Mechanical Simulation of Granular Materials
by DEM Analysis

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Abstract

A study of four constitutive contact models employed in discrete element analysis is presented. Most discrete element simulations employ simple contact models due to computational time constraints. However, few works are available in literature which evaluates the suitability of these simple models to simulate DEM applications. The influence of more complex models on bulk behavior is examined through performing a simulated quasi-static biaxial compression test and mapping out simple stress-strain relationships. Furthermore, the effects on behavior of the system while varying porosity (dense or loose) and surface friction coefficient are also investigated. Detail is given in describing the various methods used in the preprocessing stage of the granular assembly. The four contact models in consideration are: linear elastic model, non-linear Hertz-Mindlin model, rigid plastic model, and elastic-plastic model. Also presented, is an investigation into the macroscopic and microscopic mechanical behavior of a stressed assembly employing the linear elastic model. This includes stress-strain behavior and evolution of coordination number.

Introduction

Granular materials are composed of distinct particles which displaces independently from one another and interact only through contact points (Cundall 1979). This material is encountered in nature and in industrial applications, thus the importance of it cannot be overlooked. Due to its discrete nature, a loaded granular medium may display complex mechanical behaviors which cannot be explained by continuum theory (Jiang et al. 2003). Furthermore physical experiment on real granular substances are difficult due to the fact that internal forces cannot be measured without perturbing the state of the original system. The accessibility of data at any stage of the test, changing parameters such as surface
friction, particle size, or porosity, is also difficult with experiments (Cundall 1979).

An alternative approach to studying granular material is in using numerical techniques. The discrete element method (DEM) is one such technique that is simple yet powerful. It works by following the trajectory of each particle, monitoring all the forces on it, then through integrating Newton’s second law, calculates the new movement of the particles. Forces on a particle may include gravitational, electrostatic, cohesive, and most importantly, contact force due to collisions (Renzo 2004). Majority of DEM employs the simplest contact force model whereby particle interaction is represented as a linear spring-dashpot-slider system. Even though more complex and realistic models are available, the large amount of calculation in DEM makes using a simpler model more practical. However, there have been few works which have compared and assessed the simulation capabilities in using a simple contact model as opposed to a more complex one.

The Discrete Element Method

DEM is a dynamic process by which boundary disturbances propagate through the medium to create movements in the internal particles. Very small time steps are taken to represent this dynamic process numerically. It is assumed that within each time step, the forces experienced by each particle only results from its immediate neighbor (Cundall 1979). In this study, a soft contact model approach is used, whereby the physical deformation resulting from particle collisions is represented as an overlap between the particles (Figure 1a). The contact force is therefore directly related to the amount of overlap $\delta$ and a stiffness parameter $k$. This relationship is known as the force-displacement law. The contact force can then be set to Newton’s second law and the new movements of the particle can be determined through integration. The calculation cycle of DEM therefore alternates between the force-displacement law and Newton’s second law (Figure 1b).

\[ f = k\delta = m_a \]

Figure 1a. Contact overlap between two particles. Figure 1b. DEM cycle.
Contact Models

The basis for constitutive contact models assumes that the magnitude of the force is directly related to the amount of overlap. Both contact force in the normal direction and frictional force in the tangential direction are taken into consideration with the model. The four contact models considered in this study are briefly explained:

*Linear elastic:* The linear elastic model is the most intuitive and simplest way of modeling particles in contact (Renzo et al. 2004). It assumes that the force is linearly related to the particle overlap through the stiffness constant. The relationship appears as follows:

\[ f_n = k_n \delta_n \]  \hspace{1cm} (1a)

\[ f_t = k_t \delta_n \leq F_{n,max} = \mu |F_n| \]  \hspace{1cm} (1b)

In this model the only parameters considered are the normal \( k_n \) and tangential \( k_t \) contact stiffness and the friction coefficient \( \mu \).

*Non-linear elastic:* This model is based on Hertz’s elastic theory for the normal contact direction and Mindlin and Deresiewicz approximate no-slip solution for the tangential direction (Renzo et al. 2004).

\[ f_n = \frac{G}{3(1-v)} \sqrt{8R_e \delta_n^{2/3}} \]  \hspace{1cm} (2a)

\[ f_t = \frac{2 \left[ 3G^2(1-v)f_n R_e \right]^{1/3}}{2-v} \delta_n^{2/3} \]  \hspace{1cm} (2b)

Where \( R_e \), the equivalent radius is defined as: \( R_e = \left( \frac{1}{R_1} + \frac{1}{R_2} \right)^{-1} \)  \hspace{1cm} (2c)

*Rigid-plastic:* Plastic deformation of contacts was solved by Redanz and Fleck (2001) in their study of compaction of metallic cylinders. They assumed that the normal pressure \( p \) at the contacts equals a Prandtl number of three times the yield strength \( \sigma_y \).

\[ p = 3\sigma_y \]  \hspace{1cm} (3a)

\[ f_n = 3\sigma_y A_e \]  \hspace{1cm} (3b)

Where the effective contact area \( A_e \) is defined as: \( A_e = \sqrt{8\delta_e R_e} \)  \hspace{1cm} (3c)

The model assumes that the contact experiences only plastic deformation, therefore elastic deformation parameters, i.e. elastic modulus, Poisson’s ratio, are not present.
Elastic-plastic: For an elastic-plastic contact, an elastic and plastic part contributes independently to form the contact force model (Stronge 2000).

\[
f_n = f_y \left[ \frac{2\delta_n}{\delta_y} - 1 \right] \left[ 0.95 + 0.30 \ln \left( \frac{2\delta_n}{\delta_y} - 1 \right) \right] \tag{4a}
\]

with

\[
f_y = \pi (1.1Y_R^2) \left( \frac{3\pi}{4} \right) \left( \frac{1.1Y}{E^*} \right)^2 \tag{4b}
\]

The limiting overlap for elastic deformation \( \delta_y \) is defined as:

\[
\delta_y = \frac{R_c}{E^*} \left( \frac{3\pi}{4} \right) \left( \frac{1.1Y}{E^*} \right)^2 \tag{4c}
\]

with \( Y \) representing the uniaxial yield stress and \( E^* \) as the equivalent elastic modulus. This set of equations is only valid within certain elastic-plastic range defined as \( 1 < \delta_n / \delta_y < 84 \). It is assumed that within this range, the observable permanent indentation is small due to the incompressibility of the plastic deformation and that this deformation occurs within the elastic body (Hu et al. 2004).

**Biaxial Simulation**

Two boundary conditions were explored in this study. The first approach consists of a four wall enclosure around the assembly where the top and bottom wall simulated loading platens (Figure 3a). These walls were moved at very small strain rate in order to maintain a quasi-static compression. The vertical walls kept a constant consolidation stress on the sample throughout the procedure by applying a numerical servo-mechanism. This approach is similar to a laboratory biaxial compression test. Figure 2 shows a schematic representation of loading condition.

![Figure 2. Biaxial loading condition.](image-url)
The second approach (Figure 3b) simulated the biaxial test by employing a periodical boundary condition. Stress was induced within the assembly by assigning velocities to the boundary particles. After a review of both methods, the test was carried using periodical boundary condition in order to remove particle-wall boundary conditions.

Figure 3a. Wall enclosure boundary         Figure 3b. Periodic boundary

Two different specimen generation schemes were considered when creating the isotropic assembly. They were the isotropic-compression scheme and radius expansion scheme.

*Isotropic-compression* involved the random positioning of particles and moving the boundary walls until the assembly reached an isotropic stress state. Overlap between the particles was not allowed. Particle radii were randomly assigned within a specified range. Initial particle surface friction was set low to allow fluid movement of the assembly during compression. Once the desired state was achieved, the representative friction needed for the simulation was reinstated.

*Radius expansion* involves the assignment of particles to random locations with reduced radii and slowly restoring the radii of all the particles to the desired size. During expansion the consolidation stress on the vertical walls were kept constant with a servo-mechanism. The disadvantage of this method was that final radii range of the particles was difficult to set, however the porosity of the assembly was much easier to control than the isotropic compression method. It was decided that the radius expansion scheme was the more effective method when used with periodic boundary condition.
Simulated biaxial tests of ~4000 circular particles employing periodical boundary conditions were performed using DEM code. Two porosity states of 0.20 (loose) and 0.12 (dense) were considered for each of the four contact models. Two surface friction factors, 0.3 and 0.5, were also considered. The mechanical properties of the particles are as follows (Renzo 2004):

<table>
<thead>
<tr>
<th></th>
<th>Linear model</th>
<th>Non-linear models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal elastic constant</td>
<td>1.72e7</td>
<td>--</td>
</tr>
<tr>
<td>Tangential elastic constant</td>
<td>1.48e7</td>
<td>--</td>
</tr>
<tr>
<td>Young’s modulus E (GPa)</td>
<td>--</td>
<td>380</td>
</tr>
<tr>
<td>Poisson ratio v</td>
<td>--</td>
<td>0.23</td>
</tr>
<tr>
<td>Shear modulus G (GPa)</td>
<td>--</td>
<td>154</td>
</tr>
</tbody>
</table>

Table 1. Mechanical properties of the granular material.

Analysis

As a result of severe time constraints, simulations were only completed on the linear elastic model. Therefore, the analysis will focus instead on the micro and macro mechanical behaviors of the linear elastic model. The biaxial test results are presented in terms of the stress ratio and the strain as shown in Figure 5. The stress ratio \( q/p \) is defined as the deviatoric stress \( q \) divided by the mean stress \( p \), where \( q = \sigma_{22} - \sigma_{11} \) and \( p = (\sigma_{22} - \sigma_{11})/2 \).

Figure 4 and 5 compares the two different frictional states for a given porosity state. As seen in the figure, the behavior of the material in loose and dense state is essentially the same with the larger friction factor achieving a higher maximum stress ratio. Furthermore, with increasing strain, the system approaches a critical state in which the stress ratio is no longer dependent on the initial porosity. This is in good agreement with simulations run by Rothenburg (2004).

The distinction most apparent between the loose state and dense state is the amount of softening behavior. The dense state achieved a much greater softening behavior apparent in the initial peak. By setting a constant friction factor and only varying the porosity, this behavior becomes more evident (Figure 6).
Figure 4. Stress ratio versus strain for loose assembly with different friction factors.

Figure 5. Stress ratio versus strain for dense assembly with different friction factors.
The evolution of the coordination number with increasing strain is shown in Figure 7 and 8. After a strain of about 20% for the dense assembly and 10% for the loose one, the system begins to reach a steady-state where contact disintegration and creation occurs at the approximately the same rate. However, it is noted that the higher friction factor is able to reach a steady state with a lower coordination number. This is because with a higher friction factor, the tangential forces are unrestricted and the contacts will therefore freely disintegrate to some critical state. However, with lower friction factor, the range of the tangential forces is limited. This decreases the chances of contact disintegration leading to instability to occur and therefore the number of contacts that can disintegrate is also limited. With a lower contact disintegration rate, the assembly with the lower friction factor will achieve steady-state at a higher coordination number. This is in agreement with studies performed by Rothenburg (2004).
Figure 7. Coordination number versus strain for dense assembly with two friction factors.

Figure 8. Coordination number versus strain for loose assembly with two friction factors.

Conclusion

A simulated biaxial compression test on a granular assembly was performed using the discrete element method. The paper initially sought to compare the effectiveness of four constitutive models to accurately simulate the mechanical behavior of a granular
assembly. However, due to research time constraints, only one constitutive model was able to be simulated prior to this report. This report instead investigated the macro and micro mechanical behavior of an assembly employing only a linear elastic contact model. The relationship between stress and strain and coordination number and strain were examined under varying porosity and friction factors. The results of the tests were in good agreement with previous works. Contingent upon the willingness of Professor Hongwu Zhang and graduate student Jianmin Qin to further collaborate with the author, the author wishes to run the remaining three contact models in the near future when time permits.

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