Three-Dimensional Discrete Element Simulations of Direct Shear Tests

Catherine O’Sullivan  
Department of Civil and Environmental Engineering, Imperial College London, UK

Liang Cui  
Department of Civil Engineering, University College Dublin, Ireland

Keywords: Discrete element methods, direct shear test

ABSTRACT: Using discrete element methods, geotechnical engineers can create "virtual laboratories" to simulate conventional laboratory tests. In this study, three-dimensional DEM simulations of direct shear tests are coupled with equivalent physical tests on steel balls. The macro-scale response of simulations is compared with the physical test results to validate the discrete element model and to gain insight into the test itself. Once validated, the discrete element simulations can be interpreted with confidence to develop conclusions regarding the particle-scale interactions driving the macro-scale response observed in the physical tests. Contact forces, particle displacements, and local shear stresses and strains are considered here.

1 Introduction

To date, much of our understanding of soil response has developed using standard laboratory tests. The direct shear test is one of the oldest and most commonly used laboratory tests in geotechnical engineering. Research considering the direct shear test includes the experimental studies by Shibuya et al (1997) and the finite element analyses described by Dounias et al (1993) and Potts et al (1987). In a discrete element simulation, it is relatively easy to monitor the micro-mechanisms that contribute to the often complex macro-scale response of granular materials. Discrete element analyses of laboratory tests are useful as they allow researchers to analyse their assumptions regarding the material response in these element level tests.

Recent research that has explored the applicability of the distinct element method (DEM) to simulate the direct shear test has been restricted to two-dimensions (Zhang and Thornton (2002) and Masson and Martinez (2001)). However, the work of Thomas (1997) quantitatively demonstrated the limitations of using two-dimensional representations of real three-dimensional materials such as soil. Recognizing these findings the current research extends the earlier DEM studies by considering this test in three dimensions. In addition, the numerical simulations are coupled with complementary physical tests, so that the results obtained in the idealized virtual DEM environment can be compared with a realistic test environment.

This paper firstly describes a series of physical tests on stainless steel spheres. Then, following a description of the details of the DEM simulation approach, the numerical results are compared with the physical tests results. The analysis of the simulation results includes an examination of the local stresses, the particle displacements, the contact forces and the local strains. The results are...
2 Physical direct shear tests

The direct shear test apparatus used in the current study comprises a metal box of square cross section (60 mm wide), divided horizontally into two halves. During testing, the lower section of the box was moved forward at a constant velocity (0.015 mm/s) while the upper section of the box remained stationary. The force required to maintain the upper section of the box in a stationary position was measured using a load cell and proving ring. The vertical load was applied to the top of the shear box using a system of dead weights attached to a lever. The shear stress was calculated by dividing the horizontal load measured in the proving ring by the specimen cross sectional area, while the vertical stress was calculated by dividing the applied vertical load by the specimen cross-sectional area.

For the current study 0.9922 mm Grade 25 Chrome Steel Balls were selected as their geometry is accurately controlled during fabrication. The ball radii are 0.9922 mm, the density is 7.8334 x 10^{-6} kg/mm³, the shear modulus is 7.945 x 10^7 kg/(mm s²), and the Poisson’s ratio is 0.28. The inter-ball friction angle of 5.5° measured by O’Sullivan et al (2004) for equivalent balls was assumed in the current study. The ball-boundary friction angle for the apparatus used here was measured in a series of tilt tests, giving a value of 9.0°.

For each direct shear test the balls were placed in the shear box in three equal layers. Each layer had a mass of 125 g (corresponding to 3900 balls). Following placement of the balls, a number of hammer “taps” were applied to each vertical side of the box to increase the specimen density. A series of tests were performed where the density of each test specimen was carefully controlled. For each test, the height of the specimen was monitored as taps were applied to the shear box until the density was close to the required value.

The test results are illustrated in Table 1 and Figure 1. Note that the horizontal strain was calculated as the displacement of the lower section of the box divided by the box width. As illustrated in Figure 1(c), the average peak friction angle for the material was found to be 24.8°. However, as illustrated in both Figure 1(b) and Figure 1(c), there was a degree of scatter in the experimental results and, acknowledging this scatter, the peak friction angle can be said to be between 23.7° and 25.8°. Figure 1(a) indicates that in all cases there was some initial compression of the specimen prior to dilation. As is evident from Figure 1(b), the specimen response was stress dependant, with the decline in the measured shear stress values post-peak being greater at larger vertical stresses. Furthermore, the specimens with greater vertical stresses exhibited higher initial stiffness values.

3 DEM simulations

3.1 Implementation of direct shear testing in 3DDEM

The DEM code (3DDEM) used for the simulations described here is a modification of a code developed by Lin and Ng (1997) for three-dimensional ellipsoidal particles, which in turn is a modification of the Trubal DEM code (Cundall and Strack, 1979). The program uses spherical particles and is further described in O’Sullivan (2002). For the current study, the Hertz-Mindlin contact model is used to model the contact between spheres.

The method used here to simulate the direct shear test using DEM was originally proposed by O’Sullivan (2002) and is illustrated in Figure 2. During the simulation, the specimen is enclosed by ten rigid boundaries; two horizontal boundaries at the top and bottom, four vertical boundaries at the
front and back, and four vertical boundaries at the left and right of the specimen. Prior to shearing, the two back boundaries are co-planar and the two front boundaries are co-planar. Similarly, the two left boundaries are co-planar and the two right boundaries are co-planar. During shearing, one set of vertical boundaries is moved laterally with a constant velocity. An imaginary horizontal plane is constructed through the middle of the specimen. All of the particles with centroids located above this plane are checked for contact with the moving boundaries, while all of the particles with centroids located below this plane are checked for contact with the stationary boundaries. Two horizontal boundaries are introduced at the left and right edges of the shear plane to prevent spheres “falling” out of the shear box.

Table 1: Void Ratios for Physical Tests

<table>
<thead>
<tr>
<th>Test No</th>
<th>1-1</th>
<th>1-2</th>
<th>1-3</th>
<th>2-1</th>
<th>2-2</th>
<th>2-3</th>
<th>3-1</th>
<th>3-2</th>
<th>3-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Void ratio</td>
<td>0.5869</td>
<td>0.5877</td>
<td>0.5824</td>
<td>0.5907</td>
<td>0.5880</td>
<td>0.5892</td>
<td>0.5895</td>
<td>0.5886</td>
<td>0.5744</td>
</tr>
</tbody>
</table>

(Note Vertical Stresses: Tests 1-1,1-2,1-3 54.5 kPa, Tests 2-1,2-2,2-3 108 kPa, Tests 3-1,3-2,3-3 163.5 kPa)

Figure 1: Summary of the physical test results where density was controlled

The measurement sphere illustrated in Figure 2 is used to measure the average stresses in the specimen. Such a system to measure stress in discrete element simulations has been described by a number of researchers including Bardet (1998). The average stress \( \bar{\sigma}_{ij} \) in the sphere is given by

\[
\bar{\sigma}_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} f_{ij}^c l_{ij}^c \quad (i, j = x, y, z)
\]

where \( N_c \) is the number of contacts within the measurement sphere, \( V \) is the volume of the sphere, \( f_{ij}^c \) is the contact force at contact \( c \), \( l_{ij}^c = x_j^c - x_i^c \) is the branch vector connecting two contacting particles, \( a \) and \( b \) with centroids at \( x_i^c \) and \( x_j^c \).

Prior to shearing the measurement sphere is used in a “servo-controlled” system to bring the specimen into a prescribed initial stress configuration. In the “servo-controlled” system, if the stress measured within the measurement sphere, \( \sigma_{ij}^{meas} \), differs from the user-specified stress, \( \sigma_{ij}^{req} \), the boundaries perpendicular to \( i \) direction are slowly moved so that the measured stress attains the required stress values. A servo-controlled approach is also used during the test to ensure that the vertical stress, as measured along the top boundary, remains constant during shearing.
3.2. Analysis Parameters

Table 2: Input parameters for DEM simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Density</th>
<th>Shear modulus</th>
<th>Poisson ratio</th>
<th>Friction coefficient between balls</th>
<th>Friction coefficient between balls and box</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius [L]</td>
<td>0.9922</td>
<td>7.8334 x 10^3</td>
<td>7.945 x 10^7</td>
<td>0.28</td>
<td>5.5°</td>
<td>9.0°</td>
</tr>
<tr>
<td>Friction coefficient between balls</td>
<td>5.5°</td>
<td>0.28</td>
<td>7.945 x 10^7</td>
<td>0.28</td>
<td>5.5°</td>
<td>9.0°</td>
</tr>
</tbody>
</table>

Table 2 lists the input parameters used in the simulation. A comparison of the parameters listed in Table 2 with the steel ball properties listed above illustrates that the physical tests and the numerical simulations are equivalent, apart from the differences in the density value used. Density scaling is commonly used to reduce the computational cost associated with DEM simulations for quasi-static analyses (e.g. O’Sullivan et al (2004)). In the current analyses attempts were made to run the simulations without any density scaling; however, significant difficulties were encountered in bringing the system into equilibrium.

3.3. Specimen generation

The difficulties associated with generating a three-dimensional specimen to a specified void ratio for use in a discrete element analysis cannot be overstated. For the current analysis the sphere packing algorithm proposed by Jodrey and Tony (1985) was initially used to generate the specimen. The resultant specimen was however looser than the specimens tested in the labs. To densify the specimens three alternatives were considered: 1) 11700 balls with a radius of 0.9393 L were initially generated in a box of size 60 L x 60 L x 20 L. This radius was then gradually expanded to 0.9922 L, the box height was increased to 21 L, and the system was brought into equilibrium. 2) 11700 balls with a radius of 0.9922 L were initially generated in a box of size 63 L x 63 L x 21 L. All the x-coordinates and y-coordinates of the ball were multiplied by a factor of 20/21 therefore to occupy a region of 60 L x 60 L x 21 L and the system was allowed to come into equilibrium. 3) 11700 balls with a radius of 0.9922 L were initially generated in a box of size 60 L x 60 L x 30 L. A vertical body force (i.e. gravity) was applied and the system was allowed to come into equilibrium.

3.4. Direct Shear Test Simulations

For the DEM simulations the “virtual” specimens were initially subjected to isotropic stress conditions of 50,000 M/(LT^2), 100,000 M/(LT^2) and 150,000 M/(LT^2). These initial stress conditions were attained using the servo-controlled approach detailed above. Then, during shearing the upper section of the box was moved at a velocity of 0.015 L/T. The macro-scale test results are summarized in Table 3 and Figure 3. Figure 3(a) is a plot of shear stress versus horizontal strain,
and Figure 3(b) is a plot of the peak shear stress versus the normal stress.

The initial specimen compression observed in the numerical simulations (Figure 3(a)) is smaller than that observed in the physical tests (Figure 1(a)). A comparison of Figure 1(b) and Figure 3(b) indicates that the numerical simulations exhibit a stiffer response in comparison to the physical tests. As indicated in Figure 3(c) the average peak friction angle for the simulations was found to be $23.8^\circ$, (recall an average value of $24.8^\circ$ was obtained in the physical tests). As with the physical tests there is some scatter in the results and the friction angle is in the range of $23.5^\circ$ to $24.3^\circ$. The shear stresses exhibited some fluctuations during shearing as a consequence of the servo-controlled algorithm, however these stress fluctuations did not affect the overall response as they are quite short in duration.

![Graphs showing strain and stress relationships](image)

Figure 3: Summary of numerical simulation results

<table>
<thead>
<tr>
<th>Specimen Generation Method 1</th>
<th>Specimen Generation Method 2</th>
<th>Specimen Generation Method 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test No</td>
<td>Void ratio</td>
<td>Test No</td>
</tr>
<tr>
<td>1-1</td>
<td>0.5537</td>
<td>2-1</td>
</tr>
<tr>
<td>1-2</td>
<td>0.5639</td>
<td>2-2</td>
</tr>
<tr>
<td>1-3</td>
<td>0.5772</td>
<td>2-3</td>
</tr>
</tbody>
</table>

(Note Vertical Stresses: Tests 1-1, 1-2, 1-3 50000 M/(LT^2), Tests 2-1, 2-2, 2-3 100000 M/(LT^2), Tests 3-1, 3-2, 3-3 150000 M/(LT^2))

4 Analysis of micro-scale parameters

4.1 Stress analysis

Information about the inter-particle contact forces can be used in combination with Equation (1) to examine the variation of shear stress within the specimen. For this analysis, a series of rectangular boxes of varying depths were created to examine the variation in stress within the specimen during shearing. The configuration of these boxes is illustrated in Figure 4(a). In each case the center of the stress measurement box was located at the center of the specimen, and the thickness of the box, d, ranged from H/10 to 2H/5, where H is the specimen height. Figure 4(b) illustrates the variation in the shear stress $\sigma_{zx}$, as measured in the stress measurement boxes, as a function of strain. As illustrated in Figure 4(b), the measured shear stress, $\sigma_{zx}$, increases as the thickness of the measurement box decreases. For the three vertical stresses considered, the ratio of the peak
\( \sigma_{xz} \) value for \( d=1/5 \) \( H \) divided by the peak \( \sigma_{xz} \) value for \( d=2/5 \) \( H \) is consistently about 1.09, whereas the ratio of the peak \( \sigma_{xz} \) value for \( d=1/10 \) \( H \) divided by the peak \( \sigma_{xz} \) value for \( d=2/5 \) \( H \) is consistently about 1.17.

\[ \begin{array}{c}
\text{Direction of shearing} \\
\text{z} \\
\text{y} \\
\text{x} \\
d \\
H \\
\end{array} \]

Figure 4(a): Illustration of configuration of the rectangular box used to calculate local stresses

4.2. Incremental Displacements

Two orthogonal views of the incremental displacements for the simulation of specimen 3 (normal stress \( (\sigma_n) \) of 150,000 \( \text{M/(LT}^2) \)) are illustrated in Figure 5, considering the horizontal strain increment from 0.005 to 0.052. For ease of visualization only displacements exceeding the average incremental displacement are illustrated for the central fifth segment of the specimen. Referring firstly to Figure 5(a), as would be expected, most of the displacement is concentrated in the upper half of the shear box. At the left hand side of the box there is downward motion of the particles, while at the right hand side of the box there is upward motion of the particles. Comparing Figure 5(a) and Figure 5(b), it is clear that the components of the particle displacement vectors in the \( y \)-direction are small but finite in comparison to the component of these vectors in the \( x \)-direction.

\[ \begin{array}{c}
\text{(a) Front view (y = 24 L to y = 36 L)} \\
\text{(b) Side view (x = 24 L to x = 36 L)} \\
\end{array} \]

Figure 5: Incremental displacement vectors for the horizontal strain increment from 0.005 to 0.052 for two orthogonal central segments of the specimen (only displacements exceeding the average incremental displacement are illustrated)
4.3. Contact forces

Two orthogonal views of the contact force vectors for the simulation of specimen 3 ($\sigma_n$ of 150,000 M/(LT²)) at a horizontal strain of 0.052 are illustrated in Figure 6. Figure 6(a) is a front view of the specimen and Figure 6(b) is a side view of the specimen. For ease of visualisation, only contacts where the magnitude of the contact force exceeds the average contact force plus one standard deviation are considered for the central fifth segment of the specimen. The distribution of contact forces illustrated in Figure 6(a) is qualitatively similar to the distribution of contact forces obtained by Zhang and Thornton (2002) in their two-dimensional discrete element analysis of the direct shear test. The forces are transmitted diagonally across the specimen. A side view of the specimen is given in Figure 6(b). While it is difficult to identify any clear trend in the orientation of the contact force vectors from this perspective, the finite values of the components of the contact forces orientated in the y-direction is an indicator of the three dimensional nature of the problem.

4.4. Strain localization analysis

For the simulation of specimen 3 with a $\sigma_n$ of 150,000 M/(LT²), the local strain values were calculated using the non-linear homogenization technique proposed by O'Sullivan et al (2003). The strain values on a vertical plane through the center of the specimen, i.e. with $y=30$ mm are illustrated in Figure 7 for the strain increment from 0.005 to 0.052. Contours of the shear strains $\gamma_{zx}$, $\gamma_{yz}$ and $\gamma_{zy}$ as well as the volumetric strain, $\varepsilon_{vol}$, are illustrated. Considering the $\gamma_{zx}$ contours and the $\varepsilon_{vol}$ contours, the localizations along the left hand side of the box appear to be inclined. Similar inclined localizations were observed by Potts et al (1987) in finite element analyses of the direct shear test. The propagation of strain from the edges of the box is also similar to distribution of strain observed by Potts et al.

5 Discussion

This research has coupled discrete element simulations of the direct shear test with complementary physical tests on an idealised granular material. The average peak friction angle obtained in the DEM simulations matched the physical test results within 1°. The response in the simulations was slightly stiffer than the response observed in the physical tests and future analyses will attempt to identify the source of this discrepancy.

An analysis of the results of the simulations considered the local stress values, the incremental displacements, the distribution of contact forces and the local strain values. Whereas the particle displacements were predominantly restricted to the direction of shearing, significant contact forces developed orthogonal to the direction of shearing, illustrating the three dimensional nature of the material response at the particle scale. Within the specimen, the stresses are non-uniform with the shear stresses increasing closer to the zone of shearing. The local strain values are non-uniform and propagation of the shear strain and the volumetric strain contours inwards from the edges of
the boxes was observed.

Figure 7: Strain contours for horizontal strain increment 0.005 to 0.052 (Contour interval 0.05)

6 Acknowledgements

Funding for this research was provided by the Irish Research Council for Science, Engineering and Technology (IRCSET) under the Basic Research Grant Scheme. Additional partial funding was provided by the Institution of Engineers of Ireland Geotechnical Trust Fund and the President’s Research Award, UCD. Mr. George Cosgrave assisted with the laboratory tests.

7 References


