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Particle Based Multiphysics Simulation for Applications to Design of Soil Structures and Micromechanics of Granular Geomaterials

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1 General introduction

1.1 Particle based simulations in geomechanics

The soils and their constructions are bases for human life and they are designed and evaluated to satisfy the safety criteria. Nevertheless, when natural hazards such as earthquakes, tsunami or heavy rainfall attack the city or the rural area, we have trouble in preventing the earth constructions from the severe destruction. In order to minimize damage caused by the disasters, it is important to predict in advance how the earth structures collapse or how the collapses affect the surrounding area, but unfortunately it is not easy to estimate and control the complex behaviors of the soils with large deformation.

Here, geomaterials are composing of an infinite number of congested soil particles. Thus, such materials are in category of the granular materials. In general, the micromechanical behaviors of the granular materials are inherently discontinuous and heterogeneous (Jaeger et al., 1996 [1]). Additionally, liquids and gases existing in the pore space add the multiphysics nature to the micromechanics of the soils. These unique features of the soils make it more difficult for us to understand the macroscopic behaviors accurately.

To overcome such difficulties, I focus on the particle based computational mechanics which have been developed as a relatively new discipline of the computational mechanics, compared to the continuum based mechanics. The concept of the particle based in the thesis indicates two different computational models in both the solid and the fluid mechanics. Firstly, the notion expresses the computational representation of the physical particles, that is, numerical discontinuous modeling of the materials. The methods of the computational mechanics of discontinua include the Discrete Element Method (DEM) (Cundall and Strack, 1979 [2]), the Contact Dynamics (CD) (Moreau, 1988 [3]; Stewart and Trinkle, 1996 [4]), the methods of classical Molecular Dynamics (MD) (Alder and Wainwright, 1957 [5]) and the Discontinua Deformation Analysis (DDA) (Shi, 1988 [6]). These methods employing the physical particles can deal with the engineering problems and the processes where constitutive laws are not too efficient.

On the other hand, the concept of the particle based also represents the discretization methods, where the behavior of the continua is modeled as the virtual particles having the mechanical information, in other words, these particles mean the interpolation points rather than being the physical particles. Such mesh-free methods include the Smoothed Particles Hydrodynamics (SPH) (Gingold and Monaghan, 1977 [7]; Lucy, 1977 [8]), the Moving Part-
Particle Simulation (MPS) (Koshizuka and Oka, 1996 [9]), the Material Point Method (MPM) (Sulsky et al., 1994 [10]), the Lattice-Boltzmann-Method (LBM) (McNamara and Zanetti, 1988 [11]; Qian et al., 1992 [12]) and the Particle in Cell (PIC) (Brackbill and Ruppel, 1986 [13]). These methods are used extensively for not only the fluid dynamics simulations but also the solid mechanics. In some cases, these above two concepts of the physical particles and the virtual particles are connected in order to simulate the multiphysics phenomena and the multiphase flow, e.g., fluid-particle system or fluid-structure system.

![Figure 1.1 An example of the DEM simulation of the laboratory test: a one-axial compression test of the cohesive soils. The number of the soil particles is about 30,000. The contact bond model, which is described in detail in Chapter 3, is employed as the contact logic.](image)

In the thesis, I deal with the geomaterials and the geostructures as the discrete materials, and discuss the mechanism of the soils and its constructions from microscopic point of view through the particle based simulations. Interests in such numerical methods have grown in recent years with the increasing the computing power and the development of the parallelization schemes. This study investigates not only the solid phase but also the fluid phase existing at pore scale. The simulation methods mainly used in the thesis are the DEM and the LBM: the DEM is used as simulating the solid phase and the LBM is used as the fluid phase, and the coupled DEM-LBM is used for the multiphysics phenomena.
1.1. PARTICLE BASED SIMULATIONS IN GEOMECHANICS

such as seepage failure of the soils induced by the flow of the pore fluid. Examples of the DEM simulation and the coupled DEM-LBM simulation are shown in Figures 1.1 and 1.2, respectively. Here, there are two main objectives to use the particle based simulations in geotechnical engineering, as follows.

One of the objectives is to newly propose the efficient discrete element models so that the large deformation of the soil structures can be successfully reproduced. Numerical modeling in the civil engineering is often based on the continuum hypothesis, and a lot of continuum approaches have been developed to take discontinuities into account and they have produced many results (Noda et al., 2008 [14]). However, the inner discrete structure and its large deformation cannot be modeled sufficiently by such approaches. In contrast, the particle based simulations have advantages of dealing with the large displacements of the subject materials, rather than the continuum based simulations. The various application examples with the large-displacement have been carried out: landslide by the SPH (Pastor et al., 2008 [15]), crack propagation by the MPM (Daphalapurkar et al., 2007 [16]), falling rocks by the DEM (An and Tannant, 2007 [17]), sand production by the DEM coupled with the conventional CFD method (Zhou et al., 2011 [18]), tsunami simulation by the DEM coupled with the SPH (Cleary and Prakash, 2004 [19]) and so on. This is why an application of the particle based method to the practical problems leads to high motivation for the researchers and the engineers in the area of geomechanics.

The other objective is to clarify the micromechanics of the soils. There is still no comprehensive theory for granular materials including the soils that can successfully describe the behaviors of such materials. In the physical particle model, loads and deformations can be applied to the numerical samples to mimic laboratory tests (see Figure 1.1), and then the particle-scale mechanisms, which are the key to the complex overall material response, can be monitored and analyzed. In other words, the physical particle model can easily measure the contact force, the contact orientations, the particle rotations and so on (see Iwashita and Oda, 1999 [20]; Hinrichsen and Wolf, 2004 [21]; O’Sullivan, 2011 [22]). Such detailed micromechanical information is not available in the laboratory experiments or other simulation models. Furthermore, when a computational fluid model is coupled with the physical particle model (see Figure 1.2), we can microscopically investigate the multiphysics phenomena such as seepage failure, internal erosion and liquefaction of the soils. Obtained findings at micro-scale may also contribute to the constitutive laws which are being developed to describe the macroscopic complex behavior of soils.
CHAPTER 1. GENERAL INTRODUCTION

Figure 1.2  Coupled DEM-LBM simulation of the particle sedimentation in the viscous fluid inside a rectangular box. This calculation is performed on Geforce GTX TITAN. The fluid node is $200 \times 200 \times 300$ and the number of the particles is about 35,000. The ratio of the lattice space to the particle diameter is set to be 4.0. Reynolds number $Re < 1$.

1.2 Thesis outline

The main topic of the thesis is the modeling of the granular soils and its structures by means of the DEM and the LBM. This study is motivated by both (i) the geo-engineering application and (ii) the micromechanics of the soils, as explained in the previous section. This thesis consists of seven chapters: the topics of the geo-engineering application are discussed in Chapters 3 and 4, while the topics of the micromechanics are discussed in Chapters 5 and 6. An outline of the thesis is presented as follows. More detailed introductions and literature reviews are given in each chapter.

In chapter 2, I describe the basic theory of the computational techniques, i.e., the DEM and the LBM that are mainly used in this study. Overviews of the parallelization methods of these two methods on many core processors are also described. It should be noted here that all of accelerated simulation codes with parallelization used in the thesis are uniquely-developed by the author.

In chapter 3, a simple contact model for the DEM with fewer parameters is proposed so that the boundary value problems in geotechnical engineering can be studied. The interparticle contact bond model, which reproduces the behavior of cohesive geomaterials, and the rolling friction model, which expresses the interlocking effect of grain shapes with circular particles,
are introduced into the conventional collision law for the two-dimensional DEM. Both of these models require only one additional parameter. Parametric analyses, based on several direct shear tests, are performed to validate the proposed model and to obtain relationships between the DEM parameters and the failure criteria for geomaterials by means of $c$ and $\phi$. In the last section, the proposed model is extended to the three dimensions, and I briefly present an application example of the proposed model to the seismic behavior of the ripraps on the embankment dams.

In chapter 4, the shape effect of the blocks comprising a dry-stone masonry retaining wall under seismic loading is investigated through centrifuge model tests and numerical simulations using the three-dimensional DEM. The variations in block shape, namely, cubic-shape and wedge-shape, are compared. For both the physical experiments and the numerical simulations, the seismic resistivity is higher in the wall of wedge-shaped blocks than in the wall of cuboid blocks, although the total mass is larger for the wall of cuboid blocks. Therefore, a detailed investigation is performed by the discrete element model to explore the mechanism of the shape effect. I find that the surface area, which contributes to the frictional resistance between each stone block and the backfill, is the key parameter to mobilize the anti-seismic strength of a dry-stone masonry retaining wall.

In chapter 5, in order to study the effects of the rolling friction of the particles on granular packing, I present a detailed analysis of circular disk assemblies with rolling friction under macroscopic one-dimensional compression. The rolling friction of the particles produces a resisting moment to the rolling at each contact. A series of 2-D DEM simulations are performed with various values for the rolling friction parameter. I focus on several macroscopic and microstructural properties of granular media and analyze them as a function of the rolling friction. From these results, I show that the rolling resistance, which results from the rolling friction of the particles, contributes to the inhibition of the rearrangement of the particles and increases the magnitude of the fabric anisotropy under packing. In addition, from both microscopic and macroscopic points of view, I describe that the stress state in a granular packing can vary considerably depending on the rolling resistance.

In chapter 6, I have numerically investigated the boiling phenomena in order to capture the process of the seepage-induced failure of non-cohesive granular soils by means of the direct particle-fluid model, and to confirm the applicability of such a direct solution to the problems in the geotechnical engineering. The motion and collision of the solid particles are calculated by the DEM and the fluid flow of the pore fluid is directly solved at a smaller scale than the particle diameter by the LBM. By coupling DEM and LBM, the interaction
between the particle and the fluid is also calculated. As a result of the analysis of the boiling phenomena of the soils, numerically predicted value for the critical hydraulic gradient is in good agreement with the theoretical one. In addition, the rapid change of the flow pattern around the critical hydraulic gradient can be microscopically captured. From the observation of the evolution of the force chains inside the soils, I have demonstrated that the failure process of the contact networks with the increasing seepage force can be also simulated. Other possible applications of the direct particle-fluid simulation method are discussed in the last section.

In chapter 7, final conclusions on the thesis are drawn and future possible developments on the particle based methods for the geomechanics are summarized.
2 Basic theory of computational techniques

2.1 Discrete element method

The discrete element method was first developed by Cundall and Strack (1979 [2]) for rock mechanics and later applied to granular materials. The algorithm of the DEM is based on the explicit method for the equation of motion and avoids the inversion process for the stiffness matrices which is generally one of the main processes in structural analyses, such as the DDA, the CD and the Finite Element Method (FEM). Unlike a hard sphere model, moreover, in the frame of a soft sphere model such as DEM, shapes of the element and their multibody collisions can be considered. The DEM had limited application when the original method was first proposed, but recent development of the computer technologies and the parallelization techniques enable us to handle quite large number of the particles in simulations (Nishiura and Sakaguchi, 2011 [23]). Because of these advantages, the DEM is widely used as a method of discontinuous modeling in various scientific fields. The basic calculation procedure is described as follows.

![Figure 2.1 Conceptual descriptions of the DEM (a) Calculation of resultant force on particle i. (b) A pair of circular or spherical particles i and j undergoing contact.](image)

Figures 2.1 (a) and (b) show the conceptual descriptions of the DEM. In the DEM, the translational and rotational motion of a discrete particle i are dictated by the following
CHAPTER 2. BASIC THEORY OF COMPUTATIONAL TECHNIQUES

momentum equations.

\[ m_i \frac{d^2 x_i}{dt^2} = \sum F_{con} + F_{gra}, \quad (2.1) \]

\[ I_i \frac{d^2 \theta_i}{dt^2} = \sum T_{con}, \quad (2.2) \]

where \( x_i \) and \( \theta_i \) are the position vector and the rotational angle, \( m_i \) is the particle mass, \( I_i \) is the particle moment of inertia, \( F_{gra} \) is the external force induced by the gravitational acceleration, \( \sum F_{con} \) refers to the sum of the resultant interparticle force at the contacts and \( \sum T_{con} \) is the sum of the resultant moment around the center of the mass of a particle.

A contact force \( F_{con} \) is calculated by the linear-contact law in this study, i.e., the contact springs are assumed to be linear. Let us consider a pair of circular or spherical particles \( i \) and \( j \) that are close to contact, as shown in Figure 2.1 (b). The value for \( F_{con} \) acting on particle \( i \) from particle \( j \) is decomposed into its normal \( F_{con}^n \) and tangential \( F_{con}^t \) components as follows.

\[ F_{con} = F_{con}^n + F_{con}^t. \quad (2.3) \]

The contact logic is followed by the Voigt model, that is, the normal repulsive force \( F_{con}^n \) is assumed to be proportional to the overlap distance \( \delta_{ij} \), and a dissipative component is set to be proportional to the relative normal velocity, \( U_{nj}^n \), between particles \( i \) and \( j \).

\[ F_{con}^n = \left(k_n \delta_{ij} - \gamma_n U_{nj}^n\right) n_{ij}, \quad (2.4) \]

and

\[ U_{nj}^n = \left(U_{ij} \cdot n_{ij}\right) n_{ij} + \left(a_i \Omega_i + a_j \Omega_j\right) \times n_{ij}, \quad (2.5) \]

where \( k_n \) is the normal spring constant, \( \gamma_n \) is the damping coefficient and \( n_{ij} \) is the normal unit vector. \( U_{ij} \) is the relative velocity between particle \( i \) and \( j \), \( a \) and \( \Omega \) are a relative length from the mass center of the particle and an angular velocity, respectively. Such a method allowing the overlap between particles is generally referred to the soft sphere model. Parameter \( k_n \) is chosen sufficiently large enough to describe a rigid solid. The relation between the damping coefficient \( \gamma_n \) and the restitution coefficient \( e_n \) is given by

\[ e_n = \exp \left( \frac{-\pi \kappa}{\sqrt{1 - \kappa^2}} \right), \quad (2.6) \]

where the damping parameter is defined as \( \kappa = \sqrt{\gamma_n/\gamma_n^{crit}} \). The value for critical damping \( \gamma_n^{crit} \) is calculated as \( 2 \sqrt{k_n m_p} \).
2.1. DISCRETE ELEMENT METHOD

On the other hand, the tangential force $F^\text{con}_t$ is given by

$$F^\text{con}_t = k_t \Upsilon_{ij} - \gamma_t U_{ij}^t,$$

(2.7)

where $\Upsilon_{ij}$ is a tangential relative displacement defined by integrating the slip velocity $U_{ij}^t$ during the contact:

$$\Upsilon_{ij} = \int_0^t U_{ij}^t \, dt,$$

(2.8)

where the slip velocity is calculated as

$$U_{ij}^t = U_{ij} - U_{ij}^n.$$

(2.9)

Since the tangential plane varies with time, the obtained tangential force must be projected on the current tangential plane after each time step as

$$F^\text{con}_t = F^\text{con}_t - (F^\text{con}_t \cdot \mathbf{n}_{ij}) \mathbf{n}_{ij}.$$

(2.10)

The actual tangential force is followed by the Coulomb law of friction when it exceeds the friction limit $\mu |F^\text{con}_n|$ and is then given by

$$F^\text{con}_t = \mu |F^\text{con}_n| \frac{F^\text{con}_t}{|F^\text{con}_t|},$$

(2.11)

where $\mu$ is the friction coefficient. The value for the dynamic friction coefficient and the static friction coefficient assumed to be equivalent. Finally, the corresponding torque is given by

$$\mathbf{T}^\text{con} = a_i \mathbf{n}_{ij} \times F^\text{con}.$$

(2.12)

In most DEM codes, Equations (2.1) and (2.2) are integrated by means of the leap-frog method or the velocity Verlet algorithm with a time increment $\delta t^\text{dem}$ in order to update the position and the rotational angle (O’Sullivan, 2009 [22]). The value for $\delta t^\text{dem}$ is determined by the following CFL condition.

$$\delta t^\text{dem} < \delta t^\text{dem}_c = 2 \left( \sqrt{1 + \kappa^2} - \kappa \right) \sqrt{\frac{k_n}{m_p}},$$

(2.13)

where $\delta t^\text{dem}_c$ is the critical time step. However, this time step value may be too large to obtain stable solutions. The actual value for $\delta t^\text{dem}$ used for solving the momentum equations
is about one tenth of $\delta_{c_{DEM}}$.

Apart from that, for the efficient force summation (the process of calculation of $\sum F_{con}$ and $\sum T_{con}$ at each particle), I employ the Verlet list algorithm (Poschel and Schwager, 2005 [24]). This algorithm is based on a simple property of the DEM simulation: two particles being close to each other at a given time will stay close neighbors at least in the subsequent short time steps. By incorporating the Verlet list algorithm, the number of contact candidates for each particle can be reduced in advance before the contact judgment, which needs heavy computational demands.

### 2.2 Lattice Boltzmann method

The lattice Boltzmann method is one of the CFD methods and increasingly attracts researchers in many areas, such as a turbulence flow (Yu et al., 2005 [25]), a flow in porous media (Guo and Zhao, 2002 [26]) and a multi-phase flow (Chen and Doolen, 1998 [27]; Inamuro et al., 2004 [28];). In the thesis, the particle based methods include the LBM, where the velocity moments of the virtual fluid particles having finite directions are placed at each node, as shown in Figure 2.2. The behaviors of the fluid particles in the model are governed by a propagation phase and a collision phase for the velocity moments moving from node to node. Historically, the LBM was derived from the idea of the Lattice Gas Cellular automaton (LGCA) (McNamara and Zanetti, 1988 [11]) and began to be developed for variety of fluid dynamics in the early 1990’s (Qian et al., 1992 [12]; Qian et al., 1995 [29]; Chen and Doolen, 1998 [30]). The LBM is an alternative to other CFD methods, which are based on the following Navier-Stokes (N-S) equations for incompressible fluid:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{u} + \mathbf{G},$$

(2.14)

where $\mathbf{u}$ is the velocity, $\rho$ is the density of the fluid, $p$ is the pressure, $\nu$ is the kinematic viscosity and $\mathbf{G}$ is the forcing term. The conventional CFD methods numerically solve this equation by means of the Finite Volume Method (FVM), the Finite Difference Method (FDM) or the FEM.

To the contrary, the solution of the LBM is governed by Equation (2.15).

$$f_\alpha(x + c_\alpha \delta_t, t + \delta_t) - f_\alpha(x, t) = \Omega_\alpha(x, t) + G_\alpha \delta_t,$$

(2.15)

where $f_\alpha$ is the $\alpha$-th component of the velocity distribution function and $c_\alpha$ is the $\alpha$-th
2.2. LATTICE BOLTZMANN METHOD

Component of the discrete velocity. The value for $x$ is the position of the node which is being calculated and $\delta t$ is the discrete time. One of the right term for $\Omega_\alpha$ indicates the $\alpha$-th component of the collision operator and $G_\alpha$ is $\alpha$-th component of the force term. $\alpha$ 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 D2Q9 model for the two dimensions and the D3Q19 model for the three dimensions are usually used. In the D3Q19 model employed in Chapter 6, discrete velocities are defined as $c_\alpha = (0, 0, 0), (\pm c, 0, 0), (0, \pm c, 0), (\pm c, 0, \pm c), (0, \pm c, \pm c)$ for $\alpha = 0 \sim 18$, and $c = \delta x/\delta t$ where $\delta x$ is the grid space.

For the Single Relaxation Time (SRT) model (Qian et al., 1992 [12]), $\Omega_\alpha$ is given as

$$
\Omega_\alpha(x, t) = -\frac{1}{\tau}\{f_\alpha(x, t) - f_\alpha^{eq}(x, t)\}, \tag{2.16}
$$

where $\tau$ is a relaxation time coefficient and $f_\alpha^{eq}$ is the $\alpha$-th component of the equilibrium distribution function. The form of Equation (2.16) is also called as LBGK model. It is probed that the N-S equation can be approximately derived from the LBGK equation through the Chapman-Enskog expansion (McLennan, 1965 [31]) or the S expansion (Sone, 1971 [32]). Functions $f_\alpha^{eq}$ in the D3Q19 model are calculated by

$$
f_\alpha^{eq} = \omega_\alpha \rho \{1 + 3(c_\alpha \cdot u)/c^2 + 9(c_\alpha \cdot u)^2/2c^4 - 3(u \cdot u)/2c^2\}, \tag{2.17}
$$

where $\omega_\alpha = 1/3$ for $\alpha = 0$, $\omega_\alpha = 1/18$ for $\alpha = 1, 2, 3, 4, 5, 6$, and $\omega_\alpha = 1/36$ for $\alpha =$
The fluid velocity at the node is given by the vector $\mathbf{u}$, which is determined by

$$\rho \mathbf{u} = \sum_{\alpha} f_{\alpha} c_{\alpha}, \quad (2.18)$$

and where the density $\rho$ is given by

$$\rho = \sum_{\alpha} f_{\alpha}. \quad (2.19)$$

The pressure $p$ is easily computed as a function of the density using the speed of sound $c_s$:

$$p = c_s^2 \rho, \quad (2.20)$$

where $c_s$ is defined as $c_s^2 = c^2 / 3$. In the LBM, the velocity and the pressure is available in local form according to the above equations. On the other hand, relaxation parameter $\tau$ is directly related to the dynamic viscosity as follows.

$$\nu = \frac{1}{3} c^2 \delta t \left( \tau - \frac{1}{2} \right). \quad (2.21)$$

The value for $\tau$ also affects the numerical stability, and is often chosen in the range from 0.5 to 1.0.

The accuracy of LBM is evaluated by the use of the computational Mach number $M$:

$$M = \frac{\| \mathbf{u}_{\max} \|}{c}, \quad (2.22)$$

which is proportional to the Knudson number. $\mathbf{u}_{\max}$ is the maximum fluid velocity in the system. Because the compressibility error is on the order of $M^2$ (Reider and Sterling, 1995 [33]), the value for $M$ should be satisfied with $M \ll 1$.

Due to the unique features of the calculation procedures as described in the above, the LBM has a lot of advantages compared to other CFD methods. Firstly, it is relatively easy to implement the simulation code because it is completely explicit method and does not need an implicit solution for Equation (2.14). Secondly, flows inside complex boundaries can be easily managed without the boundary-fitted grids. Thirdly, the calculation is purely local at each node, that is, the method is inherently parallel.
2.3 Parallelization on many core processor

Particle based methods are closely related to the progress of the computer science. When such methods are applied to the practical engineering problems in the three dimensions, it is necessary to implement the simulation code with parallelization and vectorization on a given hardware. Recently, some new hardware for the scientific calculation has appeared and their integrated development environment has been developed. For example, the Graphics Processing Unit (GPU) as typified by NVIDIA’s products (see Figure 2.3) and the Many Integrated Core architecture (MIC) as typified by Intel Xeon Phi are widely used as a “personal super computer” for the sake of high performance computing.

For the DEM, I incorporate the acceleration algorithm on a many core architecture suggested by Nishiura and Sakaguchi (2011 [23]) and Nishiura et al. (2014 [34]) into my in-house code. This method is mainly featured by the new searching algorithm for determining the contact candidates and the efficient algorithm for summing the contact forces with a reference table. These algorithms are valid for not only the GPU but also a multi-core CPU. Due to the necessity of the introduction of such new ideas, the code with parallelization on the GPU is completely different from the serial code.

Figure 2.3 My GPGPU machines equipped with NVIDIA GeForce GTX TITAN and Tesla C2070. (a) A full view of the machines. (b) A side view. The graphic board is equipped at a position indicated by the arrow.
For the LBM, on the contrary, a major change of the basic calculation process is not needed for the implementation on the GPU. This is because the method has inherently parallel nature, as described in the previous section. I referred to the methods which are lectured by NVIDIA Corporation, 2014 [35], in order to develop my GPGPU (General-purpose computing on graphics processing units) code.

My in-house codes are follows.

**DEM-ON!** is a discrete element simulation code for the 2-D and the 3-D implemented by C++ language with OpenMP for multi-core CPU. This code can deal with the macro particle model for arbitrary shape element.

**DEMottio** is a discrete element simulation code for the 2-D and the 3-D implemented by CUDA C and C++ language for NVIDIA GPU. CUDA 4.2 is used for Tesla C2070 and CUDA 5.0 is used for GeForce GTX TITAN. Memory reduction algorithm for broad particle size distribution is installed in this code.

**LBM-ON!** is a coupled particle-fluid simulation code implemented by C++ language with OpenMP for multi-core CPU. This code is only compatible with 2-D.

**LBMony** is a coupled particle-fluid simulation code implemented by CUDA C and C++ language for NVIDIA GPU. This code is compatible with both 2-D and 3-D.
3 Failure criteria for geomaterials in simple discrete element modeling

3.1 Introduction

The conventional contact model for the discrete element method sometimes fails to express the mechanical behavior of geomaterials (Cundall and Strack, 1979 [2]). In order to apply DEM to geotechnical engineering problems, such as the calculation of the earth pressure (Maynar and Rodriguez, 2005 [36]) and the prediction of a slope failure (Wang et al., 2003 [37]), it is necessary to pay special attention to the contact model. However, the model should be as simple as possible due to the massive computational costs of the DEM in determining suitable parameters for certain ground properties: cohesion $c$ and internal friction angle $\phi$. In Chapter 3, modified versions of two models are introduced into the conventional contact model for the DEM so that the failure criteria for geomaterials can be satisfactorily reproduced with fewer parameters.

The first model is the linear contact bond model, suggested by Utili and Nova (2008 [38]) which reproduces the behavior of cohesive geomaterials in the 2-D DEM. In most bond models proposed by other researchers (ITASCA, 2004 [39]; Jiang et al., 2006 [40]), many parameters are required for a transformation from the unbonded case to the bonded case, but the Utili and Nova model (the U-N model) requires only one parameter. This bond model has the advantage of being able to minimize the micromechanical parameters needed to reproduce the cohesive behavior of geomaterials in the DEM.

The second model is the rolling friction model, suggested by Sakaguchi et al. (1993 [41]). This model expresses the interlocking effect of grain shapes with circular particles, which have the numerical efficiency resulted from simple collision detection. Otherwise, polygonal shaped particles have a disadvantage for searching contact candidates. This rolling friction model also requires only one parameter.

Parametric analyses, based on several direct shear tests, are performed to validate the proposed model. Simple relationships between the macromechanical strength parameters ($c$ and $\phi$) and the corresponding micromechanical quantities at the particle contacts are obtained so that they can be used to express the failure criteria for geomaterials in the DEM.

This chapter is organized as follows. In Section 3.2, the above two models which are introduced into the DEM simulations are described. In Section 3.3, the procedure used to
execute the numerical direct shear test is illustrated. In Section 3.4, I derive the correlations between the macromechanical parameters \((c\) and \(\phi)\) and the micromechanical parameters. Conclusions and an application example of the proposed model follow in Sections 3.5 and 3.6, respectively.

### 3.2 Contact models

#### 3.2.1 Linear contact bond model

DEM permits the neighboring particles to be bonded together by springs through which both attractive and repulsive forces can be transmitted. Among these bond models, the contact bond model, proposed by Utili and Nova, requires only one micromechanical parameter for a transformation from the unbonded case to the bonded case. This bond model is characterized by the adaptation of the Mohr-Coulomb failure criterion into the \(F_{\text{con}}^n-F_{\text{con}}^t\) plane, as shown in Figure 3.1. In the U-N model, the input parameter is \(c_\mu\) and the tensile strength \(t_\mu\) is given simply by

\[
t_\mu = \frac{c_\mu}{\tan \phi_\mu}.
\]

where \(\phi_\mu\) is the interparticle friction angle. However, according to the original definition, this model cannot deal with cases in which the particle size is changed, because the unit of input parameter \(c_\mu\) is N.

![Figure 3.1 Linear contact bond model (Utili and Nova, 2008 [38]).](image-url)
In this study, this bond model is modified and new input parameter \( t'_\mu \) N/m is employed. The tensile strength, \( t_\mu \) N, is given by

\[
t_\mu = t'_\mu (d_i + d_j)
\]  
(3.2)

where \((d_i + d_j)\) is the conceptual particle contact width. In this interparticle bond model, the restriction of the tangential contact force is determined by the following equation.

\[
F_{\text{cont}}^t < \mu \left( \frac{|F_{\text{con}}^n|}{|F_{\text{con}}^t|} \right) F_{\text{cont}}^t
\]  
(3.3)

This form is a modified version of Equation (2.11). When the contact bond breaks, the friction force is calculated on the basis of Equation (2.11).

Here, two possibilities are given when the contact strength is exceeded, namely, the fragile behavior (F), in which the contact breaks and the failure surface decreases to the failure surface of the unbonded contact, and the ductile behavior (D), in which the contact remains intact and the strength remains unaltered. Utili and Nova concluded that DF (the shear contact behavior is ductile and the normal contact behavior is fragile) was the only model suitable for reproducing \( c \) and \( \phi \) soil. Thus, I also employ the DF failure condition.

### 3.2.2 Rolling friction model

DEM simulations using circular particles tend to overestimate the magnitude of particle rotations and they are not able to produce high shear strength values. Such values may be obtained when particle rotations are inhibited, but it is recognized that DEM simulations with no particle rotation should not be applied to general boundary value problems (Committee of Mechanics for Discrete Medium, 2010 [42]). To overcome this problem, there have been several methods proposed to model rolling resistance in DEM. One way is to directly introduce geometrical effect using non-spherical particles (Matsushima et al., 2009 [43]; Ferrelec and McDowell, 2010 [44]) or bonded spherical particles (Jiang et al., 2006 [40]). Another way is to introduce a model for rolling resistance at a contact of spherical particles for simplicity in its evaluation and less computational cost (Sakaguchi et al., 1993 [41]; Iwashita and Oda, 2000 [45]). The model used in this study is a rolling resistance as a function of contact normal force and a length parameter to represent the contact area as follows.

Figure 3.2 (a) illustrates two arbitrary shaped particles \( i \) and \( j \) are compressed by \( F_{n\text{cont}}^c \) forming a contact area. We modeled this scenario in two-dimensional DEM with circular particles introducing a contact radius \( a \) on the contact plane as in Figure 3.2 (b) to char-
Figure 3.2 Conceptual description of rolling friction model (Sakaguchi et al., 1993 [41]).
3.2. CONTACT MODELS

acterize contact area. In this figure, blue and yellow dots represent contact edge points. In actual particulate materials, non-zero contact area may be caused by contact deformation or by particle shape. However in this study, \( a \) is simply given as

\[
a = br,
\]

where \( b \) is constant and \( 0 \leq b \leq 1 \). Contact radius \( a \) is proportional to particle radius \( r \) regardless of contact deformation due to \( F_{n}^{\text{cont}} \). When particles \( i \) and \( j \) have different radii \( (r_i, r_j) \), \( a \) is determined by the smaller radius to satisfy the condition in Equation (3.4).

If particles have angular velocity in either direction as dotted blue or yellow curved arrow in Figure 3.2 (c), it is translated to the rolling (solid curved arrow) on the contact plane about either of the contact edge points with corresponding color. It should be noted here that the contact plane is geometrically determined from the position and the radii of two particles in contact. Hence, we assume that the contact plane and the edge points are instantaneously fixed for one time step in DEM computation regardless of the particle rotation direction. This means that the rolling of particles \( i \) and \( j \) do not affect each other no matter in which direction \( i \) and \( j \) rotate in this model.

On the other hand, the product of \( F_{n}^{\text{cont}} \) and \( a \) always acts as anti-rolling moment \( M_r \) depicted by red curved arrows in Figure 3.2 (d) regardless of the rolling direction. Let \( \omega' \) be angular velocity of a particle without considering the anti-rolling moment, then

\[
T^{\text{rol}} = -\text{sgn}(\omega')|F_{n}^{\text{con}}|a,
\]

where \( \text{sgn}(\cdot) \) is a signum function as below.

\[
\text{sgn}x = \begin{cases} 
1 & x > 0 \\
0 & x = 0 \\
-1 & x < 0.
\end{cases}
\]

If the contact bond is assigned, the anti-rolling moment is given as

\[
T^{\text{rol}} = -\text{sgn}(\omega')|F_{n}^{\text{con}}| + t_{\mu}|a,
\]

where \( t_{\mu} \) is the normal tension strength defined in the previous subsection.

Equations (3.5) and (3.7) suggest that the anti-rolling moment works to reduce the angular velocity of each individual particle, but it never enhance to produce negative angular velocity.
For this reason, if negative angular velocity is produced by anti-rolling moment, the direction of anti-rolling moment also flips to cancel the negative angular velocity and we set the angular velocity zero. Equations (3.5) and (3.6) also tell that the anti-rolling moment never produces self-rolling without external moment from static state. It only gives the angular velocity reduction as friction. Thus we call it "rolling friction". When the rolling friction is considered, Equation (2.2) is rewritten as follows.

\[ I \frac{d^2 \theta_p}{dt^2} = \sum T^{con} + \sum T^{rol}. \]  

(3.8)

As described in this subsection, this model requires only one additional parameter \( b \). Thus, it is easy to obtain corresponding relations between the packing properties and the rolling friction of the particles.

### 3.3 Parametric analyses

Two-dimensional simulations of direct shear tests using DEM are described in detail in this section. The input parameters for the particles are listed in Table 3.1. The values for normal and tangential constant contact stiffness, \( k_n \) and \( k_t \), employed in the simulations were the same as those utilized by Nakase (see Nakase et al., 2001 [46]), as the results obtained are not influenced by these parameters in quasi-static conditions (Kadau et al., 2006 [47]). Damping was controlled by a local damping coefficient (Cundall, 1987 [48]), but the damping force has no effect on the term of gravitational acceleration. Taking into consideration the fact that a large \( b \) value (\( b > 0.5 \)) stopped particle rotation in some preliminary simulations, the input values for \( b \) were determined. Then, given that the interparticle friction angle of natural sand is reported to be about 27 deg. (Mogami, 1969 [49]), 20, 25, and 30 (deg.) were determined as input values for \( \phi_\mu \).

The particle size distribution, featuring seven different particle radii, was used to generate the DEM specimens. The scale of this grain size distribution was 50 times more than that of Zhang et al. (Zhang et al., 2007 [50]), and the range of radii was the same as that of Utili and Nova (Utili and Nova, 2009 [38]). The bottom-to-top reconstruction algorithm (Poschel and Schwager, 2005 [24]) was used to generate the packing particles geometrically in a shear box, which is 315 mm wide and 140 mm high. The width of the shear box is 70 times larger than \( D_{max} = 4.5 \) mm on the basis of the criterion of the Japanese Geotechnical Society (The Japanese Geotechnical Society, 2000 [51]). The total number of particles employed in the
3.3. PARAMETRIC ANALYSES

The numerical specimen was 4,541.

After specimen generation, the material properties were set for all particles and the specimens were consolidated by moving the top wall downward for stress control. However, contact bond parameter, $t'_\mu$, were not assigned to particles in consolidation process so that contact bond cannot be broken before shear process. After stabilization, the particles at the top and bottom layer, which are colored in black in Figure 3.3, were fixed to the wall to model rough surface boundary. At the same time, bonds were formed at all particle contacts. Finally, the direct shear tests were performed with a constant shear rate of 1.25 % shear strain per second. This shear rate ensured that quasi-static condition were always present during testing (Wang and Gutierrez, 2010 [52]). The test arrangement is also shown in Figure 3.3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m)</td>
<td>2,400</td>
</tr>
<tr>
<td>Normal contact stiffness (N/m)</td>
<td>$4.00 \times 10^7$</td>
</tr>
<tr>
<td>Tangential contact stiffness (N/m)</td>
<td>$1.44 \times 10^7$</td>
</tr>
<tr>
<td>Local damping coefficient</td>
<td>0.2</td>
</tr>
<tr>
<td>Time step (sec.)</td>
<td>$5.0 \times 10^{-6}$</td>
</tr>
<tr>
<td>$\phi_\mu$, Inter-particle friction angle (deg.)</td>
<td>20, 25, 30</td>
</tr>
<tr>
<td>$b$, Rolling friction coefficient</td>
<td>0.05, 0.10, 0.20, 0.30</td>
</tr>
<tr>
<td>$t'_\mu$, Inter-particle bond strength (N/m)</td>
<td>0, 30, 60, 120</td>
</tr>
<tr>
<td>Normal stress (kN/m)</td>
<td>50, 100, 200</td>
</tr>
</tbody>
</table>

All boundaries were simulated by rigid walls having the same contact stiffness as the particles. The coefficient of friction between the vertical walls and the particles was set to zero to reproduce the ideal experimental conditions. A series of direct shear tests was performed with different contact parameters and under different levels of vertical pressure. A total of 144 tests were run. Shear stress and normal stress were calculated by the same method as that used by Zhang et al. (Zhang et al., 2007 [50]), and the horizontal displacement and the vertical displacement were evaluated at the boundaries. All boundaries were simulated by
3.4 Correlation between $c$, $\phi$ and DEM parameters

Figure 3.4 presents the numerical results obtained from direct shear tests in the case of $t'_\mu = 30$ (N/m), $\phi_\mu = 30$ (deg.) and $b = 0.2$. In Figure 3.4 (a), the obtained shear stresses against the applied normal stress are plotted. Internal friction angle $\phi$ and cohesion $c$ are derived from Mohr-Coulomb yield line. On the other hand, Figure 3.4 (b) and Figure 3.4 (c) show the evolution of the shear stress and the volumetric strain under shearing, respectively. From these figures, a peak shear strength and a positive dilatancy can be observed. These results indicate a typical shear behavior of densely packed sands (Zhang et al., 2007 [50]; Wang and Gutierrez, 2010 [52]). This trend was obtained in all cases.

A scatter plot matrix is then illustrated in Figure 3.5 in order to evaluate the influence of each micromechanical parameter ($t'_\mu$, $\phi'_\mu$, and $b$) on the macromechanical parameters ($c$ and $\phi$) obtained from the parametric analyses. The correlations between the input parameters and the macromechanical parameters are shown in the six boxes. In addition, relationships between DEM parameters and shear strength are listed in Table 3.2. Firstly, the influence of micromechanical parameter $t'_\mu$ on $c$ and $\phi$ are described in detail. From the relation between $t'_\mu$ and $c$ in Figure 3.5 and Table 3.2, it can be easily seen that there is a strong correlation between $t'_\mu$ and $c$, i.e., cohesion increases with an increasing bond parameter $t'_\mu$. On the contrary, in the $t'_\mu - \phi$ correlation, $t'_\mu$ has little effect on $\phi$. Such
3.4. CORRELATION BETWEEN \( C \), \( \phi \) AND DEM PARAMETERS

![Graphs showing correlation between \( C \), \( \phi \) and DEM parameters.](image)

Figure 3.4 A result of direct shear simulation. (a) Shear stress vs. normal stress. A solid line indicates the Mohr-Coulomb yield line. (b) Shear stress vs. shear displacement. (c) Vertical displacement vs. shear displacement.
correlations are in accordance with the numerical data reported by the other researcher (Utili and Nova, 2009 [38]) in the literature relative to biaxial tests where the cohesion of the particle assemblage is reported to increase with an increasing bond force at each contact point. Thus, it is possible to conclude that the behavior of cohesive geomaterials can be reproduced by employing new input parameter $t'_\mu$ whose unit is N/m.

![Figure 3.5](image)

**Figure 3.5** A scatter plot matrix between DEM parameters, $t'_\mu$, $\phi_\mu$, and $b$, and shear strength, $c$ and $\phi$.

Secondly, the influence of $\phi_\mu$ on the increase in global strength is focused. From the $\phi_\mu$-$c$ relation, it can be seen that $\phi_\mu$ contributes a little to cohesion $c$. Thus, the proposed model improve the U-N model, where the effect of $\phi_\mu$ on $c$ is large. It is thought that this is resulted from introducing the new bond parameter. In the $\phi_\mu$-$\phi$ relation, $\phi_\mu$ has a little contribution to internal friction angle $\phi$ in the range of the input value for $\phi_\mu$.

Finally, the correlations between $b$ and macromechanical parameters are described. The strong correlation between the internal friction angle and rolling friction coefficient $b$ is shown in Figure 3.5 and Table 3.2. This correlation agrees well with the numerical data.
reported in the literature relative to torsional shear tests (Nakase et al., 2001 [53]) and
biaxial tests (Yamamoto, 1997 [54]). Hence, it is possible to conclude that the interlocking
effect of grain shapes can be also expressed successfully when the rolling friction model is
used in combination with the proposed contact bond model. On the other hand, in the $b$-$c$
relationship, $b$ has some effect on $c$. This implies that the interlocking effect of grain shapes
influences not only $\phi$, but also $c$.

Table 3.2 Relationships between DEM parameters and shear strength

<table>
<thead>
<tr>
<th></th>
<th>$t'_{\mu} = 0$ (N/m)</th>
<th>$t'_{\mu} = 30$ (N/m)</th>
<th>$t'_{\mu} = 60$ (N/m)</th>
<th>$t'_{\mu} = 120$ (N/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_{\mu}$ = 20 (deg.)</td>
<td>$b = 0.05$</td>
<td>$b = 0.10$</td>
<td>$b = 0.20$</td>
<td>$b = 0.30$</td>
</tr>
<tr>
<td>$t'_{\mu}$</td>
<td>$c = 5.7$</td>
<td>$c = 7.19$</td>
<td>$c = 8.7$</td>
<td>$c = 10.60$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 26.8$</td>
<td>$\phi = 31.0$</td>
<td>$\phi = 35.9$</td>
<td>$\phi = 38.8$</td>
</tr>
<tr>
<td>$t'_{\mu}$ = 30 (N/m)</td>
<td>$c = 18.6$</td>
<td>$c = 21.5$</td>
<td>$c = 21.6$</td>
<td>$c = 25.2$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 26.5$</td>
<td>$\phi = 30.6$</td>
<td>$\phi = 37.0$</td>
<td>$\phi = 38.1$</td>
</tr>
<tr>
<td>$t'_{\mu}$ = 60 (N/m)</td>
<td>$c = 30.9$</td>
<td>$c = 37.3$</td>
<td>$c = 37.0$</td>
<td>$c = 39.5$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 26.0$</td>
<td>$\phi = 30.0$</td>
<td>$\phi = 35.9$</td>
<td>$\phi = 38.9$</td>
</tr>
<tr>
<td>$t'_{\mu}$ = 120 (N/m)</td>
<td>$c = 55.7$</td>
<td>$c = 65.4$</td>
<td>$c = 70.4$</td>
<td>$c = 67.5$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 25.7$</td>
<td>$\phi = 30.0$</td>
<td>$\phi = 35.1$</td>
<td>$\phi = 38.2$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$t'_{\mu}$ = 0 (N/m)</th>
<th>$t'_{\mu}$ = 30 (N/m)</th>
<th>$t'_{\mu}$ = 60 (N/m)</th>
<th>$t'_{\mu}$ = 120 (N/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_{\mu}$ = 30 (deg.)</td>
<td>$b = 0.05$</td>
<td>$b = 0.10$</td>
<td>$b = 0.20$</td>
<td>$b = 0.30$</td>
</tr>
<tr>
<td>$t'_{\mu}$</td>
<td>$c = 7.9$</td>
<td>$c = 10.3$</td>
<td>$c = 10.2$</td>
<td>$c = 11.5$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 27.8$</td>
<td>$\phi = 32.2$</td>
<td>$\phi = 39.4$</td>
<td>$\phi = 44.8$</td>
</tr>
<tr>
<td>$t'_{\mu}$ = 30 (N/m)</td>
<td>$c = 21.1$</td>
<td>$c = 23.7$</td>
<td>$c = 30.2$</td>
<td>$c = 31.1$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 27.5$</td>
<td>$\phi = 33.2$</td>
<td>$\phi = 38.0$</td>
<td>$\phi = 44.1$</td>
</tr>
<tr>
<td>$t'_{\mu}$ = 60 (N/m)</td>
<td>$c = 35.5$</td>
<td>$c = 39.3$</td>
<td>$c = 52.1$</td>
<td>$c = 54.6$</td>
</tr>
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<td>$\phi$</td>
<td>$\phi = 26.8$</td>
<td>$\phi = 32.6$</td>
<td>$\phi = 37.0$</td>
<td>$\phi = 43.9$</td>
</tr>
<tr>
<td>$t'_{\mu}$ = 120 (N/m)</td>
<td>$c = 61.1$</td>
<td>$c = 68.6$</td>
<td>$c = 92.6$</td>
<td>$c = 96.1$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi = 26.6$</td>
<td>$\phi = 32.2$</td>
<td>$\phi = 37.5$</td>
<td>$\phi = 44.7$</td>
</tr>
</tbody>
</table>

From what was shown up to this point, it can be concluded that, in the case of the same
$\phi_{\mu}$ value, cohesion can be mainly related to $t'_{\mu}$ and contributed a little by $b$, and the internal...
friction angle can depend greatly on $b$. These trends are also shown in Table 3.2, which gives the obtained values for $c$ and $\phi$ for various micromechanical parameters in the case of $\phi_{\mu} = 20$ and 25 deg.. Moreover, according to Table 3.2, a range of obtained $\phi$ values covers the values of geotechnical engineering interest, which is more than 35 deg..

Hence, it is possible to conclude that simple relationships between the DEM parameters ($t'_{\mu}$, $\phi_{\mu}$, and $b$) and $c$ and $\phi$ are obtained, and that the failure criteria of geomaterials can be satisfactorily reproduced by the 2-D DEM. In addition, due to the simple relationships, it is possible to easily derive the micromechanical parameters needed in other boundary value problems from the known macromechanical strength parameters. If a different particle size distribution were chosen, the obtained values could be different, but the obtained relationships between the micro- and the macromechanical strength parameters may be about the same (Cambou et al., 2000 [55]). Therefore, the relationships obtained can be used for determining suitable micromechanical strength parameters when a DEM analysis is applied to geotechnical engineering problems.

It should be noted here that a careful attention is required not to choose an improper input value. For the choice of the rolling friction, the value for $b$ should be less than 0.50 in order not to stop the rotation of the particle. A large $b$ value manages to give a unusually large macroscopic strength. In addition, for the choice of the sliding friction, the value for $\phi_{\mu}$ should be less than 45 deg. so as to prevent from the increase of errors of energy balance in a granular system.

### 3.5 Application example of proposed model

In this section, an application example of the proposed model in the three dimensions is briefly presented. The analysis object is the deformation behavior of the ripraps on embankment dams. The ripraps are discrete materials of construction; they are used as a cover to protect the surface of embankment dams from storm, rainfall and weathering. When a large earthquake occurs, it is usually observed that the ripraps and the dam body jointly deform at the same time (see Figure 3.6, Fukushima et al., 2011 [56]), but the mechanism of this process has not been well understood. To clarify this mechanism, it is important to account for the discrete nature of the materials. Moreover, it is also necessary to consider not only the interaction between the ripraps, but also the interaction between the ripraps and the dam body. For these reasons, both of ripraps and dam body are modeled by the rigid particles so that the large deformation can be reproduced.
3.5. APPLICATION EXAMPLE OF PROPOSED MODEL

Figure 3.6 A field research of the deformation of the ripraps on Mitsumori dam in Fukushima (Fukushima et al., 2011 [56]).

The full view of the simulation model before input of the seismic acceleration is illustrated in Figure 3.7. Each riprap is modeled by a clumped particle, which is rigidly connected by some spherical particles. The size of the riprap is 1.0\times1.0\times6.0 m. Each riprap is composing of 32 spherical particles. The details of the model of the clumped particle are described in Chapter 4. On the other hand, the soils comprising the dam body are modeled by using the proposed model, i.e., the assemblies of the spherical particles have rolling friction and tensile strength at the contacts with other particles.

In the process of construction of the dam body, gravitational packing was performed, and then unneeded soil particles were removed so that the objective configuration of the slope can be obtained. The ratio of the slope gradient is 1:3. In order not to produce non-uniform distribution of volume fraction in height, initial packing was conducted under three time frames. The number of the packed particles of the dam body is about 200,000. The macromechanical strength, i.e., the internal friction angle and cohesion, of the numerical soils was measured by several direct shear simulations. After that, the ripraps are arranged along the slope surface, as shown in Figure 3.7. The total number of the ripraps is 2,100. The ripraps positioned at the upper and lower end of the slope are fixed with assuming as a non-slip concrete. Under above conditions, repeated seismic analyses are performed with different contact parameters, packing state, seismic magnitude. In these analyses, the parallelized algorithm for the rigid particle simulations on the sheared-memory multiprocessors (Nishiura and Sakaguchi, 2011 [23]) reported in Chapter 2 was employed so that large-scale analyses...
Figure 3.7  A snapshot of ripraps before input of seismic acceleration.
3.5. APPLICATION EXAMPLE OF PROPOSED MODEL

in three dimensions could be carried out quickly.

![Figure 3.8](image)

Figure 3.8  Seismic behavior of ripraps on the embankment dams (a) A snapshot of ripraps after input of seismic acceleration. (b) Cross-sectional view on y-z plane. (c) Time evolution of the vertical displacement $dz$ for each ripraps.

In Figure 3.8, one of the results of the analyses is reported. This is the case where the frequency is 2 Hz, the amplitude is 800 gal and the loading time is 54 s. Figure 3.8 (a) shows a snapshot of ripraps after input of seismic acceleration and Figure 3.8 (b) shows the cross sectional view of the dam body at the time of 54 s. From these figures, it can be observed that uplift occurs in the lower part of the slope and the settlement occurs in the upper part.
of the slope. This deformation induces the empty space at the upper non-slip concrete. In addition, the formation of the uplift at the bottom is linear in $x$ direction, as shown in Figure 3.8 (a).

Figure 3.8 (c) shows the evolution of the vertical displacement of the ripraps $dz$ m in a cross-section as a function of the time. The value for $y$ m in this figure indicates $y$ position of the mass center of the ripraps. These plots are at 18 s, 36 s and 54 s. It can also be seen in Figure 3.8 (c) that the uplift and the settlement increase in the lower part and in the upper part, respectively. These features obtained in the simulations are in good agreement with the actual seismic behavior observed in the field research (Fukushima et al., 2011 [56]), as shown in Figure 3.6. If a continuum approach is employed, it is difficult to reproduce such a large deformation behavior.

### 3.6 Conclusions

This study presented a simple discrete element modeling for geomaterials so that geotechnical engineering problems may be studied by DEM with fewer parameters. The modified versions of the linear contact model and the rolling friction model are newly introduced into the contact logic between the particles. Although the simple, failure criteria for geomaterials, that is, the $c$ and $\phi$ values of geotechnical engineering, are satisfactorily obtained by adding only two parameters to the conventional contact model in the 2-D DEM. Above discussions is limited in the two dimensions, but it is easy to extend the proposed model to the three dimensional condition. Moreover, the relationships between the DEM parameters and the macromechanical parameters are so simple that suitable DEM parameters can be easily determined from known $c$ and $\phi$ values.

In addition to the validation of the proposed model, 3-D discrete element simulations were performed under seismic loads in order to investigate the deformation behaviour of the ripraps on the earth dams. As a result of these analyses, the actual seismic behaviour of the ripraps on the dam body was successfully reproduced by the discontinuous approach. In future work, I am going to perform further parametric study so that the deformation mode can be predicted in advance from the slope inclination of the dam, $(c, \phi)$ of the dam body, the shape and the arrangement of the ripraps and the magnitude of the seismic load. Applications of the proposed simple contact model to other earth constructions are also the future works.
4 Effects of block shape on seismic behavior of masonry retaining wall: Numerical investigation by discrete element modeling

4.1 Introduction

Dry-stone masonry retaining walls represent a traditional form of construction which can be found all over the world, i.e., in Asia, Africa, North and Latin America, Europe and Australia (Colas et al., 2008 [57]). Such walls are composed of a lot of stones which are interlocked with each other without mortar. Their structures are very simple, but flexible and durable enough to withstand several major earthquakes over the years. Low environmental impact and economic efficiency are also advantages of dry-stone walls. However, there is still a lack of theoretical knowledge about the dry-stone construction. For this reason, although there has been an increase in interest in dry-stone construction even in recent years, it is difficult to encourage new construction projects from the scientific viewpoint. It is important, therefore, to investigate the detailed behavior of masonry walls and to give a mechanical explanation for the stability of the walls.

The stability of a stone wall depends on several factors, such as the material properties, the backfill conditions, the block arrangement, the block shapes and so on. To clarify this complex mechanism, researchers have employed various approaches, such as centrifuge model experiments (Yoshida et al., 2007 [58], 2009 [59]), real-scale tests (Yamamoto et al., 2010 [60]), the continuum numerical model (Dewoolkar et al., 2009 [61]; Colas et al., 2010 [62]), the discontinuous numerical model (Claxton et al., 2005 [63]; Kamai and Hatzor, 2008 [64]; Yoshida et al., 2007 [58]) and the homogenization theory (Mathieu et al., 2010 [65]). Although such works have produced many results, the contribution of each individual block to the overall stability of the wall has not been well discussed due to the difficulty of its quantitative measurement. There are some early efforts using numerical simulations that include the effect of the block shape of the masonry structure in two dimensions (Kamai and Haltzor, 2008 [64]; Colas et al., 2008 [57]) and in three dimensions (Furukawa et al., 2011 [66]). However, the shape effect of the blocks on the deformation behavior of the wall still has not sufficiently been discussed both from the experimental and the numerical
standpoints.

To overcome this difficulty, we firstly performed centrifuge model tests on the blocks of a castle wall to investigate its overall behavior under seismic loads using two differently shaped blocks, cubic-shaped and wedge-shaped. Then, we conducted a numerical simulation to mimic the centrifuge model tests for a detailed analysis using the three-dimensional discrete element method. The advantage of DEM as a numerical tool is its capability to simulate large deformations, which is difficult to do with a continuum-based model such as FEM.

In both the centrifuge experiments and the numerical model, the failure mode of the wall greatly differed between the two cases. The toppling type of deformation occurred in the cuboid blocks, while the swelling-like type of deformation occurred in the wedge-shaped blocks. In addition, the overall resistivity against seismic loading was found to be higher in the wedge-shaped blocks than in the cuboid blocks. Such trends obtained from the simulation agree well with those obtained from the experiments. These results indicate that it is important to take account of block shapes when masonry structures are designed from the perspective of discontinuous mechanics. Then, we investigated how each individual block shape contributes to the stability of the masonry wall.

Chapter 4 is organized as follows. In Section 4.2, I firstly highlight the centrifuge model tests and the obtained experimental results. Details of the simulation models are given in Section 4.3, while the results and a discussion are given in Section 4.4. A summary is presented in Section 4.5.

4.2 Centrifuge model test

4.2.1 Experimental method

Several centrifuge model tests at a scale of 1:33 were performed with different block shapes for the masonry wall using the centrifuge facility at Shimizu Institute of Technology (Yoshida et al, 2007 [58], 2009 [59]). Herein, two experiments are discussed; one is the case of the cuboid-shaped blocks and the other is the case of the wedge-shaped blocks. Herein, two experiments are discussed; one is the case of the cubic-shaped blocks and another is the case of the wedge-shaped blocks. Our study refers to the actual masonry construction which is found in Tokyo Imperial Palace, in other words, we model the masonry wall located at Nakano-mon Gate and Yamazato-mon Gate for the cubic-shaped block and the wedge-shaped block, respectively. The sizes of the model were determined by the scaling laws (Taler RN, 1995 [67]) in accordance with the centrifuge acceleration of 33 g, for which g is
Figure 4.1  Pictures of the centrifuge model experiment. (a) Centrifuge machine (Yoshida et al., 2007 [58]). (b) Centrifuge earth tank. (c) Model configuration in the centrifuge earth tank in the case of the wedge shaped block.
the magnitude of gravitational acceleration. Thus, the stone blocks and cobble stones used in the experiment are about one-thirty third size of the real scale. The height of the wall used in the model experiment is also reproduced by referring to the actual masonry construction, and we have determined that the height of the wall is composed of the five blocks. On the other hand, the width of the wall is determined in order to satisfactorily evaluate the three dimensional deformation through preliminary experiments, and then the aspect ratio of the wall is fixed for simplicity. Photograph and sketches of the configurations of the centrifuge model are shown in Figure 4.1 and 4.2. In Figure 4.2, the system size in the equivalent full-scale field situation is presented in addition to that in the experimental model.

The full view of the centrifuge machine is given in Figure 4.1 (a). The centrifuge earth tank, shown in Figure 4.1 (b), is 796 mm in width, 440 mm in depth and 500 mm in height. The directions of the width, the depth and the height are given in Figure 4.1 (c). In this tank, the centrifuge model consists of stone blocks, cobble stones for the backfill and surrounding soils, as shown in Figures 4.1 (c) and 4.2 (a). Such wall structures are commonly found in Japanese castles (Tanaka et al., 1998 [68]). Each stone block is made of granite. The area behind the pile of stones is filled with coarse aggregates which are smaller than 10 mm in size. It should be noted here that, in traditional method of construction of the Japanese castle, the layer of the cobble stones are artificially-compacted densely in a careful manner (Tanaka et al., 1998 [68]). Therefore, in the model experiment, these coarse aggregates for modeling the cobble stones are also compacted densely. The internal friction angle of the backfill is more than 40 deg. in a laboratory test. Since the size of the coarse aggregate is much larger than that of the sand particle, the shear strength of the former one seems to be larger than that of the latter one in the same void ratio. Then, the area of the surrounding soils is filled with Toyoura sand whose particle size distribution has an average particle diameter of \( D_{50} = 0.2 \) mm, and is compacted densely. The side walls of the tank are made of acrylic so that the inside of the container will be visible.

The arrangement of the stone blocks from the front view in the depth direction is depicted in Figure 4.2 (b). In the cuboid case, as illustrated in Figures 4.2 (b) and (c), two different sizes of blocks are employed and the masonry wall is composed of 25 blocks. The number of large blocks is 20 and the number of small blocks is 5. In the wedge-shaped case, on the other hand, there is only one size of block and the masonry wall is composed of 45 blocks. It should be noted here that the detailed displacement of each stone block during the centrifuge tests was not observed in this study. This is because it was difficult to equip measurement devices inside the model when the large deformation and the failure of the
4.2. CENTRIFUGE MODEL TEST

Figure 4.2 Sketches of model configuration for cuboid-shaped stones and wedge-shape stones. (a) Side view of models. (b) Front view of configurations of stone blocks. (c) Sizes of stone blocks.
wall were the main objects of this investigation.

In the preliminary experiments, in order to find the threshold value for the amplitude of the seismic wave just breaking the wall, triangular impulses of 0.5 s with a frequency of 60 Hz (i.e., about 2 Hz at 1 g) and with 30 waves were applied by gradually increasing the wave amplitude from 2,000 gal (i.e., about 60 gal at 1 g). As a result of the repeated experiments, it was confirmed that the threshold value in the case of the cuboid block was 6,000 gal (i.e., about 200 gal at 1 g) and that in the case of the wedge-shaped block was 11,000 gal (i.e., about 370 gal at 1 g). Thus, triangular acceleration impulses with the above amplitudes were applied repeatedly to the masonry wall until failure was reached.

![Figure 4.3 Snapshots of model experiment at initial state and at collapsing state. (a) Cuboid blocks. (b) Wedge-shaped blocks.](image-url)
4.2. CENTRIFUGE MODEL TEST

4.2.2 Experimental result

In both cases, the wall reached failure in the middle of the third seismic acceleration. This indicates that the masonry structure of the wedge-shaped blocks is stronger than that of the cuboid blocks. In fact, in a separate experiment, the wall with the wedge-shaped blocks was able to withstand three times the seismic load of 6,000 gal, which lead to collapse in the case of the cuboid blocks.

Furthermore, the failure modes of the walls are completely different from each other, as illustrated in Figure 4.3, which shows snapshots of the initial state and the collapsing state of the walls viewed from directly above. This collapsing state occurs in the middle of the third seismic acceleration. In the case of the cuboid blocks, it is observed that each separate block moves as one under seismic loads, that is, toppling failure occurs. A cross-section view of this failure mode, observed through the acrylic board, is depicted in Figure 4.4 (a).

In the case of the wedge-shaped blocks, on the other hand, a considerably different failure mode is observed in both height and width directions. Unlike the case of the cuboid blocks, the stone blocks do not move as one, but the displacements of the blocks positioned on the second step from the top exceed those of the blocks positioned on the other steps in the height direction. The feature of this failure mode, from a lateral view, is illustrated in Figure 4.4 (b). Additionally, an arch-shaped configuration is observed in the width direction and large deformation occurs in the middle.

During the tests, the deformation of the surrounding soils was very small and contributed little to the collapse of the wall. In other words, the failure of the wall was mainly due to the interaction between the stone blocks and the backfill. In fact, this trend has also been reported in field research (Murakami et al., 2012 [69]), where the stone walls of castles in Japan, damaged by a large earthquake, were investigated, and the causes of the collapse of the wall were discussed.

As described above, two major differences between the cuboid case and the wedge-shaped case have been obtained. Firstly, the stability of the wall comprised of the wedge-shaped blocks is higher than that of the wall comprised of the cuboid blocks. Secondly, toppling deformation occurs in the wall of cuboid blocks, while swelling-like deformation occurs in the wall of wedge-shaped blocks.
4.3 Discrete element simulation

A numerical simulation to mimic the centrifuge tests was performed in order to investigate the shape effect of the blocks at each individual block scale and to quantitatively understand the findings of the experiments. For the numerical approach, I chose the discrete element method to reproduce the behavior of the inner discrete structures with large deformation observed in the centrifuge model tests, since this behavior is difficult to reproduce by continuum approaches, such as the finite element method.

I performed this numerical study using my in-house code based on the conventional DEM, as described in Chapter 2. A contact force $F_{\text{con}}$ is calculated by the linear-based contact law in this study, i.e., the contact springs are assumed to be linear and $k_n / k_t = 4$ ($k_n = 1.0 \times 10^8$ N/m, $k_t = 2.5 \times 10^7$ N/m), where $k_n$ is the normal spring constant and $k_t$ is the shear spring constant, respectively. The values for the normal and the tangential viscous damping, for inhibiting the numerical oscillation, are determined to be small enough so as not to make a significant contribution of total energy dissipation to the granular system.

4.3.1 Stone blocks

The stone blocks comprising the masonry wall were modeled by the clumping of spherical particles (e.g. Itasca, 2005 [70]) to form cuboids and wedges, as illustrated in Figure 4.5. In my model, regardless of the forces acting upon them, the blocks will not break apart. Each of these clumped particles acts as a rigid body. Thus, the translational and rotational
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Figure 4.5 3D numerical model of stone blocks. (a) Small and large cuboid blocks. (b) Wedge-shaped block.

The equations of motion for block $b$ are described as follows:

$$m_b \frac{d^2 x_b}{dt^2} = m_b g + \sum_{p=1}^{N_p} (\tilde{F}^{\text{con}}_p + F^{\text{con}}_p),$$  \hspace{1cm} (4.1)

$$I_b \frac{d^2 \theta_b}{dt^2} = \sum_{p=1}^{N_p} (\tilde{T}^{\text{con}}_p + (x_p - x_b) \times F^{\text{con}}_p + T^{\text{con}}_p),$$ \hspace{1cm} (4.2)

where $x_b$ and $\theta_b$ are the translational and rotational displacement vectors, respectively, $m_b$ is the clump particle mass, $I_b$ is the clump particle moment of inertia, $N_p$ is the number of particles comprising the block, $F^{\text{con}}_p$ is the resultant force acting on particle $p$, $\tilde{F}^{\text{con}}_p$ is the externally applied force vector acting on particle $p$, $T^{\text{con}}_p$ is the resultant moment acting on particle $p$, $\tilde{T}^{\text{con}}_p$ is the externally applied moment acting on particle $p$, and $x_p$ and $x_b$ are the centroid position vectors of particle $p$ and block $b$, respectively. The moment of inertia $I_b$ at each time step is updated by the quaternion method (Pöschel and Schwager, 2004 [24]).

The large cuboid blocks are composed of 706 particles, the small cuboid blocks are composed of 386 particles and the wedge-shaped blocks are composed of 290 particles. The size of the blocks in the simulation is thirty-three times larger than that in the model experiments, which corresponds to the scale factor of the centrifuge tests. The density of the stone blocks is 2650 kg/m$^3$. The friction coefficient between the stone blocks is 0.6 (see Kasa et al., 2008 [71]).
4.3.2 Cobble stones

The cobble stones for the backfill are modeled by mixing single spherical particles with two rigidly connected particles (see Figures 4.6 (a) and (b)) so that the interlocking effect due to the shape of the cobble stones can be reproduced. In this study, I call these connected particles ”pair particles” and the normal spherical particle a ”single particle”. The pair particles are also modeled by the clumped spherical particles. The motion of the pair particles is calculated in the same manner as Equations (4.1) and (4.2).

In the previous research, using the direct shear simulation of granular assemblies, my co-worker showed that the internal friction angle of the specimen is increased by increasing the ratio of the pair particles (Yoshida, 2005 [72]). The ratio of the pair particles $\varepsilon_{\text{pair}}$ is defined as follows:

$$\varepsilon_{\text{pair}} = \frac{N_{\text{pair}}}{N_{\text{single}}},$$

(4.3)

where $N_{\text{pair}}$ is the number of pair particles and $N_{\text{single}}$ is the number of single particles. Through the introduction of pair particles, the internal friction angle can be obtained within the range of geotechnical engineering interest (more than 30 deg.).

The particles for the cobble stones have a particle size distribution of $D_{\text{max}}/D_{\text{min}} = 2$, $D_{\text{max}} = 0.30$ m and $D_{\text{min}} = 0.15$ m. The density of the cobble stones and the friction coefficient between the cobble stones are the same as for the stone blocks.

4.3.3 Surrounding soil

The deformation of the surrounding soils in the model tests was very small and contributed little to the collapse of the wall, as described in Section 4.2. Thus, for the sake of simplicity, a fixed plane boundary is substituted for the surrounding soils. The surrounding soils are assumed to have enough strength so as not to deform by the seismic loads during the nu-
numerical tests. This simple modeling has the advantages of being able to reduce the number of particles used in the simulation and requiring lower computational costs. The friction coefficient of the soil boundary between the Toyoura sand and the stone blocks or the cobble stones is 0.5 (see Katagiri, 2009 [73]).

Figure 4.7 3D discrete element model of masonry structure at initial state. (a) Cuboid block. (b) Wedge-shaped block.
4.3.4 Computational model setup

In the first process of the computational model setup, the arranged stone blocks are fixed and the spherical particles are generated in an area behind the stone wall. In this generation process, the position of each particle is chosen randomly one by one and placed one by one in such a way that there is no overlapping with the particles which have already been placed. The number of particles for the layer of cobble stones is 15,000.

After specimen generation, the material properties are set for all particles and the simulations are performed by dropping the particles into the bottom of a container under gravity. The values for the inter-particle friction coefficients during packing, $\mu_{\text{pack}}$, are in the range of 0.0 to 0.6. By using different values for $\mu_{\text{pack}}$, different packing conditions can be obtained (Fukumoto et al., 2013 [74]) for the parametric seismic analysis. This packing process is run until the void ratio of the backfill becomes constant. The simulation is run with a time step of $1.0 \times 10^{-6}$ s.

At the end of the packing process, some contacts between single particles are chosen randomly and pair particles are generated with arbitrary values for $\varepsilon_{\text{pair}}$ in the range of 0.0 to 3.0. After the generation of the pair particles, the stone blocks are permitted to move freely. The simulation model setup is over when the granular system reaches the steady state. I judge this state by the same criterion as that used in the packing process. The void ratio at this state is defined as $\varepsilon_{\text{void}}$. Figures 4.7 (a) and (b) show the initial states of the simulation model of the masonry structure in the case of the cuboid blocks and the wedge-shaped blocks, respectively.

The value for the sliding friction of the side walls made of acrylic is 0.25. All of the walls, including the soil boundaries, are fixed and do not move throughout the simulation.

4.3.5 Seismic analysis

By using the experimental results, the same seismic waves, which have been converted from the value at 33 g to the value at 1 g, are applied to the simulation model. That is, triangular acceleration impulses of 15 s with a frequency of 2 Hz, 30 waves and 200 gal, are used for the case of the cuboid blocks, while impulses with a frequency of 2 Hz, 30 waves and 370 gal are used for the case of the wedge-shaped blocks. These seismic loads are repeatedly entered into the masonry system until the wall reaches failure. In this seismic analysis, various values for $\varepsilon_{\text{pair}}$ and $\varepsilon_{\text{void}}$ are chosen in order to find a suitable condition for the backfill.
4.4 RESULTS AND DISCUSSION

The parametric seismic analysis shows that $\varepsilon_{\text{pair}}=2.5$ and $\varepsilon_{\text{void}}=0.75$ are suitable parameters which result in a good correlation with the centrifuge model tests in regard to the amount of seismic loads until failure. In both cases, when these parameters are employed, the wall reaches failure in the middle of the third seismic acceleration in the same manner as in the centrifuge tests.

Here, when smaller values for $\varepsilon_{\text{pair}}$ and $\varepsilon_{\text{void}}$ are employed, earlier failure occurs in both cases. On the other hand, when larger values for the parameters of the backfill are used, the wall can resist three times the seismic loads in both cases. Thus, the strength of the backfill can be controlled by varying the values for $\varepsilon_{\text{pair}}$ and $\varepsilon_{\text{void}}$.

To assess the strength of the backfill with these parameters, separate direct shear simulations are conducted to obtain the internal friction angle. According to the simulations, the internal friction angle is about $40^\circ$. This strength value is appropriate for the backfill filled with coarse aggregates (Yamada et al., 2009 [75]). Note that further results with a variation in $\varepsilon_{\text{pair}}$ and $\varepsilon_{\text{void}}$ are not discussed in detail here because the main focus of this chapter is to compare the experiments and the simulations from the perspective of the effects of the block shape. Only the case where $\varepsilon_{\text{pair}}=2.5$ and $\varepsilon_{\text{void}}=0.75$ is addressed in the following discussion.

Therefore, when the appropriate backfill condition have been chosen, the discrete element simulations can prove quantitative correspondence with the centrifuge model tests with respect to the amount of seismic loads until failure. Moreover, in terms of the seismic stability
and the failure mode resulting from the block shape, there is also a close numerical agreement with the experimental results, as will be described in the subsequent subsections.

Figure 4.9 Snapshots of simulation viewed from directly above at initial state and at collapsing state. The displacement of the particles of the backfill, colored in blue, is more than a half of the maximum displacement. (a) Cuboid block at 30 s. (b) Wedge-shaped block at 40 s.

4.4.1 Strength of structures

Compared to the wall of the cuboid blocks, the wall of the wedge-shaped blocks withstands larger seismic loads. This is the same as the result of the model experiments. This trend for the strength of the structure due to the block shape is observed in other parameters of the backfill $\varepsilon_{\text{pair}}$ and $\varepsilon_{\text{void}}$.

Here, in the case of the cuboid blocks, the total mass of the wall is $1.2 \times 10^5$ kg and the surface area contacting the backfill is $4.5 \times 10^2$ m$^2$. On the other hand, in the case of the wedge-shaped blocks, the total mass of the wall is $9.9 \times 10^4$ kg and the surface area contacting the backfill is $1.23 \times 10^2$ m$^2$. In other words, although the total mass of the wall of the wedge-shaped blocks is smaller than that of the wall of the cuboid blocks, the surface
area contacting the backfill of the former one is larger than that of the latter one. The surface area contacting the backfill per unit mass is $3.75 \times 10^{-4} \text{ m}^2/\text{kg}$ for the cuboid case and $1.24 \times 10^{-3} \text{ m}^2/\text{kg}$ for the wedge-shaped case. The value for the wedge-shaped case is three times larger than that for the cuboid case. This feature is in common with geosynthetic reinforced soil (GRS) retaining walls with geogrids (Miyata et al., 2012 [76]), which show high stability by means of generating high friction with the backfill. Therefore, it can be assumed that the difference in stability comes from the difference in the formation of the friction generation between the stone blocks and the backfill.

![Image of simulation snapshots](image)

**Figure 4.10** Snapshots of simulation from lateral view at initial state and at collapsing state. The displacement of the particles of the backfill, colored in blue, is more than a half of the maximum displacement. (a) Cuboid block at 30 s. (b) Wedge-shaped block at 40 s.

### 4.4.2 Deformation mode

Figure 4.8 shows the masonry walls in a state of collapse in the case of the cuboid block and the wedge-shaped block. In this figure, the snapshot for the former case is at the time of 30 s and that for the latter case is at the time of 40 s. Comparing the two snapshots, it is apparent that the failure modes are considerably different from each other. For the cuboid block, all of the blocks comprising the wall move as one and large rotational deformation is observed. On the other hand, for the wedge-shaped block, large swelling-like deformation
The failure modes viewed from directly above are shown in Figure 4.9, where the displacement of the particles of the backfill, colored in blue, is more than a half of the maximum displacement. In the cuboid block, it is also observed as viewed from above that the stone blocks move as one. In the wedge-shaped block, the displacements of the blocks positioned at the second step from the top exceed that of the blocks positioned at other steps in the height direction. Additionally, in the width direction, an arch-shaped configuration is observed, that is, the large deformation of the stone blocks occurs in the middle. Both snapshots obtained from the simulation are qualitatively in agreement with the failure mode in the model experiment, as illustrated in Figure 4.3.

Furthermore, from Figure 4.9, the distribution of cobble particles with large displacements is also different between the two cases. In the cuboid case, the cobble stones with large displacements are uniformly distributed in the width direction. In the wedge-shaped case, on the other hand, the area of the large deformation of the backfill is concentrated in the middle of the width. These distributions correspond to the positions of the stone blocks with large displacements. Therefore, it is thought that the difference in the deformation of the wall is caused by the difference in the deformation of the backfill.

Figure 4.10 shows the cross-section views in a state of collapse. These cross-sectional surfaces in the figure are cut off in \( y = 4.5 \) m and \( y = 8.5 \) m of the width direction. The particles of the backfill, colored in blue, indicate the same meaning as that in Figure 4.9. It can be clearly seen in Figure 4.10(a) that toppling failure occurs in the case of the cuboid block. In addition, from this figure, a slipped region and settlement of the upper right area of the backfill are observed in both of \( y = 4.5 \) m and \( y = 8.5 \) m. The settlement of the backfill associated with the deformation of the masonry wall is also reported in the real-scale tests with the shaking table (Yamamoto et al., 2008 [60]).

On the other hand, as shown in Figure 4.10 (b), a different failure mode is observed in the case of the wedge-shaped block. The feature of this failure mode is that the middle blocks in the height direction exceed in deformation amount. Settlement of the upper right area of the backfill is also observed in the wedge-shaped case. However, unlike the cuboid case, the amount of cobble stones with large displacement in \( y = 4.5 \) m is larger than that in \( y = 8.5 \) m. Considering both Figures 4.9 (b) and 10 (b), the deformation mode of the backfill is different from the position of the cross-sectional surface.

The evolution of the residual horizontal displacement of each stone block, as a function of elapsed time (from 5 s to 30 s) in the cuboid case, is showed in Figure 4.11. Five blocks of
4.4. RESULTS AND DISCUSSION

Figure 4.11  Evolution of residual horizontal displacement of each stone block as function of elapsed time in cuboid case. (a) Stones positioned at middle in width. (b) Stones positioned at wall vicinity.

Figure 4.12  Evolution of residual horizontal displacement of each stone block as function of elapsed time in wedge-shaped case. (a) Stones positioned at middle in width. (b) Stones positioned at wall vicinity.
the middle row in the width direction are plotted in Figure 4.11 (a) and five blocks against
the side wall in the width direction are plotted in Figure 4.11 (b). Comparing Figures 4.11
(a) and (b), it is seen that the magnitude of toppling is not different from the positions in
the width direction. The displacement of the blocks is roughly proportional to the height.
Furthermore, both of the figures indicate that the deformation mode of the cuboid case is
unchanged with elapsed time during the seismic analysis.

On the other hand, the evolution of residual horizontal displacement (from 5 s to 40 s) in
the wedge-shaped case is illustrated in Figure 4.12. Just the same as in Figure 4.11, both
of the displacements of the middle row and the wall vicinity row in the width direction are
shown. From this figure, the horizontal displacement of the blocks positioned at the second
and third steps from the top are larger than the other three blocks in the height direction.
That is, large deformation occurs at about the middle of the wall height. Additionally, the
differences in displacements in the height direction increase with increases in elapsed time.
This trend is observed in both Figures 4.12 (a) and (b).

Compared with Figures 4.12 (a) and (b), however, the value for the residual displacement of
the blocks in the middle row is larger than that of the blocks along the wall. This suggests
that large deformation occurs in the middle of the width direction in the wedge-shaped
case. This obtained numerical data corresponds to the arch-shaped configuration which is
obtained in the model experiment, as shown in Figure 4.3 (b). This deformation mode
including the width direction is characteristic of three dimensions and cannot be obtained
by a two-dimensional simulation.

Finally, in order to easily compare the deformation mode, 3-D plots of the residual dis-
placement for each case are showed in Figures 4.13 (a) and (b). The displacement of the
cuboid blocks is at the time of 30 s and that of the wedge-shaped blocks is at the time of 40
s. From the figures, the three-dimensional difference in the deformation mode obtained in
the experiment is confirmed numerically. It is validated from our discrete element approach
that the block shapes comprising the wall have a great influence on the deformation behavior
of the wall.

4.5 Conclusions and future work

In Chapter 4, I have investigated the shape effect of the blocks comprising a dry-stone
masonry retaining wall under seismic loading; one was a cubic-shaped block and the other
was a wedge-shaped block. The detailed mechanisms of the seismic resistant behavior were
investigated through the discrete element modeling which can successfully reproduce the overall behavior of masonry structures found in the physical experiments.

For both the physical experiments and the numerical simulations, the seismic resistivity was found to be higher in the wall of wedge-shaped blocks than in the wall of cuboid blocks, although the total mass was larger for the wall of cuboid blocks. This was due to the effect of the surface area contacting the backfill per unit mass. It can be assumed that the difference in stability is due to the difference in the formation of friction generation between the stone blocks and the backfill.

The deformation mode of the wall was found to be different between the two block shapes; toppling deformation occurred in the cuboid blocks, while swelling-like deformation occurred in the wedge-shaped blocks. In addition, the deformation mode of the backfill behind the stone wall was also different in each case. In particular, in the wedge-shaped case, the deformation of both the wall and the backfill is characteristic of three dimensions, that is, large deformation is concentrated in the middle of the width direction. Such deformation modes cannot be reproduced by a two-dimensional simulation.

From these results, it can be concluded that when masonry structures are simulated and designed, it is important to take account of the block shapes from the perspective of discontinuous mechanics. Furthermore, it is necessary to consider the three-dimensional deformation so that a quantitative prediction of the seismic behavior can be achieved. It should be noted here that these conclusions are based on limited conditions, that is, the size and the aspect

\[ \text{Figure 4.13  Three-dimensional plot of residual horizontal displacement of each stone block.} \]

(a) Cuboid block at 30 s. (b) Wedge-shaped block at 40 s.
ratio of the retaining wall are fixed in this study. More qualitative modeling for the masonry system is to be investigated under different conditions in future work. Additionally, I plan to focus attention on the friction formation between the stone blocks and the backfills, and to give a detailed scientific exploration to the mechanisms of the stability of the masonry wall.
The role of rolling friction in granular packing

5.1 Introduction

The dense packing of granular materials has been the focus of intense research from both numerical and experimental approaches in physics, engineering and other areas of research for decades (Jaeger et al., 1996 [1]; Goldenberg and Goldhirch, 2008 [77]; Roux, 2000 [78]; Makse et al., 2000 [79]; Mueth et al., 1998 [80]; Tighe et al., 2010 [81]; Matuttis et al., 2000 [82]; Rothenberg and Bathurst, 1992 [83]; Guises et al., 2009 [84]). Even today, however, this research topic continues to perplex physicists and engineers. It is especially important to obtain a comprehensive understanding of the properties of the initial packing, which depend on the packing conditions, because these properties are essential to the rheology of granular media.

It should be noted that such particles, consisting of granular materials, are used in many industrial fields and often have irregular shapes. Even if a particle is almost spherical in form, its surface has irregularities or asperities. Due to the features of these particles, rolling at the contacts between the particles can be resisted. Previous experimental and numerical studies have shown that the particle shape strongly affects the quasi-static mechanical behavior of granular materials (Matuttis et al., 2000 [82]; Rothenberg and Bathurst, 1992 [83]; Guises et al., 2009 [84]; Lu and McDowell, 2007 [85]; Matsushima and Chang, 2011 [86]). Therefore, it is important to take account of the effects of the rolling resistance due to particle shape when the packing properties of granular materials are discussed. However, while the importance of the rolling resistance under shear is widely accepted, the effects of the rolling resistance under packing have not been systematically investigated.

In this chapter, the packing of compressible granular assemblies with rolling friction is investigated by means of 2-D DEM (Cundall and Strack, 1979 [2]). Rolling friction means a mechanical property which produces a resisting moment to the rolling at each contact. In this study, I employ circular particles to simplify the investigation process. In order to reproduce the rolling resistance with circular particles, the rolling friction model based on a relative rotation, which introduces a contact law to the particle-particle contacts, is employed. Then, two-dimensional granular samples are deposited under gravity and compressed in a rectangular box by vertical pressure. They are analyzed at the steady state with various values for the rolling friction parameter.
Firstly, I describe that the influence of the rolling resistance on the volume fraction and the average coordination number. In addition, I investigate the distribution of contact angles, which give an indication of the fabric anisotropy. Next, I focus on the effects of the rolling resistance on the lateral stress response to a vertical stress applied on the granular system in terms of both macroscopic and microstructural properties. I employ the coefficient of earth pressure at rest as the macroscopic parameter. At the same time, I investigate the angular distribution of normal contact forces from the aspect of the microstructural properties. The relationship between these two properties of stress transmission is also described. Finally, I show the effect of the rolling resistance on the homogeneity of the force distribution in granular media.

Chapter 6 is organized as follows. In Section 6.2, I firstly describe the numerical method, the system characteristics, and the loading parameters. Details of the results of the numerical simulations and discussions are given in Section 6.3. A summary is presented in Section 6.4.

5.2 Simulation details

5.2.1 Rolling friction based on relative rotation

Several methods have been proposed to model the rolling resistance in DEM (Matuttis et al., 2000 [82]; Rothenberg and Bathurst, 1992 [83]; Guises et al., 2009 [84]; Lu and McDowell, 2007 [85]; Matsushima and Chang, 2011 [86]; Tordesillas and Stuart Walsh, 2002 [87]; Estrada et al., 2008 [88]). One method is to directly introduce the geometrical effect using non-spherical particles. Another method is to introduce a model for the rolling resistance at the contact point of the spherical particles for the simplicity of its evaluation and lower computational costs. The model used in this study is the rolling resistance as a function of the relative rotation and a length parameter is used to represent the contact area as follows. Note that this rolling friction model is slightly different from the model reported in Chapter 3.

Figure 5.1 (a) illustrates two arbitrarily shaped particles \(i\) and \(j\) are compressed by the normal contact force forming a contact area. We modeled this scenario in two-dimensional DEM with circular particles introducing a contact diameter \(a\) on the contact plane to characterize the contact area. In actual particulate materials, a non-zero contact area may be caused by contact deformation or by particle shape. In this study, however, \(a\) is simply given as

\[
a = bd, 
\]

(5.1)
where $b$ is constant and $0 \leq b \leq 1$. Contact diameter $a$ is proportional to particle diameter $d$ regardless of the contact deformation. When particles $i$ and $j$ have different diameters ($d_i, d_j$), $a$ is determined by the smaller diameter to satisfy the condition in Equation (5.1).

![Diagram](image)

Figure 5.1 Rolling friction model. **a** Contacts between irregularly shaped particles. **b** Rolling friction acting on an irregularly shaped particle which rotates. **c** Model of rolling friction with a circular particle for DEM simulations.

Taking the rolling resistance into account, the angular velocity $\omega$ for a single particle is calculated as

$$I \frac{\partial \omega}{\partial t} = \sum_{i=1}^{n} (T + T_r), \quad (5.2)$$

where $n$ is the coordination number of the particle, $I$ is the moment of inertia, $T$ is the rolling moment due to the tangential contact force and $T_r$ is the anti-rolling moment as illustrated in Figure 5.1 (b). The value of $T_r$ is expressed as

$$T_r = -af_r, \quad (5.3)$$

and $f_r$ is given in consideration of the relative rotation between two particles, $\theta_r$, as follows.

$$f_r = k_n a \theta_r, \quad (5.4)$$
where $k_n$ is the normal spring constants. Note that Equation (5.3) asserts that anti-rolling moment $T_r$ always decreases the magnitude of the angular velocity. In addition, in this model, we give no threshold to $T_r$ in order not to increase the number of input parameters. This assumption is different from other rolling friction models (Iwashita and Oda, 2000 [45]; Tordesillas and Stuart Walsh, 2002 [87]) which have a threshold for $T_r$.

Here, the signs of the relative rotation are obviously different between two particles and the degrees of that are equivalent to each other. Therefore, opposite and equal torques act on these two particles respectively and the angular momentum is conserved.

As described in this subsection, this model requires only one additional parameter $b$. Thus, it is easy to obtain the corresponding relations between the packing properties and the rolling friction of the particles.

5.2.2 Packing method

Circular particles are generated in a rectangular box, 200 mm in width and 160 mm in height (see Figure 5.2 (a)). In this generation process, the position of each particle is chosen randomly one by one and placed one by one in such a way that there are no overlaps with the particles which have already been placed. The granular system consists of 19,186 particles, which have a particle size distribution of $D_{\text{max}}/D_{\text{min}} = 3$, $D_{\text{max}} = 1.423$ mm, and $D_{\text{min}} = 0.474$ mm and a density of 2,400 kg/m$^2$. The contact springs are assumed to be linear and $k_n / k_t = 4$ ($k_n = 4.0 \times 10^7$ N/m, $k_t = 1.0 \times 10^7$ N/m), where $k_t$ is the shear spring constants. Rigid walls, whose contact parameters are identical to those of the particles, are assumed for the boundaries. The side walls are fixed and do not move throughout the simulation.

Since the aim of my study is the granular packing in the quasi-static state, I introduce local non-viscous damping (ITASCA, 2004 [39]) in order to achieve the equilibrium state. According to the definition of (ITASCA, 2004 [39]), the damping-force is added to the equation of motion. I constrain the damping to be small enough so as not to have any effect on the results presented in this paper. The non-dimensional value for the damping coefficient is 0.2. In addition, I make the damping force in such a way that it has no effect on the gravitational acceleration of the particles.

In order to study the effect of the rolling friction, different values for rolling friction coefficient $b$ are used. In the preliminary simulations, I observed no particle rotation due to compression for $b$ larger than 0.2. For this reason, I use seven values for $b$ in the range of 0.00 to 0.15. Moreover, in order to study the combined effect of the inter-particle friction and the rolling friction, three values for $\mu$, namely, 0.08, 0.36 and 0.70, are used. Here, the
Figure 5.2  Packing process for 45,658 granular particles. (a) Particles are randomly placed while avoiding overlap with each other in a rectangular area, 315 mm in width and 250 mm in height. (b) Particles are dropped into the container under the gravity. (c) The compression process is performed by applying vertical pressure to the granular system. $\sigma_v$ and $\sigma_h$ indicate the stress acting on the top wall and on the lateral wall, respectively.
value for $\mu$ of realistic granular materials is up to 1.0. Taking this fact into consideration, I determined the range in the input values for $\mu$. At contacts between the wall and the particles, the inter-particle friction and the rolling friction are set to zero for simplicity.

After specimen generation (see Figure 5.2 (a)), the material properties are set for all particles and the simulations are performed by dropping the particles into the bottom of the container under gravity (see Figure 5.2 (b)). This sedimentation process is run until the average coordination number and the volume fraction become constant. The simulations are run with a time step of $5.0 \times 10^{-7}$ s.

The granular samples are then subjected to vertical compression by the top wall for stress control (see Figure 5.2 (c)). In this process, the gravity continues to act on the samples. The default position of the top wall is determined so that the particle which has the largest height can just come into contact with the top wall. The constant confining stress acting on the top wall is 100 kN/m, i.e., the value of $\sigma_v/k_n$ is 0.0025 and the value of $(mg/D)/\sigma_v$ is about 0.00018, where $m$ is a typical particle mass, $g$ is the gravity acceleration and $D$ is a typical particle diameter. These values give the approximate deformation of the grains and the strength of gravity, respectively. In Figure 5.2 (c), $\sigma_v$ indicates the stress acting on the top wall and $\sigma_h$ indicates the stress acting on the lateral wall. The compression process is over when the system reaches a steady state. I judge this state by the same criterion as that used in the sedimentation process.

The packing process, described above, is performed with different rolling friction parameters $b$ and inter-particle friction coefficients $\mu$. A total of 21 tests are run. Granular samples are analyzed at the steady state at the completion of the compression.

5.3 Results and discussion

5.3.1 Volume fraction and average coordination number

Firstly, I describe the influence of the rolling resistance on volume fraction $\xi$. The value for $\xi$ is defined by $\xi = V_p/V$, where $V_p$ is the total volume of the particles and $V$ is the total volume of the packing. The relationship between volume fraction $\xi$ and rolling friction coefficient $b$ is reported in Figure 5.3. As expected, volume fraction $\xi$ decreases with increases in $b$ for all $\mu$ cases. This indicates that the rolling resistance inhibits the rearrangement of the particles under packing and that the volume of the voids within the granular samples increase at the steady state.

Next, I discuss average coordination number $Z$, which is the average of the contacts per
5.3. RESULTS AND DISCUSSION

particle in the contact network, \( Z = 2M/N \), where \( M \) is the total number of contacts and \( N \) is the total number of particles in the contact network. Figure 5.4 shows the relationship between average coordination number \( Z \) and rolling friction coefficient \( b \). From this plot, we can see that the value for \( Z \) consistently decreases as \( b \) increases for all \( \mu \) cases. It is thought that the decrease in \( Z \) for each \( \mu \) case is mainly due to the decrease in volume fraction \( \xi \) resulting from the rolling resistance.

Figure 5.3 Volume fraction \( \xi \) as a function of rolling friction coefficient \( b \) for several fixed values for \( \mu \).

Additionally, from the analysis in Figures 5.3 and 5.4, for \( \mu = 0.08 \), as \( b \) increases, \( \xi \) and \( Z \) decreases to plateau values of about 0.83 and about 3.9, respectively. This means that the rolling friction has an insignificant influence when the value for \( \mu \) is small. In contrast, with a large value for \( \mu \), the rate of decrease in \( \xi \) and \( Z \) is larger in the other \( \mu \) cases. That is, as \( \mu \) increases, the contribution of the rolling friction to the resisting moment becomes large under packing. This trend is in agreement with the recent work involving the investigation of the relative contributions of the inter-particle friction and the rolling friction under shear (Estrada et al., 2008 [88]).

On the other hand, Figure 5.5 shows the evolution of \( \xi \) as a function of \( Z \). From this plot,
we can see that $\xi$ increases with increases in $Z$ regardless of $\mu$ or $b$. In other words, there is a universal relation between $\xi$ and $Z$. This relation implies that the effect of $b$ on $\xi$ and $Z$ is almost equivalent to that of $\mu$ under packing. Therefore, it can be concluded that the restrain effect on the rearrangement under packing depends on the combination of $\mu$ and $b$.

![Graph](image)

Figure 5.4  Average coordination number $Z$ as a function of rolling friction coefficient $b$ for several fixed values for $\mu$.

5.3.2 Granular fabric

To investigate the granular fabric at the stable state under compression, the distribution of the contact angles, $M(\theta)$, in cases where $\mu = 0.08$ and $b = 0.02$ (□), $\mu = 0.36$ and $b = 0.05$ (○), and $\mu = 0.70$ and $b = 0.15$ (△), is plotted in Figure 5.6. In this polar diagram, contact angle $\theta \in [0, 180)$, in degrees, is measured with respect to the horizontal axis in a counterclockwise direction. For the cases where $\mu=0.08$ and $b=0.05$, the fabric is nearly isotropic. In fact, regardless of the $b$ value, this trend is identical if $\mu=0.08$. This is because the restrain effect on the rearrangement of the particles is very small in such cases. In contrast, for other two cases in Figure 5.6, the fabric shows anisotropy. These plots suggests that the magnitude of the fabric anisotropy increases with increases in $\mu$ and $b$. Therefore,
the fabric anisotropy also varies depending on the combination of \( \mu \) and \( b \).

Furthermore, from Figure 5.6, we can also see that the directions of the fabric anisotropy correspond to those of the principal stress in this compression system (i.e. the directions of \( \sigma_v \) and \( \sigma_h \), illustrated as Figure 5.2 (c)). In addition, with increasing \( \mu \) and \( b \), the contacts between the particles decrease along the direction of the minor principal stress. From these results, it can be recognized that the fabric anisotropy under packing, which results from the particle characteristics, arises along the direction of the principal stress.

### 5.3.3 Lateral stress response to the vertical stress

Next my investigation is focused on the force transmission in granular media. I employed the coefficient of earth pressure at rest, \( K \), as the expression for the lateral stress response to the vertical stress. This parameter is given in the following:

\[
K = \frac{\sigma_h}{\sigma_v},
\]

(5.5)

where \( \sigma_h \) is the lateral stress and \( \sigma_v \) is the vertical stress, which are evaluated by the lateral wall and the top wall, respectively (see Figure 5.2 (c)). The value of \( K \) indicates a macroscopic property of force transmission in granular media. Figure 5.7 shows the relationships between \( K \) and \( b \). From this figure, we can see that \( K \) decreases with increases in \( b \). It is
clear that the rolling resistance under packing has an effect on the lateral stress response to the vertical stress. My data is consistent with the experimental and the numerical studies on the effects of inter-particle bonds on the evolution of horizontal stress under vertical pressure (Yun and Evans, 2011 [89]). The rolling resistance and the cementation at the contacts are similar in that both of them prevent the rearrangement of particles under compression.

However, in the case of $\mu = 0.08$, $K$ decreases to plateau values of about 0.8 in the same way as for $\xi-b$ and $Z-b$. This is because the effect of the rolling friction is small when $\mu$ is small, as described in Sec. 3.1. That is, for $\mu = 0.08$, the properties of packing show no significant difference with the value of $b$. Moreover, the obtained results for $\mu = 0.36$ are about the same as those for $\mu = 0.70$. Therefore, only the case where $\mu = 0.36$ is addressed in the following discussion.

It should be noted that the value for $K$ is usually used in geotechnical engineering to estimate the lateral pressure as a function of depth under the ground. In addition, the value for $K$ is often described as simply being related to the angle of internal friction of granular materials $\phi$ (Duran, 1999 [90]; Jãky, 1944 [91]; Eder, 2004 [92]), whereas the value for $\phi$ is closely related to the rolling resistance (Lu and McDowell, 2007 [85]; Matsushima and Chang, 2011 [86]). Therefore, it is natural to assume that there must be some correlations
5.3. RESULTS AND DISCUSSION

Figure 5.7 Coefficient of redirection toward the wall $K$ as a function of rolling friction coefficient $b$ for several fixed values for $\mu$.

between $K$ and $b$. Indeed, my data suggest that the value of $K$ is strongly affected by the rolling resistance of the particles. This observation implies that there is a triadic correlation between $K$ and $\phi$ and $b$.

In order to investigate the origin of this macroscopic force transmission, I also study the angular variation in the normal forces from a microscopic point of view, as shown in Figure 5.8. Contact angle $\theta \in [0, 180)$, in degrees, is measured in the same manner as in Figure 5.6. In this figure, $180$ (deg.) is divided into $60$ bins of $3$ (deg.) each and the average normal force in each bin normalized by the mean normal force, $f_n(\theta)/\langle f_n \rangle$, is plotted against the mean value of that bin for $\mu = 0.36$. Previous studies have shown that this angular distribution is well fitted with just one parameter by Fourier series expressions in sheared granular assemblies (Bathurst and Rothenburg, 1989 [93]; Radjai et al., 1998 [94]; Majmudar and Behringer, 2005 [95]; Snoeijer et al., 2006 [96]). According to these studies, my data are fitted by the solid curves drawn in Figure 5.8, described by the following equation:

$$\frac{f_n(\theta)}{\langle f_n \rangle} = 1 - A \cos 2\theta, \; \theta \in [0, 180), \quad (5.6)$$

where $A$ is the fitting parameter, which corresponds to the amplitude of this "wave"-like
distribution. In other words, the value of $A$ is the magnitude of mechanical anisotropy.

Figure 5.8 Angular variation in the normal contact forces in the case of $\mu = 0.36$ for macroscopic one-dimensional compression.

From Figure 5.8, we can observe that $A$ increases with increases in $b$. In other words, the rolling resistance broadens the angular distribution of the contact forces. Figure 5.8 also shows that the contact angle carrying the largest force is 90 (deg.) and that the contact angle carrying the smallest force is 0 (deg.) in all $b$ cases. This observation suggests that the directions of these contact angles coincide with those of the principal stress in the macroscopic one-dimensional compression system. From this fact, it can be expected that the amplitude of the mechanical anisotropy contributes strongly to the value of $K$, which is defined by $\sigma_h / \sigma_v$.

In order to verify the correlation between $K$ and $A$, we observed the evolution of $K$ as a function of $A$, as shown in Figure 5.9. The solid line is a fitting line described by the following equation:

$$K = -\alpha A + \beta,$$

(5.7)
where both $\alpha$ and $\beta$ are fitting parameters. The fit of the data to Equation (5.7) shown in Figure 5.9 is very good; $\alpha = 1.391$, $\beta = 0.997$ and a coefficient of determination $R^2$ is 0.989. The fitting line indicates that the value of $K$ is about 1.0 when the magnitude of mechanical anisotropy is zero (i.e. $A = 0.0$). Here, it should be noted that we found a clear fitting by Equation (5.7) for the granular systems which have relatively anisotropic fabric due to the particle characteristics, as described in Section 3.2. In addition, both of the normal contact forces and the tangential contact forces are active in these granular systems.

When this analysis is applied to the granular system, where the fabric is isotropic and the tangential contact forces are not active, the relationship between $K$ and $A$ is derived theoretically from (Radjaï et al., 1998 [94]) as follows:

$$K = \frac{1 - \frac{1}{2}A}{1 + \frac{1}{2}A}$$

The curve for Equation (5.8) is depicted by the dotted line in Figure 5.9. Obviously, we can see that the solid line for Equation (5.7) deviates from the dotted line for Equation (5.8). It can be expected that this deviation is mainly due to the difference of the analysis conditions, i.e., whether the fabric is isotropic or anisotropic, the tangential contact forces are active or inactive and the rolling friction of the particles is present or not.

From these macroscopic and microscopic aspects, it is confirmed that the rolling resistance contributes to the stress redirection in granular assemblies. On the basis of these above findings, we can assume that such a difference in stress states, associated with the rolling resistance, is closely related to the shear strength.

5.3.4 Force distribution

Finally, in this section, the influences of the rolling resistance on the force distribution are addressed. Figure 5.10 shows the probability density distribution of normal contact force $f_n$ for $\mu = 0.36$. The normal forces are normalized by the mean normal force $\langle f_n \rangle$. In the inset, a part of function $P(f_n)$ for forces less than $\langle f_n \rangle$ is plotted. Function $P(f_n)$ decays faster for large forces (above the mean normal force) than the exponential and has no clear peak around the mean normal force. Additionally, the force distribution has an upturn at very small forces ($f_n / \langle f_n \rangle < 0.2$). Such trends can also be seen for $\mu = 0.70$. In contrast, the distributions is less sensitive with $b$ for $\mu = 0.08$, where the apparent effectiveness of the rolling resistance cannot be observed.

From the inset in Figure 5.10, we can see that the fraction of the particle-particle contacts
with very small forces increases with an increasing $b$, even though the coordination number decreases with an increasing $\mu$. This means that the number of weakly supported particles, which are often termed rattlers or floaters (O’Sullivan, 2011 [22]), increases as a result of the enhanced interlocking effect between particles due to the rolling resistance. Moreover, from Figure 5.10, it can be observed that as the $b$ increases, the force distribution becomes broad and the slope of the tail becomes smaller; the fraction of contacts which have large forces also increases. These results show that the stress distribution in a granular packing is less homogeneous in the presence of the rolling friction of the particles. The evolution of inhomogeneous stress distributions, with an increase in $b$, corresponds to the increase in the magnitude of the mechanical anisotropy, as shown in Figure 5.8.

5.4 Conclusions and future work

I performed a series of 2-D DEM simulations in order to study the effects of the rolling friction of the particles on granular packing. As a result of the analysis, I showed how the rolling resistance, which results from the rolling friction of each particle, plays a role in granular packings, as mentioned below.
Firstly, the rolling resistance was shown to influence the volume fraction and the average coordination number. The obtained data showed that the rolling resistance inhibits the rearrangement of the particles under packing, and its inhibition is almost equivalent to the inhibition effect of the sliding friction. Secondly, I investigate the granular fabric at the stable state and showed that the magnitude of the fabric anisotropy increases along the directions of the principal stresses with increases the rolling resistance. Then, I investigated the lateral stress response to the vertical stress in granular media from the perspective of both macromechanical and micromechanical properties. I found that the stress redirection also varies depending on the value of the rolling friction coefficient, i.e., the rolling resistance reduces the coefficient of earth pressure at rest and broadens the angular distribution of contact forces. In addition, it can be assumed that there are strong correlations between the rolling resistance and the stress state and the shear strength of granular materials. Finally, I showed that the probability density distribution of normal contact forces, \( P(f_n) \), is also affected by the rolling resistance. In other words, the presence of the rolling friction makes the force distribution more inhomogeneous.

In these above findings, the relationship between the stress state and the rolling resistance is particularly important. This is because the stress state is one of the indispensable factors
for evaluating the rheology of granular media. Therefore, it is necessary to take into account the rolling resistance when circular or spherical particles are employed in DEM simulations for actually non-spherical granular packing.

On the other hand, my findings also imply that the origin of lithostatic pressure, developed in gravitationally deposited granular piles, may be related to the particle shape. Note that lithostatic pressure is a component of confining pressure derived from the weight of the column of rock above a specified level. Further investigation should be done on this point. For example, I plan to analyze the angle of repose.

It should be noted that many techniques for particle packing have been proposed in DEM simulations (Feng et al., 2003 [97]). Previous research works have revealed that different packing methods have a strong influence on the arrangement of the particles (Geng et al., 2001 [98]; Voivret et al., 2007 [99]). My observations reported here are based on one of them, namely, that particles are generated randomly and dropped under gravity. Therefore, further studies by means of other packing methods should be also conducted. In addition, I am going to focus attention on the relation between the initial packing state and the subsequent shear behavior.
6 3-D direct simulation model for failure of non-cohesive granular soils with seepage flow

6.1 Introduction

The solid particle-fluid multiphase flow and its multiphysics 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 recently developed a X-ray tomography (Sukop et al., 2008 [100]; Moreno-Atanasio et al., 2010 [101]) and a high speed camera (Li et al., 2012 [102]), but their observation capacity and available information at particle-resolution are still limited.

In addition to experimental approaches, the development of numerical simulation can help our understanding of such complex particle-fluid systems (Van der Hoef et al., 2008 [103]). Because of the importance of capturing properly the interactions between particle and fluid, microscale numerical method (Glowinski et al., 2001 [104]; Gallier et al., 2014 [105]; Yu and Shao, 2007 [106]) which can deal with the fluid flow at less particle scale, as illustrated in Figure 6.1 (a), is needed. In contrast, macroscale methods (e.g. Tsuji et al., 1993 [107]), as illustrated in Figure 6.1 (b), have less computationally load and are suitable for an industrial application, but such methods require a local averaging which loses the essential details of the fluid flow. The former type of the direct methods are intently improved and new findings are obtained mainly in research fields such as chemical engineering (Ikeno and Kajishima, 2007 [108]), bio-engineering (MacMeccan et al., 2009 [109]) and soft matter physics (Kim et al., 2006 [110]).

In geomechanics, a particle-fluid system also exists in the form of solid particles and pore liquids or gases, that is 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 foundations. In previous studies, for example, 2-D or 3-D physical particle simulations coupled with Fictitious Domain Method (FDM) (Toppin et al., 2013 [111]), with Lattice Boltzmann Method (LBM)
CHAPTER 6. 3-D DIRECT SIMULATION MODEL FOR FAILURE OF NON-COHESIVE
GARANULAR SOILS WITH SEEPAGE FLOW

Figure 6.1 Schematic pictures of the coupled particle-fluid model. (a) The case where particle diameter is larger than the grid space. (b) The case where particle diameter is smaller than the grid space.

(Cui et al., 2014 [112]; Mansouri et al., 2009 [113]; Lomine et al., 2013 [114]) and with Direct Numerical simulation (DNS) (Ji et al., 2013 [115]) have been applied to the geo-engineering problems. 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.

I am also interested in the applicability of a direct numerical model to the geomechanics. In this study, I focus on the non-cohesive dense granular soils with the flow of pore liquids in three dimensions. My goal is to numerically capture the process of the seepage-induced failure from the micromechanical aspects without any macroscopic assumptions. To accomplish the objective, I have investigated the boiling phenomenon with upward seepage flow with the variety of the pressure gradient. The solid particles and the pore fluid are directly solved by using both the discrete element method and the lattice Boltzmann method. Because contacts between particles inevitably occur in dense granular assemblies, contact force and sliding friction between particles must be considered (Seto et al., 2013 [116]). In such a case, it is necessary to employ a soft sphere model such as DEM that allows overlap between the physical particles. On the other hand, LBM are employed for the seepage flow so that intricate pore geometry inside accumulated soils can be managed in a relatively simple way.
6.2. PARTICLE-FLUID NUMERICAL METHOD

without boundary-fitted meshes (Thompson et al., 1985 [117]). In addition, compared with the conventional CFD method on the basis of the Navier-Stokes equation, the LBM has an advantage of the parallelization of its code because the required calculation at each node is completely local resulted from its feature of discretization. Moreover, to calculate the interaction between the solid and the fluid, an immersed boundary approach was employed.

As a result of the analyses, numerically predicted value for the critical hydraulic gradient is in good agreement with the theoretical value, and what is more, the presented simulation model can capture the evolution of the seepage failure with the increases of pressure gradient. In particular, the rapid change of the flow pattern around the critical hydraulic gradient and the disappearing process of the contact networks can be observed from microscopic point of views.

Chapter 6 is organized as follows. In Section 6.2, I firstly highlight the physical model used in this investigation. Details of the conditions of the simulation are given in Section 6.3. Then, the results and a discussion are given in Section 6.4. A summary of the chapter is presented in Section 6.5 and a future work is suggested in Section 6.6.

6.2 Particle-fluid numerical method

6.2.1 Partially saturated lattice Boltzmann model

In order to perform the coupled particle-fluid simulations in the framework of LBM, the partially saturated lattice Boltzmann model allowing momentum transfer inside the solid phase, whose concept is originally proposed by Noble and Torczynski (1998 [118]) is used. After the proposal of the method, this approach have been improved by a lot of researchers in order to simulate complex particle-fluid systems (Owen et al., 2011 [119]; Han and Cundall, 2011 [120]; Strack and Cook, 2007 [121]). This model enables to deal with the moving solid-liquid boundary and to calculate the hydrodynamic force acting on the solid obstacle. Compared to other coupled model (Ladd, 1994a [122]; Ladd, 1994b [123]; Feng and Michaelides, 2004 [124]), 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 lattice BGK equation, as described in chapter 2, is reformulated to account for the additional parameter, $B$, and the additional term $\Omega$.

$$\Omega_\alpha(x, t) = -\frac{1}{\tau}(1 - B(x, t))(f_\alpha(x, t) - f_{eq, \alpha}(x, t)) + B(x, t)\Lambda_\alpha + G_\alpha \delta t,$$ 

(6.1)
where $B$ is given by

$$B(x, t) = \frac{\chi(x, t)(\tau - \frac{1}{2})}{(1 - \chi(x, t)) + (\tau - \frac{1}{2})},$$

(6.2)

The parameter $\chi(x, t)$ is the volume fraction of solid at each node. The value for $\chi$ varies between 0 for a completely fluid node and 1 for a completely solid node. Then, the value for $\Lambda_{\alpha}$ is calculated as follows.

$$\Lambda_{\alpha} = f_{-\alpha}(x, t) - f_{eq}(\rho, u) + f_{eq}(\rho, u^p) - f_{\alpha}(x, t),$$

(6.3)

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

The calculation procedure for $\chi$ is based on the following level-set function $H$ (Gallier, 2014 [105]).

$$\chi(x, t) = H(r - \|x - x^p(t)\|),$$

(6.4)

$$H(x) = \begin{cases} 
1, & x \geq \frac{r}{2}, \\
\frac{1}{2} \tanh(\frac{4x}{r} + 1), & \|x\| < \frac{r}{2}, \\
0, & x \leq -\frac{r}{2},
\end{cases}$$

(6.5)

where $r$ is particle radius, $x$ is the position vector at a node and $x^p$ is the mass center of the particle. The parameter $\epsilon$ is the same value as the lattice space $\delta_x$. This approximated procedure for $\chi$ has numerical efficiency rather than polygonal approximation method or sub domain decomposition method (Owen et al., 2011 [119]; Chen et al., 2013 [125]).

When two particles collide, the soft sphere model such as DEM allows them to slightly overlap. On the basis of this overlap region, contact forces are calculated in DEM solver. In the case where the LBM node positions at the overlap region, that node belongs to more than one particle. To deal with such a case, I assume that each LBM node is constrained to belongs to the particle whose mass center is closer to that node.

### 6.2.2 Collision law and motion of physical particle

The handling of the collision law and the motion of the solid particle are presented in this subsection. The collision law is governed by the DEM as described in detail in Chapter 2. In addition, the hydrodynamic force and torque resulted from seepage flow are needed for the motion of the particles. The equation of motion accounting for these forces $F^{byd}$ and
6.3. SIMULATION DETAILS

The hydrodynamic force $F_{hyd}$ is described as following equations.

$$m_p \frac{d^2 x_p}{dt^2} = \sum F^{con} + F^{gra} + F^{hyd},$$  \hspace{1cm} (6.6)

$$I_p \frac{d^2 \theta_p}{dt^2} = \sum T^{con} + T^{hyd},$$  \hspace{1cm} (6.7)

where $F^{gra}$ includes the buoyancy force. These forms are reformulated versions of Equation 2.1 and 2.2. $F^{hyd}$ and $T^{hyd}$ are given by summing up the change of momentum inside the solid phase:

$$F^{hyd} = \delta_t^2 \sum_n B_n \left( \sum_{\alpha} \Lambda_{\alpha} c_{\alpha} \right),$$  \hspace{1cm} (6.8)

$$T^{hyd} = \delta_t^2 \sum_n \left\{ (x_n - x_v) \times B_n \left( \sum_{\alpha} \Lambda_{\alpha} c_{\alpha} \right) \right\},$$  \hspace{1cm} (6.9)

where $n$ is the number of the node belonging to the solid phase of a particle.

Note that the lubrication force arising between two approaching particles is not accounted in this study. For example, lubrication models in frame of a direct numerical simulation are proposed by (Ding and Aidun, 2003 [126]; Wachs, 2009 [127]; Yeo and Maxey, 2010 [128]). However, I assume that the lubrication effect is too weak in the soil structure, in which the particles are highly concentrated, the density ratio of the solid to the fluid is large and the viscosity of the fluid is small. Thus, the proper lubrication model in the multiphase system comprising of soil particles and pore water is not considered in the following discussions.

6.3 Simulation details

Coupled DEM-LBM simulations of boiling phenomena of soils with upward seepage flow were performed in order to investigate the applicability of the particle-fluid simulations to geotechnical engineering problems. In the first process of specimen preparation before boiling simulation, the spherical soil particles are generated inside an area enclosed with six plane walls, where 1.5 mm in $x$-direction, 7.5 mm in $y$-direction and 1.5 mm in $z$-direction. In this packing process, only DEM calculation was performed in gravity field. The particles have a size distribution of $D_{max}/D_{min} = 1.33$, $D_{max} = 2.0 \times 10^{-4}$ m and $D_{min} = 1.5 \times 10^{-4}$ m in order to avoid crystallization at initial packing state. $D_{max}$ is the maximum particle diameter and $D_{min}$ is the minimum particle diameter in the granular system. The density of the soil particles $\rho_s$ is 2,8500 kg/m$^3$ and the sliding friction between the immersed particles is 0.5.
The rolling friction of the particles is not considered in this study. The contact springs are assumed to be linear and $k_n / k_t = 4 \ (k_n = 1.0 \times 10^6 \text{ N/m}, \ k_t = 2.5 \times 10^5 \text{ N/m})$, where $k_n$ is the normal spring constant and $k_t$ is the shear spring constant, respectively. The values for the normal and the tangential viscous damping, for inhibiting the numerical oscillation, are determined to be small enough so as not to make a significant contribution of total energy dissipation to the granular system. The number of the particles for the soil sample is 1049. Initial solid fraction of the packed sample, $\xi$, is 0.571. This value indicate medium dense state of granular media comprising of spherical particles (O’Sullivan, 2013 [22]).

![Figure 6.2](image.png)

Figure 6.2  Pictures of the initial configuration of the simulation model. (a) The full view of the model. (b) The cross sectional view in $yz$-plane at $x = 75\delta_x$. The area colored in white indicates the solid phase and the area colored in black indicates the fluid phase.
Figure 6.2 shows the initial configuration of the simulation model. As described in Chapter 2, D3Q19 velocity model was employed by taking into account both computational accuracy and efficiency. Gravitational force acts in negative direction of $y$-coordinate and the seepage flow streams in the opposite direction of the gravity. To generate upward flow resulted from the difference of the pressure, Zhou and He pressure boundary condition (Zhou and He, 1997 [129]) is used in lower and upper boundaries in the perpendicular direction to the flow. Other four boundaries in the same direction as the seepage flow, i.e., $xy$ and $yz$ planes, are subjected to the non-slip boundary condition by using the bounce-back scheme (Ziegler, 2013 [130]).

Lattice space $\delta_x$ is $1.0 \times 10^{-5}$ m and the system size is $150\delta_x \times 300\delta_x \times 150\delta_x$. The area occupied with the soil particles is $150\delta_x \times 200\delta_x \times 150\delta_x$. At $y=20\delta_x$, a plane bottom wall which allow the fluid to pass but does not allow the solid, which is assumed to be a metallic mesh wall, is placed. The friction conecofficient between the particles and the wall is set to 0 so as to compare the numerical result and the theoretical solution. The boundary friction is not considered in the theory of one-dimensional seepage failure of soils (Ishihara, 2001 [131]).

The fluid density $\rho_f$ is 1,000 kg/m$^3$, where the density ratio of the solid to the fluid is 2.5. Time step for fluid phase, $\delta_t$, is $1.0 \times 10^{-5}$ s and time step for solid phase is $\delta_t^{dem}$, is $2.0 \times 10^{-8}$ s. Until the fluid flow is newly updated, the hydrodynamic force acting on the solid particle is assumed to be the same value. The relaxation time coefficient $\tau$ is 0.8, and then the kinetic viscosity of the fluid, $\nu$, is $1.0 \times 10^{-6}$ m$^2$/s from Equation (2.21).

Under the above conditions, the resolution value for $D_{min}/\delta_x$ is 15. In the preliminary simulations, it is evaluated that this value satisfies the seepage flow at void spaces which is smaller than the particle diameter. In fact, some previous researches have reported that proper drag force is obtained and the variation of pore pressure is captured when the resolution value is greater than 10 (Han and Cundall, 2013 [132]; Mutabaruka et al., 2014 [133]).

With varying the hydraulic gradient $i$, series of the boiling simulation is conducted. Initially, the system is set at quiescent state with $\rho=1,000$ kg/m$^3$ and $u=0$ m/s. Total 11 cases are performed with the value for $i$ ranging from 0.170 to 0.935, $i = 0.17, 0.34, 0.51, 0.68, 0.714, 0.748, 0.782, 0.816, 0.85, 0.884, 0.918$. These values are corresponding to the ratio of the outlet pressure to the inlet pressure, 0.990, 0.980, 0.971, 0.962, 0.960, 0.958, 0.956, 0.954, 0.952, 0.950 and 0.948. All of these calculations are performed on the graphic processing unit (NVIDIA GeForce GTX TITAN). Parallelized algorithm for DEM suggested by (Nishiura and Sakaguchi, 2013 [23]) is incorporated into the coupled DEM-LBM code. Detailed parallelization methods relative to the coupling scheme on many core architecture
is not discussed in this literature.

![Graph](image_url)

Figure 6.3  (a) Variation of pressure $p$ with $y$ coordinate in the case of $i=0.51$. (b) Variation of flow velocity $u$ with $y$ coordinate in the case of $i=0.51$.

### 6.4 Results and discussion

This section discusses the applicability of the direct particle-fluid simulation method to the boiling phenomena of the soils. In order to measure progress in the flow, Figures 6.3 (a) and (b) which indicate the pore pressure variation $p_{xz}$ and the flow velocity $u_{xz}$ with $y$ coordinate in the case of $i = 0.51$ after $1.0 \times 10^4$ steps (0.1 s) are presented. The value for $p_{xz}$ and $u_{xz}$ are averaged in a $xz$ section and are normalized by the value at inlet, namely, $y = 0$. The value for $y$ is also normalized by the length in $y$ direction. According to Figure 6.3 (a), the ratio of the pressure at the outlet to that at the inlet reach a given pressure difference. It can be also shown that the hydraulic gradient justly acts on the area of $y = 0.1-0.7$, where the soil particles exist. On the other hand, from Figure 6.3 (b), we can observe that the fluid velocity at the inlet is about the same with that at the outlet. Additionally, the large velocities are distributed in the region of the soils, depending on the solid fraction. These above results indicate that the developed flow in the porous media is obtained. The
same criterion of evaluating the steady flow is used for other $i$ cases.

### 6.4.1 Critical hydraulic gradient

Figure 6.4 (a) shows the evolution of the sum of the hydrodynamic force $|F_{hyd}^y|/W_p$ acting on the soil particles in the $y$ direction as a function of $i$. The hydrodynamic force is divided by the total mass of the specimen $W_p$, which includes the buoyancy force. The boiling onset is at a time when $|F_{hyd}^y|$ is equal to $W_p$, thus the value for $i$ corresponding to $|F_{hyd}^y|/W_p = 1.0$ is the critical hydraulic gradient $i_c$ predicted from the numerical simulations. The solid line in the figure is a fitting line described by $|F_{hyd}^y|/W_p = ai + b$, where $a$ and $b$ are the fitting parameters. The range of the fitted data is $|F_{hyd}^y|/W_p < 1.0$. The fit of the data to the linear equation is very good; $a = 1.148$ and $b = 0.000$. From the approximate relation between $|F_{hyd}^y|/W_p$ and $i$, the critical hydraulic gradient $i_c$ is calculated as 0.871.

In addition, it is also evident from this figure that the hydrodynamic force is proportional to the hydraulic gradient in the range of $i < i_c$. This fact indicates that seepage force acting on the soils according to the pressure difference can be qualitatively calculated without any continuum assumptions for the seepage flow. When $i > i_c$, on the other hand, the proportional relation between the seepage force and $i$ breaks because the soils began to move and they are not fixed against the seepage flow. After the boiling onset, the seepage force acting on the soils is nearly-constant.

Here, the theoretical value for the critical hydraulic gradient $i_c^{\text{theory}}$ on the basis of the theory of one-dimensional seepage failure can be obtained from the initial solid fraction and the density ratio of the solid to the fluid. This value is given by

$$i_c^{\text{theory}} = \xi (\rho_s/\rho_f - 1.0),$$  \hspace{1cm} (6.10)

and that is calculated as 0.857. Thus, $i_c$ obtained from the simulations is almost consistent with $i_c^{\text{theory}}$. It can be concluded that this particle-fluid simulation for the seepage failure is not only qualitative but also quantitative. We believe that more highly accurate simulation can be performed when the multi-relaxation time lattice Boltzmann model (D’Humieres, 2002 [134]) is employed. In the MRT model, compared to the SRT model, the dependency of the precision of the non-slip boundary condition on the relaxation time coefficient is small.

The introduction of the MRT model to the presented coupled method is a future work.

Furthermore, Figure 6.4 (b) shows the evolution of the force, $|F_{wall}^y|/W_p$, acting on the bottom wall positioning at $y = 20\delta_x$ in the $y$ direction with the increasing $i$. The acting force is also divided by the total mass of the specimen with the same as the hydrodynamic
Figure 6.4 (a) Sum of the hydrodynamic force acting on the solid phase, $F_{y}^{\text{hyd}}$, as a function of hydraulic gradient $i$ with a linear fitting line: $y = ax + b$. The dotted line shows $F_{y}^{\text{hyd}} = W_p$. (b) Acting force on the bottom wall positioning at $y=20\delta_x$, $F_{y}^{\text{wall}}$, as a function of hydraulic gradient $i$ with a linear fitting line: $y = ax + b$. The dotted line shows $F_{y}^{\text{wall}} = 0$. 

\begin{align*}
F_{y}^{\text{hyd}}/W_p & \quad a = 1.148 \\
& \quad b = 0.000 \\
F_{y}^{\text{wall}}/W_p & \quad a = -1.146 \\
& \quad b = 0.999
\end{align*}
force in Figure 6.4 (b). The solid line in this figure is also a fitting line described by 
\( |F_{\text{wall}}|/W^p = ai + b \), where \( a \) and \( b \) are the fitting parameters. The range of the fitted data is 
\( |F_{\text{wall}}|/W^p > 0.0 \). The fit of the data to the linear equation is very good; \( a = -1.146 \) 
and \( b = 0.999 \). This plot reveals the proportional relation between \( |F_{\text{wall}}| \) and \( i \) for \( i < i_c \). 
When \( i \) is larger than \( i_c \), the value for \( |F_{\text{wall}}| \) is zero because the soil particles move together 
with the fluid flow in the positive \( y \) direction, and they are detached from the bottom plane 
assuming a metallic mesh wall. Moreover, comparison between Figures 6.4 (a) and (b) shows 
that an equilibrium in the direction of gravity, 
\( |F_{\text{hyd}}|/W^p + |F_{\text{wall}}|/W^p = 1.0 \) for \( i < i_c \), is satisfied. It should be noted that the wall friction is set to be zero in this investigation 
because the classic theory of the seepage failure does not include the effect of the boundary 
friction. Therefore, it can be thought that incompatibility between the simulation results 
and the theory occurs when the non-zero values for the wall friction are used.

6.4.2 Failure induced by seepage flow

First, the process of seepage failure in terms of the fluid flow is analyzed. In Figure 6.5, the 
distribution of the flow velocity \( |u| \) m/s in the \( yz \) plane with \( i = 0.34, 0.85 \) and \( 0.884 \) at 0.1 s 
is illustrated. The color maps of the flow velocity are at \( x = 75\delta_x \) and are corresponding to 
the cross-sectional view of the simulation model as shown in Figure 6.2 (b). The maximum 
flow velocities at each hydraulic gradient are \( 1.6 \times 10^{-3} \) m/s for \( i = 0.34 \), \( 4.0 \times 10^{-3} \) m/s for 
\( i = 0.85 \) and \( 4.5 \times 10^{-3} \) m/s for \( i = 0.884 \). These values are used as the threshold values 
to make the the color maps. In this figure, the velocities at the solid nodes are set to be 
0 because the fluid phase and the solid phase are to be readily identifiable. Note that the 
maximum flow velocity in all cases is \( 6.8 \times 10^{-3} \) m/s for \( i = 0.918 \) at 0.1 s, and this velocity 
sufficiently satisfies Equation (2.22) in Chapter 2 for guaranteeing the incompressible flow, 
\( M \ll 1 \).

As we can see from Figure 6.5, in the cases of \( i = 0.34 \) and \( 0.85 \) where \( i < i_c \), large 
velocities are distributed in the range of the porous solid. Comparison between these two 
cases shows that the velocity distributions are almost the same, although the magnitude 
of the flow increases with the increasing of \( i \). Similarity relationships of the distributions 
with each other are observed in other \( i < i_c \) cases. This feature of the velocity distributions 
along \( y \)-coordinate corresponds to Figure 6.3 (b). To the contrary, in the case of \( i = 0.884 \) 
where \( i > i_c \), as a result of the movement of the soil particles, the distribution of the flow 
velocity rapidly changes from the former two cases. It can be expected that the flow volume 
dramatically increases after exceeding the critical hydraulic gradient.
Figure 6.5  Flow velocity distributions in $yz$ plane at $x=75\delta_x$ for various hydraulic gradient $i$. In these color maps, maximum values for flow velocity, $u_{\text{max}}$, are 0.0016 m/s for $i=0.34$, 0.0040 m/s for $i=0.85$ and 0.0045 m/s for $i=0.884$. 
6.4. RESULTS AND DISCUSSION

Figure 6.6 The evolution of the inflow velocity and the soil velocity as a function of hydraulic gradient $i$.

Figure 6.7 The lateral views of the soil sample at $t = 0.0$ s and $t = 0.1$ s in the case of $i=0.918$. 
To confirm the transformation of the flow around $i = i_c$, a variation of the inflow velocity $u_{in} \text{ m/s}$ with $i$ is presented in Figure 6.6. The value for $u_{in}$ is defined as the averaged flow velocity in the $xz$ plane at $y = 10\delta_x$. $u_{in}$ for $i < i_c$ is at a steady state and $u_{in}$ for $i > i_c$ is at a time of 0.1 s. From this figure, it is shown that the inflow velocity rapidly increases in the range of $i > i_c$. In $i < i_c$, on the other hand, the inflow velocity increases at a rate proportional to the pressure differences. This linear relation represents that the obtained results are satisfied with the Darcy law in porous media. The coefficient of permeability which is derived from the slope of the line through $i < i_c$ is about $4.8 \times 10^{-4} \text{ m/s}$.

![Figure 6.8](image)

Figure 6.8 3-D visualization of the force chains between the particles for various hydraulic gradient $i$. The line thickness corresponds to the contact normal force.

In addition to the inflow velocity, the velocity of the soil samples against the hydraulic gradient is also plotted in Figure 6.6. After the boiling occurs, the soil particles move as ones in positive $y$-direction, as shown in Figure 6.7 where the lateral snapshots at $t = 0$ s and 0.1 s in the case of $i = 0.918$ are illustrated. Therefore, the velocity of the soil $< u_p > \text{ m/s}$ in the figure is defined as the averaged velocity of all particles. $< u_p >$ for $i < i_c$ is at
6.4. RESULTS AND DISCUSSION

A steady state and $< u_p >$ for $i > i_c$ is at a time of 0.1 s. From the evolution of the soil velocity, it can be observed that the soil particles start to accelerate after $i > i_c$, while they stay at rest in $i < i_c$. The plots also show that the velocities of the soil after the boiling are almost the same as the inflow velocity.

Next, the process of seepage failure in terms of the effective stress is discussed. Figure 6.8 visualizes the force chains between the soil particles in the three dimensions for various hydraulic gradient $i$ at 0.1 s. The line thickness of the force chain corresponds to the magnitude of the normal contact force. The evolution of the force chains clearly shows that the contact networks between the soil particles proceed to disappear with the increasing in the seepage force. In the theory of the one-dimensional seepage failure, the effective stress is zero when $i$ is larger than $i_c$. However, in $i = 0.884 > i_c$ of the figures, the force chains do not completely disappear and small contact forces in the soil sample are still maintained. This is mainly because the moving soil particles are associated with the collisions and contacts shortly after the boiling onset. Such a observation with respect to the contact network can be obtained when the soft sphere model is employed as a collision law, which allows to retain the contacts between the particles. Otherwise, a hard sphere model cannot reproduce the evolution of the force chains. Similar correlations are obtained in the cases where other sliding friction $\mu = 0.1$ and 0.3 are used. Thus, the friction between the particles has very few effects on the results in this investigation, in which the wall friction is ignored.

Then, to verify the validity of the simulation of the flow in porous media, numerically obtained relation between friction factor $\psi$ and particle Reynolds number, $Re$, is shown in Figure 6.9. Only the cases for $i < i_c$ are plotted because the flow inside soils cannot be evaluated after the seepage failure occurs, as described in Figure 6.5. By reference to (Inamuro et al., 1999 [135]), the friction factor $\psi$ is given by

$$\psi = \frac{\Delta p}{\rho u_{in}^2} \frac{D_e}{L} \frac{(1 - \xi)^3}{\xi}, \quad (6.11)$$

where $\Delta p$ is the pressure difference in the zone of the porous media, $D_e$ is the hydraulic diameter and $L$ is the hydraulic length. Then, $Re$ is defined as the following equation.

$$Re = \frac{u_{in} D_e}{\nu \xi}. \quad (6.12)$$

In the regime of the laminar flow, the relationship between the friction factor and $Re$ is
followed by the Blake-Kozeny equation,

$$\psi = \frac{150}{Re}.$$  \hspace{1cm} (6.13)

which is the empirical relation obtained from the laboratory test (Bird et al., 1960 [136]). The solid curve in the figure indicates Equation (6.13). It is apparent from the figure that the simulation result agrees well with the empirical equation. This agreement implies that the spatial resolution used in this investigation is enough to capture the intricate flow at pore-scale. Furthermore, $Re < 1$ for $i < i_c$ in the figure confirms the Darcy relation obtained from the Figure 6.6, since the laminar flow in porous media is defined as $Re < 1$.

### 6.5 Conclusions and future work

In this chapter, I have numerically investigated the boiling phenomena in order to capture the process of the seepage-induced failure of non-cohesive granular soils by means of the direct particle-fluid model. The motion and collision of the solid particles are calculated by
the DEM and the fluid flow of the pore fluid is directly solved at a smaller scale than the particle diameter by the LBM. By coupling DEM and LBM, the interaction with the particle and the fluid is also calculated.

As a result of the analysis of the boiling phenomena of the soils, the proportional relation between the seepage force and the pressure gradient was observed. In addition, the numerically predicted value for the critical hydraulic gradient is in good agreement with the theoretical value. I believe that the qualitative and quantitative analysis can be carried out through the presented direct particle-fluid model without continuum assumptions.

![Figure 6.10](image)

**Figure 6.10** A simulation of the internal erosion of the soils. The simulation area is $3000\delta_x \times 1000\delta_x$. The total number of the particles is about 3,500 and the total calculation step is $3.0 \times 10^6$. The descriptions are at the initial state, at 10 s and at 30 s, respectively.

Then, the process of seepage failure in terms of both the fluid flow and effective stress was also explored. From the distributions of the flow velocity and the evolution of the inlet flow, the boiling onset can be captured. In particular, I found that the rapid change of the flow pattern occurs at around the critical hydraulic gradient. On the other hand, from the
observation of the evolution of the force chains inside the soils, I have demonstrated that the contact networks inside the soils gradually disappear with the increasing the seepage force.

Above discussions are focused on only the boiling phenomena of the soils induced by the upward seepage flow, but the coupled DEM-LBM simulation method can be used for other geo-engineering problems. For example, Figure 6.10 shows that internal erosion of the cohesive geomaterials develops due to the fluid flow in the two dimensions. For the collision law, the linear contact bond model described in Chapter 3 is employed. In such a system, the seepage flow inside the solid phase is much smaller than the flow in the void space at the center. Thus, I assume that the flow inside the solid phase can be ignored. Since the flow is solved at less particle scale, the hydrodynamic force acting on the particle and the particle transport can be simulated in detail. In addition, I plan to introduce the Large Eddy Simulation (LES) model (Yu et al., 2005 [25]) or the two-phase model (Chen and Doolen., 1998 [27]: Inamuro et al., 2004 [28]) to the frame of the partially saturated LB model in order to extend the range of applications. It is thought that such a direct numerical model contributes to the deep understanding of the multiphysics phenomena in the soil mechanics from the microscopic views.
7 Summary and future prospects

The thesis presents the various analyses of the particle based methods for the soil structures and the granular geomaterials. My study is motivated by both (i) the geo-engineering application and (ii) the micromechanics of the soils. In Chapter 3, a simple contact model for the failure criteria of geomaterials were proposed and the relationships between the DEM parameter and the macroscopic parameter were shown. In Chapter 4, I applied the discrete element model to a dry-stone masonry retaining wall, and have demonstrated the shape effect of the blocks comprising the wall under seismic loading; one was a cubic-shaped block and the other was a wedge-shaped block. In Chapter 5, I performed a series of 2-D DEM simulations in order to study the effects of the rolling friction of the particles on granular packing. Through the numerical analyses, I have identified that the rolling resistance plays an important role not only in the shearing process, but also in the packing process. In Chapter 6, the efficiency of the direct particle-fluid approach for the seepage failure of granular soils was confirmed.

![Figure 7.1 A SPH simulation for the break of the column of water.](image)

In future prospects, in terms of the geo-engineering application, I am going to develop other particle based methods in order to broaden a range of applications. For example, I plan to implement the SPH, the MPM or the MPS, which are the mesh-less particle method, so that large scale geo-engineering problems may be managed more effectively. A simulation example of the SPH method for the fluid is presented in Figure 7.1. The DEM is simple
and suitable for the investigations of the micromechanics of soils, but has a limitation of applying to the practical boundary value problems. This is mainly because the physical particle model cannot consider the constitutive law at once. Fortunately, a parallelization scheme for the mesh-less particle methods is almost the same as that for the DEM. Through achieving mastery of several types of the particle based methods, we seek an accomplishment of the flexible choice of the numerical method according to the situation demands.

Figure 7.2 Granular material with a broad size distribution. The particle colored in pink has the smallest size and the particle colored in navy has the largest size. The ratio of the the smallest size to the largest size is ten.

In terms of the micromechanics of the soils, on the other hand, I plan to implement a new simulation method for the granular materials having the broad size distributions (see Figure 7.2) with seepage flow. I am going to solve this challenging issue by combining the different coupling schemes at different levels of scale. In other words, the two types of the coupled particle-fluid models, illustrated in Figure 6.1 (a) and (b), are connected for dealing with the broad size distributions. In addition to the numerical investigations, experimental observations using a X-ray tomography and a image analysis are also to be conducted.
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