Experimental quantification and DEM simulation of micro-macro behaviors of granular materials using x-ray tomography imaging

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ABSTRACT

A non-invasive experimental method and a clustering DEM model were developed in this study to investigate micro-macro behaviors of real granular materials with irregular particle shape configurations. The investigated behaviors include global deformations, failure strengths and residual strengths, stress and strain distributions, local coordination number, local void ratio, particle kinematics, and fabric orientation distributions.

The experimental method includes an approach to automatically identify and recognize multiple particles using x-ray computed tomography imaging (XCT) and an enhanced approach to digitally represent microstructures of granular materials. The digitally represented microstructure can be directly employed for numerical simulation setup. A compression test and a direct shear test on coarse aggregates were conducted and analyzed using this method. The experimental measurements were applied for the evaluation of DEM simulations.

The clustering DEM model provided in this study extends the conventional DEM model by incorporating actual microstructure of materials into simulations. Real irregular particles were represented by clusters of balls in the clustering DEM model while spherical particles were employed in the conventional DEM model. The PFC$^{3D}$ commercial software was applied for 3D DEM simulations of the compression test and the direct shear test.

Compared to the conventional DEM model, the clustering DEM model demonstrated a better capability of predicting both the micro and macro behaviors of granular materials, including dilation, strength, particle kinematics, and fabric evolution.

Fabric distribution was investigated for both the conventional DEM model and the clustering DEM model. The clustering DEM model described the fabric distribution of actual
materials more precisely. This feature enabled it to simulate micro-macro behaviors of materials more accurately.

A theoretic stress-fabric tensor relationship was also evaluated using the simulated stress and fabric distributions based on the actual microstructure of a real material. This relationship incorporated the anisotropic microstructure characteristics of the material. Whether it can better describe behaviors of granular materials was evaluated in this study.

Generally, this research provides a more inherent understanding of granular materials through both DEM simulations and experimental validations.
CHAPTER 1: INTRODUCTION

1.1 Micro and Macro Features of Granular Materials

Granular materials consist of discrete particles that interact only at contact points. Generally, all geomaterials including soils, gravels, and concretes can be treated as granular materials whose micromechanical behaviors are discontinuous and heterogeneous. Research involving granular materials has been carried out to understand engineering problems such as shear banding (Rice 1980; Bardet 1990, 1991; Iwashita 1998), liquefaction (Darve 1996; Lade 2002) and dilatation (Evesque 1993; Oda 1997). Although it has been widely recognized that microfeatures have a significant effect on the overall behavior of granular materials, the relationship between microquantities and macroproperties is not yet well known (Oda and Iwashita 1999). For instance, it has been believed that strain localization leads to shear band formation, but there is a lack of understanding of the micromechanical processes that lead to initiation of shear bands (Rice 1980; Bardet 1990). It has also been observed that different microdeformation fields may result in a same average macrodeformation field (Wang and Chang 2003), but the mechanism leading to this phenomenon is not clear. One reason to the lack of understanding is that microcharacteristics of granular materials are difficult to measure through experimental tests due to the limitation of conventional techniques in obtaining microquantities such as microdisplacements, fabric quantities, and microstrains. Although it has been qualitatively observed that particle rotations in the shear band are very significant and the microrotations of particles may be several times larger than the macrorotations (Oda and Iwashita, 1999; DeJong and Frost, 2002), these findings are limited in a 2D scheme, and few quantitative measurements of the microdeformation of granular materials are available in 3D.
Since imaging technologies, such as x-ray computerized tomography (XCT), have been employed for the non-invasive measurements of internal structures, it became feasible to investigate microfeatures of materials by experiments. Digital correlation methods, however, are required to interpret the image data obtained from experiments, and most of these procedures are still complex and time consuming. One of the challenges for 3D microcharacteristic quantification is to identify individual particles. The existing method for particle identification requires human judgment (Wang 2004). An enhanced method is needed to increase the efficiency to automatically identify and recognize 3D individual particles in experimental tests.

Fabric is of great importance to understand the micromechanical behavior of granular materials. It describes the spatial arrangement of discrete particles. Studies involving fabric anisotropy have been reported in several publications (Oda and Konoshi, 1974; Oda and Konoshi 1998). Fabric tensors were also introduced in granular mechanics to link the granular systems and continua from a deformation point of view (Oda et al. 1982; Mehrabadi et al 1982; Nemat-Nasser et al. 1984). Constitutive models derived from fabric tensors were expected to better describe behaviors of granular materials since those models incorporated the anisotropic microstructure characteristics of materials (Oda, 1989; Zysset and Curnier 1995). Few of these relations, however, have been evaluated for real material systems with irregular particles.

1.2 Continuum and Discrete Approach

With the increasing capability of computer techniques, numerical simulation becomes a more and more popular tool supplementing real tests to investigate the micromechanical behaviors of granular materials. The continuum approach and the discrete approach are two major approaches employed by numerical simulations. Some classic continuum theories have been well developed and widely used. However, continuum analysis of granular materials is very difficult because the calibration of a constitutive model includes lots of material constants.
without clear physical meaning. The discrete approach has an outstanding advantage in understanding micromechanics of granular materials through modeling granular materials as packed assemblies of discrete elements because the particle arrangement can be modeled explicitly and the material constants have clear physical meaning.

1.3 Discrete Element Method (DEM)

Introduced by Cundall (1971), the discrete element method (DEM) is one of the most popular discrete approaches which describe material behaviors directly from particle motions and interparticle forces. Although DEM was originally developed to investigate the validity of various continuum models, it becomes a powerful tool to study the behavior of granular materials by taking into account the interactions among constituents and providing deeper understanding of the granular system at the particle level (Oda 1999). As a matter of fact, it has been increasingly applied to the study of micromechanical behaviors of granular materials (Cundall and Strack 1979; Ghaboussi 1990; Thornton 1992). The fundamental algorithm of DEM is based on the finite difference formulation of the motion equations. It avoids the inversion process for stiffness matrices, which enables it to deal with a large number of particles during simulation. Cundall and Roger (1992) summarized the basic considerations in numerical modeling of discrete element systems.

The first program code based on DEM was developed by Goodman (1968) to model a complex problem with several hundred interfaces. His job could not be strictly called a discrete element method, but his work was a pioneer in this field. A FORTRAN-code called BALL was used as an aid to develop a general constitutive model for granular materials based on micromechanical considerations in the early research (Cunall and Strack 1979b). Later, Cundall and Strack (1979c) developed another FORTRAN-code, TRUBAL, to model the mechanical behavior of 3D assemblies. Other distinct element codes, UDEC (Cundall 1985), DIBS (Walton
1980), 3DSHEAR (Walton 1988) and 3DEC (Hart, R.D and Cundall 1988), PFC$^{3D}$ (Itasca 1999) were mostly developed to model physical systems for soils. Those codes used explicit time-marching to solve the equations of motions directly. Bodies were treated as either rigid or deformable while contacts were deformable. CICE (Hocking 1985) was a representative code whose method was similar to the distinct element method in the case of rigid bodies but model superposition was used for deformable bodies. DDA (Shi 1988) was a code for discontinuous deformation analysis, and it considered the contact to be rigid and the bodies to be either rigid or deformable. The momentum-exchange method, in which both the contacts and the bodies were considered rigid, was applied in frictional sliding (Hahn 1988). PFC$^{3D}$ was used in this study and will be introduced in detail in Chapter 5.

Although the current DEM approach has its outstanding advantage in studying microfeatures of particle packing, it is not sophisticated enough to be used in engineering practice. First of all, the lack of related experimental quantifications makes it difficult to evaluate the accuracy of the simulation results. Some previous studies are restricted to 2D (Ting et al 1993; Bardet 1994), while it is not clear if those findings based on 2D are still valid in 3D simulations. Secondly, few of the previous works are based on real materials. How to accurately represent a real material system with complex-shaped particles in DEM model has not yet been solved. Most of the current DEM approaches use spheres, ellipsoids, or computer generated particle configurations to represent real irregular particles in simulations (Cundall 1971; Cundall and Strack 1979; Thornton 1998; Rothenburg et al. 1989; Mirghasemi, 2002). Since real particles have complex shape, it is necessary to investigate the effect of particle shape on the simulation results. Attempts have been made to simulate elliptical systems in both 2D (Rothenburg 1992) and 3D (Lin and Ng 1997). More complicated particle shapes can be modeled using superquadrics (Williams 1991) or bonding a number of spheres together (Walton and Braun
Although some reasonable results were obtained under those simplified cases, more sophisticated models involving more complicated particle shape are expected. Some research began to consider the effect of particle shape on simulation results, but it could only predict the behavior of granular materials qualitatively (Jensen et al. 2001a, 2001b). Efforts have also been made to simulate the polygon-shaped particles or computer generated irregular particles (Mirghasem 2002; Ni 2000), but few DEM codes were developed based on the real microstructure of the material. The difference between the simulations based on simplified systems and those based on real microstructures is not yet known. How to quantitatively simulate the micromechanic properties of real granular materials, such as microdisplacement and microstrain fields induced by irregular particle shapes, is also a problem.

The clustering DEM model provided in this study incorporated the actual microstructures of materials. Many quantities such as microkinematics, strains, and stresses for irregular particles can be simulated using this model. The fabric and fabric evolution in the clustering DEM model and the conventional DEM model are particularly investigated and compared. The reason is that fabric quantitatively describes microcharacteristics of granular materials and is of great importance to the understanding of macroscopic behaviors.

1.4 Objectives

To solve the problems encountered in previous research on both experimental measurements and numerical simulations, and to improve the understanding of micro-macro mechanical behaviors of granular materials, it is important to establish an enhanced DEM model to simulate real irregular particles, and, at the same time, to develop new experimental methodologies to evaluate the simulation results. Several objectives are included in this research.

The first objective is to develop an experimental measurement method to measure the microquantities of granular materials. The experimental method should include methodologies
for 3D quantification of particle kinematics and local strains and include an enhanced approach for 3D microstructure representation of granular media. The represented microstructure should be applicable in numerical simulation. The experimental methodology should have the ability to detect and recognize multiple particles automatically. A confined compression test and a direct shear test need to be accomplished and analyzed using the experimental methodology.

The second objective is to develop a clustering DEM model to simulate behaviors of granular materials. The clustering DEM model should be able to incorporate the actual microstructure of real materials, in which real irregular particles are represented by clusters of balls. A burn algorithm needs to be developed and employed to improve simulation efficiency by reducing the required number of balls. This algorithm is critical to make the 3D clustering DEM model practical for a typical PC computer.

The third objective is to investigate microcharacteristics and macroproperties of materials using DEM simulations. A more inherent understanding of micro-macro mechanism of granular materials is expected by analyzing the simulation results. The particle shape effect should be studied by comparing the simulation results based on spherical particles and those based on irregularly shaped particles. The input microparameters of the material should be investigated and calibrated based on the macroproperties obtained from the experimental measurements.

The fourth objective is to evaluate the accuracy and validity of DEM simulations by experimental measurements. The confined compression test and the direct shear test need to be simulated by the clustering DEM model and the conventional DEM model respectively. The simulation results of the clustering DEM model is expected to give good agreement with the experimental measurements.

The last objective is to evaluate the theoretical relationship and to interpret the micro-macro behaviors of granular materials from the fabric and fabric evolution points of view. Fabric
describes the spatial arrangement of particles and associated voids. The fabric evolution in the shear zone is of great importance to understand the mechanism of shear banding. By addressing the fabric difference between the clustering DEM model and the conventional DEM model, the particle shape effect on the micromechanism of granular materials can be further understood. Fabric tensors are useful to describe the constitutive relationships of granular materials in continuum mechanics by considering the anisotropic microstructure characteristics. There are various continuum models, but few of them have been verified. This study will evaluate the stress-fabric tensor relationship provided by Mehrabadi et al. (1982), using the simulation results based on real microstructures. It is expected to give an example to apply the DEM simulations for the evaluation of theoretic predictions.

Figure 1-1 illustrates the whole schematic of the above tasks and their correlations.

1.5 Organization of the Dissertation

The contents of this dissertation are organized as following:

Chapter 1: Introduction and Literature Review

Chapter 2: Techniques of the x-ray tomography imaging and image acquiring, image processing, and analysis

Chapter 3: 3D quantification of particle displacements and local strains using x-ray tomography imaging: methodologies and measurements for compression test

Chapter 4: Experimental study of particle kinematics and strain localizations using x-ray tomography imaging: methodologies and quantifications for direct shear test

Chapter 5: DEM theory and the input microparameters calibration

Chapter 6: 3D reconstruction of irregular particles in DEM using x-ray tomography imaging

Chapter 7: DEM simulation of confined compression test and the comparison with the experimental measurements
Chapter 8: DEM simulation of direct shear test and the comparison with the experimental measurements

Chapter 9: Fabric evolution in the DEM simulation of direct shear test and an evaluation of the stress-fabric tensor relation

Chapter 10: Summary, conclusions, and recommendations for further research
Figure 1-1: Schematic of this research work
CHAPTER 2: X-RAY TOMOGRAPHY IMAGING TECHNOLOGY, IMAGE PROCESSING, AND IMAGING ANALYSIS

2.1 Introduction

Imaging technologies have been widely used in the areas of science and engineering such as medicine, physics, chemistry, material science and environment. The most popular tools include radiography, nuclear magnetic resonance (NMR), laser-aided tomography (LAT), and x-ray computed tomography (XCT). The XCT imaging was applied in this study to provide geometric information to represent irregular particles for the DEM simulations, and to provide microstructure for the 3D quantification of particle kinematics in experiments. The detailed description of this technology has been given in the publications of Desrues et al (1996), and Raynaud et al (1989). This chapter briefly introduces the advantage of XCT and its fundamental mechanism as well as the image processing and analysis. Figure 2-1 illustrates the procedure in detail of obtaining microstructure and geometric information through imaging acquisition, image processing and analysis.

2.2 X-ray Computed Tomography Imaging

X-ray computerized tomography (XCT) imaging is an advanced technique acquiring a stack of sectional images of material non-destructively. It was early used in medical diagnosis and medical science and then applied to investigate the microstructures of complex materials. Compared to the conventional destructive methods which can be applied only on the surface of a specimen, XCT has the advantage of acquiring the internal microstructure in a non-destructive manner with high accuracy (Lee and Dass 1993). Compared to other non-destructive techniques such as Magnetic Resonance Imaging (MRI, Lizak et al 1991) and Laser-Aided Tomography (Konagai et al. 1992), XCT imaging has the advantages of powerful penetrating and high sensitivity to material density. Furthermore, the specimen needs no special treatment as MRI
The high resolution of industrial XCT is up to 10 μm which provides the required resolution to measure the details at the individual particle level.

**Figure 2-3: An illustration of the procedure of image processing and image analysis**

An illustration of the mechanism of XCT is presented in Figure 2-2. When an x-ray beam is generated from the x-ray source, the intensity attenuation of the x-ray beam after penetrating a specimen is detected by the detector. During the scanning, the specimen rotates slowly, controlled by the manipulator and the detector records the attenuation profiles for each rotation. According to the attenuation of the x-ray caused by the density difference of the material, the cross-sectional gray images can be constructed numerically from the sets of recorded profiles. The ACTIS imaging system of the XCTIQS Lab in the Department of Civil and Environmental Engineering in Louisiana State University (LSU) is presented in Figure 2-3. The maximum size of specimen for this system is up to 6 inches, and the highest resolution reaches to 10μm.
resolution of 0.2mm was used in this study, which was adequate to capture the shape of coarse aggregates.

Figure 2-2: An illustration of the mechanism of x-ray tomography imaging

Figure 2-3: The ACTIS imaging system of the XCTIQS Lab at LSU
2.3 Image Processing

The gray images acquired by XCT cannot be directly used in the data analysis. Image processing is necessary to obtain the available high quality images. Image Pro Plus is employed in this study for image processing and image analysis. During this processing, gray images were transferred into binary images (black and white images) according to a threshold segmenting voids from solids. The voids are colored white while the aggregates black. In this study, the threshold was determined by human judgment through comparing the gray images and binary images, which is simple and feasible for two-phase material system. There are also other methods to determine the segmentation threshold (Roberts et al. 1984; Jain and Dubuisson 1992; Leu 1992; Lindquist et al. 1996). Additional manipulation is still needed for the binary images in order to remove the noise and completely separate the aggregates. This procedure relies on human judgment. Good quality binary images can be obtained after image processing.

2.4 Image Analysis

Image analysis is applied to obtain geometric information of aggregate cross-sections based on binary images. The geometric measurement includes mass center coordinates, area of aggregate cross-sections and bitmaps. In Bitmap, pixel value of voids is 255 while that of solids is 0. Table 2-1 gives an example of a bitmap of a binary image. The geometric data are essential for the 3D individual particle representation and microquantities quantification. The user-defined macro is helpful to deal with number of images automatically.
Table 2-1: An illustration of the pixel values in the bitmap of a binary image

<table>
<thead>
<tr>
<th>Slice No.5</th>
<th>Column</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>255</td>
</tr>
<tr>
<td>3</td>
<td>255</td>
</tr>
<tr>
<td>4</td>
<td>255</td>
</tr>
<tr>
<td>5</td>
<td>255</td>
</tr>
<tr>
<td>6</td>
<td>255</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>509</td>
<td>255</td>
</tr>
<tr>
<td>510</td>
<td>255</td>
</tr>
<tr>
<td>512</td>
<td>255</td>
</tr>
</tbody>
</table>

Note: pixel value “0” denotes aggregate, “255” denotes voids
CHAPTER 3: EXPERIMENTAL STUDY OF PARTICLE TRANSLATIONS AND LOCAL STRAINS IN COMPRESSION TEST USING X-RAY TOMOGRAPHY IMAGING

3.1 Objectives

The objective of this chapter is to develop a valid experimental method to quantify particle translational displacements and local strains for granular materials. In order to achieve this objective, the first step is to develop a method to automatically identify individual particles with irregular shapes, and then calculate particle kinematics and local strains in 3D scheme by comparing the mass center coordinates and orientations of particles before and after the test.

3.2 Experimental Quantifications

3.2.1 Materials and Experimental Setup

A compression test with lateral sponge confinement on coarse aggregates was conducted to induce the desired particle movements and structural deformation. Limestone aggregates passing 1/2” sieve but retained on 3/8” sieve were used. The aggregates were put into a transparent cylindrical container as shown in Figure 3-1 (100mm high, 103mm diameter), which was especially designed for the convenience of x-ray scanning. A piece of sponge was placed along the inside wall of the container to allow some lateral displacement so that the displacements of individual aggregates would be discernible. Using X-ray tomography imaging technology, 2D images recording the cross sections of the specimen were acquired slice by slice from bottom to top of the specimen. Then a uniform axial load was applied on the top of the aggregates. The physical properties of the load and specimen are presented in Table 3-1. After testing, the specimen was scanned by X-ray again and sectional images of the deformed microstructure were acquired. Based on the images acquired before and after the compression test, particle kinematics and local strains can be obtained using the following methodology.
Figure 3-1: The specimen for confined compression test
<table>
<thead>
<tr>
<th>Limestone Aggregates</th>
<th>Sponge</th>
<th>Container Size (mm)</th>
<th>Axial Load (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size (mm)</td>
<td>Specific Gravity</td>
<td>Number of Aggregate</td>
<td>Young's Modulus (Gpa)</td>
</tr>
<tr>
<td>9.5~12.7</td>
<td>2.674</td>
<td>173</td>
<td>37</td>
</tr>
</tbody>
</table>

### 3.2.2 Particle Identification

After gray images were acquired by XCT, the software named Image Pro Plus was used to process the gray images and obtain the digitalized geometric properties of individual particle cross sections such as the mass center coordinates, and the cross-section area. Each particle cross section \( (i) \) in each slice \( (z) \) was denoted as \( PC(i,z) \). Then the next step was to identify which particle cross sections in sectional slices belong to one particle, namely a 3D reconstruction procedure. A similarity index (SI) method to identify individual particles from a granular media was presented elsewhere (Wang et al. 2004). Further research showed that some enhancement can be made to improve the efficiency. Recognizing that the particle identification was very sensitive to mass center coordinates, a modified SI method was employed here. Two particle cross sections in two adjacent slices were considered to belong to the same particle, if a minimum SI \( (SI_{\text{min}}) \) was obtained using the following equation:

\[
SI(i,z)_{\text{min}} = \min (|x_{i,z} - x_{j,z+1}| + |y_{i,z} - y_{j,z+1}|)
\]

\[
i = 1,2,\cdots n
\]

\[
j = 1,2,\cdots m
\]

where \( n \) and \( m \) represent the number of particle cross sections in adjacent slices \( z \) and \( z+1 \); \( x \), \( y \) are mass center coordinates of the \( i \)th particle in \( z \)th slice or \( j \)th particle in \( (z+1) \)th slice. Using this equation, each particle cross section in slice \( z \) could find its corresponding cross section in slice \( z+1 \).
There still were 3 cases that would confuse the judgment in individual particle identification:

1) A new particle emerged in the \((z+1)\)th slice. In this case, no corresponding particle cross section could be found in the \(z\)th slice (shown as Figure 3-2). Then a new code was assigned to this new particle.

![Figure 3-2: Images showing new particle emerge](image)

2) Existing particle cross sections disappeared in the next slice \((z+1)\). In this case, \(n<m\). One particle cross section in slice \((z+1)\) would correspond to two or more particle cross sections in slice \(z\) with \(SI_{\text{min}}\). Then the pair cross sections \(PC(i,z)\) and \(PC(j,z+1)\) with smallest \(SI_{\text{min}}\) were considered to belong to the same particle. Any other particle cross sections in slice \(z\) corresponding to that particle cross section \(PC(j,z+1)\) were who disappeared in slice \((z+1)\), as Figure 3-3 shows.

3) Existing particle disappeared in the \((z+1)\)th slice while a new particle emerged in that slice almost at the same location (having similar mass center coordinates, shown as Figure 3-4). Then the trend of the area change of the particle cross-section at slice \(z-1\), \(z\), \(z+1\), \(z+2\) was traced. In this case, the trend must satisfy the relationship:
Area_{z-1,i} > Area_{z,i} \& Area_{z+1,i} < Area_{z+2,i} \), otherwise those cross sections were still considered to belong to the same particle.

The whole procedure is presented as a flow chart in Figure 3-5.

Figure 3-3: Images showing old particle disappear

Figure 3-4: Images showing old particle disappear and new particle emerge at the same location
Figure 3-5: Flow chart to identify individual particles

Input $X_{zi}$, $Y_{zi}$, $Z_{zi}$, $Z_{zi}$, $Area_{zi}$,

$SI_{zi} = |X_{z+1,i} - X_{zi}| + |Y_{z+1,i} - Y_{zi}|$

For particle $i$ in slide $z$, find minimum $SI_{zi}$

If more than one $P_i$ in the $z$ slide points to the same particle $P_j$ in the $z+1$ slide

Smallest $SI_{\text{min}}$?

$N_{\text{next}}_{zi} = 0$, $SI_{\text{min}} = -1$

$N_{\text{next}}_{zi} = N_{pj}$

$Area_{z-1,j} > Area_{zi}$

$Area_{z+1,k} > Area_{z+2,l}$

$SI_{\text{min}} > SI_0$?

$P_{zi} = N_{\text{next}}_{z-1,j}$

Output $P_{zi}$, Number of slides that $P_i$ occupies; $&$ Code of $P_i$, mass center, Area for each particle shown in each slide.

20
Based on the above method, a FORTRAN program was developed to identify individual particles from those measured data automatically. Each identified particle was assigned a code $k$ ($k = 1, 2, 3...$). With this code, the corresponding mass center and area of cross section $i$ for particle $k$ in image slice $z$ could be found. Table 3-2 presents the calculated $S_{\text{min}}$ between pairs of particle cross sections in slice No.70 and slice No.71. Table 3-3 presents the geometrical information for the identified cross-sections of particle No.50 in sectional slices. With those data, the microstructure of specimen could be represented, which is essential for experimental quantification and numerical simulation.

### 3.2.3 Quantification of Particle Kinematics in 3D

After being sustained a compression force, the microstructure of the granular material would change accordingly. If the change of locations and orientations of the individual particles were recorded, the kinematics of the particles could then be calculated based on mathematical relationships. For this confined compression test, the particle displacements were relative small compared to the size of the particles, and the coordinates of the mass center of individual particles changed little in radial direction. Judgment can still be made based on a SI method for recognizing individual particles. A particle similarity index ($S_{\text{Ip}}$) was defined as follows:

$$S_{\text{Ip}} = \left| x_b - x_a \right| + \left| y_b - y_a \right| + \left| z_b - \left( z_a + \frac{\Delta h}{h} \ast z_a \right) \right|$$

(3-2)

where $x_b, y_b, z_b =$ mass center coordinates of individual particles before test

$x_a, y_a, z_a =$ mass center coordinates of individual particles after test

$\Delta h =$ vertical global deformation of the specimen

$h =$ height of the specimen.
Table 3-2: Example of connection status of particle cross-sections between two adjacent slices

<table>
<thead>
<tr>
<th>Particle cross-section i</th>
<th>SI\textsubscript{min}</th>
<th>Particle cross-section j</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.31</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0.37</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>0.21</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>0.57</td>
<td>4</td>
</tr>
<tr>
<td>5</td>
<td>0.37</td>
<td>5</td>
</tr>
<tr>
<td>6</td>
<td>0.04</td>
<td>6</td>
</tr>
<tr>
<td>7</td>
<td>0.58</td>
<td>7</td>
</tr>
<tr>
<td>8</td>
<td>0.91</td>
<td>8</td>
</tr>
<tr>
<td>9</td>
<td>0.49</td>
<td>9</td>
</tr>
<tr>
<td>10</td>
<td>0.42</td>
<td>10</td>
</tr>
<tr>
<td>11</td>
<td>0.87</td>
<td>11</td>
</tr>
<tr>
<td>12</td>
<td>-1*</td>
<td>0*</td>
</tr>
<tr>
<td>13</td>
<td>0.49</td>
<td>12</td>
</tr>
<tr>
<td>14</td>
<td>0.21</td>
<td>13</td>
</tr>
<tr>
<td>15</td>
<td>1.05</td>
<td>15</td>
</tr>
<tr>
<td>16</td>
<td>0.21</td>
<td>14</td>
</tr>
<tr>
<td>17</td>
<td>0.29</td>
<td>16</td>
</tr>
<tr>
<td>18</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>19</td>
<td>0.28</td>
<td>17</td>
</tr>
<tr>
<td>20</td>
<td>0.4</td>
<td>19</td>
</tr>
<tr>
<td>21</td>
<td>0.51</td>
<td>18</td>
</tr>
<tr>
<td>22</td>
<td>1.09</td>
<td>20</td>
</tr>
<tr>
<td>23</td>
<td>0.07</td>
<td>21</td>
</tr>
<tr>
<td>24</td>
<td>0.38</td>
<td>22</td>
</tr>
<tr>
<td>25</td>
<td>0.39</td>
<td>23</td>
</tr>
<tr>
<td>26</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>

Note: This table shows that particle cross-section i in slice 70 and j in slice 71 belong to the same particle. SI is the minimum similarity index calculated between cross-section i and j. If SI\textsubscript{min} = -1 & j = 0, it means that particle disappears in slice No.71.
Table 3-3: The areas and mass centers of all cross-sections of particle No.50

<table>
<thead>
<tr>
<th>slice No. (z)</th>
<th>cross-section No. (i)</th>
<th>Area (mm$^2$)</th>
<th>center-x (mm)</th>
<th>center-y (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>57</td>
<td>11</td>
<td>5.38</td>
<td>2.75</td>
<td>38.93</td>
</tr>
<tr>
<td>58</td>
<td>11</td>
<td>27.05</td>
<td>6.63</td>
<td>37.73</td>
</tr>
<tr>
<td>59</td>
<td>12</td>
<td>74.31</td>
<td>10.15</td>
<td>37.13</td>
</tr>
<tr>
<td>60</td>
<td>11</td>
<td>89.23</td>
<td>11.49</td>
<td>36.65</td>
</tr>
<tr>
<td>61</td>
<td>11</td>
<td>96.66</td>
<td>11.87</td>
<td>36.37</td>
</tr>
<tr>
<td>62</td>
<td>12</td>
<td>96.7</td>
<td>12.11</td>
<td>36.01</td>
</tr>
<tr>
<td>63</td>
<td>12</td>
<td>85.14</td>
<td>11.58</td>
<td>35.66</td>
</tr>
<tr>
<td>64</td>
<td>13</td>
<td>75.15</td>
<td>11.44</td>
<td>35.21</td>
</tr>
<tr>
<td>65</td>
<td>13</td>
<td>63.78</td>
<td>10.88</td>
<td>34.95</td>
</tr>
<tr>
<td>66</td>
<td>14</td>
<td>53.6</td>
<td>10.19</td>
<td>34.63</td>
</tr>
<tr>
<td>67</td>
<td>14</td>
<td>44.48</td>
<td>9.13</td>
<td>33.95</td>
</tr>
<tr>
<td>68</td>
<td>14</td>
<td>38.11</td>
<td>8.76</td>
<td>33.44</td>
</tr>
<tr>
<td>69</td>
<td>15</td>
<td>30.75</td>
<td>8.36</td>
<td>33.01</td>
</tr>
<tr>
<td>70</td>
<td>15</td>
<td>23.04</td>
<td>7.45</td>
<td>32.44</td>
</tr>
<tr>
<td>71</td>
<td>15</td>
<td>15.98</td>
<td>5.98</td>
<td>31.65</td>
</tr>
<tr>
<td>72</td>
<td>16</td>
<td>9.57</td>
<td>4.74</td>
<td>31.28</td>
</tr>
<tr>
<td>73</td>
<td>16</td>
<td>4.12</td>
<td>2.8</td>
<td>31.23</td>
</tr>
</tbody>
</table>

Note: This table presents cross-section i in slice z belonging to particle No.50 and its corresponding area and mass center coordinates.
The pair of particles giving the smallest SIₚ was considered to be the same particle. If two or more particles after testing were paired to the same original particle, then their volumes were compared and the one whose volume was closest to that original particle was recognized. The above process was repeated till all the particles after testing were recognized. The detailed calculation flow chart is presented in Figure 3-6.

The volumes and mass centers of the individual particles were calculated using following equations:

\[
V_k = \sum \left( \left(\text{Area}_{z-1,i} + \text{Area}_{z,i} \right) \Delta H_{z-1,i} / 2 \right) \quad (3-3)
\]

\[
X_{c_k} = \frac{1}{V_k} \sum \left( \left(\text{Area}_{z-1,i} + \text{Area}_{z,i} \right) \Delta H_{z-1,i} \left( X_{z-1,i} + X_{z,i} \right) / 4 \right) \quad (3-4)
\]

\[
Y_{c_k} = \frac{1}{V_k} \sum \left( \left(\text{Area}_{z-1,i} + \text{Area}_{z,i} \right) \Delta H_{z-1,i} \left( Y_{z-1,i} + Y_{z,i} \right) / 4 \right) \quad (3-5)
\]

\[
Z_{c_k} = \frac{1}{V_k} \sum \left( \left(\text{Area}_{z-1,i} + \text{Area}_{z,i} \right) \Delta H_{z-1,i} \left( Z_{z-1,i} + Z_{z,i} \right) / 4 \right) \quad (3-6)
\]

where \( \Delta H \) = space between two adjacent slice

\( V_k \) = volume of particle \( k \)

\( Xc, Yc, Zc \) = mass enter coordinates of particle \( k \).

The particle translations can then be calculated as

\[
\text{DISP}_k = \sqrt{u_k^2 + v_k^2 + w_k^2} \quad (3-7)
\]

where \( u = Xc^a - Xc^b ; v = Yc^a - Yc^b ; w = Zc^a - Zc^b \), and the superscript “a” denotes after the deformation and “b” denotes before the deformation.
Input $X_{z,i}, Y_{z,i}, Z_{z,i},$ Area $z,i, P_{z,i}, H_{z,i}$

\[ V_k = \sum (\text{Area}_{z,j} + \text{Area}_{z,j})H_{z+1,j}/2 \]
\[ X_c_k = \frac{1}{V_k} \sum (\text{Area}_{z,j} + \text{Area}_{z,j})H_{z+1,j}(X_{z,j} + X_{z,j})/4 \]
\[ Y_c_k = \frac{1}{V_k} \sum (\text{Area}_{z,j} + \text{Area}_{z,j})H_{z+1,j}(Y_{z,j} + Y_{z,j})/4 \]
\[ Z_c_k = \frac{1}{V_k} \sum (\text{Area}_{z,j} + \text{Area}_{z,j})H_{z+1,j}(Z_{z,j} + Z_{z,j})/4 \]

\[ SI_p = |X^b_c - X^a_c| + |Y^b_c - Y^a_c| + |Z^b_c - (Z^a_c + \Delta h/k \cdot Z^a_c)| \]

Pair of particles giving the minimum $SI_p$?

\[ P(P_k^b) = P_k^a \]

If two $P_k^a$ points to the same original particle

\[ P(P_k^b) = P_k^a \]

Output

Particle $P_k^a$ (after test) corresponding to original particle $P_k^b$;
Displacements of particle $P_k$ in $x, y, z$ direction after test.

Figure 3-6: Flow chart to recognize particles after test
The Particle rotation (microrotation) vector \( \vec{\Omega} \) can be obtained from the following relation:

\[
\Delta \vec{\Omega} = \vec{\Omega}_b - \vec{\Omega}_a
\]

(3-8)

where \( \Delta \vec{\Omega} \) = particle rotation vector.

\( \vec{\Omega}_b \) = orientation of the individual particle in initial configuration

\( \vec{\Omega}_a \) = orientation of the individual particle in deformed configuration.

### 3.2.4 Computation of Micromotions and Local Strains in 3D

A two-dimensional (2D) experimental method was developed by Wang et al (1999) to measure the particle translational displacements and rotations by comparing images of the cross sections of a specimen acquired before and after the test. The measured displacements were then used to compute the local strains in a 2D scheme. The studied material was a weakly bonded granular material (asphalt concrete). Figure 3-7 presents the algorithm of the method, and details about the method can be found elsewhere (Wang et al. 1999). The 2D method can be extended to 3D by including the motions in z direction. Local strains can be computed following the Finite Element Method (FEM). When four adjacent particles form a tetrahedron (4 nodes, i.e. Figure 3-8), the local strain components can be computed by treating the four mass centers as the four nodes of the tetrahedron element, using the following equations:

\[
\varepsilon_x = \frac{\partial u}{\partial x} = a_1; \quad (3-9.a)
\]

\[
\varepsilon_y = \frac{\partial v}{\partial y} = b_2; \quad (3-9.b)
\]

\[
\varepsilon_z = \frac{\partial w}{\partial z} = c_3 \quad (3-9.c)
\]
\[ \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) = \frac{b_1 + a_1}{2}; \]  

(3-9.d)

\[ \varepsilon_{xz} = \frac{1}{2} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) = \frac{a_3 + c_1}{2}; \]  

(3-9.e)

\[ \varepsilon_{yz} = \frac{1}{2} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) = \frac{b_3 + c_2}{2} \]  

(4) \hspace{2cm} (3-9.f)

where \( a_0, a_1, a_2; b_0, b_1, b_2; c_0, c_1, c_2 \) can be obtained by solving the following linear equations:

\[
\begin{bmatrix}
1, x_i, y_i, z_i \\
1, x_j, y_j, z_j \\
1, x_k, y_k, z_k \\
1, x_l, y_l, z_l
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2 \\
a_3
\end{bmatrix}
= 
\begin{bmatrix}
u_i \\
v_j \\
v_k \\
v_l
\end{bmatrix}; \hspace{2cm} (3-10.a)
\]

\[
\begin{bmatrix}
1, x_i, y_i, z_i \\
1, x_j, y_j, z_j \\
1, x_k, y_k, z_k \\
1, x_l, y_l, z_l
\end{bmatrix}
\begin{bmatrix}
b_0 \\
b_1 \\
b_2 \\
b_3
\end{bmatrix}
= 
\begin{bmatrix}
v_i \\
v_j \\
v_k \\
v_l
\end{bmatrix}; \hspace{2cm} (3-10.b)
\]

\[
\begin{bmatrix}
1, x_i, y_i, z_i \\
1, x_j, y_j, z_j \\
1, x_k, y_k, z_k \\
1, x_l, y_l, z_l
\end{bmatrix}
\begin{bmatrix}
c_0 \\
c_1 \\
c_2 \\
c_3
\end{bmatrix}
= 
\begin{bmatrix}
w_i \\
w_j \\
w_k \\
w_l
\end{bmatrix}; \hspace{2cm} (3-10.c)
\]

The global strains of the entire specimen are measured by:

\[ \varepsilon_1 = \frac{\Delta h}{h} \]  

(3-11.a)

\[ \varepsilon_2 = \varepsilon_3 = \frac{\Delta r}{r} \]  

(3-11.b)

\[ \varepsilon_{12} = \varepsilon_{13} = \frac{\varepsilon_1 - \varepsilon_2}{2} \]  

(3-11.c)

where \( \Delta h, h = \) vertical displacement and the height of the specimen;

\[ \Delta r, r = \) displacement in the radial direction and the radius of the specimen. \]
Figure 3-7: Illustration of the algorithm for measuring the translational and rotational displacements and strains (Wang et al. 1999)

Figure 3-8: Illustration of 3D motions of 4 adjacent particles during compression test
The global volumetric strain is defined as:

\[ \varepsilon_v = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = \varepsilon_1 + 2\varepsilon_2 \]  \hspace{1cm} (3-12)

The global volumetric strain can also be calculated from the sum of weighted local volumetric strain by the following equation:

\[ \varepsilon_v = \sum V_{\beta} \varepsilon^l_{\beta} = \sum V_{\beta} (\varepsilon^l_{1\beta} + \varepsilon^l_{2\beta} + \varepsilon^l_{3\beta}) \]  \hspace{1cm} (3-13)

where \( \varepsilon_v \) = global volumetric strain calculated from local volume strain

\( V_{\beta} \) = volumetric fraction of each local volume to the total volume

\( \varepsilon^l_{i} \) = local strain in tetrahedron i.

Comparing the global volumetric strain calculated by direct measurements and that calculated by weighted local volumetric strains, the local strain quantification methodology can be evaluated.

3.3 Experimental Results Analysis

Following Equation 3-3, 3-4, 3-5 and 3-6, the mass center coordinates and volumes of individual aggregates were calculated. The displacements of those aggregates were calculated by Equation 3-7. The calculated mass center coordinates and the displacements for 30 individual particles are shown in Table 3-4. The initial sample porosity \( n \) was calculated as following:

\[ n = 1 - \frac{V_s}{V_T} \]  \hspace{1cm} (3-14)

where \( V_s \) = volume of solids, \( V_T \) = volume of the entire specimen. The volume of solids could be calculated by two different methods. Using bulk specific gravity, it was calculated by the classic equation \( V_s = \frac{m_s}{G_s \times G_w} \), where \( m_s \) = mass of particles; \( G_s \) = bulk specific gravity; \( G_w \) = mass of a unit volume of water. Using area of particle cross sections obtained by image analysis, the
volume of each particle $V_p$ could also be calculated by Equation 3-3. The volume of solids was then calculated as $V_s = \sum V_p$. The sample porosity calculated was 49.6% by bulk specific gravity and 50.3% by image analysis. Their difference is very small, thus the data obtained from imaging technology are valid to certain degree for further calculation.

The local macrostrains in each tetrahedron, calculated by Equation 3-9 are shown in Table 3-5. The local strains $\varepsilon_x$ at height $z = 45 \sim 55$ mm were projected on x-y plane, which are presented as contour in Figure 3-9. It was found that strain $\varepsilon_x$ showed a tendency of dilation from center to edge but there still was a small contraction at the edge due to the boundary confinement. Figure 3-10 presents the contour of strain $\varepsilon_z$ at $y = 45 \sim 55$ mm projected on x-z plane. Most of the regions show a tendency of strain contraction and most of the contraction occurred at the top of the specimen. Strain dilation also exists in the center region.

In Figure 3-10, a vertical line was drawn at $x = 50$ mm from top to bottom, and the values of local strain $\varepsilon_z$ at the vertical line were read every 10 mm (i.e. $dz = 10$ mm). Then the total deformation of z direction can be calculated as $\Delta z = \sum \varepsilon_z dz = -9.2 \text{mm}$, which is close to the measured vertical deformation, 9.8 mm. The global volumetric strain calculated by Equation 3-12 is 0.047 while that calculated by equation 3-13 is 0.052, which is also close to each other. Thus the methods to quantify the local strains are validated to certain degree.

3.4 Summary and Conclusions

Using x-ray tomography imaging, methodologies for individual particle representation, particle kinematics and local strain quantification were developed for the results analysis of a compression test. These methodologies make it practical to investigate the macro-micro behavior of granular materials by experiments. The quantified particle translational displacements and
local strains are reasonable. With these methodologies, it becomes feasible for experimental validation of the continuum theory in true 3D and the quantitative accuracy of numerical simulation.

Table 3-4: The mass center coordinates and the displacements for individual particles obtained from experimental test

<table>
<thead>
<tr>
<th>Agg.No.</th>
<th>Coordinates of the Mass center (mm)</th>
<th>Displacement in x,y,z direction (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>x</td>
<td>y</td>
</tr>
<tr>
<td>1</td>
<td>46.15</td>
<td>29.55</td>
</tr>
<tr>
<td>2</td>
<td>56.19</td>
<td>34.22</td>
</tr>
<tr>
<td>3</td>
<td>39.01</td>
<td>33.28</td>
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<tr>
<td>4</td>
<td>29.51</td>
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<td>5</td>
<td>65.51</td>
<td>37.97</td>
</tr>
<tr>
<td>6</td>
<td>50.78</td>
<td>47.22</td>
</tr>
<tr>
<td>7</td>
<td>72.69</td>
<td>47.58</td>
</tr>
<tr>
<td>8</td>
<td>30.07</td>
<td>48.18</td>
</tr>
<tr>
<td>9</td>
<td>41.34</td>
<td>50.11</td>
</tr>
<tr>
<td>10</td>
<td>61.13</td>
<td>52.16</td>
</tr>
<tr>
<td>11</td>
<td>70.06</td>
<td>56.57</td>
</tr>
<tr>
<td>12</td>
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<td>63.49</td>
</tr>
<tr>
<td>13</td>
<td>51.54</td>
<td>60.31</td>
</tr>
<tr>
<td>14</td>
<td>53.85</td>
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<td>66.35</td>
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<td>52.25</td>
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<tr>
<td>17</td>
<td>38.80</td>
<td>42.14</td>
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<tr>
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<td>34.35</td>
<td>66.85</td>
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<td>57.04</td>
</tr>
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<td>69.94</td>
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</tr>
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<td>50.64</td>
<td>44.38</td>
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Note: this table only presents calculated results of 30 particles.
Table 3-5: The local macrostrains and macrorotations from experimental test

<table>
<thead>
<tr>
<th>No.</th>
<th>$\varepsilon_x$</th>
<th>$\varepsilon_y$</th>
<th>$\varepsilon_z$</th>
<th>$\varepsilon_{xy}$</th>
<th>$\varepsilon_{yz}$</th>
<th>$\varepsilon_{xz}$</th>
<th>$\Delta\alpha$</th>
<th>$\Delta\beta$</th>
<th>$\Delta\gamma$</th>
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<td>-0.12</td>
<td>0.05</td>
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</tr>
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<td>-0.21</td>
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<td>0.12</td>
<td>0.23</td>
<td>0.14</td>
<td>-0.07</td>
</tr>
</tbody>
</table>

Note: this table only presents calculated results of 30 particles.
Table 3-6: Comparison of coordination number between DEM simulation and experiment measurements

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiments</th>
<th>DEM-Sphere</th>
<th>DEM-Irregular Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>coordination number(before test)</td>
<td>4.930</td>
<td>3.030</td>
<td>4.930</td>
</tr>
<tr>
<td>coordination number(after test)</td>
<td>6.130</td>
<td>6.710</td>
<td>6.650</td>
</tr>
<tr>
<td>change</td>
<td>1.200</td>
<td>3.680</td>
<td>1.720</td>
</tr>
</tbody>
</table>

Table 3-7: Comparison of macroproperties between DEM simulation and experimental measurements

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiments</th>
<th>DEM-irregular</th>
<th>%Relative diff.</th>
<th>DEM-sphere</th>
<th>%Relative diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical contraction(mm)</td>
<td>9.800</td>
<td>9.230</td>
<td>5.816</td>
<td>12.300</td>
<td>25.510</td>
</tr>
<tr>
<td>Radial dilation(mm)</td>
<td>0.780</td>
<td>0.730</td>
<td>6.410</td>
<td>1.090</td>
<td>39.744</td>
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<tr>
<td>Global Volume Strain</td>
<td>-0.041</td>
<td>-0.039</td>
<td>4.368</td>
<td>-0.044</td>
<td>6.652</td>
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<td>change of porosity</td>
<td>0.024</td>
<td>0.023</td>
<td>5.859</td>
<td>0.027</td>
<td>13.858</td>
</tr>
</tbody>
</table>
Figure 3-9: $\varepsilon_x$ contour in XY plane-experimental result
Figure 3-10: $\varepsilon_z$ contour in XZ plane-experimental results
CHAPTER 4: EXPERIMENTAL STUDY OF PARTICLE KINEMATICS AND STRAIN LOCALIZATION IN THE DIRECT SHEAR TEST

4.1 Objectives

A Direct Shear Test was conducted and analyzed in order to achieve two objectives. The first one was to develop a new 3D methodology to quantify particle orientations, particle rotations, and strain localizations in the shear band. The second objective was to use the methodology to obtain the microstructure of the specimen and to investigate particle kinematics, localized strains, global strength, and global deformations in the post failure stage.

4.2 Introduction

Shear banding is a localized phenomenon occurring in a limited zone in loaded materials where sufficient deformation is spontaneously accumulated. The appearance of shear banding alters behaviors of geomaterials so considerably that it can not be neglected in both experimental tests and theoretical studies (Oda 1999). Much research has been conducted to study features of the shear band. However, previous research on shear band has mainly been limited to macroscopic properties such as the shear band angle (Vardoulakis 1980; Bardet 1991), thickness (Muhlhaus and Vardoulakis 1987), and local void ratio change (Desrues et al. 1996). The microproperties of the shear band were not studied until recent decades due to the lack of ability to measure the microquantities in earlier days. Oda (1997) and Oda and Kazama (1998) reported findings about the microstructure developed in the shear band: extremely large voids were observed in shear bands; particle orientation changed sharply at the shear band boundaries; a high gradient of particle rotation can be developed in a relatively narrow zone. Their studies contributed to the development of micromechanical theories about the shear band but their material systems were limited to ideal disks. Since natural materials are composed of 3D
irregular particles, how the particle shape affects shear banding in 3D needs to be investigated. Thanks to the development of image technologies, the 3D quantification of irregular particle kinematics becomes possible. To study the microcharacteristics of shear banding at the post-failure stage, a direct shear test was conducted on coarse aggregates. The test procedure followed American Society for Testing and Materials Standards (ASTM, 1991). The sample was scanned by XCT both before and after shearing. The original microstructure and the deformed microstructure of the material were then acquired. Following the 3D quantification method, the particle translations, rotations, as well as local strains were obtained.

4.3 Materials and Experimental Setup

River gravels passing the 1/2”-sieve and retaining on the 3/8”-sieve were used as loaded materials. The physical properties of materials are presented in Table 4-1. A Direct Shear Apparatus EL28-007 series was used for this test, as illustrated in Figure 4-1. Normal forces applied were 2 kg, 12 kg, 32 kg, and 52 kg, respectively. The relative lateral displacement was 9 mm. Displacement rate equaled to 0.12mm/sec.

<table>
<thead>
<tr>
<th>Material</th>
<th>Agg. Size (mm)</th>
<th>Agg. Specific Gravity</th>
<th>Young's Modulus</th>
<th>Weight (g)</th>
<th>Porosity (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crushed River Gravel</td>
<td>9.5–12.7</td>
<td>2.528</td>
<td>60 Gpa</td>
<td>1878</td>
<td>44.4</td>
</tr>
</tbody>
</table>

A special shear box was designed for the test with a size of 5” × 5” × 2.5” (127 mm × 127 mm × 63.5 mm). It was made from plexiglas which can be penetrated easily by x-rays (Figure 4-2). The size of the shear box was carefully chosen to meet the requirement of both the ASTM standard D3080-90 (1991) and the XCT machine. The ASTM standard requires that the width of the shear box should not be less than 10 times the maximum particle size.
Figure 4-1: The ELE direct shear apparatus EL28-007 series

Figure 4-2: The shear box and the material used in the direct shear test
Aggregates were put into the shear box and compacted by a 5 lb compact hammer until the desired unit weight was obtained. A normal force was then applied on the top of the specimen. The top box was fixed, and the bottom box was pushed along the horizontal direction. The relative lateral displacement and shear force between two boxes were monitored automatically during shearing by a data acquisition system named Wave book/512™ 12-bit 1MHZ, as illustrated in Figure 4-3. The specimen (shear box with compacted crushed aggregates) was scanned by XCT before and after shearing. Figure 4-4 presents the sectional gray images acquired by XCT.
4.4 3D Quantification of Particle Rotations

Using the sectional images obtained before and after shearing, it is able to quantify particle translations, rotations, as well as local strains. The methodology to quantify particle translations and local strains has been presented in Chapter 3. The method to quantify particle rotations is developed in this section. Three tasks need to be achieved in order to quantify particle rotations, i.e. particle boundary detection, particle orientation quantification, and particle reorganization after the test.
4.4.1 3D Detection of the Particle Boundary

After gray images were acquired by XCT, they were converted into binary images (black/white images) through image processing. Each binary image was divided into $512 \times 512$ grids which represent 26214 pixels. Each pixel was assigned a value representing the level of grayness or brightness of this pixel, ranging from 0 (which means completely black), to 255 (which means completely white). In each image slice, connected pixels with a value of 0 on the same row were considered as a subparticle, and its beginning and end columns were recorded (refer to Table 4-2 in this Chapter and Table 2-1 in Chapter 2).

Table 4-2: Illustration of identifying particle cross section in one image slice

<table>
<thead>
<tr>
<th>Slice No.5</th>
<th>Column</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 2 3 4 5 6 ... 509 510 512</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>P1</td>
</tr>
<tr>
<td>4</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td></td>
</tr>
<tr>
<td>Row 6</td>
<td>... ... ... ... ... ... ... ... ... ... ...</td>
</tr>
<tr>
<td>509</td>
<td>P3</td>
</tr>
<tr>
<td>510</td>
<td>P4</td>
</tr>
<tr>
<td>512</td>
<td></td>
</tr>
</tbody>
</table>

Comparing two subparticles at the neighbor rows with beginning columns of $BC(i,k)$ and $BC(i+1,j)$ and the end columns $EC(i,k)$ and $EC(i+1,j)$, if any one of the following formulas was
satisfied, subparticle \( k \) in row \( i \) and subparticle \( j \) in row \( i+1 \) were considered to belong to the same particle.

\[
\begin{align*}
BC(i + 1, j) &< BC(i, k) < EC(i + 1, j) \\
BC(i + 1, j) &< EC(i, k) < EC(i + 1, j) \\
BC(i, k) &< EC(i + 1, j) < EC(i, k) \\
BC(i, k) &< BC(i + 1, j) < EC(i, k)
\end{align*}
\]  

(4-1)

Connected subparticles in each slice were considered as one particle cross section and were assigned a sole code \( N_z \) (refer to table 4-2). The subscript “\( z \)” denotes slice number. Then each particle cross section was specified in terms of the slice number \( Z \), the beginning row \( R_b \) and the end row \( R_e \) (the value is between 1 and 512), as well as the beginning column and the end column \( C_e \) (the value is between 1 and 512) of each row that it occupied.

Using software Image Pro Plus, the mass center and the area of each particle cross section could be obtained. Following the procedure provided in Chapter 3 (compression test), based on the mass center and the area transition of the particle cross section, particle cross sections in sectional slices belonging to the same particle were identified (refer to Table 4-3).

The particle boundary points were recorded by a boundary function

\[
P(Z, N_z) = f(R_b, R_e, C_b, C_e, Z)
\]  

(4-2)

where \( z = \text{slice No;} \) \( N_z = \text{code assigned for particle cross sections in each slice} \)

The global coordinates of each boundary point could also be written as

\[
\begin{align*}
x(P) &= R \\
y(P) &= C \\
z(P) &= Z
\end{align*}
\]  

(4-3)

where \( R = \text{number of row} \)

\( C = \text{number of column} \)

\( Z = \text{number of slice}. \)
Table 4-3: Description of particle boundary occupied in sectional image slices

<table>
<thead>
<tr>
<th>Particle No.8</th>
<th>Begin Slice=1,</th>
<th>End Slice=9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slice No1</td>
<td>Column</td>
<td>Rb</td>
</tr>
<tr>
<td></td>
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<td>234</td>
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<td></td>
<td>108</td>
<td>227</td>
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<td></td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Slice No2</td>
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<td>231</td>
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<tr>
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<td>100</td>
<td>228</td>
</tr>
<tr>
<td></td>
<td>101</td>
<td>228</td>
</tr>
<tr>
<td></td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Slice No3</td>
<td>89</td>
<td>230</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>227</td>
</tr>
<tr>
<td></td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Slice No9</td>
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<td></td>
<td>107</td>
<td>229</td>
</tr>
<tr>
<td></td>
<td>108</td>
<td>231</td>
</tr>
</tbody>
</table>
4.4.2 Procedure of 3D Quantification of Particle Rotations

The particle rotation (microrotation) vector $\vec{\Omega}$ can be calculated from following relation:

\[ \Delta \vec{\Omega} = \vec{\Omega}_b - \vec{\Omega}_a \]  

(4-4)

where $\Delta \vec{\Omega}$ = particle rotation vector

$\vec{\Omega}_b$ = orientation of the individual particle in initial configuration

$\vec{\Omega}_a$ = orientation of the individual particle in deformed configuration.

The orientation of the individual particle is defined as the orientation of the feret length (maximum length) of that particle. When the boundary points of each particle were known, its feret length could be calculated using the equations below:

\[ d_i = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \]  

(4-5)

\[ L_{\max} = \max(d_i) \quad i = 1, 2, \ldots, n \]

where $d_i$ = distance between boundary point $i$ and $j$, ($i \neq j$)

$L_{\max}$ = feret length of individual particle.

The orientation angle of feret length is calculated as:

\[ \theta_x = \cos^{-1}\left(\frac{x_b - x_e}{L_{\max}}\right) \]  

(4-6a)

\[ \theta_y = \cos^{-1}\left(\frac{y_b - y_e}{L_{\max}}\right) \]  

(4-6b)

\[ \theta_z = \cos^{-1}\left(\frac{z_b - z_e}{L_{\max}}\right) \]  

(4-6c)

\[ \theta \in (0, \pi) \]

where $b, e$ = particle surface points which give the maximum distance
\[ \theta = 3 \text{ components of orientation angle.} \]

The difficulty became how to identify the pair of surface points after the particle had certain movement. Because of the unavoidable error gained from the image processing, the feret length calculated before the test and that after the test may not be exactly the same. Similarly, the pair of surface points detected after the test may not the same as that detected before the test, which directly leads to a miscalculation of the particle orientation. To improve the accuracy, the methodology below was developed to reduce the risk of misidentifying pair of surface points.

Step 1: Following a procedure similar to the one used in chapter 3, identify the particles after they have movements.

Step 2: For particle \( i \) before the test, find its feret length according to the particle outline and identify two end points \( e1, e2 \) and one midpoint \( m \) in feret length. Via the midpoint, draw an imaginary line perpendicular to the feret length, crossing the particle surface at point \( v1 \) and point \( v2 \) respectively. Calculate the distance from point \( v1 \) to \( m \) and the distance from point \( v2 \) to \( m \) (refer to Figure 4-5a).

Step 3: For particle \( i \) after the test, following the same procedure used in Step 2, find three possible feret lengths and their perpendicular lines as well as the corresponding end points and midpoints. Calculate the distances from the end points to the midpoints respectively (Figure 4-5 b).

Step 4: Define a similarity index of orientation \( (SIO = |L_{v1,m}^a - L_{v1,m}^b| + |L_{v2,m}^a - L_{v2,m}^b|) \), where \( L = \) distance from the end point of perpendicular line to the midpoint; superscript “\( a \)” denotes status after the test, and superscript “\( b \)” denotes status before the test. Comparing the three calculated SIO, choose the smallest one. The feret length giving the smallest SIOs (SIO\(_{\text{min}}\)) is considered as the same feret length detected before test.
Figure 4-5: An illustration of the procedure to find the true feret length after test

Step 5: Calculate the distances from two end points of the identified feret length to the particle mass center, choosing the one giving bigger distance as the initial point and the other one as the end point. Following equation 4-3, calculate the orientation angle.

Step 6: Screen the particles whose orientation may not be correctly identified using the above method. If the $SIO_{min}$ is very big, it is probable that all three feret lengths are not the same as that detected before the test. This happens when the quality of images is poor and the error accumulated from image processing is so big that the represented particle completely loses its original shape. In this case, the particle is not considered for the orientation calculation. Another index $IA$ is also defined to adjudge the case that the particle is very round and its feret length is not significantly longer than other lengths. $IA = \frac{L_{\text{max}}}{L_{v1,v2}}$, where $IA = \text{index of angularity}; L_{\text{max}} =$ feret length of the particle; $L_{v1,v2} =$ length perpendicular to the feret length and across the
midpoint of feret length (Figure 4-5). If \( IA < 1.5 \) is satisfied, the particle will not be considered for the orientation calculation.

4.5 Evaluation of Strain Localization

Strain localization can be evaluated by the ratio of the local strains to the global strains of the entire specimen. The dimensionless global strains were calculated by the following equations:

\[
\varepsilon_1 = \frac{\Delta h}{h}; \varepsilon_2 = \frac{\Delta l}{l}; \varepsilon_3 = \frac{\Delta w}{w} \tag{4-7a}
\]

\[
\varepsilon_{12} = \frac{\varepsilon_1 - \varepsilon_2}{2}; \varepsilon_{13} = \frac{\varepsilon_1 - \varepsilon_3}{2}; \varepsilon_{23} = \frac{\varepsilon_2 - \varepsilon_3}{2} \tag{4-7b}
\]

where \( \Delta h \) = vertical deformation of the specimen

\( h \) = height of the specimen

\( \Delta l, \Delta w, l, w \) = lateral deformation and the length of the specimen.

The degree of strain localization can be defined as the effective local strains normalized by the effective global strain (defined as \( \varepsilon = \sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{13}^2} \)).

4.6 Experimental Results Analysis

4.6.1 Image Data Validation

The space between two adjacent images was 1.3mm, about 1/10 of the maximum particle size. Totally 90 images were obtained for the specimen before the test and 94 images after the test. Using x-ray tomography imaging and the 3D particle identification procedure, the mass center and volume of each particle were obtained. Some of the calculated results are presented in Table 4-4. The specimen porosity calculated by image analysis was 44.8%, which was very
close to the measured value 44.4%. Thus, the data obtained from image analysis are valid to be used for further analysis.

Table 4-4: The mass center coordinates and the displacements of individual particles (experimental measurement)

<table>
<thead>
<tr>
<th>Particle No.</th>
<th>mass center coordinates</th>
<th>Displacement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>x</td>
<td>y</td>
</tr>
<tr>
<td>1</td>
<td>47.15</td>
<td>29.11</td>
</tr>
<tr>
<td>2</td>
<td>81.65</td>
<td>29.81</td>
</tr>
<tr>
<td>3</td>
<td>62.48</td>
<td>32.34</td>
</tr>
<tr>
<td>4</td>
<td>116.66</td>
<td>31.61</td>
</tr>
<tr>
<td>5</td>
<td>34.84</td>
<td>33.93</td>
</tr>
<tr>
<td>6</td>
<td>104.96</td>
<td>33.41</td>
</tr>
<tr>
<td>7</td>
<td>91.91</td>
<td>30.72</td>
</tr>
<tr>
<td>8</td>
<td>73.39</td>
<td>32.24</td>
</tr>
<tr>
<td>9</td>
<td>53.76</td>
<td>38.57</td>
</tr>
<tr>
<td>10</td>
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<td>38.76</td>
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<td>51.67</td>
</tr>
<tr>
<td>18</td>
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<td>51.80</td>
</tr>
<tr>
<td>19</td>
<td>126.67</td>
<td>53.12</td>
</tr>
</tbody>
</table>

4.6.2 Global Properties Analysis

In this chapter, the global properties are those calculated for the entire specimen, the local macroproperties are those calculated for the tetrahedron formed by four nodes of particles, and the microproperties are those calculated at the particle level. The change of the sample porosity after the test was 2.27%. There were 5mm vertical dilatancy and 9mm relative displacement between two shear boxes after the test. The curve of the void ratio after the test along the height of the deformed specimen was plotted in Figure 4-6. The void ratio near the shear plane is apparently larger than others, and the void ratio outside the shear band is near the initial specimen void ratio (0.81).
The curve of the shear strength versus the lateral displacement is presented in Figure 4-7. In this figure, the shear strength of the specimen was found increased gradually to peak strength then decreased sharply to a relatively stable value. This value is named the residual strength, which means the specimen still has certain residual strength even if its structure has been damaged. This status is named the post-failure stage. Figure 4-8 presents the strength envelope which was obtained by finding the peak shear stress under different normal stress values. The peak shear stress increased with the increase of the normal stress. The bulk friction angle is defined as the slope of the curve, which was $40.1^\circ$ in this study.

**4.6.3 Particle Kinematics in the Shear Zone**

Particle translational displacements in the post-failure stage were calculated following the 3D quantitative methodology presented in Chapter 3. The illustration of the particle translational displacement is presented in Figure 4-9. It is found that most particles in the upper shear box had both significant vertical dilations and lateral movements, while those in the lower part almost had no vertical movements. The particle rotations were calculated using the method provided in the beginning of this chapter. Some particles used in the test are cubic-shaped, i.e. no significant feret length. They were not considered for further analysis. Fortunately, those particles were randomly distributed in the specimen and the lost data would not affect the statistical analysis of microfeatures of the specimen.

To know the evolution of microfeatures in the shear zone, the microkinematics including particle displacements and particle rotations in column A, B and C (refer to the monitoring system in Figure 4-10), were plotted in Figure 4-11 and 4-12. The normal force was 20 N and the peak shear force was 63 N in this case. In Figure 4-11, the particle displacement changed little at the height about 0 to 40 mm and it decreased in a uniform gradient with the increase of the
height. At the height about 80 mm it reached to a small value and changed little beyond that height. The shear zone can be defined by the two twist points (refer to Figure 4-11). In Figure 4-12, the three curves give the same trend, reaching peak value near the shear plane (at height 60 mm). It was found that particles in the middle height of the specimen had bigger magnitudes of rotations while those in the upper and lower part had smaller values (Figure 4-12). This is because a shear plane was defined by the interface of the upper and lower boxes, and most of the energy was absorbed by particles closer to that plane. The transaction of interparticle force mostly occurred in a zone, i.e. shear zone, explaining the significance of the particle rearrangement in the shear zone. It is interesting to notice that the shear zone thicknesses (about 40 mm) defined by the distribution of particle displacement and that of particle rotations are close to each other. Then a conclusion can be drawn that translations and rotations of irregular particles have equal contribution to the formation of shear zone, which was also supported by the experimental observation of Oda (1977) on disks.

Figure 4-6: The variation of the void ratio with the height of the specimen
Figure 4-7: The strength envelope under a normal stress of 1.78 Kpa

Figure 4-8: The variation of the shear force with time
4.6.4 Local Macrorotations and Microrotations

A 3D linear interpolation of special discretization approach was used to calculate the local strains and local rotations. One application of this method in the finite element analysis was described by Zienkiwicz and Taylor (2000). It has been believed to give a good match to the globally applied strain values (O’Sullivan, et al. 2003). The detailed methodologies have been described in Chapter 3. The calculated results were presented in Table 4-5. Comparing the microrotations (particle rotations) and the local macrorotations (tetrahedron rotations), it is found that two values can be very different. Thus the equation used in the second gradient theory which employing local rotations may not correctly describe the micromechanism of granular materials.
Figure 4-10: Illustration of the monitoring system of the direct shear test
Figure 4-11: Distribution of particle displacements in Column A, B and C

Figure 4-12: Distribution of particle rotations in Column A, B and C
Table 4-5: The microrotations and local macrorotations from the experimental test

<table>
<thead>
<tr>
<th>No.</th>
<th>Local Rotation</th>
<th></th>
<th>Particle Rotation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Δα(rad)</td>
<td>Δβ(rad)</td>
<td>Δγ(rad)</td>
<td>magnitude</td>
</tr>
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<td>0.00</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
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<td>0.03</td>
</tr>
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<td>0.01</td>
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<td>-0.01</td>
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<td>-0.08</td>
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</tbody>
</table>

Note: some particles had no significant max length and were not considered in the orientation calculation using the developed method.

4.6.5 Local Strains

The quantified effective local strains and degree of strain localization are presented in Table 4-6. The strain contours were plotted in Figure 4-13~ Figure 4-30. From the contours, it was found that the strain was highly heterogeneously distributed in the specimen. The strains presented significant localization, showing both dilatancy and contraction. The zone of strain dilatancy and strain contraction can be very close to each other. Most of the contraction occurred at the edge of the specimen because of the boundary confinement.
Table 4-6: The local macrostrains obtained by experimental test

<table>
<thead>
<tr>
<th>No.</th>
<th>$\varepsilon_x$</th>
<th>$\varepsilon_y$</th>
<th>$\varepsilon_z$</th>
<th>$\varepsilon_{xy}$</th>
<th>$\varepsilon_{yz}$</th>
<th>$\varepsilon_{xz}$</th>
<th>$\varepsilon_{eff}$</th>
<th>degree of strain localization</th>
</tr>
</thead>
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<td>0.02</td>
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<td>-0.06</td>
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<td>0.07</td>
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</tr>
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<td>-0.02</td>
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<td>-0.04</td>
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<td>0.00</td>
<td>0.02</td>
<td>0.15</td>
</tr>
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Figure 4-13: $\varepsilon_x$ contour in y-z plane
Figure 4-14: $\varepsilon_y$ contour in y-z plane
Figure 4-15: $\varepsilon_z$ contour in y-z plane
Figure 4-16: $\epsilon_{xy}$ contour in y-z plane
Figure 4-17: $\varepsilon_{yz}$ contour in y-z plane
Figure 4-18: $\varepsilon_{xz}$ contour in y-z plane
Figure 4-19: $\varepsilon_x$ contour in x-z plane
Figure 4-20: $\varepsilon_y$ contour in x-z plane
Figure 4-21: $\varepsilon_z$ contour in x-z plane
Figure 4-22: $\varepsilon_{xy}$ contour in x-z plane
Figure 4-23: $\varepsilon_{yz}$ contour in x-z plane
Figure 4-24: $\varepsilon_{xz}$ contour in x-z plane
Figure 4-25: $\varepsilon_x$ contour in x-y plane
Figure 4-26: $\varepsilon_y$ contour in x-y plane
Figure 4-27: \( \varepsilon_z \) contour in x-y plane
Figure 4-28: \( \varepsilon_{xy} \) contour in x-y plane
Figure 4-29: $\varepsilon_{yz}$ contour in x-y plane
Figure 4-30: $\varepsilon_{xz}$ contour in x-y plane
4.7 Summary and Conclusions

A methodology to quantify particle orientations and particle rotations was developed in this chapter. The quantification procedure, including particle boundary identification, particle orientation quantification, and particle reorganization, was applied for the analysis of the direct shear test. The specimen porosity calculated from image analysis agreed well with the measured value.

A significant shear band was detected by investigating particle kinematics and the void ratio distribution after shearing. The shear zone thickness defined by the distribution of particle displacements and that of particle rotations is consistent with each other. The strain was significantly localized in the specimen, showing both dilation and contraction. The zone of strain dilation and strain contraction can be very close to each other. The quantified microrotations and local macrorotations were quite different, indicating that the equation used in the second gradient theory which ignored particle rotations may not correctly describes the micromechanism of granular materials.
5.1 Objectives

The first objective of this chapter is to introduce the fundamental mechanism of DEM. The second objective is to present the background for stress and strain rate measurements, and damping principles in PFC$^{3D}$. The third objective is to calibrate the input parameters for DEM simulations.

5.2 Fundamental Mechanism of DEM

The distinct element method (DEM) models materials as a packed assembly of discrete particles. It allows an understanding of the micromechanics of granular materials at the particle level. The particles are usually simplified as disks or spheres in the conventional DEM approach. Each particle is assumed to be a rigid body, but slight overlap is allowed at the contact points. Relative movements between particles in conjunction such as separation or slippage are allowed during the simulation. Superparticles with arbitrary shape can be modeled by clusters of spheres.

The fundamental mechanism of DEM is summarized in the following section.

In the DEM simulation, the interaction of particles is treated as a dynamic process with states of equilibrium developing whenever the internal forces balance. It can be used to model dynamic or semi-static problems. For a granular material, if the stress varies slowly with time, it can be treated as a semi-static system and the inertia term may be negligible. The contact forces
and displacements of a stressed assembly of particles are calculated by tracing the movements of individual particles and solving Newton’s Equation of Motion:

\[ M \ddot{x} + D \dot{x} + R(x) = F \]  

(5-1)

where \( \ddot{x}, \dot{x}, x \) = linear acceleration, velocity, and displacement vectors respectively; \( M \) = mass; \( D \) = damping; \( R \) = internal restoring force; \( F \) = external force. The calculations are performed alternatively by applying Newton’s Second Law to the particles and the force-displacement law to the contacts. The former is used to determine the motion of each particle arising from the contact, and the latter is used to update the contact force arising from the relative motion at each contact. The force-displacement law allows two components of force to act with the corresponding components of the displacement, respectively, via the normal stiffness and shear stiffness. The following equations and explanations are abstracted from the menu book of PFC\textsuperscript{3D} (Itasca 1999).

The contact force is decomposed into the normal force and shear force at the contact point.

\[ F_i = F_i^n + F_i^s \]  

(5-2)

where \( F_i, F_i^n, F_i^s \) = contact force vector, normal contact force vector and shear contact force vector respectively.

The normal contact force vector is calculated by:

\[ F_i^n = K^n U^n n_i \]  

(5-3)

where \( K^n \) = normal stiffness, \( U^n \) = overlap, \( n_i \) = unit normal vector of the contact plane.

The shear force to vector is calculated by:

\[ \Delta F_i^s = -K^s \Delta U_i^s \]  

(5-4)
where $K^s =$ shear stiffness, $\Delta U_i^s =$ the increment of shear displacement. For the linear contact model, the two contact stiffnesses are assumed to act in series. The contact normal stiffness is given by $K_n = \frac{k_n^A k_n^B}{k_n^A + k_n^B}$. The contact shear stiffness is given by $K_s = \frac{k_s^A k_s^B}{k_s^A + k_s^B}$, where the superscripts A, B denote two entities in contact.

Assuming contact occurs between particles $A$ and $B$ with radii $r^A$ and $r^B$ respectively, as shown in Figure 5-1, then the relative displacement in normal component and tangential component can be expressed respectively as:

$$\Delta U_n^{AB} = (\Delta x^A - \Delta x^B) \cdot n^{AB} \quad (5-5)$$

$$\Delta U_s^{AB} = (\Delta x^A - \Delta x^B) \cdot t^{AB} + r^A \Delta \omega^A + r^B \Delta \omega^B \quad (5-6)$$

where $\Delta x^A, \Delta x^B =$ the translational displacement of particle $A, B$; $n^{AB}, t^{AB} =$ the unit normal vector and tangential vector on particle $A$ at the contact point respectively; $\Delta \omega^A, \Delta \omega^B =$ rotations about the center of particle $A$ and $B$.

$$n^{AB} = (x^B - x^A) / d^{AB} \quad (5-7)$$

where $x^A, x^B =$ position vector of the center of particles $A$ and $B$; $d^{AB} =$ distance between the centers of particles $A$ and $B$ and $d^{AB} = |x^B - x^A|$. As long as $d^{AB} < r^A + r^B$ is maintained, particles $A$ and $B$ overlap with each other and there is a contact force between them, as shown in Figure 5-2.

Considering the simplest model for the relationship between the contact force and the amount of overlap, the normal component of contact force can be expressed as following:

$$F_n^{AB} = K_n (r^A + r^B - d^{AB}) \quad (5-8)$$
The incremental form of the normal contact force can be expressed in terms of the incremental relative displacement between particles A and B as following:

\[ \Delta F_n^{AB} = K_n \Delta U_n^{AB} \]  \hspace{1cm} (5-9)

Both of above equations can be used in computer codes; however, more accurate results based on the first one can be expected since no repetition of addition is needed as in the incremental calculation based on the latter equation. However, to obtain the tangential component of the contact force, the incremental form should be used because a slippage is allowed to occur during the calculation and the tangential component of the contact force depends on the history of the relative displacement while not determined by the current locations of disks. For a slipping contact point, the value of \( K_n \) should be set to zero; otherwise, it would take a constant value in the simplest linear model. Assuming a Mohr-Coulomb condition, then slip occurs only when the below inequality is satisfied:

\[ |F_t^{AB}| > c + F_n^{AB} \tan \phi \mu \]  \hspace{1cm} (5-10)

where \( c \) = cohesion coefficient; \( \phi \mu \) = angle of interparticle friction. At every slipping contact point, the above inequality can be modified as:

\[ F_t^{AB} = \frac{F_t^{AB}}{|F_t^{AB}|} (c + F_n^{AB} \tan \phi \mu) \]  \hspace{1cm} (5-11)

When the body force \( b^A \) is applied to particle A, the resultant static force applied to particle A is:

\[ F^A = -\sum_B \left( F_{nB}^{AB} n^{AB} + F_{tB}^{AB} t^{AB} \right) + b^A \]  \hspace{1cm} (5-12)

The moment about the center of particle A is

\[ M^A = -r^A \sum_B F_t^{AB} \]  \hspace{1cm} (5-13)
To get a step-by-step solution, Newton’s equation should be converted into a set of finite difference formulations which contain terms at time $t$ and time $t + \Delta t$ separately at the right and left side of the equations. This process requires a huge memory space and long computing time in the case that the number of independent variables is large. Some simplification needs to be made to save time and speed the calculation process. DEM adopts a simplified conversion scheme that only takes the mass matrix $M$ into consideration, and the granular element method, proposed by Kishino (1988), simplified the equation as stiffness matrix control only. In DEM,
the translational and rotational accelerations of particle A can be determined by a simplified Newton’s Second Law:

\[ \frac{\partial^2 x^A}{\partial t^2} (t) = \frac{F^A}{m^A} \]  \hspace{1cm} (5-14)

\[ \frac{\partial \omega^A}{\partial t} (t) = \frac{M^A}{I^A} \]  \hspace{1cm} (5-15)

where \( m^A \) = mass of particle A; \( I^A \) = moment of inertia of particle A.

At time \( t+\Delta t/2 \), the translational and rotational velocities of particle A can be expressed in the finite difference regime.

\[ \frac{\partial x^A}{\partial t} (t + \Delta t / 2) = \frac{\partial x^A}{\partial t} (t - \Delta t / 2) + x^A (t) \]  \hspace{1cm} (5-16)

\[ \frac{\partial \omega^A}{\partial t} (t + \Delta t / 2) = \frac{\partial \omega^A}{\partial t} (t - \Delta t / 2) + \omega^A (t) \]  \hspace{1cm} (5-17)

And the position and rotation vector can be expressed as following:

\[ x^A (t + \Delta t) = x^A (t) + \frac{\partial x^A (t + \Delta t)}{\partial t} \Delta t \]  \hspace{1cm} (5-18)

\[ \omega^A (t + \Delta t) = \omega^A (t) + \frac{\partial \omega^A (t + \Delta t)}{\partial t} \Delta t \]  \hspace{1cm} (5-19)

A damping system should be included in the basic equation for a stable calculation because DEM utilizes the calculation algorithm based on the equilibrium equation of motions. It can be introduced either in the form of a dashpot model between particles or as a damping mechanism applied directly to individual particles. For the former damping system, the viscosity coefficients \( \eta_n \) and \( \eta_t \) are applied in the normal and tangential directions, and the damping forces between particles A and B are given as \( \eta_n \Delta u_n^{AB} / \Delta t \) and \( \eta_t \Delta u_t^{AB} / \Delta t \) respectively. As long as a damping mechanism applied directly to a particle, the conventional viscous model can be adopted, that is, the velocity of the particle produces a proportional damping force in the
opposite direction to the velocity vector. Other damping mechanism reduces the static force and moment applied to the particle by a damping coefficient $\alpha$,

$$F_d = -\alpha \Delta x^4 / |\Delta x^4| |F^4|$$  \hspace{1cm} (5-20)

$$M_d = -\alpha (\Delta \omega^4 / |\Delta \omega^4| |M^4|)$$  \hspace{1cm} (5-21)

where $F_d, M_d =$ reduced static force and moment (Oda 1999).

5.3 Mechanism Employed in PFC$^{3D}$

Particle Flow Code in 3 Dimensions (PFD$^{3D}$) is used to model the movement and interaction of rigid particles. It is an efficient tool to model complicated problems in solid mechanics and granular flow. PFC$^{3D}$ has several advantages: 1) only spheres are used, thus the contact detection is much simpler and more efficient; 2) large displacements can be modeled; 3) clusters are allowed to break. PFC$^{3D}$ allows finite displacements and rotations of discrete bodies, including complete detachments, and recognizes new contacts automatically as the calculation progress. It can be viewed as a simplified implementation of DEM because of the restriction to spheres. However, spheres can be slaved into clumps to serve as superparticles with irregular shapes. Spheres within a clump may overlap to any extent and each clump behaves as a rigid body with deformable boundaries (Itasca 1999). The following section introduces the measurement mechanism, which is summarized from the manual of PFC$^{3D}$.

5.3.1 Stress Measurement

In a DEM model, the term “stress” refers to the average stress in a specific volume since it is in fact a quantity in a continuum theory and does not exist at each point in an assembly of discrete particles. Newton Second’s Law and Force-Displacement Law act only between particles in the microscale. Thus it is necessary to covert the particle behavior at the micro level to a continuum term using an average process. Measurement spheres are used in PFC$^{3D}$ to define
local volumes so that a number of quantities such as the porosity, coordination number and stress can be calculated within the volume. The stress distribution in an assembly can be obtained by defining a number of measurement spheres at different locations in the assembly and calculating the average stress in each measurement sphere.

The average stress tensor in a volume $V$ is defined by:

$$
\bar{\sigma}_{ij} = \frac{1}{V} \int_{V} \sigma_{ij} \, dV
$$

(5-21)

where $\bar{\sigma}_{ij} =$ average stress tensor; $\sigma_{ij} =$ stress tensor acting throughout the volume $V$. For a particulate material, stresses exist only in particles, thus above formulation can be replaced by:

$$
\bar{\sigma}_{ij} = \frac{1}{V_{np}} \int_{np} \bar{\sigma}_{ij} \, dV_{p}
$$

(5-22)

where $\bar{\sigma}_{ij} =$ average stress tensor in particle $P$; $Np =$ number of particles; $V_{p} =$ volume of particle $P$. Assuming the stresses in each particle are continuous and in equilibrium, the average stress tensor in a particle can be written as:

$$
\bar{\sigma}_{ij} = \frac{1}{V_{p}} \int_{V_{p}} \bar{\sigma}_{ij} \, dV_{p} = \frac{1}{V_{p}} \sum_{Nc} \left[ x_{i}^{c} - x_{i}^{p} \right] n_{i}^{c-p} F_{j}^{c}
$$

(5-23)

where $x_{i}^{c}, F_{j}^{c}, x_{i}^{p} =$ the location, force at contact $c$ and location of particle $p$ respectively; $n_{i}^{c-p} =$ the unit-normal vector directed from the particle centroid to the contact location, and is a function of both the contact and particle. A correction factor $C$ is needed to compute the average stress when applying the above formulations because only the particles with centroids contained within the measurement sphere are considered in the above computation process.
where: \( n \) = porosity of the assembly; \( N^p \) = number of particles; \( V^p \) = volume of particle \( P \); \( V_m \) = volume of the measure sphere. Applying Equations 5-24 and 5-23 to Equation 5-22, we can obtain the expression of the average stress:

\[
\bar{\sigma}_{ij} = C \sum_{N_p} \sum_{N_c} |x_i^c - x_i^p| n_{i}^{c,p} F_j^c
\]

where \( x_i^c, F_j^c, x_i^p \) = location, force at contact \( c \) and location of particle \( p \) respectively; \( n_{i}^{c,p} \) = unit-normal vector directed from the particle centroid to the contact location; \( C \) = correction factor; \( Np \) = number of particles; \( Nc \) = number of contacts (Itasca 1999).

### 5.3.2 Strain Rate Measurement

Because the velocity field in voids of an assembly is non-zero, the strain rate cannot be expressed as an average strain rate directly in terms of the velocity field. Instead, a strain-rate tensor based on a best-fit procedure is determined, which can minimize the error between the predicted and measured velocity of all balls within the measurement sphere. A velocity-gradient tensor \( \dot{\alpha}_{ij} \) is referred as the strain-rate tensor for a given measurement sphere:

\[
\dot{\alpha}_{ij} = \dot{e}_{ij} - \omega_{ij}
\]

\[
\dot{e}_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i})
\]

\[
\omega_{ij} = \frac{1}{2}(v_{j,i} - v_{i,j})
\]

where \( \dot{\alpha}_{ij} \) = strain rate tensor; \( \dot{e}_{ij} \) = rate-of-deformation tensor; \( \omega_{ij} \) = spin tensor; \( v_{i,j} \) = velocity gradient.
The predicted relative velocity can be written as

\[
\dot{v}_i^{(p)} = \alpha_{ij} \dot{x}_j^{(p)}
\]  
(5-27)

\[
\dot{x}_j = x_j^{(p)} - \bar{x}_j
\]  
(5-28)

where \(x_j^{(p)}\) = central location of particle \(p\); \(\bar{x}_j\) = mean position of the \(N_p\) particles in the measurement sphere, \(x_j = \frac{\sum x_i^{(p)}}{N_p}\).

The error for the predicted value is given by:

\[
SS = \sum_{Np} \left[ \dot{v}_i^{(p)} - \dot{V}_i \right]^2 = \sum_{Np} \left( \dot{v}_i^{(p)} - \dot{V}_i \right) \left( \dot{v}_i^{(p)} - \dot{V}_i \right)
\]  
(5-29)

where \(SS\) = sum of square of the deviation between predicted and measured velocities. \(\dot{v}_i^{(p)}\) = predicted relative velocity of particle \(P\); \(\dot{V}_i^{(p)}\) = measured relative velocity of particle \(P\); \(N_p\) = number of particles within the measurement sphere (Itasca 1999).

5.3.3 The Principle of Damping

Damping is applied during the simulation to help to dissipate energy in the case that the frictional sliding is not active or not sufficient to achieve the stable state solution within a certain reasonable number of cycles. In PFC\(^3D\), the damping force is introduced into the equation of motion to damp the accelerating motion only. The damping operates by removing kinetic energy twice per cycle. The damping force is controlled by the damping coefficient \(\alpha\) .

\[
\alpha_{dc} = \pi D_f
\]  
(5-30)

\[
D_f = \frac{\Delta W_i / W_i}{4\pi}
\]  
(5-31)
where $\alpha_{dc}$ = damping coefficient; $D_f$ = fraction of critical damping; $\Delta W(i)$ = energy removed per cycle, $W(i)$ = mean kinetic energy at the instant of removal.

This form of damping has several advantages: 1) only the accelerating motion is damped, thus no erroneous damping forces arise from the steady-state motion; 2) the damping coefficient $\alpha$ is non-dimensional, thus it is convenient to apply to particles in any direction; 3) the damping coefficient is independent of frequency, therefore with same damping coefficient, different regions in the assembly with different natural periods are damped equally (Itasca 1999).

5.3.4 The Clump Logic

The Clump logic is provided by PFC$^{3D}$ to slave group of balls, which is helpful to model irregular particles. Contacts within a clump are skipped while those external to the clump are not affected in the calculation. Though contact forces are not generated between the slaved balls during cycling, those occurred when a clump is created or when a ball is added to the clump will be preserved. In a word, once a clump is generated it acts as a rigid particle which would never break apart no matter how much force is applied on it (Itasca 1999). The mass properties of a clump are calculated using the following equations:

$$m^{clp} = \sum_{i=1}^{N_p} m^p$$  \hfill (5-32)

$$x^{clp}_i = \frac{1}{m} \sum_{i=1}^{N_p} m^p x^p_i$$  \hfill (5-33)

$$I^{clp}_{ii} = \sum_{i=1}^{N_p} \left\{ m^p (x^p_i - x^{clp}_i)^2 + \frac{2}{5} m^p \left( R^p \right)^2 \right\}$$  \hfill (5-34)

$$I^{clp}_{ij} = \sum_{i=1}^{N_p} \left\{ m^p (x^p_i - x^{clp}_i)(x^p_j - x^{clp}_j) \right\} \quad (j \neq i)$$  \hfill (5-35)

where $m^p$, $m^{clp}$ = mass of the ball and clump, respectively.
\( \chi^p, \chi^{clp} \) = mass center coordinates of the ball and clump, respectively

\( I^{clp} \) = product of inertia (Itasca 1999).

The resultant force of a clump is calculated as:

\[
F_{i}^{clp} = \sum_{i}^{N_p} \left( F_i + \sum_{i}^{N_c} F_{i}^{pc} \right)
\]

(5-34)

where \( F_{i}^{clp} \) = resultant force of a clump

\( F_{i} \) = external applied force acted on sphere

\( F_{i}^{pc} \) = force acting on the ball \( P \) at a contact point.

The resultant moment of a clump is calculated as:

\[
M_{i}^{clp} = \sum_{i}^{N_p} \left( M_i + \varepsilon_{ijk} (\chi_j^p - \chi_j^{clp}) F_k + \sum_{i}^{N_c} \varepsilon_{ijk} (\chi_k^c - \chi_k^{clp}) F_{i}^{pc} \right)
\]

(5-35)

where \( M_{i}^{clp} \) = resultant moment of a clump

\( M_i \) = external applied moment acting on ball \( P \)

\( F_k \) = resultant force acting on sphere \( P \) at centroid

\( F_{k}^{pc} \) = force acting on sphere \( P \) at contact point (Itasca 1999).

5.4 Input Microparameters Calibration for DEM Simulations

The basic algorithm of the DEM approach is based on the finite difference formulations of particle motions, thus the microproperties instead of macroproperties of materials are required in the simulation. However, the conventional experiments can only provide the macroparameters such as Young’s modulus and Poisson’s ratio of a material. For a material with the known macroproperties and simple packing arrangement, its microparameters may be predicted from the commonly measured macroproperties (Jenkins and Strack 1993; Thornton 1997). But for the
material with an arbitrary packing, a microproperty specification procedure is needed to obtain the microparameters such as the particle stiffness and particle friction coefficient. In this procedure, the relationship between the microparameters and the macroproperties response can be established by adjusting the input microparameters in a serial of simulations. The microparameters of the synthetic material can then be determined by matching its macroproperty response to a particular physical material based on the obtained relationship. This procedure is also called the microparameter calibration. Though the synthetic material may also be sensitive to the particle size and packing arrangement, the effect of the particle size can be eliminated by employing appropriate scaling relations when specifying model parameters in the simulation. The packing arrangement has only a minor effect if the packing geometry is not too extreme (Itasca 1999). Besides the particle stiffness and particle friction coefficient, other parameters such as the particle gradation, the damping coefficient, and the wall stiffness were also investigated in order to know how much they may affect the simulation results.

A direct shear test was simulated and the relationships between the input parameters and the shear strength were obtained. The assembly used in the simulation was composed of 1280 spheres. The mass centers and volumes of spheres were chosen based on the result of image analysis for a real specimen used in the experimental test, which has been described in Chapter 3. Figure 5-3 presents the microstructure of the synthetic specimen used in the simulation. The shear boxes were simulated by nine rigid walls with two wings attached to the edge of the upper and the lower box (Illustrated in Figure 5-4). The wings were used to prevent particles from escaping from the box during shearing. A rigid load plate was placed on the top of the particles which can move up and down during compressing and shearing. The compression stress was kept constant during shearing by adjusting the velocities of load plate using a numerical servomechanism (Itasca 1999). Similar to the experimental procedure of the direct shear test, the
position of the upper box was fixed and the lower box was moved forward at a rate of 0.02 mm/time step along the horizontal direction until the relative displacement reached 50.0 mm. The shear force was monitored by measuring the resultant force occurred at wall No. 4 as well as wall No. 7.

5.4.1 Effect of the Number of Particles

In order to study the effect of the number of particles, different sample sizes were used while the particle size and specimen initial porosity were kept unchanged in a serial of simulations. The range of particle size was chosen from 9.5 mm to 12.9 mm. The number of particles would vary when different sample sizes were used, thus the effect of the particle number in fact reflects the sample size effect. The particles were randomly packed and compacted under a constant normal load (5.78 kPa). Figure 5-5 presents the variation of the shear strength with the particle number. The shear strength was represented by the ratio of the peak shear stress and the normal stress ($\tau/\sigma$). It decreased sharply with the increase of the particle number when the particle number was smaller than 1000. But when the particle number was increased beyond 1000, the shear strength changed little. Thus the smallest representative sample size should be 1000 particles. 1280 particles are adequate to obtain a stable result.

Figure 5-3: The microstructure used in the simulation of the direct shear test
Figure 5-4: The illustration of the shear box used in the simulation

Figure 5-5: The relationship between the shear strength and number of particles

\[ \sigma = 5.78 \text{ kPa} \]
5.4.2 Effect of the Particle Stiffness

To investigate the effect of the particle stiffness, a serial of simulations were performed by adjusting the particle stiffness. The ratio of the normal stiffness to the shear stiffness \((K_n/K_s)\) was first set to 1.0. Then the particle normal stiffness was chosen as \(1 \times 10^3, 1 \times 10^4, 1 \times 10^5, 1 \times 10^6, 1 \times 10^7, 1 \times 10^8\) N/m respectively in each simulation. Figure 5-6 presents the relationship between the peak shear force and the particle stiffness. Figure 5-7 presents the same relationship but plotted in the logarithmic scale. A twist point is apparently in both curves. The shear strength increases almost linearly with the increase of the particle stiffness when \(K_n\) is smaller than \(1 \times 10^6\) but the slope of the curve drops suddenly when \(K_n\) is around \(1 \times 10^7\) N/m. The particle normal stiffness was chosen as \(5.0 \times 10^5\) N/m and the ratio of the shear stiffness to normal stiffness \(K_s/K_n\) was chosen from 0.1 to 20.0 to study the effect of particle shear stiffness. The normal stress was set to 57.8 kPa in these simulations. The variation of peak shear force with the shear stiffness is presented in Figure 5-8. It was found that the shear strength increased with the increase of the particle shear stiffness. The particle shear stiffness was then set to \(5.0 \times 10^5\) N/m and the \(K_s/K_n\) was chosen from 0.05 to 100 to study the effect of the particle normal stiffness. Figure 5-9 presents the variation of the shear strength with the particle normal stiffness. This curve had the similar shape with that in Figure 5-8, which indicates that the particle normal stiffness and the particle shear stiffness have an equal contribution to the shear strength in the simulation.

5.4.3 Effect of the Wall Stiffness

The change of the wall stiffness would affect the contact force between the balls and walls. In order to know whether its effect is significant or not, a different ratio of wall stiffness to particle stiffness \((K_{nw}/K_{np})\) was chosen from 1.0 to 5.0 in a serial of simulations. Figure 5-10 presents the variation of peak shear force with the ratio \(K_{nw}/K_{np}\). It is found that the peak shear
force has only slight change when different ratio was used in the simulation thus the effect of this ratio is believed not significant on the shear strength of granular material.

Figure 5-6: The relationship between the shear strength and the particle stiffness

Figure 5-7: The relationship between the shear strength and the particle stiffness (in logarithmic scale)
Figure 5-8: The variation of the shear strength with the particle shear stiffness

Figure 5-9: The variation of the shear strength with the particle normal stiffness
5.4.4 Effect of the Wall Friction

The wall friction was chosen from 0.1 to 1.0 in order to know its effect. The change of the shear strength with the wall friction is presented in Figure 5-11. It is found that the peak shear force varies within 40 N~50 N when different wall friction was chosen. This gradient of variation is minor compared to the effect of particle stiffness.
5.4.5 Effect of the Particle Friction Coefficient

The particle friction coefficient is another intrinsic parameter required by PFC\textsuperscript{3D}. It differs from the bulk friction angle in that it relates to the friction generated between the particle surfaces when one particle slides slowly over another. Particle friction coefficient varying from 0.1 to 2.0 was used in a serial of simulations to study its effect. A suitable particle friction coefficient can be chosen for further simulations when the desired bulk friction angle is matched with that measured in the conventional experimental test. The variation of the peak shear force with the particle friction coefficient under a normal stress of 1.78 kPa is presented in Figure 5-12. It increases with the increase of the particle friction coefficient, and their relation is non-linear. A power equation is appropriate to describe their relation. Figure 5-13 presents the shear strength envelopes under different particle surface friction coefficients. Using linear interpretation, the slope of the shear strength envelopes gives the bulk friction angle. The variation of bulk peak friction angle with the particle friction coefficient is presented in Figure 5-14. Figure 5-15 presents the change of bulk residual friction angle with the particle friction coefficient.

![Figure 5-12: The variation of peak shear force with the particle friction coefficient](image)

\[
y = 2.2128x^{0.2171} \\
R^2 = 0.9996
\]
Figure 5-13: The peak shear strength envelope under different particle friction coefficient

Figure 5-14: The residual shear strength envelope under different particle friction coefficient
5.4.6 Effect of the Damping Coefficient

Damping is applied during the simulation to help to dissipate energy in case that frictional sliding is not active or not sufficient to achieve the stable state solution within a certain reasonable number of cycles. The damping force is controlled by the damping coefficient. Damping coefficients varying from 0.01 to 0.5 was used in a serial simulation. The variation of the peak shear force with the damping coefficient is presented in Figure 5-16. The change of peak shear force is small when the damping coefficient changed from 0.0 to 0.5. It was also noticed that it cost more time to achieve an equilibrium situation when a smaller damping coefficient was used. This is reasonable because more time needs to be spent on energy dissipation when a smaller damping coefficient is used in the simulation.
Figure 5-16: The relationship between the shear force and the damping coefficient
CHAPTER 6: 3D REPRESENTATION OF IRREGULAR PARTICLES IN DEM SIMULATIONS USING X-RAY TOMOGRAPHY IMAGING

6.1 Basic Idea of Clustering

An irregularly shaped particle can be represented by clusters of very small balls. Figure 6-1 illustrates the basic idea of clustering. Small balls can be generated and slaved together according to the configuration of an irregular particle. In PFC3D, each cluster behaves as a rigid body with a deformable boundary. Contacts internal to the cluster are skipped while any contact force that exists when a cluster is created or when a sphere is added to the cluster will be preserved during iteration cycles. The mechanism has been introduced in Chapter 5. For the detail of PFC3D, please refer to the Itasca manual 2.0 (Itasca 1999).

![Figure 6-1: The illustration of representing irregular particles using clustering of balls](a) (b)

6.2 Algorithm to Represent a Real Particle with Irregular Shape

6.2.1 3D Representation of Particles in DEM Simulation Based on X-ray Tomography Images

Sectional bitmaps of specimens were used for the 3D representation of irregular particles in DEM simulations. The bitmaps were obtained by image processing and image analysis which have been described in Chapter 2. Each bitmap was divided into 512×512 pixels. Each pixel is assigned a value representing the level of grayness or brightness of this pixel, ranging from 0
which means completely black (represent solid), to 255 which means completely white (represent void). Small balls were generated in DEM simulations to represent those pixels whose values are 0. The balls comprising the same particle were slaved together using the clump logic provided by PFC\textsuperscript{3D}, and then the entire aggregate skeleton of the specimen can be rebuilt. The procedure is illustrated in Figure 6-2.

A very large number of small balls are needed to represent the microstructure of a specimen using one ball to represent one pixel. As a result, huge memory and time are required for one simulation. The approximate maximum number of balls that can be generated in PFC\textsuperscript{3D} for different RAM is shown in Table 6-1. It is approximately a linear relationship. For a typical PC computer with 1G RAM, the predicted approximate maximum number of balls is about 600,000. Table 6-2 shows the PFC\textsuperscript{3D} runtime calculation rates for different computers and operating systems. For instance, when Pentium III and Win95 are used, the calculation rate is 0.0273 sec/ball/1000steps. If 100,000 balls are involved and the cycle time is 10000 steps, then the total time should be 0.0273*100,000*10000 = 27,300,000 sec/10 steps = 7,600 hr/1000 steps, which makes it impractical to perform such a simulation. Even using a more advanced computer and operating system, the calculation time could still be a problem when large number of balls is involved. Thus it is imperative to find a way to reduce the required number of balls when representing a complex material system. Two burn algorithms are developed for this purpose.

<table>
<thead>
<tr>
<th>Available RAM (MB)</th>
<th>Approx. maximum number of particles*</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>10,000</td>
</tr>
<tr>
<td>72</td>
<td>50,000</td>
</tr>
<tr>
<td>145</td>
<td>100,000</td>
</tr>
</tbody>
</table>

*compacted state (Contacts require more memory than balls.)

Source from PFC 3D manual 2.0 (Itasca, 1999)
Table 6-2: PFC\textsuperscript{3D} runtime calculation rates

<table>
<thead>
<tr>
<th>Computer</th>
<th>Operating System</th>
<th>sec/ball/1000 steps (x 10\textsuperscript{-2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentium III (500 MHz)</td>
<td>Win95</td>
<td>2.73</td>
</tr>
<tr>
<td>Pentium II (450 MHz)</td>
<td>WinNT</td>
<td>3.03</td>
</tr>
<tr>
<td>Pentium II (400 MHz)</td>
<td>Win95</td>
<td>3.31</td>
</tr>
<tr>
<td>Pentium II (300 MHz)</td>
<td>Win95</td>
<td>3.43</td>
</tr>
<tr>
<td>Pentium II (266 MHz)</td>
<td>WinNT</td>
<td>5.19</td>
</tr>
<tr>
<td>Pentium II (266 MHz)</td>
<td>Win95</td>
<td>5.28</td>
</tr>
<tr>
<td>Pentium Pro (200 MHz)</td>
<td>Win95</td>
<td>7.16</td>
</tr>
<tr>
<td>Pentium-S (150 MHz)</td>
<td>Win95</td>
<td>12.5</td>
</tr>
</tbody>
</table>

Source from PFC 3D manual 2.0 (Itasca 1999)

Figure 6-2: The illustration of representing the particles using x-ray tomography imaging

(a) Geomaterial

(b) One layer cut from the specimen

(c) Particle cross-section in the layer

(d) Small balls are used to replace pixels in composing the particles
• Burn Algorithm 1-the boundary approach

To aid in understanding, a 2D illustration of applying Burn Algorithm 1 for one particle is presented in Figure 6-3. A similar procedure can be applied for the 3D case.

Step 1: For a given cluster of balls which are used to represent an irregular particle, identify the boundary of the cluster.

Step 2: For each ball, draw an imaginary circle using its mass center coordinate as the centroid, and expand the circle until it is tangent to the inner boundary of the cluster. Compare the circles, and find the largest one, named as \( C_i \). Remove the small balls whose mass center coordinates lie in or on the boundary of \( C_i \).

Step 3: For the other balls, repeat step 1 and step 2, finding circle \( C_2 \) and removing small balls whose center lies in or on the boundary of \( C_2 \).

(a) Cluster of Small balls with equal radius is used to represent the particle

(b) Remove smalls balls whose center in the biggest circle \( C_1 \)

(c) Continue remove smalls balls whose center in the second biggest circle \( C_2 \)

(d) Generate balls \( C_1, C_2, C_3 \ldots \)

Figure 6-3: The illustration of applying Burn Algorithm 1 (the boundary approach)
Step 4: Repeat the third step and find the nth circle \( C_n \) till the radius of \( C_n \) is not larger than the radius of small balls.

Step 5: Generate new balls using the center and radius of \( C_1, C_2...C_n \) respectively. Most of the small balls are then replaced by those larger balls.

The above procedure is repeated for all clusters so that the entire aggregate skeleton can be rebuilt in this way. Assume the number of small balls is \( N_s \), the number of balls after applying the burn algorithm is \( N_l \), then the reduced number of balls \( N_r \) can be calculated as: \( N_r = N_s - N_l \)

- Burn Algorithm 2-the cubic package approach

The cubic package approach is based on the idea that every eight cubic packed balls can be approximated by one ball whose radius is two times bigger. Because the space between two adjacent image slices is usually bigger than the dimension of the pixel, there would be a “gap” between two layers of balls if one pixel is replaced by one ball (illustrated as Figure 6-4). In order to form a cubic package, more layers of balls must be added to fill the “gap” and the diameter of the ball needs to be chosen according to the dimension of the space. For example, if the space between two adjacent images is 6 pixels, two layers of balls with diameter equaling to 3 pixels can be generated to fill the space. Then the following procedure is required to burn the cubic packed balls.

Step 1: Search all the balls which are used to represent a particle, identifying cubic packed 8-ball-groups (four balls in the top and four balls in the bottom). Using the center coordinates of the cubic packages and the double radius of the small ball, generate larger balls to replace those 8-ball-groups.

Step 2: Repeat step 1 till desired number of balls are satisfied.

The above procedure is illustrated in Figures 6-5 and 6-6.
Figure 6-4: The 3D application of Burn Algorithm 2
(Bigger balls are generated to fill the space between two separated layers)
6.3 Representation Results and Comparisons between Two Burn Algorithms

Figure 6-7 presents the 2D visualization of an irregular particle represented by clusters of balls without ball-burning. Figure 6-8 presents the 2D visualization of the same particle after applying Burn Algorithm 1 (the boundary approach). Figure 6-9 is the 2D visualization of the same particle after applying Burn Algorithm 2 (the cubic package approach). Comparing those visualizations, it was found that the boundary approach represented the particle shape outline more precisely, but the ball package was arbitrary, and the mass of the cluster was more heterogeneous. The comparison of results of two algorithms is presented in Table 6-3. For Figure
6-9, the required number of small balls was 207 while only 67 balls were needed after applying Burn Algorithm 1, and 19 balls were needed after applying Burn Algorithm 2. Totally, 68% balls were reduced for Burn Algorithm 1 and 91% were reduced for Burn Algorithm 2. The required time for applying of the two algorithms was 0.2 min and 0.1 min respectively when a typical PC with 1G RAM and 2G CPU was used.

Figure 6-6: The steps to represent an irregular particle using Burn Algorithm 2

a) The particle is rebuilt by layers of balls

b) Bigger balls generated to fill the “gap”

c) Smaller balls are replaced by bigger balls

d) Final replacement result shown in 3D
Figure 6-7: Representation of an irregular particle without ball-burning (2D)
Figure 6-8: Representation of an irregular particle using Burn Algorithm 1 (2D)
Figure 6-9: Representation of an irregular particle using Burn Algorithm 2 (2D)

Table 6-3: Comparison of the effect of two burn algorithms

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Burn Algorithm</th>
<th>Number of Balls</th>
<th>Required Time(min)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Before</td>
<td>After</td>
</tr>
<tr>
<td>2D</td>
<td>burn1</td>
<td>207</td>
<td>67</td>
</tr>
<tr>
<td></td>
<td>burn2</td>
<td>207</td>
<td>19</td>
</tr>
<tr>
<td>3D</td>
<td>burn1</td>
<td>3837</td>
<td>1261</td>
</tr>
<tr>
<td></td>
<td>burn2</td>
<td>3837</td>
<td>147</td>
</tr>
</tbody>
</table>
The 3D visualization of a real irregular particle is presented in Figure 6-10. 3837 balls were required to represent this particle. The 3D visualization of the same particle represented by cluster of balls after applying Burn Algorithm 1 and Burn Algorithm 2 are presented in Figure 6-11 and Figure 6-12 respectively. When Burn Algorithm 1 was applied, 1261 small balls were used to reconstruct the particle, and only 141 balls were used when Burn Algorithm 2 was applied. 67% balls were reduced by Burn Algorithm 1, and 96% were reduced by Burn Algorithm 2. The required time for Burn Algorithm 1 was about 100 minutes and that for Burn Algorithm 2 was about 1 minute when a typical PC with 2G CPU and 1G RAM was used. The time for applying Burn Algorithm 1 was too long to make it practical in 3D simulation. The reason was that the calculating iteration is greatly increased in 3D case for Burn Algorithm 1.

Figure 6-13 illustrates a reconstructed specimen composed of 52 particles. Millions of balls were first required to represent those particles while only 38578 balls were needed after applying burn algorithm 2.

Figure 6-10: Visualization and representation of an irregular particle using cluster of balls (3D)
Figure 6-11: Representation of irregular particles after applying burn algorithm 1 (3D)
Figure 6-12: Representation of irregular particles after applying burn algorithm 2 (3D)
6.4 Effect of the Burn Algorism

The change of sample porosity in each step for particle representation was calculated to determine the effect of Burn Algorithm 2. The initial sample porosity was 49.6% and increased to 50.3% after image analysis. It reached to 70.5% after representing particles using cluster of balls without ball-burning. And it was increased to 72.0% after applying Burn Algorithm 2. It means that though totally 22.4% solid volume has been lost when using clusters of balls to represent irregular particles, ball-burning only contributed 1.5% (refer to Table 6-4). Using small balls to represent image voxels (three dimensional pixels) was the main reason that caused the loss of particle volume. One way to compensate the effect of the volume loss is to increase the ball density so that the particle mass could be close to the true value. Since the contacts within
any cluster were ignored and each cluster behaved as one rigid particle, the existence of voids within a cluster would not significantly affect the simulation results.

Table 6-4: Change of sample porosity due to each operation in simulation setups

<table>
<thead>
<tr>
<th>operation</th>
<th>sample porosity%</th>
<th>change %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measure from classic equation</td>
<td>49.600</td>
<td></td>
</tr>
<tr>
<td>Measure from image technology</td>
<td>50.300</td>
<td>0.700</td>
</tr>
<tr>
<td>represent particle without ball-burning</td>
<td>70.500</td>
<td>20.200</td>
</tr>
<tr>
<td>represent particle with ball-burning</td>
<td>72.000</td>
<td>1.500</td>
</tr>
<tr>
<td>sum</td>
<td>22.400</td>
<td></td>
</tr>
</tbody>
</table>

6.5 Summary and Conclusions

A practical method was developed in this chapter to represent real irregular particles in DEM simulations. The basic idea of clustering was demonstrated and the method to incorporate the real microstructure into the DEM simulation was explained. Two burn algorithms were developed to represent the irregular particles using a smaller number of balls. Both of the burn algorithms demonstrated the ability to reduce the required balls significantly. The boundary approach (Burn Algorithm 1) described the particle shape outline more precisely, but the ball package was arbitrary and the masses of clusters were heterogeneous. The cubic package approach (Burn Algorithm 2) had the advantage of representing the irregular particle more homogenously with less time cost. The PFC^3D^ representation results showed that the cubic package approach was more effective to reduce calculation time and save memory.
CHAPTER 7: DEM SIMULATION OF THE COMPRESSION TEST

7.1 Objectives

One objective of this study is to simulate the global and local strains, global and local deformations and microkinematics using the clustering DEM model and the conventional DEM model. The simulation results are compared with the experimental measurements to evaluate the accuracy of the simulations by two models. The other objective is to investigate the contribution of irregular particle shapes to micro-macro behaviors of granular materials. This objective is achieved by comparing the simulation results based on real irregularly-shaped particles and those on ideal spherical particles.

7.2 PFC$^{3D}$ and DEM Simulation Setup

To study particle shape effect on the micro-macro behavior of granular materials, commercial software PFC$^{3D}$ was used to perform DEM simulation on irregular particles and on spherical particles respectively. The microstructure of the specimen used in the confined compression test was incorporated into the simulation. Irregular particles were represented by clusters of balls. Balls within a cluster may overlap to any extent and each cluster behaves as a rigid particle with deformable boundaries in PFC$^{3D}$ (Itasca 1999). The Burn Algorithm 2 (the cubic package approach) developed in Chapter 6 was applied to reduce the required number of balls so that the computation efficiency was greatly improved. The rebuilt specimen composed of 173 particles in PFC$^{3D}$ was shown in Figure 7-1. Without the burn algorithm, 5,995,450 small balls would be required to represent those particles. It is impractical for a typical PC computer to handle such a huge number of balls. But after ball-burning, only 30,161 small balls were used to represent those particles. The spherical particles were generated using the particle mass centers and volumes calculated from experimental measurements in Chapter 3 by Equations 3-3, 3-4, 3-5,
and 3-6. The specimen composed of spherical particles was assigned the same physical properties as that composed of irregular particles. The represented specimen using spherical particles was presented in Figure 7-2.

![Represented microstructure by clusters of balls](image)

**Figure 7-1: Represented microstructure by clusters of balls**

In the simulation, the particles were reconstructed in a cylindrical container and a rigid load plate was placed on the top of the specimen. The load plate was made from hundreds of strongly bonded balls that would never break apart during the simulation. An axial force was applied directly on the load plate. The physical properties of the particles, boundary, and compact force were assigned the same as those used in the confined compression test. An elastic stiffness boundary was used to simulate the soft lateral confinement, so that certain lateral movement was allowed during the simulation.
Figure 7-2: Represented microstructure by spherical particles

7.3 Simulation Results Analysis

The sample porosity calculated from image technologies (50.3%) was somewhat larger than the experimental measurement (49.6%) because there was a small area loss of particle cross sections due to separating individual particle cross sections during image processing. Though there was no significant difference between two calculated porosities, the separating operation could lead to a decrease of the effective coordination number (defined as the average contact number per particle) and may affect the effective interparticle force transaction. Thus it was necessary to expand the particle cross section slightly in the simulation so that the loss of contacts could be compensated in a certain degree. The expansion was completed based on the
configurations of particles so that the particle shapes were not changed significantly after expansion. The initial effective coordination number calculated before the expansion was 1.38, and that calculated after the expansion was increased to 4.93. The change of effective coordination number in the compression test was calculated based on the expanded original aggregate skeleton and the deformed one (Table 7-1). The simulated coordination number based on irregular particles and spheres were also calculated and compared. It was found that the change of coordination number based on spheres (0.027) was bigger than that based on the real structure (0.023). The change of porosity by the experimental measurement was 2.4%, and that by the simulation was 2.3% based on irregular particles and 2.7% based on spheres. The simulation results are compatible with the phenomenon that materials composed of round particles have better workability to be compacted than those composed of irregularly shaped particles (Roberts et al. 1996).

Table 7-1: Comparison of the coordination number between the DEM simulations and the experimental measurement

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiments</th>
<th>DEM-Sphere</th>
<th>DEM-Irregular Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>coordination number(before test)</td>
<td>4.930</td>
<td>3.030</td>
<td>4.930</td>
</tr>
<tr>
<td>coordination number(after test)</td>
<td>6.130</td>
<td>6.710</td>
<td>6.650</td>
</tr>
<tr>
<td>change</td>
<td>1.200</td>
<td>3.680</td>
<td>1.720</td>
</tr>
</tbody>
</table>

The particle motions and strains were monitored in the simulation after applying the force. The particle translational movements by simulations and by experiment were illustrated in Figures 7-3 ~ 7-5. Most of the simulated irregular particle movements occurred in the vertical direction and the movements occurred at the lower part of the specimen were very small, which had a similar trend as the experimental observations. Simulated movements of spherical particles are more erratic. The simulated magnitudes of particle translations versus experimental
measurements were plotted in Figures 7-6 and 7-7. It was found that most of the points based on irregular particles located around the equality line (45° line), while those based on spherical particles were much more scattered, indicating that the simulated irregular particle translations had better agreement with the experimental observations than those based on spherical particles. The points based on irregular particles still had some discrepancy from the experimental results. It may be caused by several reasons. First of all, using clusters of balls to represent irregular particles, the mass centers and mass momentums of represented particles are slightly different from that of real aggregates. Secondly, the quality of the images was not good enough, which increased the difficulty to identify the boundary of individual particles. And because of this, some represented particles might not keep their original shape. Thirdly, the boundary conditions are difficult to be accurately described using a small number of balls. Despite the discrepancy, it is worth noticing that the simulation based on real aggregate shapes did improve the agreement with the experimental observations.

Figure 7-3: Illustration of particle translational movements-experimental results
Figure 7-4: Illustration of particle translational movements-simulation on irregular particles

Figure 7-5: Illustration of particle translational movements-simulation on spherical particles
Figure 7-6: Simulated magnitudes of spherical particle translations vs. experimental measurements

Figure 7-7: Simulated magnitudes of irregular particle translations vs. experimental measurements
Figures 7-8 ~ 7-10 presents the contour of volumetric strains $\varepsilon_v$ at $z = 45 \sim 55$ mm by two simulations and by the experiment, which have been projected in x-y plane. It was found that all 3 contours showed strain dilation in the center part of the specimen and small strain contraction around the edge. The contour based on irregular particles had better agreement with the experimental observation, i.e. their contour shapes were closer to each other and have a similar feature of strain localization. The contour based on spherical particles was much different.

Figures 7-11 ~ 7-13 presents the contour of volumetric strains at $y = 45 \sim 55$ mm, which have been projected in x-z plane. For the experimental results, most of the strain contraction occurred at the top of the specimen and there was certain strain dilation at the middle part. The simulation results based on irregular particles had the similar trend with the experimental observations. But the contour based on spherical particles showed strain contraction almost in the entire specimen except certain regions, and the strain contraction was more significant than the experimental results.

As for the macroproperties, the comparison between the simulated results and experimental results are presented in Table 7-2. The vertical deformation of the entire specimen was 9.2 mm, close to the experimental measurement, i.e. 9.8 mm. Their relative difference was 5.8%, which was calculated as the percentage of ratio of the absolute difference between two results to the experimental result. The radial dilatancy of the specimen was measured using acquired images before and after the test. Diameters of specimen images scanned at the top, middle, and bottom of the specimen were measured and averaged. The difference of the averaged specimen diameter measured before and after the test is the radial dilatancy. For the simulation on irregular particles, the simulated radial dilatancy of the specimen (9.2 mm) was close to the experimental measurement (9.8 mm), with a relative difference of 6.4%. The relative difference between the simulated global volume strain (-0.039) and the experimental measurements (-
0.041) was 4.3%. The simulation on spherical particles yielded a global vertical deformation of 12.3 mm with a relative difference of 25.5%, a radial dilation of 1.1 mm with a relative difference of 9.7%, and a global volume strain of -0.044 with a relative difference of 6.6%. Though their global volumetric strains exhibit no significant difference, the simulated global deformations based on spheres overestimated the specimen deformation and those based on real irregular particles are in good agreement with the experimental observations. The compatibility of simulated properties based on irregular particles with the experimental observations suggests that the DEM simulation incorporating real microstructure of material is a valid approach to predict the deformation of granular materials.

![Figure 7-8: \(\varepsilon_v\) contour in x-y plane (experimental results)](image-url)
Figure 7-9: $\varepsilon_v$ contour in x-y plane (simulations on irregular particles)
Figure 7-10: $\varepsilon_v$ contour in x-y plane (simulations on spherical particles)
Figure 7-11: $\varepsilon_v$ contour in x-z plane (experimental results)
Figure 7-12: $\varepsilon_v$ contour in x-z plane (simulations on irregular particles)
Figure 7-13: $\varepsilon_v$ contour in x-z plane (simulation on spheres)
Table 7-2: Comparison of macroproperties between the DEM simulations and experimental measurement

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiments</th>
<th>DEM-irregular particle</th>
<th>%Relative diff.</th>
<th>DEM-sphere</th>
<th>%Relative diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical contraction (mm)</td>
<td>9.800</td>
<td>9.230</td>
<td>5.816</td>
<td>12.300</td>
<td>25.510</td>
</tr>
<tr>
<td>Radial dilation (mm)</td>
<td>0.780</td>
<td>0.730</td>
<td>6.410</td>
<td>1.090</td>
<td>39.744</td>
</tr>
<tr>
<td>Global Volume Strain</td>
<td>-0.041</td>
<td>-0.039</td>
<td>4.368</td>
<td>-0.044</td>
<td>6.652</td>
</tr>
<tr>
<td>change of porosity</td>
<td>0.024</td>
<td>0.023</td>
<td>5.859</td>
<td>0.027</td>
<td>13.858</td>
</tr>
</tbody>
</table>

7.4 Summary and Conclusions

Using clusters of balls to represent irregular particles, the material with actual microstructure was simulated by the clustering DEM model. Comparing the simulation results based on spherical particles and those based on irregular particles, it is found that particle shape has a significant effect on both micro and macro properties of granular materials. At the microlevel, it influences the contact interaction between particles. Thus, the particle movements and microstrain field would be different for materials consisting of particles with different shape configurations. At the macrolevel, it affects the deformation and strength of materials.

The simulation employing the conventional DEM model (based on spheres) overestimated the vertical contraction and the radial dilation of the material. The simulated spherical particle translations showed significant discrepancy from the experimental measurements. The simulation by the clustering DEM model (based on irregular particles) had agreement with the experimental observations both at the micro and macro levels.
CHAPTER 8: DEM SIMULATION OF THE DIRECT SHEAR TEST

8.1 Objective

The objective of this chapter is to investigate the particle shape effect on shear banding using DEM simulations. In order to achieve this objective, the conventional DEM simulations (based on spherical particles) and the clustering DEM simulations (based on irregularly shaped particles) will be discussed and compared to the experimental measurements. The comparisons include global macroproperties (such as the global deformations, failure strength, and residual strength), local macroproperties (such as the stress and strain distribution, local coordination number, and local void ratio), and the microcharacteristics (such as the particle kinematics, and fabric orientation distributions).

8.2 Introduction

Shear banding is a common phenomenon encountered in granular materials when the stress reaches a peak value and then drops sharply to a residual state and the deformation localizes suddenly into a narrow zone. In engineering practice, Coulomb’s failure law is usually assumed to govern the evolution of the shear band, but it may not truly describe the mechanism of the shear band. In fact, the basic micromechanism leading to the formation of a shear band is not well understood even though research has been carried out in this area by both experimental studies and numerical methods (Cundall et al. 1982; Yoshida et al. 1994; Oda and Kazama 1998; Iwashida and Oda 1998).

Numerical methods become more and more popular in this area due to their advantage to directly simulate the microprocess of shear band development in different stages. DEM is one of the effective numerical methods, which was originally developed to investigate the validity of various continuum models so that the appropriate model can be identified and incorporated into
the Finite Element (FE) analysis to solve the engineering problems (Oda 1999). It was later increasingly used in the study of behaviors of granular materials because of its ability of investigating granular material systems at the microlevel (Cundall and Strack 1979; Ghaboussi 1990; Thornton 1992). Though DEM has been recognized as a promising tool, the difficulty to model the real microstructures has limited its application. Most of the historical DEM simulations were performed using idealized particle systems such as spheres and ellipses (Cundall and Roger 1992; Routhenberg 1989; Lin and Ng 1997). Since more complicated fabrics and contact patterns exist among irregular particles (Oda et al. 1985), simulations based on idealized particles may not capture the inherent microfeatures of materials. Efforts have been made to simulate polygon-shaped particles or computer generated irregular particles (Mirghasemi 2002; Ni 2000), but few DEM codes are developed based on the real microstructure of a material. Even though the simulations were based on irregular particles (Mirghasemi et. al. 2002; Golchert 2004), the accuracy of the simulation results was unknown because few experimental measurements of microproperties were available, and the validity of a numerical method is doubted if there is no corresponding experimental data to support the simulation results. This chapter provides an evaluation of the capability of the clustering DEM model and the conventional DEM model by comparing the simulation results with the experimental observations.

8.3 DEM Simulation Setup

Particle Flow Code in Three-Dimensions (PFC\textsuperscript{3D}) was used to perform DEM simulations on irregular particles or/and on spherical particles. The microstructure of the specimen used in the direct shear test was incorporated into the simulations. Irregular particles were represented by clusters of balls using the clump mechanism of PFC\textsuperscript{3D} (Itasca 1999). Each cluster behaves as a rigid particle with deformable boundaries and contacts of balls within a cluster are ignored in the
calculation. The burn algorithm (the cubic package approach) was applied to reduce the required number of balls. The detailed discussion of the particle representation and burn algorithm has been presented in Chapter 6. The rebuilt specimen was composed of 1280 particles in PFC3D and is illustrated in Figure 8-1. About 200,000 small balls were used to represent those irregular particles. The spherical particles were generated using the particle mass centers and volumes calculated from experimental measurements. The represented specimen using spherical particles was presented in Figure 8-2.

The shear boxes were simulated by nine rigid walls with two wings attached to the upper and lower box edge (Illustrated in Figure 8-3). The wings were used to prevent particles from escaping from the box during shearing. A rigid load plate was placed on the top of the particles which can move up and down during compressing and shearing. The compression stress was kept constant during shearing by adjusting the velocities of the load plate using a numerical servo-mechanism (Itasca 1999). Similar to the experimental procedure of the direct shear test, the position of the upper box was fixed and the lower box was moved forward at a rate of 0.02 mm/ time step in the horizontal direction until the relative displacement reached 50 mm (A larger relative displacement was allowed in order to obtain a fully developed strength curve). The shear force was monitored by measuring the resultant force occurring at the wall No. 4 and wall No. 7 (Figure 5-4 in Chapter 5). The vertical displacement was monitored by measuring the displacement of the load plate.

The physical properties of the particles, shear boxes, and compact force were assigned according to those used in the direct shear test (presented in Table 3-1). The local void ratio was measured layer by layer. Each layer has a thickness of 1/6 of the height of the specimen. The monitoring system is illustrated in Figure 8-3. The individual particle displacements and rotations as well as local stresses and strains were monitored and calculated. The evolution of
fabric quantities such as distribution of branch vector (the vector connecting the centers of two neighboring particles), coordination number (average contact number vector per particle), and contact normal (normal direction to the contact plane between two contacted particles) were also monitored, which will be discussed in detail in Chapter 9.

Figure 8-1: 3D visualization of microstructure of the material composed by irregular particles

Figure 8-2: 3D visualization of microstructure of the material composed by spheres
8.4 Analysis of Simulation Results

The simulation results include the predictions of macroproperties and microproperties of the specimen composed of spheres and those composed of real irregular particles. The global macroproperties discussed in this chapter are related to the features of the entire specimen such as shear strength, global deformation, and bulk friction angle. The local macroproperties are related to the characteristics monitored in the local volumes which can be either tetrahedrons formed by four adjacent particles (refer to Figure 2-8 in Chapter 2) or the measuring layers of the specimen (refer to Figure 8-3). The microproperties are related to kinematics and contacts of individual particles. The comparisons of global macroproperties between the experimental measurement and simulations are presented in Table 8-1. The comparisons of microproperties between the experimental measurements and simulations are presented in Tables 8-2 ~ 8-4. Figure 8-4 presents the microstructure after shearing for the simulation based on spheres. Figure 8-5 presents the microstructure after shearing for the simulation based on irregular particles.

Table 8-1: The comparison of global macroproperties between the experimental measurement and simulations

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiment</th>
<th>DEM-irregular particle</th>
<th>%Relative diff.</th>
<th>DEM-sphere</th>
<th>%Relative diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical Dilation (mm)</td>
<td>5.00</td>
<td>4.50</td>
<td>10.00%</td>
<td>-3.70</td>
<td>174.00%</td>
</tr>
<tr>
<td>change of porosity</td>
<td>0.02</td>
<td>0.02</td>
<td>10.44%</td>
<td>-0.02</td>
<td>175.99%</td>
</tr>
<tr>
<td>peak shear force</td>
<td>63.47</td>
<td>67.63</td>
<td>6.55%</td>
<td>41.85</td>
<td>34.06%</td>
</tr>
<tr>
<td>Residue shear force</td>
<td>21.60</td>
<td>25.31</td>
<td>17.18%</td>
<td>32.77</td>
<td>51.71%</td>
</tr>
<tr>
<td>peak friction angle</td>
<td>40.15</td>
<td>40.51</td>
<td>0.90%</td>
<td>39.96</td>
<td>0.48%</td>
</tr>
<tr>
<td>Residue friction angle</td>
<td>34.26</td>
<td>32.55</td>
<td>5.00%</td>
<td>30.84</td>
<td>9.99%</td>
</tr>
</tbody>
</table>
Figure 8-3: Illustration of the monitoring system of the direct shear test (particle kinematics were monitored in Column A, B and C, local void ratios and fabric vectors were measured in each layer)
Table 8-2: The comparison of coordination number simulation results and experimental measurements

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiments</th>
<th>DEM-Sphere</th>
<th>DEM-Irregular Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>coordination number(before test)</td>
<td>5.77</td>
<td>5.72</td>
<td>3.61</td>
</tr>
<tr>
<td>coordination number(after test)</td>
<td>5.24</td>
<td>5.40</td>
<td>3.08</td>
</tr>
<tr>
<td>change</td>
<td>-0.53</td>
<td>-0.32</td>
<td>-0.53</td>
</tr>
</tbody>
</table>

Table 8-3: The comparison of particle translational displacements between simulation results and experimental measurements

<table>
<thead>
<tr>
<th>Particle No.</th>
<th>experiment</th>
<th>Simulation (sphere)</th>
<th>Simulation (irregular particle)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>dx  dy  dz</td>
<td>dx  dy  dz</td>
<td>dx  dy  dz</td>
</tr>
<tr>
<td>1.00</td>
<td>0.14 -8.51 0.16</td>
<td>-1.57 -4.68 -0.52</td>
<td>-2.01 -10.05 -0.30</td>
</tr>
<tr>
<td>2.00</td>
<td>0.12 -8.65 0.23</td>
<td>-2.88 -7.16 -3.60</td>
<td>-0.51 -8.92 -0.34</td>
</tr>
<tr>
<td>3.00</td>
<td>0.15 -8.45 0.29</td>
<td>-5.66 -8.04 -2.17</td>
<td>0.01  -9.35  -0.13</td>
</tr>
<tr>
<td>4.00</td>
<td>0.01 -8.84 0.26</td>
<td>-6.98 -9.96 -1.25</td>
<td>0.41  -8.95  -0.23</td>
</tr>
<tr>
<td>5.00</td>
<td>0.18 -8.39 0.08</td>
<td>-2.26 -9.00  1.24</td>
<td>0.15  -9.58  -0.95</td>
</tr>
<tr>
<td>6.00</td>
<td>0.27 -8.51 -0.12</td>
<td>-5.25 -8.99  1.01</td>
<td>0.49  -9.09  -0.03</td>
</tr>
<tr>
<td>7.00</td>
<td>0.07 -8.71 0.14</td>
<td>-2.52 -8.51 -0.47</td>
<td>-0.18  -8.76 -0.39</td>
</tr>
<tr>
<td>8.00</td>
<td>0.22 -8.53 0.27</td>
<td>-5.43 -8.43 -1.97</td>
<td>-0.31  -9.17 -0.25</td>
</tr>
<tr>
<td>9.00</td>
<td>0.31 -8.53 0.09</td>
<td>-3.29 -5.14  0.30</td>
<td>-0.39  -9.99 -0.30</td>
</tr>
<tr>
<td>10.00</td>
<td>0.12 -8.84 0.03</td>
<td>-2.70 -11.54 -0.21</td>
<td>-0.11  -8.99 -0.26</td>
</tr>
<tr>
<td>11.00</td>
<td>0.26 -8.53 0.04</td>
<td>-1.47 -4.37  1.65</td>
<td>-0.85  -9.26 -0.41</td>
</tr>
<tr>
<td>12.00</td>
<td>0.20 -8.85 0.16</td>
<td>-1.62 -9.68 -1.64</td>
<td>0.13   -8.74 -0.27</td>
</tr>
<tr>
<td>13.00</td>
<td>0.27 -8.45 0.11</td>
<td>-1.32 -8.21 -0.01</td>
<td>-0.32  -9.59 -0.05</td>
</tr>
<tr>
<td>14.00</td>
<td>0.28 -8.63 0.18</td>
<td>-3.62 -8.53  0.61</td>
<td>-1.09  -8.93 -0.26</td>
</tr>
<tr>
<td>15.00</td>
<td>0.52 -8.47 0.39</td>
<td>-3.12 -7.69 -2.41</td>
<td>-0.40  -9.73 -1.37</td>
</tr>
<tr>
<td>16.00</td>
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<td>-1.51 -10.79  0.01</td>
<td>-0.83  -8.75 -0.84</td>
</tr>
<tr>
<td>17.00</td>
<td>0.34 -8.52 0.04</td>
<td>-1.53 -8.68  1.19</td>
<td>-0.04  -10.18 -0.03</td>
</tr>
<tr>
<td>18.00</td>
<td>0.31 -8.61 0.08</td>
<td>2.01  -9.28 -0.61</td>
<td>-0.79  -8.90 -0.41</td>
</tr>
<tr>
<td>19.00</td>
<td>0.18 -8.83 0.18</td>
<td>-0.71 -10.95 -2.42</td>
<td>0.15   -9.42 -0.50</td>
</tr>
</tbody>
</table>

Note: this table only presents calculated results of 19 particles
Table 8-4: The comparison of particle rotations between simulated results and experimental measurements

<table>
<thead>
<tr>
<th>No.</th>
<th>Δα (rad)</th>
<th>Δβ (rad)</th>
<th>Δγ (rad)</th>
<th>Δα (rad)</th>
<th>Δβ (rad)</th>
<th>Δγ (rad)</th>
<th>Δα (rad)</th>
<th>Δβ (rad)</th>
<th>Δγ (rad)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.11</td>
<td>-0.06</td>
<td>0.10</td>
<td>0.34</td>
<td>0.13</td>
<td>0.17</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>-0.01</td>
<td>-0.02</td>
<td>0.00</td>
<td>0.02</td>
<td>-0.04</td>
<td>0.09</td>
<td>-0.04</td>
<td>-0.01</td>
<td>-0.31</td>
</tr>
<tr>
<td>3</td>
<td>0.03</td>
<td>0.01</td>
<td>0.01</td>
<td>-0.01</td>
<td>0.00</td>
<td>-0.03</td>
<td>-0.12</td>
<td>-0.07</td>
<td>0.07</td>
</tr>
<tr>
<td>4</td>
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<td>0.01</td>
<td>0.07</td>
<td>0.02</td>
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<td>0.12</td>
<td>0.02</td>
<td>-0.02</td>
<td>0.01</td>
</tr>
<tr>
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<td>-0.28</td>
<td>0.14</td>
<td>-0.12</td>
<td>0.06</td>
<td>-0.03</td>
<td>0.07</td>
<td>-0.04</td>
</tr>
<tr>
<td>6</td>
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<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.08</td>
<td>0.06</td>
<td>-0.02</td>
<td>0.00</td>
</tr>
<tr>
<td>7</td>
<td>0.06</td>
<td>0.00</td>
<td>0.07</td>
<td>0.15</td>
<td>0.07</td>
<td>0.01</td>
<td>-0.01</td>
<td>-0.07</td>
<td>0.04</td>
</tr>
<tr>
<td>8</td>
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<td>0.01</td>
<td>0.00</td>
<td>-0.04</td>
<td>0.04</td>
<td>0.00</td>
<td>-0.09</td>
<td>0.06</td>
<td>-0.08</td>
</tr>
<tr>
<td>9</td>
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<td>-0.05</td>
<td>-0.04</td>
<td>0.15</td>
<td>0.10</td>
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<td>0.01</td>
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<td>0.00</td>
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<td>0.03</td>
<td>-0.03</td>
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<td>0.21</td>
</tr>
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<td>-0.01</td>
<td>0.02</td>
<td>-0.09</td>
<td>0.04</td>
</tr>
<tr>
<td>12</td>
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<td>-0.05</td>
<td>-0.03</td>
<td>-0.03</td>
<td>-0.09</td>
<td>0.00</td>
<td>-0.04</td>
<td>-0.05</td>
</tr>
<tr>
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<td>0.09</td>
<td>-0.01</td>
<td>0.04</td>
<td>-0.01</td>
<td>0.02</td>
<td>0.06</td>
<td>0.01</td>
</tr>
<tr>
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<td>-0.01</td>
<td>0.02</td>
<td>0.01</td>
</tr>
<tr>
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<td>0.01</td>
<td>-0.08</td>
<td>-0.01</td>
<td>-0.16</td>
<td>0.16</td>
<td>-0.09</td>
<td>-0.01</td>
<td>0.00</td>
<td>0.06</td>
</tr>
<tr>
<td>16</td>
<td>0.03</td>
<td>-0.08</td>
<td>0.03</td>
<td>-0.08</td>
<td>-0.11</td>
<td>0.04</td>
<td>0.06</td>
<td>0.03</td>
<td>-0.05</td>
</tr>
<tr>
<td>17</td>
<td>0.05</td>
<td>-0.03</td>
<td>0.08</td>
<td>0.05</td>
<td>0.16</td>
<td>-0.06</td>
<td>0.03</td>
<td>0.05</td>
<td>-0.05</td>
</tr>
<tr>
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<td>0.01</td>
<td>0.03</td>
<td>0.05</td>
<td>-0.05</td>
<td>0.00</td>
<td>-0.14</td>
<td>0.00</td>
<td>-0.04</td>
</tr>
<tr>
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<td>0.04</td>
<td>0.06</td>
<td>-0.03</td>
<td>0.05</td>
<td>-0.06</td>
<td>-0.07</td>
<td>0.05</td>
<td>0.07</td>
</tr>
</tbody>
</table>

Note: this table only presents calculated results of 19 particles
Figure 8-4: Visualization of the sample after shearing
(Simulation on spheres)
Figure 8-5: Visualization of the sample after shearing
(Irregular particle)
8.4.1 The Prediction of Global Macroproperties of the Material

- Shear strength

As shown in Table 8-1, the peak shear strength is 63.5 N for the experimental measurement, 41.8 N for the simulation of spheres (the conventional DEM model), and 67.6 N for the simulation of irregular particles (the clustering DEM model). The residual shear strength is 21.6 N for the experiment measurement, 25.3 N for the simulation on spheres, and 32.8 N for the simulation on irregular particles. The clustering DEM model gave a more accurate prediction of the peak shear strength and residual strength than the conventional DEM model.

- Bulk friction angle

Figure 8-7 presents the peak strength envelopes obtained by the experimental measurement and the simulations. The peak bulk friction angle can be obtained by measuring the slope of the curve in Figure 8-7. The peak bulk friction angle is 40.1° for the experimental measurement, 39.9° for the simulation on spheres, and 40.5° for the simulation on irregular particles. Figure 8-8 presents the residual strength envelopes obtained by the experimental measurement and the simulations. The envelope based on the simulation of irregular particles presents no significant difference from that based on the experimental measurement. The residual friction angle is 34.3° for the experimental measurement, 32.6° for the simulation on irregular particles, and 30.8° for the simulation on spheres. The predictions of bulk friction angle based on both simulations showed consistency with the experimental measurement. But for the residual friction angle, the simulation based on irregular particles showed better agreement with the experimental measurement, and the simulation based on spheres much underestimated the residual friction angle of the material.
Figure 8-6: The peak strength envelopes based on the experimental measurement or/and simulations

Figure 8-7: The residual strength envelopes based on the experimental measurement or/and simulations
• Volumetric dilation and change of sample porosity and local void ratio

Though there was relative displacement between the upper and lower box, only the vertical displacement was counted for the global volumetric dilation of the specimen. The vertical dilation of the specimen is 5.0 mm for the experimental measurement and 4.5 mm for the simulation on irregular particles (Table 8-1). There is a 3.7 mm vertical contraction, instead of dilation, for the simulation on spheres. Apparently, the simulation based on irregular particles showed better agreement with the experimental measurement. As a result of vertical displacement, the sample porosity increased to 47% for the experimental measurement, increased to 46% for the simulation on irregular particles, and decreased to 43% for the simulation on spheres. The change of sample porosity after shearing predicted by simulation on irregular particles showed good agreement with the experimental result.

The local void ratio after shearing was measured in the local volume of the deformed specimen by the following equation:

\[
e_i = \frac{\sum V^p}{V_i - \sum V^p}
\]  

(8-1)

where  \(e_i\) = void ratio calculated in each local space

\(V^p\) = particle volume in local space

\(V_i\) = local volume.

Because the irregular particles were approximated by clusters of balls, and voids existed within a cluster, the particle volume calculated by the total volume of balls in the simulation would underestimate the actual particle volume. Since the voids within the clusters were not counted for the bulk void ratio, the actual volume of particles (the particle volume measured by image
analysis), instead of the sum of the ball volume, should be used for the calculation of the void ratio for the represented irregular particles. Figure 8-8 presents the distributions of the void ratio along the height of the deformed specimen based on the experimental measurements and two simulations. The void ratio based on the simulation of irregular particles presented apparently larger values around the shear plane and smaller values apart from the shear plane which is consistent with the experimental observation. The void ratio distribution based on the simulation of spheres did not present such a pattern, or was erratic, indicating that no significant shear zone was formed in the simulation on spheres. Oda (1997) reported a similar finding when a conventional 2D DEM model was used to perform the simulation. He modified the conventional model by taking into account the rotational resistance at contact point and then a shear zone was observed in his simulation. It is interesting to notice that a good prediction of shear band formation was also obtained using the clustering DEM model, which employed a simple linear elastic particle contact. The reason may be that the interlock between the irregular particles in fact has provided a rotational resistance at the contact point.

Figure 8-8: The distributions of void ratio along the height of the deformed specimen
8.4.2 The Prediction of the Local Macroproperties of the Material

- Local stress and local strain

Since the stress only exists within particles, the local stress in a tetrahedron is calculated as the average stress of four adjacent particles which form the tetrahedron. Assuming the stress in each particle is continuous and in equilibrium, the average stress tensor in a particle \( p \) can be written as (Itasca 1999):

\[
\bar{\sigma}_{ij}^{p} = \frac{1}{V_{p}} \int_{V_{p}} \bar{\sigma}_{ij}^{p} dV_{p}
\]

\[
= \frac{1}{V_{p}} \sum_{c} \left| x_{i}^{c} - x_{i}^{p} \right| n_{i}^{c,p} F_{j}^{c}
\]

(8-2)

where \( x_{i}^{c}, F_{j}^{c}, x_{i}^{p} \) = location, force at contact \( c \), and location of particle \( p \) respectively; \( n_{i}^{c,p} \) = unit normal vector directed from the particle centroid to the contact location, and is a function of both the contact and the particle position.

The local stress can be then calculated using the following equation (Itasca 1999):

\[
\bar{\sigma}_{ij} = \frac{1}{V_{t}} \sum_{N_{p}} \frac{\bar{\sigma}_{ij}^{p} V_{p}}{V_{p}}
\]

(8-3)

where \( \bar{\sigma}_{ij}^{p} = \) average stress tensor in particle \( P \)

\( N_{p} \) = number of particles

\( V_{p} \) = volume of particle \( p \)

\( V_{t} \) = volume of tetrahedron \( t \).

The local strains were calculated following the method provided in chapter 2 by the following relations (Wang et al. 1999):

\[
\varepsilon_{x} = \frac{\partial u}{\partial x}
\]

(8-4a)
\[
\varepsilon_y = \frac{\partial v}{\partial y} \quad (8-4b)
\]
\[
\varepsilon_z = \frac{\partial w}{\partial z} \quad (8-4c)
\]
\[
\varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \quad (8-4d)
\]
\[
\varepsilon_{xz} = \frac{1}{2} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \quad (8-4e)
\]
\[
\varepsilon_{yz} = \frac{1}{2} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \quad (8-4f)
\]

The volumetric strain is defined as
\[
\varepsilon_v = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \quad (8-5)
\]

The volumetric stress is defined as
\[
\sigma_v = \sigma_1 + \sigma_2 + \sigma_3 \quad (8-6)
\]

The simulated and measured volumetric strain fields are presented in Figures 8-9 ~ 8-17. The simulated volumetric stress fields based on irregular particles are presented in Figures 8-18 ~ 8-20. All of those simulated contours showed that the stresses or and strains were not uniformly distributed in the specimen and that the stress fields did not coincide with the strain fields. The highly non-uniform strain distributions were also observed for the experimental measurements. The simulated strain contours based on irregular particles presented similar strain localization with experimental observations while those based on spheres presented very different strain localizations. The local stresses were not measured in the experiment due to the lack of equipment. But it is still interesting to investigate the simulated stress fields and the simulated strain fields based on irregular particles. Two conclusions can be drawn based on the simulation results: 1) there seems to be no simple relationship between the applied normal stress
and the stress distribution in the specimen; 2) the volumetric strain and the volumetric stress are generally not consistent with each other although they may have certain agreement in a small zone. These conclusions seem be supported by the experimental work of Allersma (2005) who presented similar observations in a direct shear test on crushed glass using the photoelastic measuring method.

Figure 8-9: The volumetric strain contour viewed in x-y plane (experimental measurement – measured at height $z = 50 \sim 70$ mm)
Figure 8-10: The volumetric strain contour viewed in x-y plane (simulation on irregular particles-measured at height z = 50 ~ 70 mm)
Figure 8-11: The volumetric strain contour viewed in x-y plane
(simulation on spheres-measured at height $z = 50 \sim 70$ mm)
Figure 8-12: The volumetric strain contour viewed in y-z plane (experimental measurement – measured at x = 70 ~ 90 mm)
Figure 8-13: The volumetric strain contour viewed in y-z plane (simulation on irregular particles– measured at x = 70 – 90 mm)
Figure 8-14: The volumetric strain contour viewed in x-z plane
(simulation on spheres – measured at x = 70 ~ 90 mm)
Figure 8-15: The volumetric strain contour viewed in x-z plane (experimental measurement – measured at y = 70 ~ 90 mm)
Figure 8-16: The volumetric strain contour viewed in x-z plane (simulation on irregular particles – measured at y = 70 ~ 90 mm)
Figure 8-17: The volumetric strain contour viewed in x-z plane
(simulation on spheres – measured at y = 70 – 90 mm)
Figure 8-18: The volumetric stress contour viewed in x-y plane (simulation on irregular particles – measured at $z = 50 \sim 70$ mm)
Figure 8-19: The volumetric stress contour viewed in x-z plane
(simulation on irregular particles – measured at x = 70 ~ 90 mm)
Figure 8-20: The volumetric stress contour viewed in y-z plane
(Simulation on irregular particles – measured at x = 70 ~ 90 mm)
• Local macrorotation and microrotation

The local macrorotation is the macrorotation calculated in a tetrahedron which is formed by four adjacent particles. The three components of macrorotations are calculated as (Wang et al. 1999):

\[
\omega_z = \frac{1}{2} \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \quad (8-7a)
\]

\[
\omega_x = -\frac{1}{2} \left( \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) \quad (8-7b)
\]

\[
\omega_y = \frac{1}{2} \left( \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) \quad (8-7c)
\]

The detailed method to calculate the local macrorotation is presented in Chapter 2. The microrotation is the rotation of an individual particle, which can be calculated by Equation 2-19 given in Chapter 2. The simulated value of local macrorotations and microrotations are presented in Table 8-5. Those values were found to be quite different. It is reasonable because the local macrorotation didn’t consider the particle spin. Since the particle spin has been observed in the experiments, the second order gradient theory which ignores the particle spin may not correctly describe the behaviors of granular materials.

• Coordination number

The global coordination number is defined as the average contact number per particle measured in the entire specimen. Similarly, the local coordination number is the average contact number per particle measured in a local volume. The coordination number has been believed to be intimately related to the void ratio of the specimen (Bernal and Mason 1960; Oda 1977). Figure 8-21 presents the local coordination number measured in each layer for the experimental results and simulation results. The simulated coordination number based on irregular particles
presents smaller values in the middle height of the specimen and larger values in the upper and lower heights of the specimen, which showed agreement with the experimental measurements. However, the curve based on the simulation of spheres did not present significant variation along the height of the specimen. The global coordination number before shearing is 5.77 based on the experimental measurements, 5.72 based on the simulation on irregular particles, and 3.61 based on the simulation on spheres. It is apparent that a decrease of the coordination number was caused directly by simplifying irregular particles as spheres in the conventional DEM model, which then led to an under-prediction of the shear zone in the simulation. The clustering DEM model avoided this defect by representing irregular particles using clusters of balls so that it was able to keep a global coordination number close to the experimental measurement.

Table 8-5: The comparison of local macrorotations between simulated results and experimental measurements

<table>
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<th>Δβ(rad)</th>
<th>Δγ(rad)</th>
<th>Δα(rad)</th>
<th>Δβ(rad)</th>
<th>Δγ(rad)</th>
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<td>0.65</td>
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8.4.3 The Prediction of the Microproperties of the Material

- Particle kinematics

The particle translational movements and rotational movements were monitored during the simulation. Figures 8-22, 8-23, and 8-24 illustrated the simulated irregular, simulated spherical, and experimentally measured particle translational movements respectively. In the figure based on experimental results, particles in the lower box moved mostly along the horizontal direction (the direction along which two boxes had relative movement) except those located very close to the shear plane. Particles in the upper box displayed significant vertical dilation. The simulations based on irregular particles gave a similar trend as the experimental observations while those based on spheres showed very erratic particle translational movements.

Figure 8-21: The variation of local coordination number along the height of the specimen.
To compare the accuracy of the prediction of particle kinematics between two simulations, the magnitudes of simulated particle translations versus the experimental measurements were plotted in Figures 8-25 and 8-26. It was found that most of the points based on irregular particles located around the equality line (45° line) while those based on spherical particles were much more scattered, indicating that the simulation based on irregular particles predicted the particle kinematics more accurately than those based on spherical particles. The points for irregular particles still showed some discrepancy from the experimental results. The error possibly resulted from the methodology of approximation and the image processing, which have been described in Chapter 6. The magnitudes of simulated particle rotations versus the experimental measurements were plotted in Figures 8-27 and 8-28. It was found that the points based on irregular particles are closer to the 45° line and those based on spheres are very much scattered, indicating that the clustering DEM model has the capability to predict the particle rotation more accurately than the conventional DEM model.

Figure 8-22: The illustration of particle translational movements (Simulation on spheres)
Figure 8-23: The illustration of particle translational movements (Simulation on irregular particles)

Figure 8-24: The illustration of particle translational movements (Experimental measurement)
Figure 8-25: The comparison of particle displacements between the simulation on irregular particles and the experimental measurement.

Figure 8-26: The comparison of particle displacements between the simulation on spheres and the experimental measurement.
Figure 8-27: The comparison of particle rotations between the simulation on irregular particles and the experimental measurement.

Figure 8-28: The comparison of particle rotations between the simulation on spheres and the experimental measurement.
• Particle kinematics in the shear zone

To evaluate the prediction of the shear zone by two DEM models, the microkinematics including particle displacements and particle rotations in Columns A, B, and C (refer to the monitoring system in Figure 8-5), were plotted in Figure 8-29 (for spheres) and Figure 8-30 (for irregular particles). In Figure 8-29a, the spherical particle displacements showed significant fluctuations between 2 mm and 20 mm from top to bottom in Column A and Column B. There is no significant twist point detected in the displacement transition curve. In Figure 8-29b, the spherical particle rotations are also erratic. Large particle rotations occurred not only near the shear plane but also at the other part in Columns A and B. In a word, no significant shear zone has been formed in the simulation based on spheres. In Figure 8-30a, the transition of irregular particle displacements presented two significant twist points. Between the two points, the particle displacement decreased almost linearly with the increase of the height but beyond the two twist points, its value changed little. The thickness of the shear zone is about 50 mm, similar to the experimental observation. In Figure 8-30b, the irregular particle rotation is small at the upper and lower part of the specimen, and it reached peak value near the shear plane. The zone of interest defined by particle displacements has no significant difference with that defined by particle rotations, which has an agreement with the experimental observations (Figure 4-11 and 4-12).

8.5 Summary and Conclusions

In this chapter, simulations of the direct shear test based on spheres or/and irregular particles were discussed and analyzed. The simulation results including global properties, local behaviors, and microbehaviors by the conventional DEM model and the clustering DEM model were compared and evaluated by the experimental measurements. Although both models presented the ability to predict the bulk friction angle, the conventional DEM model failed to
predict other important behaviors such as the shear strength, vertical dilation, strain localization, and the microkinematics of the granular material.

Figure 8-29: The particle kinematics measured in Column A, B and C (Simulation on spherical particles)

a) Particle displacement distribution along the height of the specimen

b) Particle rotation distribution along the height of the specimen

Figure 8-29: The particle kinematics measured in Column A, B and C (Simulation on spherical particles)
b) Particle rotation distribution along the height of the specimen

Figure 8-30: The particle kinematics measured in Column A, B and C (Simulation on irregular particles)
On the contrary, the clustering DEM model presented good prediction of both macro and micro behaviors of the material by incorporating its real microstructure.

It was found that the coordination number by reconstructing the microstructure using spheres was much smaller than that using irregular particles, which indicates that particle shape affects the contact interactions between particles significantly. This is the main reason that the clustering DEM model can predict the micro-macro behaviors of granular materials more accurately.

By investigating the simulated stresses and strains based on the real microstructure, it is reasonable to believe that the stress and strain relation in granular materials after failure can be more complicated than we thought. There seems no unique relationship between the volumetric strain and the volumetric stress as well as between the applied normal stress and the stress distribution in the specimen.

9.1 Objective

The first objective of this chapter is to investigate the relationship between the microcharacteristics and the macrobehavior of granular materials from a fabric point of view. To achieve this objective, the predictions of fabric evolution using the conventional DEM model and the clustering DEM model will be compared with the experimental observations. The second objective is to evaluate the theoretical relationship between the fabric tensor and the stress tensor using the simulation results.

9.2 Introduction

Fabric describes the arrangement of discrete particles and associated voids (Brewer 1964). It is related to strength and deformation of granular materials through affecting load transfer between particles. The fabric evolution in the shear zone is of great importance to the understanding of the mechanism of shear banding. It has been observed that fabric anisotropy is induced when stress reaches the peak value (Oda and Konoshi 1974). It has also been found that the fabric anisotropy is necessary to generate a new structure in the shear band at the post failure state (Oda and Konoshi 1998). Fabric tensors were introduced in granular mechanics to describe the spatial arrangement of the particles and particle interaction patterns quantitatively. The fabric tensors include the contact normal vector tensor (Oda et al. 1982), the branch vector tensor (Mehrabadi et al. 1982) and the combined contact normal and branch vector tensor (Nemat-Nasser et al. 1984). They are useful to link the granular systems and continua from the deformation viewpoint. The 2D and 3D quantification of fabric quantities have been given by Oda (1972) and Wang et al. (2004) respectively. However, how those fabric quantities are
related to the stress and strain development in the shear band is not well studied. Mehrbadi and Nemat-Nasser (1983) developed a stress-fabric tensor relationship through a statistical consideration of the contact forces between contacting spheres. A strain-fabric-stress tensor relationship (Cowin 1985) has also been applied in continuum mechanics. Though various fabric constitutive relationships have been developed, the validity of these relationships for 3D irregular particles needs to be verified. An evaluation of the stress-fabric tensor relationships using the simulation results based on real microstructures provided in this study presents a potential application of DEM simulations for theoretical validations.

9.3 Definition and Measurement of Fabric Quantities

The commonly used parameters for fabric analysis include coordination number, contact normal vector and its distribution, branch vector and its distribution, and particle orientation and its distribution. These terms are defined as follows:

- Coordination number: the average number of contacts per particle
- Contact normal vector: the unit vector normal to the contact plane at the contact point (refer to Figure 9-1)
- Contact normal distribution: the number of contacts in different orientations
- Branch vector: the unit vector connecting the mass centers of the two contacted particles
- Branch vector distribution: the number of branch vector in different orientations
- Particle orientation distribution: the number of particles with its longest dimensions in different orientations.

The contact plane, which is tangential to the surfaces of both contacting particles, is critical to the load transfer between particles. For spherical particles, there is only one contact point between two contacting spheres, and the unit contact normal vector is equal to the unit
branch vector. The contact plane can be easily determined based on the two mass centers of contacting spheres.

![Diagram](image_url)

Figure 9-1: A 2D illustration of the branch vector, the contact normal and the contact plane. (branch vector connects mass center O1 and O2; contact plane is tangential to the particle surfaces; the contact normal vector is normal to the contact plane.)

However, for irregular particles, there can be several contact points between two contacting particles, and the unit contact normal vector and the unit branch vectors can be quite different (refer to Figure 9-2). Because irregular particles were represented by clusters of balls, the contacts between two irregular particles were in fact the contacts between balls located on the boundary of two particles. No matter how many contact points were formed between those balls, only one contact was counted as the effective contact. The position of an effective contact was approximated by the mean position of balls in contact at the boundary of two particles, and the
effective contact normal vector was approximated by the mean contact normal vector of those balls. The branch vector of two contacting particles was determined by the mass centers of two particles. In order to investigate the local fabric rearrangement, the specimen was evenly divided into 6 layers, i.e. each layer has the same dimension and volume. In each layer, the fabric quantities were measured and analyzed. The fabric quantities for the experimental test could also be measured indirectly in this way by incorporating the original and the deformed microstructure into PFC\(^3\)D.

Figure 9-2: A 3D illustration of branch vector, contact normal and contact plane for spheres and irregular particles
9.4 Branch Vector Distribution, Contact Normal Distribution, and Particle Orientation Distribution

Following the method provided by Wang et al. (2004), the distribution of unit orientation of the branch vector, contact normal vector, and feret length vector (particle orientation) can be evaluated by counting the frequency of those vectors falling into different orientation regions. The orientation regions were determined by evenly dividing the half space (z>0) into 12 regions (shown as Figure 9-3 and Figure 9-4). The distribution of the unit vectors can be obtained by counting the number of vectors that fall in the regions. Regions 1, 2, 3 and 4 were close to the z-axis; Regions 7, 8, 11, and 12 were close to the x-axis; and the regions 5, 6, 9, and 10 were close to the y-axis. To help the demonstration, Regions 1, 2, 3, and 4 were together named as Zone Z; Regions 7, 8, 11, and 12 were together named as Zone X; and Region 5, 6, 9, and 10 were together named as Zone Y.

Figure 9-3: A 3D illustration of the half orientation regions
Tables 9-1~9-7 present the distribution of the branch vector in different layers based on the experimental measurements and two simulations. The distributions of unit fabric vectors in each layer before shearing are plotted in Figure 9-5 for the particle orientation vector, in Figure 9-6 for the contact normal vector, and in Figure 9-7 for the branch vector. Only three orientation zones are illustrated in each figure in order to know the fabric concentration in $x$, $y$, or $z$ direction. The fabric vectors were found not uniformly distributed in the specimen since the fabric distribution in different layers can be quite different. It was also found that distributions of the branch vector based on two simulation setups presented no significant difference from that based on the experimental measurements, none of which show significant orientation concentration. The reason was that the initial distributions of particle mass centers in both simulations, which were critical to the calculation of branch vectors, were controlled by the experimental measurements. However, the distributions of unit contact normal vector were quite different for two simulations. The distribution of contact normal of spheres was actually the same as the
distribution of its branch vector. Neither of them had significant orientation concentration. However, this was not true for irregular particles (refer to Figure 9-2). The distribution of contact normal vector based on the simulation of irregular particles presented a significant concentration in Zone Z, and its particle orientation distribution presented a concentration in either Zone X or Zone Y in each layer, which was consistent with the experimental observations. It was apparent that the clustering DEM model gave a good representation of the microstructure of the actual specimen in terms of both contact normal vector and branch vector distribution while the conventional DEM model failed to present such a consistency.

The change of fabric distributions after shearing is plotted in the Figures 9-8, 9-9 and 9-10 for branch vector, Figures 9-11 and 9-12 for contact normal vector, and Figures 9-13 and 9-14 for particle orientation vector. For the distribution of branch vector based on the simulation of irregular particles, there is a decrease of frequency in Zone Z and an increase in Zone X or Zone Y, indicating that the branch vectors tended to rearrange during shearing from the direction perpendicular to the shear plane to the direction parallel with the shear plane. The closer to the shear plane, the more significant such tendency was. A similar phenomenon was observed for the distribution of contact normal vector and particle orientation, which is in agreement with the experimental observations. For the distribution of branch vector based on the simulation of spheres, the change of the frequency after shearing seemed erratic. It should be pointed out that the absolute value change of fabric frequency distribution predicted by the clustering DEM model did not exactly coincide with the experimental observations. However, it presented an important capability to investigate the rearrangement of irregular particles in 3D during shearing, which is critical to the understanding of the post failure behavior of real granular materials. The discrepancy between the numerical predictions and the experiment could be caused by both the
error accumulated in the experimental measurement and the approximation made in this approach.

Table 9-1: The distribution of the branch vector in different measurement layers (experimental measurement)

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Table 9-2: The distribution of the branch vector in different measurement layers (simulation on irregular particles)

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Table 9-3: The distribution of the branch vector in different measurement layers (simulation on spheres)

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Table 9-4: The distribution of the contact normal vector in different measurement layers (experimental measurements)

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Table 9-5: The distribution of the contact normal vector in different measurement layers (simulation on irregular particles)

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Table 9-6: The distribution of the particle orientation vector in different measurement layers (experimental measurement)

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<td>12</td>
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<td>10</td>
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<td>58</td>
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</tr>
</tbody>
</table>
Table 9-7: The distribution of the particle orientation vector in different measurement layers (simulation on irregular particles)

<table>
<thead>
<tr>
<th>region</th>
<th>region</th>
<th>layer1</th>
<th>layer2</th>
<th>layer3</th>
<th>layer4</th>
<th>layer5</th>
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<tbody>
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<td>5</td>
<td>1</td>
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<td>2</td>
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<td>10</td>
<td>7</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>6</td>
<td>2</td>
<td>2</td>
<td>4</td>
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<td>4</td>
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<td>14</td>
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<td></td>
</tr>
<tr>
<td>x</td>
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<td>8</td>
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<tr>
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<td>3</td>
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</tr>
<tr>
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<td>4</td>
<td>3</td>
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<td>24</td>
<td>20</td>
<td>16</td>
<td>19</td>
<td>19</td>
<td>26</td>
<td></td>
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<tr>
<td>total</td>
<td>50</td>
<td>62</td>
<td>61</td>
<td>56</td>
<td>45</td>
<td>65</td>
<td></td>
</tr>
</tbody>
</table>
Figure 9-5: The distribution of the particle orientation vector in each layer before shearing (Comparison between experimental observations and simulation results)
Figure 9-6: The distribution of the branch vector in each layer before shearing
(Comparison between experimental observations and simulation results)
Figure 9-7: The distribution of the branch vector in each layer before shearing (Comparison between experimental observations and simulation results)
9.5 Fabric Tensor Analysis

Fabric tensor is generally defined as the average tensor product of the unit vectors of the fabric quantities such as the contact normal vector, the branch vector, and the particle orientation vector. It is often used in continuum mechanics to describe the spatial arrangement of particles and voids in granular systems, and it is very useful to link the granular systems and continua. Furthermore, fabric tensors make it possible to incorporate the anisotropic microstructure characteristics of the material into the constitutive model, which is expected to better describe the behavior of the material (Oda 1989; Zysset and Curnier 1995). Hilliard (1962, 1967) provided a method to determine fabric tensors based on stereological principles. Kanatani (1984, 1985) developed cartesian tensor formulations to represent the distribution function $f(n)$ of any fabric quantities, which is useful to back calculate the fabric tensors. An estimation of $f(n)$ using second order fabric tensor is presented using the following equation (Wang 2004):

$$f(n) = \frac{C}{4\pi} \left[ 1 + \phi_y n_i n_j \right]$$

(9-1)

where $C = \int_{\Omega} f(n)dn$, $\Omega$ denotes the spherical domain of integration.

$n_i =$ unit vector of a domain, $i=1, 2, 3$

$f(n) =$ distribution function representing the orientation distribution

of any fabric quantities

$\phi_y =$ any second order fabric tensor.

The measured distribution of the fabric quantities $f(n)_m$ can be used to calculate fabric tensors by Newton’s method, i.e. minimizing the square differences between the measured and predicted distributions as follows (Wang 2004):
\[
\frac{\partial}{\partial \phi_{pq}} \left( \sum \left( f(n)_{m} - \frac{C}{4\pi} \left[ I + \phi_{ij} n_i n_j \right] \right)^{2} \right) = 0
\]  
(9-2)

The above formulation in fact includes six independent linear equations since there are six unknown terms for a symmetric second order tensor. \( C \) values are the total number of fabric quantities for the experiment measurements and simulation results, and are presented in Table 9-8. The unit vectors \( n_i \) of the 12 regions are presented in Table 9-9. The calculated fabric tensors are presented in Tables 9-10 and 9-11.

Figure 9-8: Change of frequency of particle orientation vectors in each layer after shearing. A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (experimental observations)
Figure 9-9: Change of frequency of particle orientation vectors in each layer after shearing. A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (simulation on irregular particles)
Figure 9-10: Change of frequency of branch vectors in each layer after shearing
A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (experimental observations)
Figure 9-11: Change of frequency of branch vectors in each layer after shearing. A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (simulation on irregular particles)
Figure 9-12: Change of frequency of branch vectors in each layer after shearing. A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (simulation on spheres)
Figure 9-13: Change of frequency of contact normal vectors in each layer after shearing. A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (experimental observations)
Figure 9-14: Change of frequency of contact normal vectors in each layer after shearing. A negative value indicates frequency decreased in that zone and a positive value indicates that frequency increased in that zone. (Simulation on irregular particles)
Table 9-8: The C values used for the calculation of fabric tensors after shearing

<table>
<thead>
<tr>
<th>fabric terms</th>
<th>C experiment</th>
<th>Simulation-irregular particle</th>
<th>Simulation-sphere</th>
</tr>
</thead>
<tbody>
<tr>
<td>branch</td>
<td>1288</td>
<td>1786</td>
<td>972</td>
</tr>
<tr>
<td>contact normal</td>
<td>1288</td>
<td>1786</td>
<td>972</td>
</tr>
<tr>
<td>particle orientation</td>
<td>246</td>
<td>331</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Table 9-9: The representative unit vector $n_i$ of the 12 orientation regions

<table>
<thead>
<tr>
<th>region</th>
<th>n1</th>
<th>n2</th>
<th>n3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.2706</td>
<td>0.2706</td>
<td>0.9239</td>
</tr>
<tr>
<td>2</td>
<td>0.8636</td>
<td>0.3536</td>
<td>0.3827</td>
</tr>
<tr>
<td>3</td>
<td>0.3536</td>
<td>0.8536</td>
<td>0.3827</td>
</tr>
<tr>
<td>4</td>
<td>-0.2706</td>
<td>0.2706</td>
<td>0.9239</td>
</tr>
<tr>
<td>5</td>
<td>-0.3536</td>
<td>0.8536</td>
<td>0.3827</td>
</tr>
<tr>
<td>6</td>
<td>-0.8536</td>
<td>0.3536</td>
<td>0.3827</td>
</tr>
<tr>
<td>7</td>
<td>-0.2706</td>
<td>-0.2706</td>
<td>0.9239</td>
</tr>
<tr>
<td>8</td>
<td>-0.8536</td>
<td>-0.3536</td>
<td>0.3827</td>
</tr>
<tr>
<td>9</td>
<td>-0.3536</td>
<td>-0.8536</td>
<td>0.3827</td>
</tr>
<tr>
<td>10</td>
<td>0.2706</td>
<td>-0.2706</td>
<td>0.9239</td>
</tr>
<tr>
<td>11</td>
<td>0.3536</td>
<td>-0.8536</td>
<td>0.3827</td>
</tr>
<tr>
<td>12</td>
<td>0.8536</td>
<td>-0.3636</td>
<td>0.3827</td>
</tr>
</tbody>
</table>

Table 9-10: The calculated contact normal vector tensors in different local volumes

<table>
<thead>
<tr>
<th>local volume</th>
<th>Contact normal tensor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Phi_{11}$</td>
</tr>
<tr>
<td>layer 1</td>
<td>-0.2240</td>
</tr>
<tr>
<td>layer 2</td>
<td>-0.0820</td>
</tr>
<tr>
<td>layer 3</td>
<td>0.1374</td>
</tr>
<tr>
<td>layer 4</td>
<td>-0.1018</td>
</tr>
<tr>
<td>layer 5</td>
<td>-0.0639</td>
</tr>
<tr>
<td>layer 6</td>
<td>-0.2777</td>
</tr>
<tr>
<td>global</td>
<td>0.1171</td>
</tr>
</tbody>
</table>
Table 9-11: The calculated branch vector tensors in different local volumes

<table>
<thead>
<tr>
<th>local volume</th>
<th>( \Phi_{11} )</th>
<th>( \Phi_{12} )</th>
<th>( \Phi_{13} )</th>
<th>( \Phi_{21} )</th>
<th>( \Phi_{22} )</th>
<th>( \Phi_{33} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>layer 1</td>
<td>0.0186</td>
<td>-0.3869</td>
<td>-0.3064</td>
<td>0.0636</td>
<td>0.2667</td>
<td>-0.1899</td>
</tr>
<tr>
<td>layer 2</td>
<td>0.4285</td>
<td>-0.2888</td>
<td>0.0845</td>
<td>0.0593</td>
<td>0.4051</td>
<td>-0.5193</td>
</tr>
<tr>
<td>layer 3</td>
<td>0.1886</td>
<td>-0.7861</td>
<td>-0.1116</td>
<td>-0.3078</td>
<td>0.3382</td>
<td>-0.0283</td>
</tr>
<tr>
<td>layer 4</td>
<td>0.0366</td>
<td>-0.6008</td>
<td>0.1049</td>
<td>-0.2720</td>
<td>0.5450</td>
<td>0.0680</td>
</tr>
<tr>
<td>layer 5</td>
<td>0.1422</td>
<td>-0.4303</td>
<td>0.1666</td>
<td>-0.2749</td>
<td>0.4688</td>
<td>-0.0161</td>
</tr>
<tr>
<td>layer 6</td>
<td>0.0105</td>
<td>-0.4327</td>
<td>-0.4696</td>
<td>-0.0761</td>
<td>-0.1824</td>
<td>-0.0714</td>
</tr>
<tr>
<td>global</td>
<td>-0.1055</td>
<td>0.1737</td>
<td>0.0721</td>
<td>0.0013</td>
<td>0.2247</td>
<td>-0.0379</td>
</tr>
</tbody>
</table>

9.6 Several Useful Fabric Relationships

9.6.1 Stress-Fabric-Strain Tensor Relationship

The fabric tensor can be applied in continuum constitutive models to describe the stress and strain relationship by taking into account anisotropic characteristics of materials. An elastic stress-strain relationship (Cowin 1985) can be defined as following:

\[
\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \tag{9-3}
\]

where \( \sigma_{ij} \) = stress tensor

\( C_{ijkl} \) = elasticity tensor, which is a function of the fabric tensor

\( \varepsilon_{kl} \) = strain tensor.

The general form of \( C_{ijkl} \) was given by Truesdell and Noll (1965), which assumed that the elasticity tensor was a function of the second rank fabric tensor.

9.6.2 Strain-Fabric Tensor Relationship

The fabric tensor can be related to the deformation rate tensor and the spin tensor which are used to describe the strain characteristics of materials in continuum mechanics. The
relationship between the overall deformation rate and the contact normal tensor and the relationship between the spin tensor and the contact normal tensor were given by Mehrabadi and Nemat-Nasser (1983):

\[
D_{ij} = \frac{1}{2} (E_{ik} J_{kj} + E_{jk} J_{ki})
\]

(9-4a)

\[
W_{ij} = \frac{1}{2} (E_{ik} J_{kj} - E_{jk} J_{ki})
\]

(9-4b)

where \( D_{ij} \) = overall deformation tensor

\( W_{ij} \) = spin tensor

\( E_{ik} \) = strain rate tensor

\( J_{ik} \) = contact normal tensor.

### 9.6.3 Stress-Fabric Tensor Relationship

The fabric tensor can also be directly related to the overall stress by regarding the overall stress tensor and the fabric tensor as coaxial tensors (Mehrabadi et al. 1982), using the following equations:

\[
\sigma_{ij} = \alpha_0 J_{ij} + \alpha_1 J_{ik} J_{kj}
\]

(9-5a)

\[
\sigma_{ij} = \beta_0 F_{ij} + \beta_1 F_{ik} F_{kj}
\]

(9-5b)

where, \( \alpha_0, \alpha_1 \) and \( \beta_0, \beta_1 \) = functions of the invariants of the stress tensor

\( J_{ij} \) = contact normal tensor

\( F_{ij} \) = branch vector tensor.
9.7 3D Evaluation of the Stress-Fabric Relationship

The stress-fabric relationships described by Equation 9-4 have been validated by experiments on 2D photoelastic granules with oval cross sections (Oda et al. 1982). But whether it is applicable for 3D real irregular particles is not known. With the simulated stresses and fabric quantities on irregular particles, the 3D validity of those equations can be evaluated by comparing the isotropic stress using the classic calculation and those using fabric quantities.

An isotropic overall stress is defined as the following equation:

\[
\bar{\sigma} = \left( \sigma_{11} + \sigma_{22} + \sigma_{33} \right)
\]  

(9-6)

The overall stress is calculated as (Oda 1999)

\[
\sigma_{ij} = \frac{1}{V} \sum_{np} \sigma_{ij}^p dv^p
\]  

(9-7)

Substituting Equation 9-7 into Equation 9-6, the overall isotropic stress can be calculated directly from the isotropic stress in particles using the following conventional equation:

\[
\bar{\sigma} = \frac{1}{V} \sum_{np} \sigma_{ii}^p dv^p
\]  

(9-8)

Substituting Equation 9-5a into Equation 9-6, the isotropic overall stress can be calculated by the contact normal tensor using the following equation:

\[
\bar{\sigma} = \left( \alpha_0 (J_{11} + J_{22} + J_{33}) + \alpha_1 (2J_{11}J_{12} + 2J_{12}J_{12} + J_{22}J_{22} + 2J_{23}J_{23} + J_{33}J_{33}) \right)
\]  

(9-9a)

Substituting Equation 9-5b into Equation 9-6, the isotropic overall stress can also be calculated by the branch vector tensor:

\[
\bar{\sigma} = \left( \alpha_0 (F_{11} + F_{22} + F_{33}) + \alpha_1 (2F_{11}F_{12} + 2F_{12}F_{12} + F_{22}F_{22} + 2F_{23}F_{23} + F_{33}F_{33}) \right)
\]  

(9-9b)

In order to obtain the material constants \(\alpha_0, \alpha_1\), several local isotropic stresses and local fabric tensors were measured and substituted into Equation 9-9. Several material constants \(\alpha_0, \alpha_1\) can
be calculated by solving those linear equations. The results are presented in Table 9-12. Using the average value of calculated $\alpha_0, \alpha_1$, the overall isotropic stress at peak was calculated as 1.73 kPa by Equation 9-9a and 8.84 kPa by Equation 9-9b. The overall isotropic stress calculated by the conventional Equation 9-8 was 1.13 kPa. The calculation using branch vector tensor by Equation 9-9b much overestimated the isotropic stress, and the calculation using the contact normal tensor by Equation 9-9a was close to the conventional calculation.

Table 9-12: The material constants and the calculated isotropic stress using fabric tensors

<table>
<thead>
<tr>
<th>measure volume</th>
<th>Calculation from branch vector tensor</th>
<th>Calculation from contact normal tensor</th>
<th>Calculation from particle stresses</th>
</tr>
</thead>
<tbody>
<tr>
<td>layer1,2</td>
<td>$a0 = -0.00015$ $\alpha l = 563.4$</td>
<td>$a0 = -0.0061$ $\alpha l = 1614.9$</td>
<td>N/A</td>
</tr>
<tr>
<td>layer3,4</td>
<td>$a0 = -0.00011$ $\alpha l = 1935.9$</td>
<td>$a0 = -0.0052$ $\alpha l = 4305.1$</td>
<td>N/A</td>
</tr>
<tr>
<td>layer5,6</td>
<td>$a0 = -0.00002$ $\alpha l = 34369.0$</td>
<td>$a0 = -0.0030$ $\alpha l = -1010.6$</td>
<td>N/A</td>
</tr>
<tr>
<td>isotropic stress (kPa)</td>
<td>8.8400</td>
<td>1.7300</td>
<td>1.13</td>
</tr>
</tbody>
</table>

9.8 Summary and Conclusion

The fabric quantities including branch vector, contact normal vector, and particle orientation vector were measured for two DEM models. The distributions of fabric quantities in each model were obtained by counting the frequency of fabric vectors falling into different orientation regions. The distributions of the branch vector based on two simulation setups presented no significant difference. The reason is that the initial distributions of particle mass centers in both simulations were controlled similarly to the experimental measurements. However, the distributions of the unit contact normal vector are quite different for two simulations due to the effect of particle shape. Compared to the conventional DEM model, the
clustering DEM model gave a better representation of the fabric distribution of the specimen, which made it capable to simulate the 3D rearrangement of irregular particles during shearing more accurately.

The fabric tensors for simulation on irregular particles were calculated based on the observed fabric distributions. Those terms are useful for the evaluation of constitutive relationships of granular materials. The stress-fabric relationships were evaluated using simulated data, which gave an example for another useful application of DEM simulations. The stress-contact normal tensor relationship was evaluated valid in a certain degree, but the stress-branch vector relationship seemed unsuitable for the description of irregular particles.
CHAPTER 10: SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

10.1 Summary

This research developed a 3D clustering DEM model to simulate the material strength and dilations, particle kinematics, and fabric evolution of granular materials and developed a non-invasive experimental method to evaluate the simulation results. The microstructures acquired by x-ray tomography imaging were employed for both experimental quantifications and DEM simulations.

New methodologies were included in the non-invasive method for 3D representation of irregular particles and 3D quantification of particle kinematics and local strains. These methodologies were applied for the results analysis of the compression test and the direct shear test.

A microproperty specification procedure was performed to calibrate the input microparameters. The effect of input parameters including particle stiffness, particle friction coefficient, particle size, damping coefficient, wall stiffness, and friction coefficient were investigated by preliminary simulations.

The clustering DEM model represented real irregular particles by clusters of small balls. Two burn algorithms were developed and compared in order to model the irregular particles more effectively. Simulations of the compression test and direct shear test were performed and analyzed. The effect of particle shape was investigated by comparing the simulations based on spheres and those based on irregular particles. The irregular particles and the spherical particles were generated using the exact particle mass centers and volumes by the experimental measurements so that the two synthetic materials had similar aggregate skeletons but different particle shape configurations. For the simulations of the compression test, the predictions of
behaviors of materials included particle translations, local strains, global deformations, and global strains. For the simulation of the direct test, the prediction included particle translations, particle rotations, fabric distributions, fabric evolution, thickness of shear zone, local stresses and strains, global strength, and deformations.

The theoretical stress-fabric tensor relation was evaluated by DEM simulation results.

10.2 Conclusions

This study achieved the objectives to simulate the micro-macro behavior of granular material with irregular particle shape configurations and to develop an experimental quantification method to evaluate the simulated results. The following conclusions are drawn according to the findings of this study.

1) The non-invasive experimental method developed in this study is practical for 3D representation of irregular particles and quantification of particle kinematics and local strains. The quantified particle displacements and local strains are proved reasonable by matching global deformations. The particle-recognizing procedure relies on the mass center of particle cross sections, and it is applicable to those experimental tests in which particles have relatively small displacements compared to their sizes. For those that may experience large particle displacement, the suggestion is to compare images acquired at different time intervals during the structural evolution; then the recognizing procedure can be applied to each stage. The methodology for the quantification of particle rotations is not applicable to particles without significant ferret length.

2) The clustering DEM model developed in this study presented the capability to predict particle kinematics, fabric evolutions, stress distributions, and strain distributions of granular materials. The employment of the burn algorithm saved significant computation time by enabling the representation of irregular particles using much fewer balls.
input parameters for the clustering DEM model have physical meaning and are easy to calibrate compared to those for continuum models. Particle stiffness and particle surface friction angle have the most significant effect on the material strength. Other parameters, such as the ratio of wall stiffness to the particle stiffness, wall friction coefficient, and damping coefficient, have little effect on simulation results.

3) The particle shape has significant effect on the micro-macro behavior of granular materials. Compared to the conventional DEM model (using spheres), the clustering DEM model (using irregular particles) predicted material strength, particle motions and fabric evolutions more accurately. The simulated microkinematics based on spheres presented a significant discrepancy from the experimental measurements, indicating that the conventional model may not correctly describe the micromechanisms of the material.

4) From a fabric distribution viewpoint, the clustering DEM model gave a more accurate representation of material fabrics than the conventional DEM model. This ability made the clustering DEM model able to simulate the 3D rearrangement of irregular particles more precisely.

5) Using the simulation results of the clustering DEM model, the stress-contact normal tensor relationship was proved valid to a certain degree, while the stress-branch vector relationship seemed unsuitable for the description of the 3D constitutive relation of irregular particles.

10.3. Recommendations for Further Study

10.3.1 Improving the Accuracy of the Simulations

Although the clustering DEM model has demonstrated the ability to predict the microkinematics of the granular material, some discrepancies still exist between simulation predictions and experimental measurements. Factors that may influence the accuracy of the
simulation results include the quality of images, the accuracy of image processing and image analysis, the approximation of particle shape, and the accuracy of parameter calibrations. High-quality images are critical to the accurate representation of the microstructure which is important to the DEM simulation and the experimental quantification. High-resolution imaging technology together with carefully prepared specimens would be helpful to obtain qualified images. The success of the burn algorithm decreased the accuracy of particle shape representation though it improved the efficiency of simulation. There seems to be a dilemma between the accuracy of the model and the efficiency of the simulation. However, when a supercomputing resource is available, the accuracy of the model can be improved by using more balls to represent real irregular particles.

The particle stiffness and the particle friction coefficient significantly affect the prediction of microkinematics and macrodeformations. Currently, there is no standard experimental method to obtain the microparameters. The calibration of microparameters must rely on the macroproperties of materials. The macroproperties used in this study are the bulk friction angle and the peak-strength of materials. If more macroproperties were available and a better calibration procedure was employed, the calibrated parameters would describe the microproperties of materials more accurately.

10.3.2 Improving the Capability of the Clustering DEM Model

In this study, the clustering DEM model investigated the influence of particle shape on the micro-macro behavior of granular materials. It also has the potential to study the effect of particle roughness, non-linear behavior, and even a three-phase material system.

- Particle roughness

Particle surface roughness is an important factor that may affect the micro-macro behaviors of materials. Compared to the smooth surface, the contact area between rough
surfaces is extremely small. The contact interaction pattern in the microscale as well as the macro deformation and strength can also be different for particles with rough surfaces.

- **Non-linear contact model**

  A linear elastic contact model was used in this study. It is sound for materials composed of rigid particles with a smooth surface. However, a non-linear elastic contact or plastic contact could exist between particles with asperities and rough surfaces. The non-linear behaviors of the particles need to be considered in further research.

- **Three-phase system**

  A two-phase system including particles and voids was employed in the current 3D clustering DEM model, but it has the potential to model properties of multiple-phase systems such as asphalt concrete. Each phase can be modeled by clusters of small balls with corresponding stiffness. The effect of asphalt binder can be simulated by the contact bond and parallel bond provided in PFC\textsuperscript{3D}. A 2D application of this feature was presented in the research work of You and Buttler (2002) who developed their own 2D clustering DEM model (also called the MDEM model) to predict the modulus of asphalt concrete in low temperature.

### 10.3.3 Other Applications of the Experimental Measurement Method

The quantification methodologies can also be applied in other experiments on granular materials. The quantified particle kinematics and local strains can be used for the evaluation of the validity of continuum theories such as the second-order gradient theory.
REFERENCES


Darve, F., Liquefaction phenomena of granular materials and constitutive stability, Engineering Computations (Swansea, Wales), v 13, n 7, p 5-28, 1996.


Rothenburg, L., Micromechanical features of granular assemblies with planar elliptical particles, Geotechnique v 42, 79-95, 1992.


Thornton, C. Applications of DEM to process engineering problems, Engineering Computations (Swansea, Wales), v 9, n 2, Apr, p 289-297, 1992.


NOMENCLATURE

The following symbols are used in this dissertation:

\( C \)  Total number of observed fabric quantities

\( C_f \)  Correct factor for calculation of average stress in the measure sphere

\( D_f \)  Fraction of critical damping

\( d_i \)  Distance between boundary points of one particle

\( DISP \)  Particle translational displacement

\( \dot{e}_{ij} \)  Rate-of-deformation tensor

\( F \)  Contact force vector between particles

\( F_i^n \)  Normal contact force vector between particles

\( F_i^s \)  Shear contact force vector between particles

\( G_s \)  Bulk specific gravity

\( G_w \)  Mass of a unit volume of water

\( \Delta H \)  Space between two adjacent image slices

\( \Delta h \)  Vertical global deformation of the specimen

\( h \)  Height of the specimen

\( I^A \)  Moment of inertia of particle \( A \)

\( I^{clp} \)  Product of inertia of clump

\( L_{\text{max}} \)  Feret length of individual particle

\( \Delta l \)  Lateral deformation of specimen

\( K^n \)  Particle Normal stiffness

\( K^s \)  Particle shear stiffness
$N_R$  Row number in image bitmap

$N_C$  Column number in image bitmap

$N_Z$  Image slice number

$M^A$  Moment about the center of particle $A$

$m_{clp}$  Mass of clump

$m^p$  Mass of ball

$m_s$  Mass of solids

$N_p$  Number of particles

$N_c$  Number of contacts.

$N_p$  Number of particles

$n$  Porosity of the assembly

$n_i$  Unit normal vector of the contact plane

$n^{AB}$  Unit normal vector at the contact point

$r$  Radius diameter of specimen.

$\Delta r$  Displacement in the radial direction of specimen

$SI$  Similarity index of particle cross sections

$SI_p$  Similarity index of particle

$t^{AB}$  Tangential vector at the contact point

$U^n$  Relative displacement between contacting particles

$\Delta U_i^s$  Increment of particle shear displacement

$u$  Particle displacement at x direction

$V$  Global volume
\( v \)  
Particle displacement at \( y \) direction

\( v_{i,j} \)  
Velocity gradient tensor

\( V_{fi} \)  
Volumetric fraction of each local volume to the total volume

\( V_p \)  
Volume of particle \( P \)

\( V_m \)  
Volume of the measure sphere

\( V_s \)  
Total volume of particles

\( V_T \)  
Volume of the entire specimen

\( \Delta W_{(i)} \)  
Energy removed per cycle of calculation

\( W_{(i)} \)  
Mean kinetic energy at the instant of removal.

\( w \)  
Particle displacement at \( z \) direction

\( x^p \)  
Mass center coordinates of ball

\( x^{clp} \)  
Mass center coordinates of clump

\( x \)  
Mass center coordinates of individual particles after test

\( \dot{x} \)  
Particle translational velocity

\( \ddot{x} \)  
Particle translational acceleration

\( \Delta x^A \)  
Translational displacement of particle \( A \)

\( \alpha_{dc} \)  
Damping coefficient

\( \alpha_{yi} \)  
Strain rate tensor

\( \varepsilon \)  
Effective global strain

\( \varepsilon_i \)  
Global strain

\( \varepsilon_V \)  
Volumetric strain

\( \varepsilon_i^l \)  
Local strain
\( \theta \)  
Particle orientation angle

\( \sigma \)  
Global strain

\( \sigma' \)  
Local strain

\( \Delta \Omega \)  
Particle rotation vector

\( \Omega \)  
Orientation of the individual particle in initial configuration

\( \Delta \omega^A \)  
Rotations about the center of particle \( A \)

\( \dot{\varpi} \)  
Particle rotational velocity

\( \ddot{\omega} \)  
Particle rotational acceleration

\( \omega_{ij} \)  
Spin tensor
APPENDIX I: FORTRAN CODE FOR 3D PARTICLE IDENTIFICATION

Note: This code was developed for identifying individual particles from sectional images of the specimen automatically. The identification was based on the particle cross-section mass centers and areas. Only a representative portion of this code is presented. Please contact me for the complete code.

DIMENSION SMASSX(174,150),SMASSY(174,150)
DIMENSION PERMT(174,150),AREA(174,150),NOV(174)
DIMENSION KCOUNT(150),KOUT(174,150),SIMIN(174,150)
DIMENSION KKNEXT(174,150),FERET(174,150),IZBAD(174)
DIMENSION IPU(174,150),IPD(174,150)
DIMENSION NOP(174,150),IPBZ(3000),IPEZ(3000)
DIMENSION IPNO(3000,174),ICOUNT(150)
DIMENSION SMX(3000),SMY(3000),SMZ(3000)
CHARACTER OPENPATH*28
CHARACTER InEXT*4,InNAME1*4,InNAME2*2
CHARACTER INFILE1*39, INFILE2*37
CHARACTER OUTPATH*27,OUTEXT*4,OUTNAME1*3,OUTNAME2*3
CHARACTER OUTNAME3*2,OUTFILE3*38,OUTFILE4*33
CHARACTER OUTFILE1*37, OUTFILE2*38,OUTNAME4*2
CHARACTER FNUMBER*3
CHARACTER FNUMBEQ*4
OPENPATH='C:\location\inputdat\SIdata\'
OPENPATH='C:\location\inputdat\SIdata\'
InNAME1='NOSI'
InNAME2='SI'
InEXT='.DAT'
OUTPATH='C:\LOCATION\OUTDAT\bf_test\'
OUTEXT='.TXT'
OUTNAME1='PSI'
OUTNAME2='PIZ'
OUTNAME3='MCC'
OUTNAME4='MC'
OUTFILE4=OUTPATH//OUTNAME4//OUTEXT

NSLICE=90
SIMA=20.
SIMAX=2.5

DO 5 IZ=1,NSLICE
IZZ=IZ
K0=INT(IZ/100)
K=48+IZ-K0*100
KK=INT((IZ-K0*100)/10)
KI=K-KK*10

FNUMBER=CHAR(48+K0)//CHAR(48+KK)//CHAR(KI)

INFILE1=OPENPATH//InNAME1//FNUMBER//InEXT

C WRITE(*,*)' INFILE1=',INFILE1

C PAUSE

OPEN(IZZ,FILE=INFILE1,STATUS='OLD')

READ(IZZ,6) NOV(IZ)

WRITE(*,*)' IZ=',IZ

6 FORMAT(16x,I4)

CLOSE(IZZ)

NOVIZ=NOV(IZ)

5 CONTINUE

PAUSE' 0000000000'

DO 8 IZ=1,NSLICE

WRITE(*,*)' IZ=',IZ

IZZ=IZ

K0=INT(IZ/100)

K=48+IZ-K0*100

KK=INT((IZ-K0*100)/10)

KI=K-KK*10

FNUMBER=CHAR(48+K0)//CHAR(48+KK)//CHAR(KI)

INFILE2=OPENPATH//InNAME2//FNUMBER//InEXT
OPEN(IZZ,FILE=INFILE2,STATUS='OLD')

C WRITE(*,*)' INFILE2=',INFILE2

C PAUSE

READ(IZZ,*) (AREA(IZ,I),SMASSX(IZ,I),SMASSY(IZ,I),
# FERET(IZ,I),PERMT(IZ,I),I=1,NOV(IZ))

CLOSE(IZZ)

8 CONTINUE

DO 925 IZ=1,NSLICE-1

DO 916 II=1,NOV(IZ)

KCOUNT(II)=0

916 CONTINUE

DO 921 I=1,NOV(IZ)

SII=100000.

DO 918 J=1,NOV(IZ+1)

SIP=ABS(SMASSX(IZ,I)-SMASSX(IZ+1,J))+
# ABS(SMASSY(IZ,I)-SMASSY(IZ+1,J))

IF(SIP.LT.SII) THEN

SII=SIP

KNEXT=J

END IF

918 CONTINUE

KKNEXT(IZ,I)=KNEXT

SIMIN(IZ,I)=SII
OPEN(IZZ, FILE=OUTFILE3, STATUS='NEW')
WRITE(IZZ,*) 'PARTICLE', IP, ', BS', IBZ(IP), ', ES', IPZ(IP)
DO 1886 IZ=IBZ(IP), IPZ(IP)
   IS=IPNO(IP, IZ)
   ZZ=(IZ)*.5407
WRITE(IZZ, 1885) IZ, AREA(IZ, IS), PERMT(IZ, IS), SMAXX(IZ, IS),
               # SMASY(IZ, IS), ZZ
1886 CONTINUE
CLOSE(IZZ)
1888 CONTINUE
1885 FORMAT(5X, I8, 5F10.2)
OPEN(1, FILE=OUTFILE4, STATUS='NEW')
WRITE(*,*) OUTFILE4
PAUSE
WRITE(1, 1668) (KS, IBZ(KS), IPZ(KS), SMX(KS), SMY(KS),
               # SMZ(KS), KS=1, KTOTAL)
1668 FORMAT(5X, 3I8, 3F8.2)
CLOSE(1)
END
APPENDIX II: FORTRAN CODE FOR 3D PARTICLE BOUNDARY DETECTION

Note: This code was developed for detecting particle boundary for the need of particle rotation quantification. The detection was based on image bitmaps. Only a representative portion of this code is presented. Please contact me for the complete code.

DIMENSION SMASSX(94,160),SMASSY(94,160),FERET(94,160)
DIMENSION PERMT(94,160),AREA(94,160),NOVP(94)
DIMENSION IPNO(1280,94),IPZB(1280),IPZE(1280)
DIMENSION IP(94,160)
DIMENSION IA(94,512,512),IB(94,512,160),IE(94,512,160)
DIMENSION N1(94,512),JCOUNT(160)
DIMENSION NOV(94),NV(94,512,160)
DIMENSION NOL(94,1280),KTEMP(1280)
DIMENSION LB(94,1280),LEND(94,1280)
DIMENSION IPRB(1280,94),IPRE(1280,94)
DIMENSION IPCB(1280,94,512),IPCE(1280,94,512)
DIMENSION NNAREA(94,1280)

CHARACTER OPENPATH1*33,OPENPATH2*34,InEXT*4
C  CHARACTER OPENPATH1*28,OPENPATH2*28,InEXT*4
CHARACTER InNAME1*4,InNAME2*2,InNAME3*4,InNAME4*3
C  CHARACTER INFFILE1*39, INFFILE2*37,INFFILE3*39,INFFILE4*38
CHARACTER INFIL1*44, INFIL2*42, INFIL3*45, INFIL4*38
CHARACTER OUTPATH*27, OUTEXT*4, OUTPATH2*26
CHARACTER OUTNAME2*3, OUTFILE2*37
C CHARACTER OUTFILE1*29, OUTNAME1*3
CHARACTER FNUMBER*3, inext2*4, FOUT1*33, FOUT2*36
CHARACTER FNUMBERQ*4
C INPUT DATA
C …This portion is not presented
OPENPATH1='C:\location\inputdat\SIDATA_TEST\'
C OPENPATH1='C:\location\inputdat\SIDATA\'
InNAME1='NOSI'
InNAME2='SI'
InEXT='\DAT'
Inext2='\bit'
OPENPATH2='C:\location\inputdat\BITDATA_TEST\'
C OPENPATH2='C:\location\inputdat\BITDAT\'
InNAME3='PBIT'
InNAME4='PIZ'
OUTPATH='C:\LOCATION\OUTDAT\VD_TEST\'
OUTPATH2='C:\LOCATION\OUTDAT\VBOUND\'
C OUTPATH='C:\LOCATION\OUTDAT\BF_TEST\'
C OUTPATH2='C:\LOCATION\OUTDAT\BBOUND\'
OUTEXT='\TXT'
C  OUTNAME1='PSI'
OUTNAME2='PBD'

NSLICE=94
KTOTAL=1280
C  …This portion is not presented

DO 1888 IPP=1,KTOTAL
IZZ=100
  K0=INT(IPP/1000)
  K=48+IPP-K0*1000
  KK=INT((IPP-K0*1000)/100)
  KI=INT((IPP-K0*1000-KK*100)/10)
  KQ=INT(IPP-K0*1000-KK*100-KI*10)
  FNUMBERQ=CHAR(48+K0)//CHAR(48+KK)//CHAR(KI)//CHAR(48+KQ)
  OUTFILE2=OUTPATH2//OUTNAME2//FNUMBERQ//OUTEXT
C  K0=INT(IPP/100)
C  K=48+IPP-K0*100
C  KK=INT((IPP-K0*100)/10)
C  KI=K-KK*10
C  FNUMBER=CHAR(48+K0)//CHAR(48+KK)//CHAR(KI)
C  OUTFILE2=OUTPATH2//OUTNAME2//FNUMBER//OUTEXT
OPEN(IZZ,FILE=OUTFILE2,STATUS='NEW')
WRITE(IZZ,*) ' PARTICLE',IPP,' BEGIN SLICE=',IPZB(IPP),
# ' END SLICE=',IPZE(IPP)

DO 1885 KZ=IPZB(IPP),IPZE(IPP)

write(IZZ,* ) ' SLICE=',KZ,' BEGIN LINE=',IPRB(IPP,KZ),#
# ' END LINE=',IPRE(IPP,KZ)

WRITE(IZZ,1887) (I,IPCB(IPP,KZ,I),IPCE(IPP,KZ,I),
# I=IPRB(IPP,KZ),IPRE(IPP,KZ))

1885 CONTINUE

1887 FORMAT(1X,3I8)

CLOSE(IZZ)

1888 CONTINUE

END
APPENDIX III: PFC$^3$D CODE FOR 3D IRREGULAR PARTICLE REPRESENTATION IN DEM SIMULATION

Note: This code was developed for presenting irregular particles in the clustering DEM simulation. The irregular particles were represented by clusters of small balls using this code. Only a representative portion of this code is presented. Please contact me for the complete code.

;fname gen_particle
new

;-------------------------
def get_data ;--------------input geometric information of individual particles
array aa(100000)
array xx0(100000) yy0(100000) zz0(100000)
array vol(1280)
path='C:\\location\\outdat\\bbound\\'
pmm=0
idc2=0
space=round(2*0.6744*512.0/158.0); convert minimiter to pixel value
;space=4.0
section
loop n1(0,1)
loop n2(0,9)
loop n3(0,9)
loop n4(0,9)
pmm=pmm+1
if pmm>num_agg
    ;command
    ;pause
    ;end_command
exit section
end_if
if n1=0
    if n2=0
        if n3=0
            if n4=0
                n4=1
            end_if
        end_if
    end_if
end_if
fname=path+'PBD'+string(n1)+string(n2)+string(n3)+string(n4)+'.txt'
status=open(fname,0,1)
status=read(aa,10000)
status=close
nn=0
nb=0
next_n=2

b_dep=parse(aa(1),5)
e_dep=parse(aa(1),8)

addp=1

loop dep (b_dep,e_dep)

roll=parse(aa(next_n),8)-parse(aa(next_n),5)+1

loop n_roll1 (1,roll1)

rol=next_n+n_roll1

ny=parse(aa(rol),3)-parse(aa(rol),2)

; if n_roll1=1 ; extend the boundary 1 pixels
; loop ynn(1,addp)
; loop col(-addp,ny+addp)

; nb=nb+1
; yy0(nb)=parse(aa(rol),1)-ynn
; zz0(nb)=dep*space
; xx0(nb)=parse(aa(rol),2)+col

; end_loop
; end_loop
; end_if

loop col(-addp,ny+addp)

nb=nb+1

yy0(nb)=parse(aa(rol),1)
zz0(nb)=dep*space
xx0(nb)=parse(aa(rol),2)+col
end_loop
;if n_roll=rol1
;loop ynn(1,addp)
;loop col(-addp,ny+addp)
;nb=nb+1
;yy0(nb)=parse(aa(rol),1)+ynn
;zz0(nb)=dep*space
;xx0(nb)=parse(aa(rol),2)+col
;end_loop
;end_loop
;end_if
end_loop
if dep<b_dep
next_n=2
else
if dep<=e_dep
n_roll=parse(aa(next_n),8)-parse(aa(next_n),5)+1
next_n=next_n+n_roll+1
end_if
end_if
command
;print dep n_rol next_n
    end_command
end_loop
idc1=idc2+1
re_particle
npixel=npixel+nb
vol(pmm)=string(nb*(1/5.12)^2*(2*0.6744*512.0/158.0))
vol_p=npixel*(1/5.12)^2*(2*0.6744*512.0/158.0)
end_loop
end_loop
end_loop
end_loop
end_section
end

;------------
;Some subroutines are not presented
;-----------------------------
;
def re_particle
nr=1
bd=12
find_ballgroup1
if cmm1>1
;gen_newball1
find_ballgroup2_1
if cmm2>=1
find_ballgroup2_2
gen_newball2_1
if cmm3>=1
gen_newball2_2
end_if
nnp=nnp+1
pn='par'+string(nnp)
range_ball
end_if
end_if
end

;-------------
def output
array xyz(5000)
status=open('outvem16.dat',1,1)
loop w(1,nxy)
xyz(w)=string(x(w))+' '+string(y(w))+' '+string(z(w))+' '+string(rb(w))
end_loop
status=write(xyz,nxy)
status=close
end
set max_balls 100000
set num_agg=2
plot add clump
plot add axes brown
plot set rotation (30 0 30)
get_data
agg_vol
;save gen_shear_extend.sav
;quit
APPENDIX IV: PFC$^3$D CODE FOR SIMULATION OF COMPRESSION TEST BY CLUSTERING DEM MODEL

Note: This code was developed for the simulation of the compression test. The clustering DEM model was developed and embedded. Only a representative portion of this code is presented. Please contact me for the complete code.

;fname rotation_irregularshape.dat

;the units used in this simulation: mass (g), length(mm), time(sec)

;density (kg/m$^3$=0.000001g/mm$^3$)

; stiffness(0.001N/mm=N/m), force(0.001N)

new

restore gen_bbound_extendb3.sav

call fishcall.fis

;------------------

def inside_walls

w_sstiff=3.62e7

w_nstiff=3.62e7

s_stiff=1.25e9

n_stiff=1.25e9

rwall_in=0.5*55

lwall_in=-0.5*55

alpha=22.5

beta =10.0

nn=360.0/alpha
ztwall=100.0
zbwall=0.0
tot_vol_in=(ztwall- bwall)*nn*0.5*rwall_in*cos(0.5*alpha*degrad)*2*
&rwall_in*sin(0.5*alpha*degrad)
loop n(1,nn)
  angle1=n*alpha
  angle2=(n-1)*alpha
  angle_a=90+0.5*alpha
  angle_b=180-beta-angle_a
  length1=abs(rwall_in*sin(angle_a*degrad)/(sin(angle_b*degrad)))
  xwall1=length1*cos((angle1+beta)*degrad)+50.0
  ywall1=length1*sin((angle1+beta)*degrad)+50.0
  xwall2=length1*cos((angle2-beta)*degrad)+50.0
  ywall2=length1*sin((angle2-beta)*degrad)+50.0
  command
  wall id =n ks=s_stiff kn= n_stiff face (xwall1 ywall1 ztwall) (xwall1 ywall1 zbwall) (xwall2 &
ywall2 zbwall) (xwall2 ywall2 ztwall)
  end_command
end_loop
end

;--------------
;subroutines are not presented
macro zero_vel 'ini xvel 0 yvel 0 zvel 0 xspin 0 yspin 0 zspin 0 range aggregate'
macro zero_disp 'prop xd=0 yd=0 zd=0 range aggregate'
set agg_num=173
plot add wall white
plot add axes brown
plot set rotation (30 0 30)
plot set center 5 10 5
plot set dis 600
plot show
inside_walls
outside_walls
prop_aggregate
set servo1=0
meas_sphere
position_measure
set grav 0 0 -9.8
cws
cyc 2000
del wall 101
load_plane
;save rot_shape_extenda.sav
;pause
set fishecall FC_CYC_TOP rot_measure
;set fishcall FC_CYC_TOP local_strain

solve average=0.05

cyc 350000

set servo1=1

position_measure

strain_measure1

outdata1

outdata2

outdata3

save rot_shape_extend_2.sav
APPENDIX V: PFC$^{3D}$ CODE FOR SIMULATION OF DIRECT SHEAR TEST BY CLUSTERING DEM MODEL

Note: This code was developed for the simulation of the direct shear test. The clustering DEM model was developed and embedded. Only a representative portion of this code was presented. Please contact me for the complete code.

;fname directshear.dat (irregular shape)
;the units used in this simulation: mass (kg), length(m), time(step), density(kg/m$^3$)
; stiffness(N/m), force(N) pressure(N/m$^2$)

new
restore gen_shear_m1.sav
call fishcall.fis

;----------------------------------------------
def make_walls
max_x0=0.0
max_y0=0.0
max_z0=0.0
min_x0=1000.0
min_y0=1000.0
min_z0=1000.0
bp=ball_head
loop while bp#null
if b_x(bp)-b_rad(bp)>=max_x0
max_x0=b_x(bp)-b_rad(bp)
end_if
if b_y(bp)-b_rad(bp)>=max_y0
    max_y0=b_y(bp)-b_rad(bp)
end_if
if b_z(bp)+b_rad(bp)>=max_z0
    max_z0=b_z(bp)+b_rad(bp)
end_if
if b_x(bp)+3.0*b_rad(bp)<=min_x0
    min_x0=b_x(bp)+3.0*b_rad(bp)
end_if
if b_y(bp)+3.0*b_rad(bp)<=min_y0
    min_y0=b_y(bp)+3.0*b_rad(bp)
end_if
if b_z(bp)-b_rad(bp)<=min_z0
    min_z0=b_z(bp)-b_rad(bp)
end_if
bp=b_next(bp)
end_loop

length1=0.2*length+0.5*0.001*(158-105)
length2=0.4*length+0.5*0.001*(158-105)
length3=0.6*length+0.5*0.001*(158-105)
length4=0.8*length+0.5*0.001*(158-105)
length5=1.0*length+0.5*0.001*(158-105)

w_nstiff=1.0e3
w_sstiff=1.0e3
extend=width/4

x0=min_x0
y0=min_y0
x1=max_x0
y1=max_y0
zb=min_z0

zm=0.5*(max_z0-min_z0)+min_z0
zt1=height+extend
zt2=1.0*height+extend
zt12=max_z0
xt0=x0-extend
xt1=x1+extend
yt0=y0-extend
yt1=y1+extend

y11=1.5*length+0.5*(0.158-length)
y6=-0.5*length+0.5*(0.158-length)

command

wall id=1 face(x0,y0,zm) (x1,y0,zm) ( x1,y0,zb) (x0,y0,zb)

wall id=2 face(x0,y0,zm) (x0,y0,zb) ( x0,y1,zb) (x0,y1,zm)
wall id=3 face(x1,y0,zb) (x1,y0,zm) (x1,y1,zm) (x1,y1,zb)
wall id=4 face(x1,y1,zb) (x1,y1,zm) (x0,y1,zm) (x0,y1,zb)
wall id=5 face(x0,y0,zb) (x1,y0,zb) (x1,y1,zb) (x0,y1,zb)
wall id=6 face(x0,y0,zm) (x1,y0,zm) (x1,y6,zm) (x0,y6,zm)
wall id=7 face(x0,y0,zt2) (x1,y0,zt2) (x1,y0,zm) (x0,y0,zm)
wall id=8 face(x0,y0,zt2) (x0,y0,zt2) (x0,y1,zt2) (x0,y1,zm)
wall id=9 face(x1,y0,zt2) (x1,y0,zt2) (x1,y1,zt2) (x1,y1,zm)
wall id=10 face(x1,y1,zt2) (x1,y1,zt2) (x0,y1,zt2) (x0,y1,zm)
wall id=11 face(x0,y1,zm) (x1,y1,zm) (x1,y11, zm) (x0,y11, zm)
wall id=12 face(xt0,yt0,zt12) (xt0,yt0,zt12) (xt1,yt1,zt12) (xt1,yt0,zt12)

wall id=1 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=2 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=3 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=4 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=5 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=6 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=7 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=8 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=9 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=10 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=11 kn=w_nstiff ks=w_sstiff fric=0.1
wall id=12 kn=w_nstiff ks=w_sstiff fric=0.1
def get_ss ; determine average stress and strain at walls

    ydisp1=w_y(w1)
ydisp2=w_y(w2)
    xdif = w_x(w8) - w_x(w9)
ydif = w_y(w7)
zdif = w_z(w12)
    wyforce4=w_yfob(w4)
    wyforce8=w_yfob(w8)
    wyforce9=w_yfob(w9)
    wyforce7=w_yfob(w7)
    wyforce10=w_yfob(w10)
    wxforce4=w_xfob(w4)
    wxforce8=w_xfob(w8)
    wxforce9=w_xfob(w9)
    wxforce7=w_xfob(w7)
    wxforce10=w_xfob(w10)
    shearforce=0.5*(wyforce4-wyforce7)
    new_xwidth = width + xdif
    new_ywidth = length + ydif
    new_height = 0.5*height + zdif
wsxx = 0.5*(w_xfob(w8) - w_xfob(w9)) / (new_ywidth * new_height)

wsyy = w_yfob(w7) / (new_xwidth * new_height)

wszz = w_zfob(w12) / (new_xwidth * new_ywidth)

wexx = 2.0 * xdif / (width + new_xwidth)

weyy = 2.0 * ydif / (width + new_ywidth)

wezz = 2.0 * zdif / (0.5*height + new_height)

wevol = wexx + weyy + wezz

end

; ----------------------------------------------------
def get_gain ; determine servo gain parameters for top wall motion

alpha = 0.05 ; relaxation factor

; count = 0

; avg_stiff = 0

; cp = contact_head ; find avg. number of contacts on lateral walls

; loop while cp # null

; if c_ball2(cp) = w1

; count = count + 1

; avg_stiff = avg_stiff + c_kn(cp)

; end_if

; if c_ball2(cp) = w2

; count = count + 1

; avg_stiff = avg_stiff + c_kn(cp)

; end_if
if c_ball2(cp) = w3
  count = count + 1
  avg_stiff = avg_stiff + c_kn(cp)
end_if
if c_ball2(cp) = w4
  count = count + 1
  avg_stiff = avg_stiff + c_kn(cp)
end_if
cp = c_next(cp)
end_loop
ncount = count / 4.0
avg_stiff = avg_stiff / count
gxy = alpha * (height * width) / (avg_stiff * ncount * tdel)

count = 0
avg_stiff = 0
cp = contact_head  ; find avg. number of contacts on top/bottom walls
loop while cp ≠ null
  if c_ball2(cp) = w5
    count = count + 1
    avg_stiff = avg_stiff + c_kn(cp)
  end_if
  if c_ball2(cp) = w12
if wszz#0
    www=c_ball2(cp)
    count = count + 1
    avg_stiff = avg_stiff + c_kn(cp)
    command
    ;print count
    ;pause
    end_command
end_if
end_if

cp = c_next(cp)
end_loop

ncount = count

if count # 0
    avg_stiff = avg_stiff / count
    gz = alpha * (width * length)/ (avg_stiff * ncount * tdel)
else
    gz=0.1
end_if
command
print count gz
;pause
end_command
def servo
  get_ss ; compute stresses & strains
  ydisp=ydisp+w_y(w1)
  udx = gxy * (wsxx - sxxreq)
  w_xvel(w4) = udx
  w_xvel(w2) = -udx
  udy = gxy * (wsyy - syyreq)
  w_yvel(w1) = udy
  w_yvel(w3) = -udy
  if z_servo = 1 ; switch stress servo on or off
    udz = gz * (wszz - szzreq)
  command
    print udz gz wszz count
    ; pause
  end_command
  w_zvel(w5) = udz
  w_zvel(w12) = udz
end
end

; ------------------------------------------------------------------------

def iterate
loop while 1 # 0

n_cyc=n_cyc+1

gain

; if abs((wsxx - sxreq)/sxreq) < sig_tol then
; if abs((wsyy - syreq)/syreq) < sig_tol then
; if wszz > szzreq

    if abs((wszz - szzreq)/szzreq) < sig_tol then
        exit
    end_if

; end_if

; end_if

; end_if

; end_if

command
cyc 100

print udz gz wszz count

end_command

; if n_cyc=10

; command

; clump release

; zero_vel

; make_clump

; cyc 100

; end_command
; n_cyc=0
; end_if
end_loop
end

; ----------------------------------------------------
def wall_addr
    w1 = find_wall(1)
    w2 = find_wall(2)
    w3 = find_wall(3)
    w4 = find_wall(4)
    w5 = find_wall(5)
    w7 = find_wall(7)
    w8 = find_wall(8)
    w9 = find_wall(9)
    w10 = find_wall(10)
    w12= find_wall(12)
end

;-------------------
def strength_m
n_cyc=0
section
loop while 1#0
    n_cyc=n_cyc+1

ii=out('current lateral disp='+string(ydisp2))
ii=out('current shearforce='+string(shearforce))
if ydisp2 <=-9.0e-3
    exit section
end_if
command
cyc 10
end_command
if n_cyc=1000
    end_if
end_loop
end_section
sigma1=wszz
shearforce=wforce8
end
;--------------------------
def make_clump
loop ncl(1,nnp)
pcl='par'+string(ncl)
command
clump id=ncl perm range pcl
end_command
end_loop
def set_ini

shearforce_0=shearforce
wyforce4_0=wyforce4
wyforce7_0=wyforce7

end

def accel_platens

; ----- Accelerates the platens to achieve vel of _vfinal in _nsteps, using _nchunks
; zero_vel

_nsteps=2000
_nchunks=200
_vfinal=0.02
_close=0

_niter = _nsteps / _nchunks

loop _chk (1, _nchunks)
  if _close = 1 then
    _vel = _chk*(_vfinal/_nchunks)
  else
    _vel = -_chk*(_vfinal/_nchunks)
  end_if
\[ _\text{mvel} = -_\text{vel} \]

command

wall id 1 yv _\text{vel}
wall id 2 yv _\text{vel}
wall id 3 yv _\text{vel}
wall id 4 yv _\text{vel}
wall id 5 yv _\text{vel}
wall id 11 yv _\text{vel}
cycle _\text{niter}
end_command
end_loop
end

; Some subroutines are not presented
set grav 0 0 -9.8
set num_agg=1280
set width=105.0e-3 height=120.0e-3 length=107.0e-3
;set safety_fac=0.25
;set ball_fric=0.7
macro zero_vel 'ini xvel 0.0 yvel 0.0 zvel 0.0 xspin 0.0 yspin 0.0 zspin 0.0'
macro zero_disp 'prop xd=0.0 yd=0.0 zd=0.0 range agg'
plot add axes brown
plot add wall white id on
;plot show
porosity
make_walls
set switch=0.0
position_measure
prop_aggregate
save directshear_irr_varstiff1_0.sav
;set switch=0
;zero_vel
;cyc 5
;zero_vel
;cyc 5
clump release
zero_vel
make_clump
wall_addr
prop fric 0.7
SET szzreq=1780.15 sig_tol=0.005
set fishcall FC_CYC_TOP servo
get_ss
iterate ;................ get top wall stresses to requested state
set switch=2
position_measure
save directshear_irr_varystiff1_1.sav

group part1 range \ y=(y0,length1)
group part2 range \ y=(length1,length2)
group part3 range \ y=(length2,length3)
group part4 range \ y=(length3,length4)
group part5 range \ y=(length4,length5)

plot add clump outline on shade off range group part2
plot add clump outline on shade off range group part4
plot add clump outline on shade on range group part1
plot add clump outline on shade on range group part3
plot add clump outline on shade on range group part5

hist id=1 shearforce
hist id=2 wszz
hist id=3 ydisp2
hist id=4 wyforce4
hist id=5 wyforce7
hist id=6 wyforce8
hist id=7 wyforce10
hist id=8 wxforce4
hist id=9 wxforce8
hist id=10 energy body
hist id=11 energy boundary
hist id=12 energy fric
hist id=13 energy kinetic
hist id=14 energy strain
set fishcall FC_CYC_TOP rot_measure
plot add hist -5 vs -3
clump release
zero_vel
make_clump
set_ini
accel_platens
;clump release
;zero_vel
;make_clump
strength_m
set swich=1
position_measure
micro_measure
strain_measure
outdata
out_disp
out_rot
out_strain
out_stress
save directshear_irr_varystiff1_2.sav
cyc 30000
save directshear_irr_varystiff1_3.sav

cyc 30000
save directshear_irr_varystiff1_4.sav

cyc 100000
save directshear_irr_varystiff1_5.sav

; hist write 1 vs 3 skip 50 file irr_2.his

; quit
APPENDIX VI: THE DATA OBTAINED IN THE REPEATED EXPERIMENTAL TESTS

Table 3-8: The data obtained from the repeated compression tests

<table>
<thead>
<tr>
<th>Results</th>
<th>Test 1</th>
<th>Test 2</th>
<th>Test 3</th>
<th>avg.</th>
<th>std.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical contraction (mm)</td>
<td>10.10</td>
<td>9.50</td>
<td>9.80</td>
<td>9.80</td>
<td>0.30</td>
</tr>
<tr>
<td>Radial dilation (mm)</td>
<td>0.75</td>
<td>0.80</td>
<td>0.80</td>
<td>0.78</td>
<td>0.03</td>
</tr>
<tr>
<td>Porosity (before)</td>
<td>0.49</td>
<td>0.50</td>
<td>0.49</td>
<td>0.50</td>
<td>0.00</td>
</tr>
<tr>
<td>Porosity (after)</td>
<td>0.47</td>
<td>0.48</td>
<td>0.47</td>
<td>0.47</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 4-7: The data obtained from the repeated direct shear tests

<table>
<thead>
<tr>
<th>Results</th>
<th>Test 1</th>
<th>Test 2</th>
<th>Test 3</th>
<th>avg.</th>
<th>std.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical Dilation (mm)</td>
<td>5.60</td>
<td>4.70</td>
<td>4.70</td>
<td>5.00</td>
<td>0.52</td>
</tr>
<tr>
<td>Porosity (before)</td>
<td>0.45</td>
<td>0.44</td>
<td>0.44</td>
<td>0.44</td>
<td>0.01</td>
</tr>
<tr>
<td>Porosity (after)</td>
<td>0.47</td>
<td>0.47</td>
<td>0.47</td>
<td>0.47</td>
<td>0.00</td>
</tr>
<tr>
<td>peak shear force</td>
<td>64.56</td>
<td>62.48</td>
<td>63.40</td>
<td>63.48</td>
<td>1.04</td>
</tr>
<tr>
<td>Residue shear force</td>
<td>23.70</td>
<td>19.50</td>
<td>21.80</td>
<td>21.67</td>
<td>2.10</td>
</tr>
<tr>
<td>peak friction angle</td>
<td>40.00</td>
<td>41.90</td>
<td>38.50</td>
<td>40.13</td>
<td>1.70</td>
</tr>
<tr>
<td>Residue friction angle</td>
<td>34.80</td>
<td>34.50</td>
<td>33.50</td>
<td>34.27</td>
<td>0.68</td>
</tr>
</tbody>
</table>
VITA

Yanrong Fu received her Bachelor of Science degree in civil engineering from Tongji University, Shanghai, China, in July 1998. She got her Master of Science degree in Civil Engineering from the same university in April 2001. She joined the Department of Civil and Environmental Engineering, Louisiana State University, and started her doctoral program in August 2001. While pursuing her doctorate degree, she served as graduate assistant in a research program in pavement materials and image techniques. Her research involves microstructure and damage quantification, characterization, and visualization of materials; image techniques and digital analysis in evaluation of pavement materials and geomaterials; numerical simulation and constitutive modeling of micro-macro behaviors of materials. She expects to receive the degree of Doctor of Philosophy at the December 2005 Commencement.