Meso-Scale Framework for Modeling Granular Material Using Computed Tomography

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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][2][3] or disks [4][5][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][9][10][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 happen 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 as a whole was noted by McDowell and Bolton [13], who determined that grain strength governs the strength and dilatancy of crushable soils. Additionally, in their work studying the role of grain fragmentation in the mechanical behavior of a granular material under cyclic loading, Harireche and McDowell [14] found that it in fact provides a mechanism for plastic hardening of granular materials. The significant role of grain fragmentation on the plastic behavior of soil prove the importance of including grain fracturing in the meso-scale modeling of granular materials.

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 [13] and Nakata et al [17] who also determined the the stress corresponding to catastrophic splitting is inversely proportional to the nominal diameter of the grain. However, their approaches to calculate the stress at failure used assumptions and simplifications, such as assuming 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]. Again, these approaches do not take into account actual grain morphology.

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.

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 2D and 3D explicit Lagrangian finite element code that models the interaction of discrete bodies, such as individual sand grains, using the Simple Common Plane contact algorithm. While ABAQUS/Standard is also a 2D and 3D Lagrangian finite element code that allows for parallel computation, it utilizes implicit solution techniques. The finite element library of GEODYN-L only includes first order (linear),

solid elements, whereas the ABAQUS/Standard library includes both first and second order (quadratic) 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 for FEM as well as the mesh refinement of those elements. If the grain is represented by a stiffer mesh, due to the implementation of a coarser meshing scheme or lower order elements, the stress within the grain will be underestimated, leading to retarded fracture initiation. Grain fracture initiates at surface flaws positioned near the points of contact between grains, where stresses are high. To accurately capture the stress distribution inside the grain itself, a finer mesh is required at the surface of the grain, however a coarser mesh can be used away from the grain surface to decrease the total number of elements per grain and increase computational efficiency. This yields a proposed discretization approach in which an outer portion of the grain (shell) is represented by a fine mesh and the inner portion of the grain (core) is represented by a coarse mesh. In this work, grain fracture and fragmentation is not included in the numerical analysis, however, due to the importance of the phenomenon on the behavior of the granular material, it will be included in future work. The results of analyses presented below have been used to understand the effect of mesh refinement, element type, and coordination number on stresses near the high stress concentrations at the

grain contact, which will then be used to initiate grain fracture and fragmentation. The coordination number of a grain is the number of contact points on an individual grain by neighboring grains. Using idealized spheres, example configurations of grains and corresponding coordination numbers is provided in Fig. 1.

3.1.1. Input Tomography Geometry

A tomographically imaged sample of Ottawa sand grains was reduced to a 1.712 mm x 1.73 mm x 1.296 mm cube. The cube contained 12 full grains and 12 partial grains bisected by the cube boundaries. The grains within the cube were discretized using Simpleware into a coarse and fine mesh, with 54,243 and 235,858 total linear tetrahedral elements (approximately 2,200 and 10,000 elements per grain), respectively, shown in Fig. 2.

The two discretizations were subjected to one-dimensional confined compressive loading. Deviatoric stress is applied by axial displacement of the top plane in the negative X direction at a constant velocity corresponding to an axial strain rate of $5.8 \times 10^4 \text{ s}^{-1}$. The effect of strain rate was investigated and found to have no influence on the resulting stresses within the particles. The total displacement applied to the sand grain sample was 0.100 mm corresponding to 5.8% axial strain in the X direction. A summary of the material properties used in the analyses is presented in Table 2. The plastic stress-strain relationship of the sand grain material was assumed to follow Johnson-Cook power law strain hardening, with the material properties used in these analyses determined from the stress-strain relationship presented in the nanoindentation tests of quartz sand performed by Subramanian et al [19]. It should be noted that the maximum equivalent stress (~3.0 GPa) corresponding to the catastrophic grain splitting, presented in Table 1, is less than the yield stress (6.85 GPa) of the proposed material model indicating that the material of the grains themselves remains elastic prior to splitting.

To demonstrate both the effect of mesh refinement and confirm the need for the shell-core discretization approach previously discussed, the variation of the equivalent stress along a line defined by the normal contact between two grains (as illustrated in Fig. 3) is shown in Fig. 4. As anticipated, the finer mesh resulted in equal or higher stresses at the contact point with increased applied axial stress due to the stiff behavior of the coarser mesh. However the finer mesh required 180 CPU-Hrs while the coarser mesh required only 60 CPU-Hrs. These results emphasize the need for *efficient* discretization in which a finer mesh is located along the surface of grains where contact will occur such as the shell-core approach described previously. Additionally, it should be noted that the maximum equivalent stress observed in the entire assembly of grains, shown in Fig. 5, reaches the maximum equivalent stress corresponding to catastrophic splitting of the grains (~3.0 GPa) with less than 1.0% axial strain applied. This illustrates the need to include grain fracture and fragmentation in numerical analyses even with small applied strains.

A larger cube from an imaged Ottawa sand specimen, shown in Fig. 6, was analyzed under both one-dimensional confined and unconfined compression loading. The cube had dimensions of 4.458 mm x 4.458 mm x 4.458 mm and contained 99 full and 228 partial grains. The same material properties as the smaller specimen were utilized. Each full grain contained approximately 8,600 linear tetrahedral elements for a total of 1,905,481 elements in the specimen. Therefore the mesh refinement was similar to that of the finely discretized small sample previously analyzed. Increasing the specimen size also increased the computational time required to complete the analyses to 1500 CPU-Hrs. The resulting axial stress-strain curves from the large specimen analyses are shown in Fig. 7. While grain rearrangement occurs throughout duration of the analyses, significant grain rearrangement, determined by monitoring the kinetic

energy of the grains at the nodes, was observed between 1% and 2% axial strain resulting in the dip in the axial stress-strain curves. High equivalent stresses concentrated at points of contact were also seen in grains of the larger specimen. In reviewing the variation of the contact stress with the coordination number on individual grains, example maximum contact stresses at 5% axial strain provided in Table 3, it is seen that with a higher the coordination number the maximum contact stress on an individual grain decreases nonlinearly, as was also observed by Gu and Yang [5]. This nonlinear relationship indicates that as the coordination number increases, the maximum contact stress on the particle decreases converging to a limit such that an increase in coordination number will not decrease the maximum contact stress significantly. This relationship also means that granular materials with higher densities are less likely to experience particle fragmentation due to decreased stress concentrations at contact points between grains. These findings are consistent with those of Hagerty et al [25], who determined that particle crushing increases with decreasing density in 1D high pressure compression tests. As previously mentioned, the accuracy of the predicted stress distribution at points of contact can also be influenced by element type. A higher order element, such as a quadratic tetrahedral element, will more accurately predict the stress distribution within a grain with a fewer number of elements than the linear tetrahedral element used in these analyses. Additionally the lower order element may cause locking at nodes again increasing the stiffness of the mesh and underestimating the stress concentrations. Unfortunately, a higher order element is not currently available in GEODYN-L. Future work for this research includes the implementation of finite elements, which minimize the effect of locking, such as higher order elements.

3.1.2. Idealized Spherical Geometry

Since higher order elements are currently available in the finite element code ABAQUS/Standard, analyses using this code were performed to investigate the effects of element type and mesh refinement on the stress distribution through the grain. For simplification, the grain was represented as a 0.700 mm diameter sphere of linear elastic material with an elastic modulus of 70 GPa and Poisson's ratio 0.30. The grain was considered to have a coordination number of 2 (see Fig. 1) with the contact forces assumed to be 50 N, based on the splitting force of a grain this size, and represented as a pressure over a circular area with a 3D parabolic distribution. The distribution and area of the contact pressure was calculated according to Hertz/Huber theory of contact between elastic spheres as outlined by Schönert [26].

Seven finite element discretizations of linear and quadratic tetrahedral elements using the shell-core approach were implemented, varying from 381 to 183,455 elements, as shown in Table 4.

To evaluate the ability of each meshing scheme to most accurately capture the stress distribution through the grain, the equivalent stress distributions along a path corresponding to the centerline of the spherical grain along the Y-axis are shown in Fig. 8. The distance along the centerline is normalized by the radius of the sphere, so that 0 corresponds to the center, +1 corresponds to the surface in the positive Y direction, and -1 corresponds to the surface in the negative Y direction.

The ability of a finer mesh to more accurately capture the stress distribution is most noticeable in the comparison of results using linear elements. A coarser discretization increases the overall stiffness of the continuum, decreasing the stress experienced by the grain. Using the stress to determine grain fracture initiation, a coarser discretization would over-predict the capacity of the grain. Comparing the linear and quadratic stress distributions, more than 28,000 linear tetrahedral elements (39,000 nodes / 117,000 degrees of freedom) are required to most accurately

predict stress near contacts, whereas 6,800 (11,000 nodes / 33,000 degrees of freedom) quadratic tetrahedral elements can be used instead. Decreasing the number of elements and number of nodes also decreases the number of degrees of freedom in the model, decreasing the computational effort and time required for analysis. Since the analysis of actual grain assemblies are large models requiring significant computational time, a decrease in this number of degrees of freedom in the model would allow for faster results and larger assemblies analyzed. These results also indicate that the highest stress gradient occurs within approximately a 30% radial distance from the surface suggesting that the shell of finer elements have a thickness corresponding to 30% of the grain radius, or 15% of the grain diameter.

3.2. Effect of coordination number

In addition to varying the discretization and element type, a study on the effect of the grain's coordination number was also performed. In the granular matrix, individual grain coordination numbers can vary from 2 to 10 and affect the stress distribution within the grain. The grains within a looser packed matrix will have a lower coordination number, whereas the grains within a more densely packed matrix will have a higher coordination number. Again, neighboring grains were not explicitly modeled, but contact forces between grains were represented by pressures as described above, with the magnitude of the forces determined by assuming a 50 N contact force from the upper grain and calculating the resultant reaction forces from the lower grains. The resulting equivalent stress distributions along a path corresponding to the vertical centerline of the spherical grain are shown in Fig. 9. The maximum equivalent stress in the bottom half of the grain decreases from 5.5 GPa to 3.2 GPa (41%) as the coordination number increases from 2 to 6. Again the decrease in contact stress with increasing coordination number, corresponding to an increase in density, is observed. The radial distance of the highest stress

gradient from the surface decreases from 30% to 20% of the spherical radius. Therefore the thickness of the shell required decreases with increasing coordination number.

4. Conclusions

The following conclusions are made to facilitate more accurate and efficient numerical analyses of granular material at the meso-scale:

- In this study, a new procedure is developed to precisely model the meso-scale structure of granular materials using high resolution computed tomography, advanced thresholding and digitization to model a complex geometry of particles and contacts using a viable number of finite elements, and a framework for solving boundary value problems involving complex loading.
- Due to the high stress gradient near the grain surface where contact occurs and fragmentation initiates, a discretization approach in which a shell of finer elements with a depth of 15% of the grain diameter and core of coarser elements more efficiently calculates the stress distribution through the grain.
- Stresses greater than those typically observed at catastrophic grain splitting are seen at small applied axial strains in the current study, since formulation of particle fracture has not been developed, illustrating the need to include fracture and fragmentation in future studies.
- Higher order elements should be implemented to decrease computational time of large assemblies of grains while maintaining accuracy.
- A higher coordination number, such as those observed in a densely packed assembly of grains, decreased the depth of the high stress gradient from the surface, requiring a thinner shell of fine meshing near the surface of grains.

This work focuses on the quasi-static loading of 1D compression. Additional research should be performed to better understand the effect of dynamic loadings, such as that from a projectile penetrating the granular assembly, which cause high gradients of deformation in a short period of time likely leading to significant particle fragmentation.

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Tables and Figures

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 & Bolton [13]
1.55	silica sand	74.4	2.87	Nakata et al [17]

Table 2. Properties used in GEODYN-L Analyses (Subramanian et al [19])

Property	Value
Elastic Modulus (GPa)	66.9
Poisson's Ratio	0.18
Yield Stress (GPa)	6.85
Hardening Constant	13.1
Hardening Exponent	0.656

Table 3. Example Maximum Equivalent Stress and Coordination Number at 5% Axial Strain of Larger Specimen

Coordination Number	Maximum Equivalent Stress (GPa)
4	7.9
5	5.7
6	4.8
7	4.2

Table 4. Mesh Attributes of Spherical Single Grain Analyses

Mesh	Elements	Nodes	Element Type
A	183455	32419	linear
A	183455	252150	quadratic
B	160971	28663	linear
B	160971	222154	quadratic
C	27667	5114	linear
C	27667	38850	quadratic
D	10120	2199	linear
D	10120	15473	quadratic
E	6811	1655	linear
E	6811	11076	quadratic
F	1010	353	linear
F	1010	2019	quadratic
G	381	126	linear
G	381	732	quadratic

Fig. 1. Coordination Number Configurations of Spherical Single Grain

Fig. 2. Coarse and Fine Mesh of Small Ottawa Sand Specimen used in GEODYN-L Analyses

Fig. 3. Contact Line Between Two Grains

Fig. 4. Variation of Equivalent Stress Along Contact Line With Discretization

Fig. 5. Maximum Equivalent Stress in Assembly of Small Specimen With Respect to Applied Axial Strain

Fig. 6. Mesh of Large Ottawa Sand Specimen used in GEODYN-L Analyses

Fig. 7. Axial Stress-Strain from 1D Loading of Large Specimen

Fig. 8. Effect of Mesh Refinement and Element Type on Stress Distribution within Spherical Single Grain Subjected to Varying Coordination Number of Contacts. Mesh Attributes for Each Analysis Provided in Table 4

Fig. 9. Effect of Coordination Number on Stress Distribution within Spherical Single Grain

Figure 1

Figure 2

Coarse

Fine

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9