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Research Paper

Meso-scale framework for modeling granular material using computed tomography

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ABSTRACT

Numerical modeling of unconsolidated granular materials is comprised of multiple nonlinear phenomena. Accurately capturing these phenomena, including intergranular forces and grain deformation, depends on resolving contact regions several orders of magnitude smaller than the grain size. Here, we investigate a method for capturing the morphology of the individual particles using computed X-ray tomography, which allows for accurate characterization of the interaction between grains. Additionally, the ability of these numerical approaches to determine stress concentrations at grain contacts is important in order to capture catastrophic splitting of individual grains, which has been shown to play a key role in the plastic behavior of the granular material on the continuum level. Samples of Ottawa sand are numerically modeled under one-dimensional compression loadings in order to determine the effect of discretization approaches, such as mesh refinement, on the resulting stress concentrations at contact points between grains. The effects of grain coordination number and finite element type selection on these stress concentrations are also investigated.

1. Introduction

An analytical approach to modeling granular materials subjected to various loadings, such as one-dimensional compression or triaxial compression, contains many complexities at the meso-scale or particle level. The influence of the varying multifaceted morphologies and the mechanical behavior of the individual grains under high impact loadings, including grain fracture and fragmentation, which has been shown to play a key role in the plastic behavior of the sand, are not taken into account with current methodologies. The discrete element method (DEM) is often chosen to model the discrete particles of a granular assembly. However, for simplicity, many chose to use idealized spheres [1–3] or disks [4–6] to represent sand grains and an arbitrary packing of sand grains based on a predetermined packing density. This is far from how sand grains are truly shaped and geometrically oriented. Cho et al. [7] discussed the significant impact that actual grain shape has on the stiffness and strength of the sand as a continuum. Thus including the actual grain morphology in numerical modeling will allow us to better capture the behavior of the granular assembly. Recently, tomography image based modeling, which utilizes the realistic microstructure of porous material, is starting to be used to simulate flow through porous media [8–11]. Matsushima et al. [12] have used a method of combining several spheres to model the irregular shape of a grain based on X-ray tomography data for DEM simulation. It is also now possible to obtain finite element mesh of tomography image data for FEM simulation.

Additionally fracturing and fragmentation of particles have been shown to affect the plastic behavior of the granular material and is expected to occur near the locations of high stresses, such as the near end platens for quasi-static 1D compression or where a projectile penetrates the sand at a high speed causing high gradients of deformation. The influence of grain fracture and fragmentation on the behavior of a soil was investigated by McDowell and Bolton [13], who determined that grain strength governs the strength and dilatancy of crushable soils. Plastic hardening of granular materials due to fracture and fragmentation was also observed under cyclic loading by Harireche and McDowell [14]. Given the significant role of grain fragmentation on the plastic behavior of soil, it is important that detailed modeling of these processes accurately computes the stress concentrations within the particles leading up to rupture events.

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Experimental studies on the fragmentation of individual sand grains have been performed by others in which grains were placed between two flat platens, and the breakage force corresponding to the splitting of the grain into at least two similarly sized pieces was identified as the "splitting force". A summary of these forces is shown in Table 1. Using the idealized sphere approach described in Section 3.1.2, the maximum equivalent stress corresponding to the grain size and force at catastrophic splitting was determined and is also presented in Table 1. In this table and all other results presented in this paper, equivalent stress is calculated according to the von Mises stress criterion. The maximum stress is taken to be the maximum elemental stress (calculated at the centroid of each tetrahedral element in the mesh) observed within discretized grains and is typically located at the edge of the contact area between grains, as expected by Hertz contact theory [15]. These results indicate that the force required to split a grain typically increases with the nominal diameter of the grain. A similar size dependence has been seen by Brzesowsky et al. [16], McDowell and Bolton [13] and Nakata et al. [17] who also determined the stress corresponding to catastrophic splitting is inversely proportional to the nominal diameter of the grain. However, their method of computing the failure stress assumed an idealized spherical grain or calculating the stress as $\sigma = F/d^2$, where F is the force at failure and d is the initial diameter of the grain, based on the method presented by Jaeger [18].

One current approach to account for grain fracturing is to represent each grain as an agglomerate of spherical discrete elements [14,19], utilizing a specified bond strength between elements of an agglomerate to mimic the resistance of the grain to fragmentation. However, a disadvantage of this approach is the loss of the individual grain's continuous surface and the angularities of the surface, which is necessary to properly simulate the normal and tangential contact forces between grains.

This paper establishes that the grain topology may be important to understand how grains orient themselves and rotate/slide/rearrange during elastic loading. Additionally, in order to understand how grains fracture, we must first understand how they load elastically. Hertz' seminal work on the subject has been used to estimate stresses in sand grains using DEM methods or idealized particle shapes. However, it is important to investigate how to utilize the detailed information obtained using X-ray computed tomography. Conventional notions of mesh refinement are not as straightforward since the grain surface topology will change (affecting the contact areas and emerging force chains) along with the stress concentrations within the grain material. In this paper, numerical modeling of sand grains at the meso-scale, taking into account actual grain morphology, is examined. Modeling considerations and the ability of the numerical approach to capture high stress concentrations that lead to grain fracture and fragmentation are discussed for efficient and accurate computational efforts.

2. Methods and computer codes used

2.1. Obtaining grain morphology

The utilization of actual grain morphology, obtained with X-ray computed tomography, in lieu of simplified shapes such as spheres, allows for a more realistic representation of the granular material at the meso-scale. In this proposed meso-scale approach, X-ray computed tomography of naturally occurring Ottawa sand (20/40) was obtained using a microfocus X-ray system at Helmholtz-Zentrum-Berlin (HZB). Dry Ottawa sand was placed in an aluminum cylindrical container and compacted allowing the sand specimen to reach its densest state at void ratio of 0.52, which is approximately 100% relative density (D_r). For tomography, 1000 projections were obtained over 360° total rotation of the container, and a filtered backprojection algorithm was used to reconstruct the data.

The reconstructed data set went through a series of image processing algorithms, e.g. noise filtering (median 3D), thresholding to binary image, and watershed separation, to separate any touching particles. A similar procedure was illustrated in Kim et al. [8]. The image processing was performed in the environment of *Avizo* [20]. The segmented sand grain images were converted to finite element mesh in Simpleware+FE [21]. The binary image data was initially converted to a very fine mesh based on the approach of Young et al. [22]. However the mesh can be optimized to reduce the number of elements while maintaining the original grain surface structures.

2.2. Image processing and mesh codes

Avizo is a software application that allows users to process 2D images, such as those obtained using tomography, and build 3D visualizations. Simpleware+FE is a software that utilizes the images, such as those created in Avizo, to generate a finite element mesh using smoothing algorithms to preserve the topology of the grain surfaces and allowing users to specify meshing techniques.

2.3. Finite element codes

Two codes that utilize the finite element method (FEM) were used in this paper: GEODYN-L [23] and ABAQUS/Standard [24]. GEODYN-L is a parallel 3D explicit Lagrangian finite element code with contact, including Discrete Element Method (DEM) coupling through the Simple Common Plane contact algorithm [28]. GEODYN-L is well-suited for large-scale contact problems including large material deformations. We also use ABAQUS/Standard as a 3D parallel Lagrangian finite element code for implicit time-stepping for static loading and higher order elements.

3. Effect of mesh refinement and coordination number at meso-scale

3.1. Effect of mesh refinement

At the granular level, stress distributions within the grains, which indicate the likelihood of grain fracturing, are obtained using FEM. This approach assumes that the grain is a singular continuous entity subjected to the forces imposed on it by surrounding grains. The stress distribution within an individual grain is utilized to determine if the grain has reached a stress level leading to fragmentation or splitting. The magnitude of the calculated stress within a grain can be influenced by the type of element chosen

Table 1
Splitting force of sand grains.

Diameter (mm)	Sand	Splitting force (N)	Maximum equivalent stress (GPa)	Reference
0.50	Silica sand	33.1	2.51	McDowell [27]
0.65	Silica sand	30.9	1.55	Nakata et al. [17]
1.00	Silica sand	59.0	2.96	McDowell [27]
1.00	Calcareous sand	61.9	1.92	McDowell and Bolton [13]
1.55	Silica sand	74.4	2.87	Nakata et al. [17]