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Research Paper

3D finite element modelling of force transmission and particle fracture of sand

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ABSTRACT

Global compressive loading of granular media causes rearrangements of particles into a denser configuration. Under 1D compression, researchers observed that particles initially translate and rotate which lead to more contacts between particles and the development of force chains to resist applied loads. Particles within force chains resist most of the applied loads while neighbor particles provide lateral support to prevent particles within force chains from buckling. Several experimental and numerical models have been proposed in the literature to characterize force chains within granular materials. This paper presents a 3D finite element (FE) model that simulates 1D compression experiment on F-75 Ottawa sand. The FE mesh of particles closely matched 3D physical shape of sand particles that were acquired using 3D synchrotron micro-computed tomography (SMT) technique. The paper presents a quantitative assessment of the model, in which evolution of force chains, fracture modes, and stress-strain relationships showed an excellent agreement with experimental measurements reported by Cil et al. Alshibli (2017).

1. Introduction

Granular materials are composed of discrete solid particles that interact with each other in a complex fashion. Under 1D compression, it is well-known that particles within a granular media are held together and jammed into a complex network of mutual compressive forces. There are regions of high contact stresses transmitted through some of the particles to form what is known as force chains that resist global loads applied at boundaries. Conversely, other particles experience low contact stresses and provide support for particles within force chains against buckling. Force chains were visualized using photo-elastic materials [2–10]. Besides photo-elasticity, many methods have been utilized in the last few decades to characterize and visualize force chains in granular material. To mention a few, Radjai et al. [11,12] implemented contact dynamics simulations to study the statistical distribution of contact forces inside a confined packing of 2 D circular rigid disks. Tordesillas [13] quantitatively examined force chain buckling and shear banding of 2D densely-packed cohesionless granular assembly subjected to quasi static biaxial compression using discrete element method (DEM). Similarly, Zhang et al. [14] used DEM to investigate the role of force chains in granular materials under both quasi static biaxial loading and dynamic impact loading. Coppersmith et al. [15] introduced the scaler q model to characterize force chains within a specimen composed of spherical beads in which the dominant physical mechanism leading to force chains was assumed to be the fluctuation in the force distribution that was attributed to variations in the contact angles and the constraints imposed by the force balance on each bead [16–18]. Bouchaud et al. [19] proposed phenomenological equations, also known as the oriented stress linearity model, to describe force propagation within a granular medium. Edwards and Grinev [20] proposed a new approach that employs statistical-mechanical concepts to describe the probability of contact force distribution in granular material. In summary, most of recent studies reported in the literature on force network and force chains in granular assemblies were implemented on either 2D disks or 3D spherical particles [21–25]. However, there is a lack of studies that consider the exact 3D shape of natural sand grains in a granular assembly.

There are many 3D computational models to simulate laboratory experiments on granular material which can provide quantitative global stress-strain predictions that are difficult to verify experimentally at the particle scale (e.g., stress and strain tensor components for each particle). Most of these computational models were developed based on DEM or continuum theories. The DEM was first introduced by Cundall and Strack [26] to numerically model the movement and interaction between discrete rigid particles in a granular assembly. Henceforth, DEM has been widely implemented in numerous numerical models to model the fracture of granular materials since it captures the discrete nature of particles. McDowell and Harireche [27] modelled soil

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particles in DEM as agglomerates of balls bonded togather to simulate fracture of individual soil particles, then succcesfully simulated oedometer tests on sand and showed that yielding coincides with the onset of bond breakage [28]. Ng [29] introduced a new boundary condioton (i.e. hydrostatic boundary condition) in DEM to simulate the chamber fluid presure in a triaxial compression test on ellipsoidal shape particles. Cheung and O'Sullivan [30] described algorithms to simulate the lateral boundary conditions imposed by the latex membrane used in physical triaxial tests in both 2 D and 3D DEM simulations. Belheine, Plassiard [31] applied DEM to model compression triaxial test on 3D spherical packing of particles with a rolling resistance to account for surface roughness of particles. O'Sullivan and Cui [32] simulated the response of specimens containing about 15,000 steel spheres subject to load–unload cycles in quasi-static triaxial tests to explore the particle-scale mechanics during the load reversals. Lu and Frost [33] modelled triaxial compression tests on agglomerates of sand particles that were assembled as unbreakable 2-circular clumps to achieve better interlocking between particles which yeilded more stable and efficient force chains. Hasan and Alshibli [34] used clumped spheres to simulate the 3D axisymmetric triaxial compression experiment on JSC-1A lunar regolith at different densities and confining pressure in which a significant increase in peak and critical state friction angles was well predicted at near-zero confining pressure simulations. Yang et al. [35] developed a discrete element and multiscale modeling methodology to represent granular media at their particle scale as they interact with solid deformable bodies, such as soil-tool, tire, penetrometer and pile. Cil and Alshibli [36] successfully modelled the fracture of individual silica sand particles in granular assemblies by adopting the bonded particle model concept within the framework of DEM. Kawamoto, Andò [37] outlined the level set discrete element method (LS-DEM) which is a discrete element method version that is able to simulate systems of particles with arbitrary shape using level set functions as a geometric basis.

Alternatively, the continuum-based approach assumes an elasto-plastic material and applies constitutive relations to predict the overall stress-strain relationships. This method was originally implemented in numerical modeling of soil since the original work of Roscoe et al. [38] and Drucker et al. [39]. Since then, it has been adopted in several constitutive models that can effectively predict stress-strain relations of granular material. Generally, both discrete and continuum models have successfully provided effective stress-strain predictions of behavior of granular materials. Nonetheless, continuum-based models still ignore the influence of the discrete natural of particles and assume a continuum material. On the other hand, DEM assumes rigid non-deformable particles and virtually calculates particle-level stress-strain estimations based on contact forces that are calculated with respect to a pre-defined numerical contact model. Thus, a combined approach that addresses both the continuum and discrete behavior of granular material has been established in recent years which is known as finite element-discrete element method (FEM-DEM). It adopts FEM to simulate the constitutive behavior of discrete particles, in which each discrete particle is meshed into deformable finite elements. Simultaneously, the conventional steps of DEM, including time integration, and contact detection are still applied to track the motion and interaction of individual particles. Mahabadi, Grasselli [40] implemented the FEM-DEM to simulate the behaviour of a layered rock sample under standard laboratory Brazilian disk test. Mahabadi, Cottrell [41] used FEM-DEM to numerically simulate the behaviour of Brazilian disc specimens as observed in laboratory during dynamic, high-strain rate, indirect tensile tests. Lisjak and Grasselli [42] applied a new dissipative contact interaction algorithm in FEM-DEM framework to simulate the energy loss that is observed during rock fall impacts taking into account friction, fracturing, and non-conservative forces. Rougier et al. [43] modelled Split Hopkinson Pressure Bar (SHPB) Brazilian experiments using an improved variant of FEM-DEM. Mahabadi, Lisjak [44] described a FEM-DEM numerical code for geomechanical applications. Recently, Druckrey and Alshibli [45] successfully simulated the frature of individual silica particles using the general concept of FEM-DEM within Abaqus software framework. However, to the authors best knowledge, the FEM-DEM concept has not been adopted to model the 3D behaviour of multi-particle granular assemblies. This paper implements the concept of FEM-DEM to simulate 1D compression experiment on sand using Abaqus FE code. 3D images of sand particles that were acquired using Synchrotron Micro-Computed Tomography (SMT) were used to create the 3D FE mesh. The implemented model captures the 3D physical shape of particles (morphology and particle-level characteristics) as discrete objects (discretization effect) that deform based on a FE framework (continuum behavior within each particle). A qualitative and quantitative assessment is presented by comparing the evolution of force chain, fracture modes, and stress-strain predictions with experimental results.

2. Experiment description and image acquisition

Cil et al. [1] conducted 1D compression experiment on a uniform natural silica sand known as F-75 Ottawa sand where only grain sizes between US sieve #40 (0.420 mm) and sieve #50 (0.297 mm) were used in the experiment. Sand particles were deposited inside a thick-walled acrylic mold with an inner diameter of 1 mm. The specimen had an initial height of about 2 mm. The experiment was conducted at beamline 1-ID of the Advance Photon Source (APS), Argonne National Laboratory (ANL), Illinois, USA. A special apparatus was used in which both 3D X-ray diffraction (3DXRD) and 3D SMT scans were acquired at different loading stages. The combination of 3DXRD and SMT techniques offers a unique approach to track individual particles and measure their lattice strains simultaneously. SMT scans were acquired using 70.5-keV X-ray energy while rotating the specimen at 0.2° angular increments over 180° at 0.65 s exposure time to construct a full 3D image with a spatial resolution of 1 μm/voxel. Similarly, 3DXRD scans were acquired at the same energy as the SMT scans while rotating the specimen at 1° angular intervals over 180° at a constant speed. Cil et al. [1] reported experimental measurements of the averaged lattice strain within each sand particle based on 3DXRD data and then evaluated the lattice stress tensor for each particle. They also investigated the evolution and mode of fracture of sand particles using the high-resolution 3D SMT scans.

The initial SMT image of Cil et al. [1] was used in this paper to develop the FE model that captures the exact shape of sand particles. The initial SMT image was processed using AVIZO Fire 9.3 software in which 35 particles were identified as separate objects and numerical labels (1–35) were assigned to each particle. AVIZO Fire 9.3 software was then used to crop each particle individually and its surface mesh was then generated and saved as stereo-lithography (STL) file producing 35 STL files (one for each particle). A few smoothening and simplification cycles were applied on each surface image to generate a surface mesh with approximately 800 triangles per particle. Fig. 1 shows an axial slice of the initial SMT scan and the surface meshes for all particles.

3. Finite element (FE) model description

Abaqus 6.14 was implemented to perform the FE simulations. It provides two different solvers: Explicit and Implicit. Explicit Abaqus solves for a state of dynamic equilibrium by constructing diagonal (lumped) element mass matrices to be used in computing nodal accelerations ($\ddot{u}$) at the beginning of each time increment as:

$$\ddot{u}_{(i)} = (M^{-1})(P_{(i)} - I_{(i)}) \tag{1}$$

where M is the mass matrix, P is the applied load vector, I is the internal force vector, and subscript i refers to the time increment number in an explicit dynamic step. The explicit solver integrates nodal accelerations that were calculated at time t using the explicit central-