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PS-MRT LATTICE BOLTZMANN MODEL FOR DIRECT SIMULATION OF GRANULAR SOILS AND SEEPAGE FLOW

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Abstract. We proposed a direct numerical simulation model of granular soils and seepage flow by combining the discrete element method and the lattice Boltzmann method. The MRT model was introduced in order to obtain stable solutions of fluid flow under high Reynolds number condition. The PS model, which retains a local operation at each fluid node and keep from intensive increasing the computational costs for the calculation of collision term, was also introduced as a solid-fluid coupled model. We show the effectiveness of the PS-MRT lattice Boltzmann model through several validation tests.

1 INTRODUCTION

The solid particle-fluid multiphase flow and its multi-physics phenomena can be found in a lot of scientific fields: fluidization in chemical engineering, transport of blood cell in bio-engineering, sedimentation and erosion in environmental sciences, sand production in resource engineering and so on. These physical phenomena are not well understood because of the wide variety and the complexity of the particle-fluid or the particle-particle interactions. The particle-fluid systems are often experimentally observed by using an X-ray tomography [1] [2] and a high speed camera [3], but observation capacity and available information at particle-resolution by using such apparatuses are still limited.

In addition to experimental approaches, the development of numerical simulation can help our understanding of such complex particle-fluid systems. Because of the importance of capturing properly the interactions between particle and fluid, micro-scale numerical method which can deal with the fluid flow at less particle scale is needed. In contrast, macro-scale methods have less computationally load and are suitable for an industrial application, but require a local averaging which loses the essential details of the fluid flow. The former type of the direct methods is intently improved and new findings are obtained mainly in research fields such as chemical engineering, bio-engineering and soft matter physics.

In geo-mechanics, a particle-fluid system also exists in the form of solid particles and pore liquids or gases, which are characteristic of non-Brownian and highly concentrated suspensions. A deep understanding of such a system is a key to predict and control the various phenomena, such as sand boiling, weathering of rocks, internal erosion and liquefaction of foundation. However, compared to other research fields, there are still a few 3-D applications of a direct particle-fluid solution in geotechnical engineering or civil engineering, despite the importance of consideration of the particle-fluid interaction. The 3-D condition is especially important for the soil structure because an additional special treatment to handle the zero permeability is required for a 2-D congested granular system.

In this study, we proposed an effective direct simulation method in three dimensions for both soils and seepage flow by using the DEM (Discrete Element Method) and the LBM (Lattice Boltzmann Method). Firstly, in order to stabilize the flow analysis and to improve the accuracy of the non-slip boundary condition, the MRT (Multiple Relaxation Time) model [4] was introduced into the LBGK equation, which is also called the SRT (Single Relaxation Time) model and is standard solution of the non-compressible fluids. Secondlly, PS (Partially Saturated) model [5] was chosen as a solution of the moving boundary, which can maintain the inherent parallel nature of the lattice Boltzmann equation. These two LB models and the DEM were combined, and the validation of the PS-MRT LB model was performed through several types of simulations.

2 MRT LB MODEL FOR SEEPAGE FLOW

The lattice Boltzmann method is one of the CFD methods and an alternative to the N-S equation. In the LBM, the velocity moments of the virtual fluid particles, **f**, having finite directions are placed at each node, and the behaviors of them are governed by a propagation phase and a collision phase from node to node. When the velocity moments have Q directions, **f** is defined as $\{f_\alpha \mid \alpha=0,1,\ldots Q\text{-}1\}$, where α is the number of the discrete velocities depending on the choice of the model for the velocity moment. With the consideration of the precision and the numerical efficiency, the D3Q19 model for the three dimensions is used in this study. The solution of the LBM is governed by the following lattice Boltzmann equation.

$$\mathbf{f}(\mathbf{x}+\mathbf{c}\delta_t, t+\delta_t)-\mathbf{f}(\mathbf{x},t)=\mathbf{\Omega}(\mathbf{x},t)+\mathbf{G}\delta_t. \tag{1}$$

The value for **x** is the position of the node which is being calculated, t is the time, δ_t is the discrete time and δ_x is the grid space. **c** is the grid velocity, which is calculated by δ_x/δ_t. One of the right term for $\mathbf{\Omega}$ indicates the collision operator and **G** indicates the forcing term. For the SRT (single relaxation time) LB model [6], which is a standard solution of the LBM, $\mathbf{\Omega}$ is given as

$$\mathbf{\Omega}(\mathbf{x},t)=-\tau^{-1}\mathbf{I}\left(\mathbf{f}(\mathbf{x},t)-\mathbf{f}^{eq}(\mathbf{x},t)\right), \tag{2}$$

where τ is the relaxation time coefficient, **I** is the identity matrix and $\mathbf{f}^{eq}$ is the equilibrium distribution function in the velocity space. The kinetic viscosity of the fluid ν is calculated by $c^2\delta_t(\tau\text{-}0.5)/3$.

Here, it is well known that the SRT model often results in numerical instability when fluids have relatively low viscosities. Especially, serious instability problemes occur in three dimensional flows in the case where physics may not be adequately resolved due to compurtational constraints. In order to obtain the numerical stability, we introduce the MRT (multiple relaxation time) model [4] as an alternative to the SRT model. In the MRT model, by choosing different time scales to represent changes in the various physical processes due to collisions, the stability of the LBM can be significantly improved. The collision operator for the MRT model is as follows.

$$\mathbf{\Omega}(\mathbf{x},t) = -\mathbf{M}^{-1}\hat{\mathbf{S}}\left(\mathbf{m}(\mathbf{x},t) - \mathbf{m}^{eq}(\mathbf{x},t)\right), \tag{3}$$

where $\mathbf{M}$ is a $Q \times Q$ matrix which linearly transform the velocity space, $\mathbf{f}$, to the moment space, $\mathbf{m}$: $\mathbf{f} = \mathbf{M}^{-1}\mathbf{m}$, $\mathbf{m} = \mathbf{M}\mathbf{f}$. $\hat{\mathbf{S}}$ is the diagonal matrix where $\hat{\mathbf{S}}$ = **diag** (0, s1, s2, , s4, 0, s4, 0, s4, s9, s2, s9, s2, s9, s9, s9, s9, s16, s16, s16). $\mathbf{m}^{eq}$ is the equilibrium distribution function in the moment space. It should be noted here that the value for s9 is equal to τ, and other diagonal components of $\hat{\mathbf{S}}$ is arbitrarily-assigned.

3 PS-MRT LB MODEL FOR PARTICLE-FLUID COUPLING

In order to perform the coupled particle-fluid simulations in the framework of the LBM, the PS (partially saturated) model allowing momentum transfer inside the solid phase, whose concept is originally suggested by Noble and Torczynski [5], is used. This model enables to deal with moving solid-liquid boundary and to calculate the hydrodynamic force acting on the solid obstacle. Compared to other coupled model [7] [8] [9], this method has advantages of being able to retain a local operation at each node and of keeping from intensive increasing the computational costs for the calculation of collision term. In this approach, the collision operator in the SRT model as shown in Equation (1) is reformulated to account for the solid fraction at a node, B, and the additional term, $\mathbf{\Lambda}$.

$$\mathbf{\Omega}(\mathbf{x},t) = -\left(\mathbf{I} - \hat{\mathbf{B}}\right)\left(\mathbf{f}(\mathbf{x},t) - \mathbf{f}^{eq}(\mathbf{x},t)\right) + \hat{\mathbf{B}}\mathbf{\Lambda}(\mathbf{x},t), \tag{4}$$

where $\hat{\mathbf{B}}$ is the diagonal matrix whose diagonal components are B and $\mathbf{\Lambda}$ is the additional term considering the velocities of the nodes inside the solid phase. Then, the value for $\mathbf{\Lambda}_\alpha$, which is the α-th component of $\mathbf{\Lambda}$, is given as follows.

$$\Lambda_\alpha = f_{-\alpha}(\mathbf{x}, t) + f_{-\alpha}^{eq}(\rho, \mathbf{u}) + f_\alpha^{eq}(\rho, \mathbf{u}_p) - f_\alpha(\mathbf{x}, t), \tag{5}$$

where $\mathbf{u}_p$ is the velocity of the solid including both translation and rotation motion of the corresponding particle. The notation -α is the opposite direction of α. According to above equations, when $|\mathbf{u}_p| = 0$ and $B = 1$, the bounce-back rule, i.e., the non-slip condition at solid-fluid boundary is obtained.

When the PS model is introduced into the MRT model, the collision operator is given as the following equation.

$$\mathbf{\Omega}(\mathbf{x},t) = -\left(\mathbf{I} - \hat{\mathbf{B}}\right)\mathbf{M}^{-1}\hat{\mathbf{S}}\left(\mathbf{m}(\mathbf{x},t) - \mathbf{m}^{eq}(\mathbf{x},t)\right) + \hat{\mathbf{B}}\mathbf{\Lambda}(\mathbf{x},t). \tag{6}$$

We call this equation PS-MRT LB model in this study. Equation (6) also retains a local operation at each node in the same as Equation (4). For this reason, it is easy to parallelize the LB solution in the frame of PS-MRT LB model.

4 COLLISION LAW AND MOTION OF SOIL PARTICLE

The handling of the collision law and the motion of the soil particle are presented in this subsection. The collision law for a contact force $\mathbf{F}^{con}$ and a contact torque $\mathbf{T}^{con}$ is governed by the DEM, where the contact logic is followed by the Voigt model. The normal repulsive force is assumed to be proportional to the overlap distance, and a dissipative component is set to be proportional to the relative normal velocity between particles. For the calculation of the tangential force, in addition to the same way as the normal force, the Coulomb law of friction is also considered. The value for $\mathbf{F}^{con}$ and $\mathbf{T}^{con}$ are given by summing up the change of momentum inside the solid phase

All of the calculations in the following subsections are performed on the graphic processing unit (NVIDIA GeForce GTX TITAN). Parallelized algorithm for the DEM suggested by Nishiura and Sakaguchi [10] is incorporated into the coupled particle-fluid code. Detailed parallelization methods relative to the coupling scheme on a many core architecture is not discussed in this literature.

5 DRAG FORCE ON SOIL PARTCLE

At the first step in the validation of the PS-MRT LB model, we simulate the obstacle flow, as shown in Figure 1, and obtain the correlation between drag force coefficient C_D and Reynolds number Re. Fluid flows are generated in positive direction of y-coordinate by imposing a constant velocity boundary condition on one side of zx plane, while the other side of zx plane is free outflow boundary. Grid space δ_x is 1.0×10^{-5} m and the system size is $150\delta_x \times 300\delta_x \times 150\delta_x$. Diameter of the sphere d is $30\delta_x$. The density of the fluid ρ_f is 1000 kg/m^3 and the kinetic viscosity of the fluid ν is 1.0×10^{-6} m^2/s.

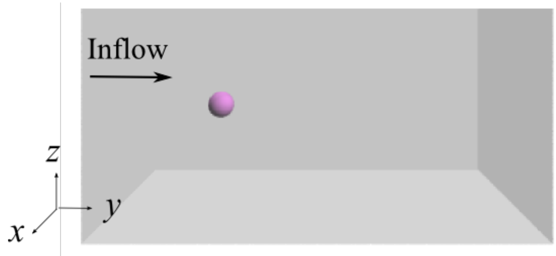

Figure 1: Model setup for the drag force acting on the sphere

As a result of the analysis, the relationships between C_D and Re for the PS-SRT model and the PS-MRT model are plotted in Figure 2. From this figure, it is shown that drag force coefficient C_D obtained from the numerical simulation is corresponding with the empirical equation: $C_D = 24/Re + 6/\ (1+Re^{-0.5}) + 0.4$. Compared with two models, stability solution can be obtained in the range of $Re < 150$ in both cases, and remarkable differences between two models are not observed.

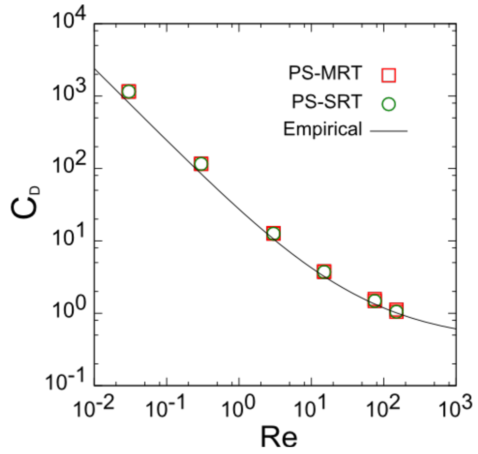

Figure 2: Drag force coefficient C_D vs. Reynolds number *Re*

6 SEEPAGE FLOW IN GRANULAR SOILS

At the next step in the validation of the PS-MRT LB model, we obtain the correlation between friction factor in porous media ψ and Reynolds number *Re*. Figure 3 shows the model setup for the seepage flow in granular soils, which are prepared by the packing analysis by using the DEM. The number of soil particles consisting of the porous media is about 1,000 and the diameter of the soil particle *d* is $16\delta_x$. Fluid flows are generated in positive direction of *y*-coordinate by imposing a constant velocity boundary condition on one side of *zx* plane, while the other side of *zx* plane is free outflow boundary, in the same manner as the analysis of the previous subsection. Grid space δ_x is 1.0×10^{-5} m and the system size is $128\delta_x \times 196\delta_x \times 128\delta_x$. The area occupied with the soil particles is $128\delta_x \times 128\delta_x \times 128\delta_x$. The density of the fluid ρ_f is 1000 kg/m^3 and the kinetic viscosity of the fluid ν is 1.0×10^{-6} m^2/s.

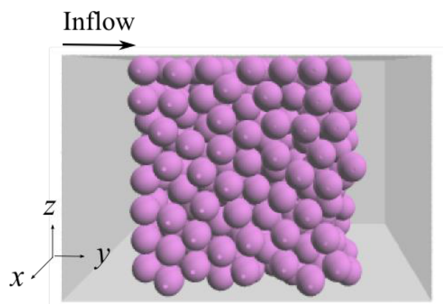

Figure 3: Model setup for the seepage flow in granular soils

Figure 4 shows the relationships between ψ and *Re* with the empirical equations: ψ = 150/*Re* (*Re*<10, Blake-Kozeny eq.), ψ = 150/*Re*+1.75 (10<*Re*<10^3, Ergun eq.). From the figure, the PS-MRT LB model can simulate the flow in the porous media in the range of *Re* < 30. By contrast, the PS-SRT LB model cannot obtain stability solution more than *Re* = 2.

Thus, the PS-MRT LB model has an adavantages to stably simulate in the flow inside the complex boundary.

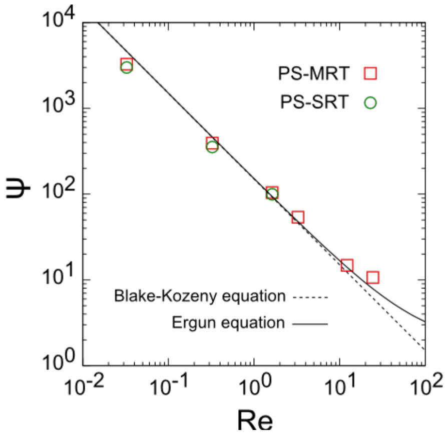

Figure 4: Model setup for the drag force acting on the sphere

7 PARTICLE SETTLING

The last simulation, as shown in Figure 5, illustrates the ability of the PS-MRT LB model to handle large systems of O(10^4). The number of the soil particles is 12,000 and the particle diameter d is $4\delta_x$. Grid space δ_x is 4.0×10^{-5} m and the system size is $160\delta_x \times 160\delta_x \times 250\delta_x$. The density of the fluid ρ_f is 1000 kg/m^3, the density ratio of the solid to the fluid is 2.5, and the kinetic viscosity of the fluid ν is 1.0×10^{-5} m^2/s. The Stokes settling velocity is 2.1×10^{-3} m/s and Reynolds number Re is about 0.3.

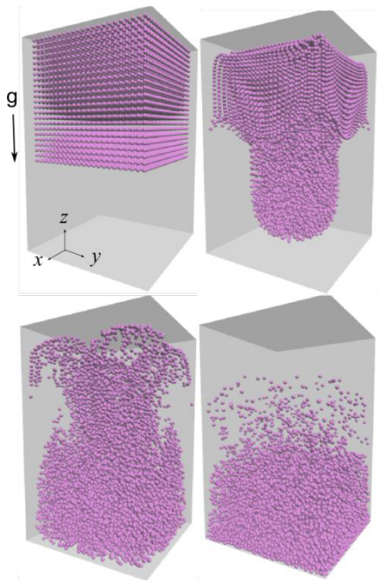

Figure 5: Snapshots of the simulation of particle settling

Figure 5 shows some snapshots during the settling simulation for different elapsed time. The core of the soil particles first swiftly settles followed by the rest of the particles. On the other hand, particles near the vertical walls fall very slowly because the strong interaction occurs between particles and walls. This type of particle settling can be observed in the previous research [11], in which a fictitious domain approach is employed for the coupling method. Therefore, the PS-MRT LB model also can obtain qualitative numerical results in such a large particle-fluid system.

8 CONCLUSIONS

In geo-mechanics, a particle-fluid system exists in the form of solid particles and pore liquids or gases, which are characteristic of non-Brownian and highly concentrated suspensions. For such complex particle-fluid systems, the PS-MRT LB model can be one of the effective way to directly solve both the soil particles and the seepage flow at pore scale. If some parallelization schemes are installed into the simulation code, we can apply the direct numerical model to not only the two-dimensional but also the three-dimensional phenomena.

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