scheme was proposed by Noble and Torczynski [24] to overcome fluctuations of hydrodynamic forces calculated by the modified Bounce Back technique. In this method, the particle is represented by solid nodes, the solid boundary nodes and interior solid nodes. The fluid nodes near solid boundary nodes are defined as fluid boundary nodes. For illustration, a diagram of IMB is plotted in Figure 1. Four sorts of nodes: solid boundary nodes, interior solid nodes, fluid boundary nodes and normal fluid nodes, are, respectively, marked in red, yellow, green and blue. In order to retain the advantages of LBM, namely the locality of the collision operator and the simple linear streaming operator, an additional collision term, Ω_i^S, for nodes covered partially or fully by the solid is introduced to the standard collision operator of LBM. The modified collision operator for resolving the fluid-solid interaction is given by

$$\Omega = -\frac{\Delta t}{\tau}(1-B)\left[f_i(x,t) - f_i^{eq}(x,t)\right] + B\Omega_i^S \tag{5}$$

where B is a weighting function that depends on the local solid ratio ε, defined as the fraction of the node area (see Figure 1).

$$B = \frac{\varepsilon(\tau - 0.5)}{(1-\varepsilon) + (\tau - 0.5)}$$

The additional collision term is based on the bounce-rule for nonequilibrium part and is given by

$$\Omega_i^S = f_{-i}(x,t) - f_i(x,t) + f_i^{eq}(\rho, U_S) - f_{-i}^{eq}(\rho, u) \tag{6}$$

where U_S is the velocity of the solid node (see Figure 1) and u is the fluid velocity of each node.

2.3.1 Computational procedure

Although the IMB scheme has been successfully implemented in the coupled DEM-LBM technique, the detailed procedure of IMB was seldom reported. Herein, we give a robust algorithm of IMB scheme to bridge the gap between the basic theory and practical application.

As mentioned before, there are four sorts of nodes: solid boundary nodes, interior solid nodes, fluid boundary nodes and normal fluid nodes, in the IMB scheme. The challenge of IMB procedure is how to efficiently identify the fluid and solid boundary node associated to each

solid particle. The detailed implementation of the proposed Boundary-Trace method (see Figure 2) is described as follows:

Step1: identify solid boundary nodes

1) Before tracing boundary nodes, set all nodes as fluid nodes.
2) Locate the first solid boundary node A from the coordinate of the sphere centre O(x0,y0). In LBM, the coordinate system is set based on grids, the coordinates of all nodes are integers. Rounding x0 leads to the X coordinate, ix, of A. then calculate the Y coordinate, (y0-dy), of P. Rounding (y0-dy) leads to iy. If iy less than (y0-dy), Y coordinate of A is (iy+1); otherwise Y coordinate of A is iy. Mark node A as the first solid boundary node.
3) To trace the next solid boundary node, two direction flags need to be introduced. One is the current direction flag which points to the direction of next searching. The other is the reference direction flag. The direction priority order is West (W)-North (N)-East (E)-South (S)-West (W). In the program, W is represented by 1 and 5; N by 2 and 6, E by 3 and S by 4. Initially, both current and reference direction flags are set as 1 (W).
4) Move the marker to the next node toward the direction of current direction flag. Check whether the new node is inside the particle. If it is outside the particle, move the maker back to the previous position and lower the current direction priority by adding 1 for next searching. Check the difference of current direction flag and reference direction flag. If the current direction flag subtracted by 2 equals to the reference direction flag, lower the reference direction priority by adding 1. If the new node is inside the particle, check whether it is a fluid node. If the new node is a fluid node, mark it as a solid boundary node. And upgrade the current direction priority by subtracting 1 for next searching. If the value of current direction flag is less than the reference direction flag, make the current direction flag is the same as the reference direction flag.
5) Continue tracing other solid boundary nodes according to 4) until the first solid boundary node is reached again.

Step2: identify fluid boundary nodes

1) After sorting out all solid boundary nodes, the first fluid boundary node B can be located by the similar method for identifying A.
2) Similarly, current and reference direction flags are employed. The direction priority order is the same as that in solid boundary nodes. Initialise current direction flag as 1 (W) and reference as 2 (N).
3) Move the marker to the next node toward the direction of current direction flag. Check whether the new node is outside the particle. If it is inside, upgrade the current direction priority by subtracting 1 for next searching. If it is outside, mark it as a fluid boundary node. Update reference direction priority though reference=current+1. Check the next node along reference direction. If the next node along reference direction is inside the particle, lower the current direction priority by adding 1 for next searching. Otherwise, check the next node along the current direction. If it is inside the particle, upgrade the current direction by subtracting 1.
4) Trace next fluid boundary node according to 3) until the first fluid boundary node is reached again.

Step3: identify interior solid nodes

1) The nodes inside the particle except solid boundary nodes can be marked as interior solid nodes.

3 Periodic Boundary Condition

To illustrate PBC in fluid-particle systems in detail, the two-dimensional migration problem of particles from the left to the right towards the horizontal direction in an infinite tube will be taken as an example.

Apparently, a simulation of the transportation of millions of particles in a sufficiently long tube is challenging. To study the distribution of particles in equilibrium, a finite model with periodic boundary conditions (See Figure 3) can be utilised to replace the real model. As marked in Figure 3a, four periodic particles, A to D, are lying at the left or right boundaries. These four particles all have two components marked in black and purple, respectively. When part of a particle (see A) exceeds the right boundary, it will enter the domain from the left boundary. When the centre point of a particle (see B) moves beyond the right boundary, the major component (in black) of particle B will be shown at the left boundary.

The treatment of PBC for DEMLBM mainly includes three parts: the interaction and periodic migration of solid particles, the fluid-solid coupling at the periodic boundary and the periodic flow of fluid. The implementation of PBC for DEMLBM can be accomplished in several ways. One efficient framework for DEMLBM, where an immersed moving boundary scheme is adopted for the fluid-solid coupling, is proposed as follows in this study.

1) Solid part

This part can be directly implemented as the treatment of PBC in DEM. The first step is to determine the maximum diameter (Dmax) of particles in this problem and to search the periodic particles within the area determined by Dmax (see read line area in Figure 3b). Then, identifying periodic particles and recording them using two arrays, defined as the left group and the right group. Next, when processing contact detection, the following situation should be considered. If the contactor (e.g. particle C or D) belongs to the periodic particles in the left (or right) group, potential interactions with the periodic particles (e.g. D or C) lying in the right (or left) group also need to be considered. This can be achieved by performing contact detection between its corresponding virtual particles and periodic particles in the right (or left) group. If interaction exists, the associated force or stress will be calculated using penalty functions and added into the resultant force, which is used to update the particle motion of the contactor. Finally, move the particle which exceeds the boundary of the problem to the position of the corresponding virtual particle, when updating the particle position.

2) Fluid part

This process is slightly different from the PBC in LBM. Fluid nodes at periodic boundaries should be examined, because some fluid nodes belonging to solid particles at the opposite boundary are not real fluid nodes. Then, loop over periodic fluid nodes at inlet or outlet, propagate associated fluid components (fluid particles) to periodic nodes at outlet or inlet if they are not solid nodes.

3) Fluid-solid coupling

In this part, only the PBC for the immersed moving boundary scheme, the commonly used fluid-solid coupling scheme in DEMLBM, will be illustrated. The fluid-solid coupling is

achieved by processing interactions between the fluid boundary nodes and the solid boundary nodes of a particle in the IMB scheme. For a periodic particle near the problem boundary, its solid boundary or/and fluid boundary nodes may be outside the active domain. The solid/fluid boundary nodes exceeding the domain of the problem will be replaced by the corresponding solid/fluid boundary nodes of the associated virtual particle. Besides, the solid ratio of a boundary node and moment applied to this particle are calculated from the geometry parameters of the corresponding virtual particle. As for the interior nodes of a periodic particle, the treatment is similar.

4 Validations and Discussions

The fracturing process involves the injection of fluid at a pressure sufficiently high to break down the rock. Proppant slurries are then pumped into the induced fracture to keep it open so that the hydrocarbon production from the well can be significantly enhanced. While most proppants are simply made of silica or ceramics, advanced proppants like ultra-lightweight proppant is also desirable and behaves as neutrally buoyant particle since it reduces proppant settling and requires low viscosity fluids to transport.

For ductile rocks and shale reservoirs, a viscous fracturing fluid is injected to create the conventional bi-wing fracture system. When a low viscosity fluid is used, the transport of conventional proppant suspension is limited only to the fracture tips. When using slick water, it is difficult to transport conventional ceramic proppants deep into the fracture network [25]. Parker and Sanchez [26] have found that exotic proppant materials such as ultra-lightweight and thermoplastic alloys could be carried deeper into the formation. In this application, the coupled DEMLBM technique is applied to study the migration of neutrally buoyant circular cylinders in plane Poiseuille flow of a Newtonian fluid.

4.1 Single particle case

The migration of single neutrally buoyant particle has been extensively investigated both experimentally and numerically. For fluid flow of high Reynold number, such as Re>1300, the equilibrium position of the particle approaches the central line of a symmetric tube [27, 28]. In this study, to greatly decrease the computing cost a square tube, 10 mm in side, instead of an infinite tube is adopted, and periodic boundary conditions are applied to the left inlet and the right outlet for the solid particle, fluid and fluid-solid interactions (See Figure 4). A circular cylinder particle with 1 mm diameter is initially placed at 5, 6, 7, 8 or 9 mm in height, respectively. The lattice space adopted is 0.1 mm, thus the problem domain is divided into 100×100 grids. The time step used is 3.333×10-8 s. In order to achieve the neutrally buoyant condition, the density of the solid particle is set to be the same as the fluid (water).

During the whole simulation, the particle whose vertical position is over 5 mm moves in a periodic mode in the horizontal direction (see Figure 6); while the particle migrates vertically towards the central line (Y=50) until it reaches an equilibrium state (see Figure 5 and 7). It is noticed that the particle initially placed at the central line tends to move slightly away from the central line. More discussion on the transportation of a single neutrally buoyant particle can be found in the references [27,28].

In order to demonstrate the computational efficiency of the proposed PBC scheme, a large model (see Figure 8a) with the same model parameters is simulated except that the horizontal length is 40 mm. The initial vertical position of the solid particle is 9 mm. The comparison of the vertical movement of the particle in two models of different sizes is given in Figure 9.

The equilibrium positions in vertical direction are consistent. It can be found that the equilibrium time used in the small model is shorter than that in the large model. It is respectively 1.67 s and 2.59 s in the small and large model. In addition, the computing cost of the small model takes about 21 h 31 min on the personal computer (Intel Core i5-3450 CPU@3.10 GHz), while it takes 95 h 26 min for the large model. Compared with the large model, the small model saves at least 77.5% of the computing time.

4.2 Multiple particles case

In this case, we model the motion of 105 neutrally buoyant circular discs in a pressure-driven Poiseuille flow. The domain of the problem under consideration is 0.1 m × 0.04 m. The top and bottom boundaries are walls where no-slip boundaries are imposed. A hydraulic gradient between the left inlet and the right outlet is applied. At the beginning, the particles are positioned uniformly (see Figure 10a) and all the particle velocities are zero. Their radii range from 1.5 mm to 2.5 mm. The lattice space adopted is 0.5 mm, thus the problem domain is divided into 200×80 grids. The time step used is 8.333×10-7 s. In order to the achieve neutrally buoyant condition, the density of the solid particle is set to be the same as the fluid (water). The velocity contour and particle positions at different instants are given in Figure 10.

It can be found that once the pressure is applied at the left inlet the fluid and the solid particles start to move from left to right. At the 12500-th time step some particles (marked in pink) move out of the right boundary and re-enter the domain from the left inlet. This process will repeat with time. The variations of the velocity profile of fluid and particles at different instants in the lattice coordinate system are shown in Figure 11. Both fluid and particles velocities increase from the boundary to the central line of the tube and the maximum velocity increase with time until the system reaches an equilibrium state. The distribution of the average solid fraction at the beginning and the equilibrium state in the vertical direction is presented in Figure 12. Initially, the solid particle is almost uniformly distributed in the Y direction and the solid fraction is around 0.15. When the transportation of particles reaches an equilibrium state, the distribution of the solid is almost normal.

In the single particle transport case, the accuracy of the PBC is validated with the experimental observation [27]. The computing cost is greatly reduced by implementing PBC in fine-grid fluid solver. In the second benchmark test, the applicability of the PBC for DEMLBM involving many particles is well demonstrated. Because of the proposed periodic boundary condition, the behaviour of neutrally buoyant particles in an infinitely long tube can be studied using a finite tube with less particles. Besides, the inherent shortcoming of DEMLBM, the expensive computing cost, can be significantly improved.

5 Conclusions

Although the DEMLBM technique has been proven to be a promising research tool for resolving fluid-particle coupling, its expensive computing cost, particularly for 3D simulations, limits the application of DEMLBM to large-sized problems. In this paper, a PBC for the DEMLBM technique was proposed. The accuracy of the PBC was validated through the quantitative single particle test. Whilst, its applicability was examined by the qualitative multiple particles transport case. The proposed PBC is well demonstrated through these two test cases and experimental observations. Currently, only 2D PBC procedure is given in this paper, the implementation of 3D PBC is straightforward.

However, programming the PBC for DEMLBM with IMB scheme is not easy. It need to repeatedly search the fluid boundary and solid boundary nodes for the solid particles within the periodic domain and process their interactions at each time step.

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