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, Alshibli [1].

Keywords: Force chains, fracture, sand, contact stresses

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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, Jean [11] [12] implemented contact dynamics simulations to study the statistical distribution of contact forces inside a confined packing of 2D 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, Nguyen [14] used DEM to investigate the role of force chains in granular materials under both quasi static biaxial loading and dynamic impact loading. Coppersmith, Liu [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, Cates [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 particles in DEM as agglomerates of balls bonded together to simulate fracture of individual soil particles, then successfully simulated oedometer tests on sand and showed that yielding coincides with the onset of bond breakage [28]. Ng [29] introduced a new boundary condition (i.e. hydrostatic boundary condition) in DEM to simulate the chamber fluid pressure 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 2D 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 yielded 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, Yu [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, pile, etc. 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, Andô [37] outlined the level set discret 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, Schofield [38] and Drucker, Gibson [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, Knight [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 fracture 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.

**EXPERIMENT DESCRIPTION AND IMAGE ACQUISITION**

Cil, Alshibli [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 second 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, Alshibli [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, Alshibli [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. Figure 1 shows an axial slice of the initial SMT scan and the surface meshes for all particles.

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:

$$\ddot{u}_{(i)} = (M^{-1})(P_{(i)} - I_{(i)})$$  \hspace{1cm} (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-difference integration algorithm to advance the velocity solution ($\dot{u}$) to time $t + \Delta t/2$ and the displacement solution ($u$) to time $t + \Delta t$ as:

$$\dot{u}_{(i+\frac{1}{2})} = \dot{u}_{(i-\frac{1}{2})} + \frac{\Delta t_{(i+1)} + \Delta t_{(i)}}{2} \ddot{u}_{(i)}$$  \hspace{1cm} (2)

$$u_{(i+1)} = u_{(i)} + \Delta t_{(i+1)} \dot{u}_{(i+\frac{1}{2})}$$  \hspace{1cm} (3)
Where \( u \) is a degree of freedom (displacement or rotation). The central-difference integration algorithm is explicit in a sense that kinematic state is advanced using the known values of \( \dot{u}_{(i-\frac{1}{2})} \) and \( \ddot{u}_{(i)} \) from the previous time step. The explicit solver can perform analysis on a large number of small inexpensive time increments to ensure that the central-difference integration rule is stable. However, if large increments are used then the solution becomes unstable and diverges rapidly.

Alternatively, Implicit Abaqus solves for a state of static equilibrium in which Newton-Raphson algorithm is implemented for each time increment \( i \) to satisfy equilibrium. In each time increment \( i \), the implicit solver assumes an estimate of the solution at iteration \( n \) to be \( u^n_i \) (subscript refers to time increment number \( i \) and superscript refers to iteration number \( n \)). As a result, a Taylor series expansion about this estimate can be expressed as:

\[
Kc = P - I
\]

Where \( c \) is the correction factor and \( K \) is the system’s tangent stiffness matrix which can be expressed as:

\[
K = \frac{\partial l}{\partial u} - \frac{\partial P}{\partial u}
\]

The implicit solver modifies the incremental displacement \( \Delta u_i \) after each iteration \( n \) using the following expression:

\[
\Delta u_{(i)}^{n+1} = \Delta u_{(i)}^{n} + c_{(i)}^{n}
\]

Iterations are repeated for each increment until the solution converges to equilibrium within a pre-defined tolerance. This implies that force and moment equilibrium are satisfied at each node. Lastly, as nodal displacements are calculated, then both the implicit and explicit solvers compute
nodal forces based on classical FE approach using stiffness matrices (i.e. \( f = ku \)) and evaluate strain-stress values for each element.

Sand is as a granular material consists of discrete particles that interact with each other through contacts and undergo large deformations. The most challenging task in such quasi-static FE simulation is the contact detection and possible mesh distortion. At first look, the implicit solver appears to be more appropriate for the quasi-static analysis reported in this paper. However, iterating in each time increment to solve the system of non-linear differential equations (Equation 4) adds limitations on the capability of the implicit solver to detect, track, and modify location of contacts during each iteration step. Alternatively, the assumption of lumped masses in the explicit solver results in diagonal mass matrices that produce a system of linear differential equations that can be solved without iteration. This provides the explicit solver a powerful advantage to be implemented in such quasi-static problems with many contacts and large deformations. In other words, even though a given FE analysis on sand grains may require a large number of small time increments in the explicit package, the analysis can still be more computationally efficient in Explicit Abaqus since large geometric changes due to contacts will require many iterations in each implicit Abaqus time increment to achieve equilibrium. A common practice to speed up the explicit solver simulations in such rate-sensitive quasi-static problems is to apply a mass scaling factor that magnifies the mass of particles. An estimate of time increment size \( (\Delta t) \) in Explicit Abaqus can be expressed as:

\[
\Delta t = \frac{\sqrt{\rho / E}}{L^e}
\]

Where \( \rho \) is the material density, \( E \) is the modulus of elasticity, and \( L^e \) is the smallest element length. Therefore, an increase in mass (density) will increase the size of time increments that will
result in reducing the total time scale of the simulation run. For example, an artificial increase in particles density by a factor $f^2$ will increase the size of time incrementation $\Delta t$ by a factor of $f$. For the simulation reported in this paper, a mass scaling factor of $10^6$ was used to achieve a total simulation time of approximately one hour. In addition, Abaqus takes advantage of parallel processing for the explicit solver that further speeds up the FE simulations. The kinetic energy of the deforming particles through the simulation was also checked to be less than 5% of the internal energy to ensure that the simulation yields an appropriate quasi-static response. Note that this limit was not fulfilled in the early stages of the simulation since deformable particles were moving freely until contacts were established to stabilize the granular system.

Meshed surface images (STL files) were imported into explicit Abaqus through a plug-in tool. For each particle, the surface triangular elements were converted into 4-node tetrahedral elements producing solid filled particles. An isotropic elastic material model was assigned to elements of sand particles. Young’s modulus of elasticity and Poisson’s ratio of silica sand were assumed to be 91.1 GPa and 0.118, respectively [46]. Then, particles were assembled (preserving the location of each particle to closely match the initial SMT image) into a discrete rigid mold and bounded by two discrete rigid end caps. A discrete rigid part represents a part that exhibits negligible deformation relative to the rest of the model and are ideally suited in Abaqus to model tooling such as punch, mold, roller, cap, etc. The principal advantage of using discrete rigid parts over deformable parts is the computational efficiency enhancement. Rigid parts in Abaqus are associated with a node, called the rigid body reference point, in which its motion governs the motion of the entire rigid body. Therefore, the motion of a rigid part is completely determined by boundary conditions applied at the reference point rather than expensive element-level calculations. Rigid parts in Abaqus have no element output variables due to the absence of element-
level calculations. However, the only output from rigid elements is the motion of the nodes as well as nodal reaction forces. The mold and end caps diameters were assigned to be 1.04 \textit{mm} and 1.02 \textit{mm}, respectively, which is similar to the experimental setup based on measurements from the initial SMT scan.

Explicit Abaqus General Contact Algorithm was adopted to define interaction properties between particles, particle-mold, and particle-end cap. The algorithm allows defining an inclusive surface that contains all exterior faces of deformable and rigid parts. In each configuration (i.e. time increment), the algorithm searches for slave node penetration including node-into-face and node-into-rigid surface penetration. For node-into-face contacts, forces which are a function of the penetration distance are applied to the slave nodes to oppose the penetration, while equal and opposite forces act on the master surface at the penetration point. Contact forces acting on the master surface are then distributed to the surface nodes. Similar formulation is implemented for node-into-rigid surface contacts with the equal and opposite contact forces always assigned to the rigid surface at the penetration point (i.e. reaction forces). Contact properties were assigned as part of contact interaction definition and were linked to the general contact domain. The paper adopted the penalty contact formulation to simulate interactions between particles in which slippage is constrained by a tangential friction coefficient (\(\mu\)) and hard normal behavior. The value of \(\mu\) is attributed to the true angle of friction (\(\phi_\mu\)) that represents friction properties between mineral surfaces of the material (quartz for silica sand used in the experiments). \(\phi_\mu\) is assumed to be approximately 22\(^\circ\) based on values reported in the literature for silica sand [47] which yields a value of 0.4 for the friction coefficient \(\mu\) (i.e. \(\tan 22^\circ \approx 0.4\)). On the other hand, the normal behavior is attributed to the “spring” stiffness that relates the contact force to the penetration distance. For hard normal contact, a stiffness value is chosen automatically by Explicit Abaqus.
such that the effect on time increments is minimal (i.e. allowed penetration is not significant in most of the analysis). Similar properties and formulation were estimated for particle-mold and particle-end cap interactions.

To mimic the experiment, the mold and bottom end cap were fixed with zero degrees of freedom while the top end cap was permitted to move in the vertical direction with one degree of freedom. The FE simulation was divided into two stages: seating and compression. In the seating stage, a seating load of 1 $N$ was applied incrementally to the top cap in the vertical direction to introduce contacts between particles resulting in approximately 25 $\mu$m vertical displacement. A 1 $N$ load is a high seating value relative to the specimen dimensions. However, it is physically a very small measurement that was barely induced when contact occurs between the loading plate and top end cap in the experiment. In FE simulations, a 1 $N$ load was still barely enough to establish the contact between the top end cap and top particles. Furthermore, a seating load of 1 $N$ was considered in the FE simulation to mimic the experiment. After seating the specimen in the FE simulations, the top end cap was programmed to move in the vertical direction at a constant rate of 0.2 $\text{mm/min}$ similar to the experimental loading rate.

Fracture of sand particles significantly affects the behavior of a granular assembly. The discrete nature of particles is a major factor that plays a significant role in understanding the mechanics of granular materials. This has already been proven by published research using DEM models. The discrete nature of particles can be characterized using several parameters such as sphericity, roundness, grain size distribution, etc. Each of these parameters is highly influenced by fracture of particles. In other words, fracture of particles in a loaded granular assembly completely change particles’ sphericity, roundness, size, size distribution, etc. Accordingly, the mechanics of the granular assembly (e.g. global stress-strain response) is highly affected. A comprehensive
understanding of sand response under loading cannot be fully understood without considering particle fracture phenomenon. A straightforward approach to simulate fracture of sand particles in Explicit Abaqus is by applying the element deletion method based on a pre-defined damage criterion. The paper adopted the brittle cracking model, which is a damage criterion where the material behavior is dominated by brittle tensile cracking. The brittle cracking model implements Rankine criterion to detect crack initiation where a crack forms when the maximum principal tensile stress exceeds a pre-defined maximum tensile strength limit ($\sigma_{tu}^l$). The crack surface is assumed to be normal to the direction of maximum principal tensile stress and the characteristic crack length is determined based on the considered element type and formulation (e.g. typically equal to the length of a line across an element for linear type mesh). This imposes mesh dependency on crack propagation while crack initiation is less sensitive to mesh refinement. The model aims to simulate behavior of particles under 1D compression which is more likely to be affected by crack initiation rather than crack propagation. Several trials were performed to calibrate the value of $\sigma_{tu}^l$ based on comparison with experimental results (SMT scans), and calibration load-displacement curve of the top end cap. An optimum value of $\sigma_{tu}^l$ was determined to be 750 MPa which yields the load-displacement calibration curve shown in Figure 2. The specimen behavior through the simulation is also depicted in Figure 3.

It is important to emphasize that studies reported in literature suggest lower values for tensile strength of silica sand particles than the 750 MPa which was used in the FE simulations. For example, Cil and Alshibli [36] constructed the Weibull Probability Distribution Function for tensile strength of silica sand grains according to experimental data and evaluated the 37% characteristic tensile strength of silica sand particles to be about 138 MPa. In the FE simulation conducted in this paper, the 750 MPa is the maximum limit of principal tensile stress that elements
can reach before deletion occurs. However, not all elements in the particle reached this limit when fracture occurs (i.e. stress localization exists within the particle itself). On the other hand, the averaged maximum tensile stress of all elements in the particle was observed to be much less than 750 MPa.

RESULTS

Force chains

Explicit Abaqus provides contact forces at surface nodes for each particle. Initially, the surface of each particle was individually examined to determine surface nodal sets associated with each contact. Accordingly, contact forces of nodal sets forming each contact were summed up in which an equivalent contact force value was determined to act at the center of nodes. A weighted average of nodes’ location with nodal contact forces as factor of importance was considered as the center of nodal sets associated with each contact (i.e. equivalent contact force location). Force equilibrium of each sand particle is fulfilled. In addition, pairs of contact forces were checked to be approximately equal in magnitude and opposite in direction. Location of contact pairs was also checked to match with minor differences (i.e. ±0.5 μm). For further explanation on calculation of equivalent contact forces, Figure 4 shows an example of equivalent contact force calculation (magnitude, direction, and location) for contact $C_{10-11}$ (contact between particle 10 and 11) at about 7% global axial strain.

As contact forces were quantified, transmission of forces was observed to occur through two main force chains. Force chains were detected based on maximum contact forces, particle assembly, stress concentrations, and quasi-linearity. The flow of major contact forces between the top and bottom end caps was tracked to identify force chains. For particles to be in a force chain,
they must experience large stresses compared to other supporting particles. Since maximum principal stresses in the conducted simulations are mostly compressive stresses and Abaqus code adopts a compression-negative sign convention, the maximum principal stress absolute ($\sigma_{abs.}$) was considered in stress level comparison between particles. In Abaqus, $\sigma_{abs.}$ is defined as the largest value between the maximum and minimum principal stresses regardless of sign convention. In other words, particles associated with force chains must have $|\bar{\sigma}_{abs.}^l| > \frac{1}{R} \sum_{i=1}^{R} |\bar{\sigma}_{abs.}^l|$, where $\bar{\sigma}_{abs.}^l$ is the particle-level averaged maximum principal stress absolute of particle $i$ and the summation runs over all particles in the assembly $R$. It is also important to emphasize on the quasi-linearity term in which the trajectories of $\bar{\sigma}_{abs.}$ for particles within a force chain must line up. A detailed description of the procedure followed in detection of force chains can be found in [48]. The evolution of the two force chains is visualized in Figure 5 at different loading stages showing colored mesh contours of Von Mises Stress distribution through particles associated with force chains that were also experimentally identified in [1] based on particles with maximum averaged principal lattice strains. Figure 6 shows force chains based on 3DXRD experimental measurements versus FE model. It can be observed that force chains that were identified by the FE model match within minor differences with force chains based on experiments, especially for the middle and bottom particles. Note that Cil, Alshibli [1] were unable to analyze the 3DXRD data for particle 31 due to possible crystal defects and the particle was only visualized in the SMT scans. Therefore, particle 31 may have caused the difference between the experiment and model quantified force chain II.

The two force chains were detected separately (i.e. no common particles) with approximately one particle separation distance (i.e. about 400 $\mu$m). Nonetheless, common supporting particles were observed to exist at certain vertical levels allowing interaction between the two detected force
chains. For example, Figure 7 demonstrates parts of force chain I and II at about 7% global axial strain with particle 26 acting as a common supporting particle. Elemental trajectories of $\sigma_{abs}$ are also plotted for each particle to illustrate stress flow within the two force chains. It can be observed from Figure 7 that particle 26 not only braces force chain I at particle 11 and force chain II at particle 34, but also provides a bridge that insures stress flow between both force chains which results in a preferential direction of $\sigma_{abs}$ trajectories toward the horizontal plane.

A comparison between loading of particles associated with detected force chains versus other particles was assessed in Figure 8. Figure 8(a) isolates particle 11 with its surrounding particles (particles 12, 4, 26, and 10) and displays nodal contact forces at about 7% global axial strain. It is important to note that particles 12, 11, and 10 are associated with force chain I, while the other two particles (particles 4 and 26) are supporting particles. It can be observed from Figure 8(a) that contact forces between force chain particles are higher in value relative to contact forces with supporting particles. For further assessment, two particulate assemblies, each consists of 3 particles, were isolated in Figure 8(b) at about 7% global axial strain and plotted with $\sigma_{abs}$ trajectory for each element. Note that both assemblies were selected at almost the same vertical level preserving their relative location as demonstrated in Figure 8(b). Particles in the first assembly (i.e. particles 6, 12, and 11) were associated with force chain I, while particles in the second assembly (i.e. particles 17, 21, and 16) were not associated with any of the detected force chains. It can be noticed from Figure 8(b) that the assembly with force chain particles is subjected to higher stresses as well as a higher degree of line up of $\sigma_{abs}$ trajectories in global compression direction (i.e. vertical direction). Again, this emphasizes on stress concentration and quasi-linearity terms that were adopted in detection of force chains.

Fracture Mode
Particles within force chains are more likely to fracture first as they experience higher contact stresses than other supporting particles. The FE simulation shows that Particle 6 in force chain I and particle 31 in force chain II are the first two particles to fracture. To assess the capabilities of the implemented fracture model, several particles (Particles 6, 31, 13, 27, and 28) with major fracture (fractured into two or more fragments) were tracked in the acquired SMT scans, isolated, and compared with FE model predictions. Figure 9 visualizes experimental versus model fracture of selected particles where an excellent agreement was found between FE model prediction and experimental fracture modes.

For further assessment of fracture mode, particles 6 and 31 (first particles to fracture in force chains I and II) were isolated and visualized with surrounding particles before and after fracture as depicted in Figure 10. It can be observed that particles 6 and 31 fractured via two different failure modes. Referring to Figure 10(a), particle 6 fractured due to bending effect in which simple vertical supports were provided near edges by particles 12 and 5 while load was applied vertically at almost mid-length by particle 8, similar to a simply supported beam. As a result of bending effect, tensile stresses initiated in the bottom region of particle 6 which in turn caused the fracture. On the other hand, particle 31 was observed to be more confined between multiple particles in which load is transmitted vertically through the force chain by particles 32 and 1 while particles 27, 17, and 35 provided lateral supports against force chain buckling [Figure 10(b)]. Particle 31 is supported by multiple particles that resulted in more even distribution of stresses through the whole particle elements which lead to particle fracture into several fragments (crushing) rather than breaking into just two major fragments as the case for particle 6. It can be observed from Figure 10(b) that fracture initiated from contact points between particle 31 and particles 1 and 32 which are all associated with force chain II.
**Stress-strain relationships within individual particles**

FE is considered as a powerful numerical modeling method since it provides quantitative estimations of stress and strain fields at each element. 3DXRD and SMT techniques have been successfully implemented to experimentally track and measure stress and strain within particles in a granular assembly [1, 24, 49]. However, such experimental particle-level measurements are still considered challenging since they require advanced and unique testing facilities. In this paper, stress and strain components of elements constituting each particle were averaged based on elements’ volumetric weights and an estimate of strain and stress tensor components per particle were computed as:

\[
\bar{E} = \frac{\sum_{i=1}^{m} e_i V_i}{\sum_{i=1}^{m} V_i}
\]

Where \( \bar{E} \) is the particle-level averaged stress or strain tensor component, \( e \) is the stress or strain component of the individual element \( i \), \( V \) is the volume of the considered element \( i \), and the summation runs on all elements \( (m) \) forming the particle. Note that Abaqus sets the volume of failed elements to 0 when the moment deletion occurs. Otherwise, volume of elements was exported in parallel with stress or strain components at each time step to compute the average estimate value. As estimates of particle-level averaged stress and strain tensors were evaluated, principal values and directions were then computed to be the tensorial eigenvalues and eigenvectors, respectively. For example, Figure 11 shows the evolution of averaged principal stresses and strains of Particles 6 and 31 with respect to global axial strain. For particle 6, experimental measurements of principal stresses and strains that were reported in [1] are also plotted in Figure 11 which show a close match with the FE model predictions. Again, it is important to emphasize that particle 6 did not fracture at particle-level averaged maximum
principal stress of 750 MPa (i.e. value set for $\sigma_{tu}$) but at a much lower value around 70 MPa versus experimental fracture around 90 MPa. This can be directly related to the localization of stresses within the particle itself. Beside particle-level averaged stress and strain estimates, FEM also provides the distribution of such estimates within the particle volume which can be used for further assessment of stress localization within the particle itself. For example, Figure 12 shows a histogram of maximum principal tensile stresses of particles 6 and 31 normalized by element numbers where a high percentage of elements within particle 6 are exposed to higher principal tensile stresses. Concurrently, elements exposed to low principal tensile stress are still more likely to exist within particle 6 than particle 31 (i.e. histogram steps of particle 31 levels more than particle 6). This can be explained by the two different fracture modes of particle 6 and 31. Particle 6 fractured as a result of tensile stress localization induced by bending effect due to bridging action. On the other hand, particle 31 fractured into multiple fragments by crushing due to higher confinement. Consequently, it is more likely to find more elements far from stress localization region within Particle 6 which are exposed to lower stresses. In other words, crushing action in particle 31 creates a better distribution of stresses between elements which levels down the histogram steps.

**SUMMARY AND CONCLUSIONS**

A FE approach that addresses the discrete nature of sand particles was adopted to simulate the 3D behavior of sand under 1D compression. The proposed approach captures 3D particles morphology and the effect of the discrete nature of sand in a continuum framework. 3D morphology of discrete particles was captured by extracting the exact shape of sand particles from the initial SMT scan images. Particles were individually meshed in AVIZO Fire 9.3 and were then used to generate the FE model in Explicit Abaqus. A deformable isotropic linear elastic material
model was used to investigate the behavior of sand particles. Transmission of vertical load was tracked to characterize force chains. The model captured the evolution of force chains to transmit the load between the top and bottom end caps while some of surrounding particles provided support against force chain buckling. The FE model gave an excellent prediction of force chains that compared well with experimental measurements based on 3DXRD data [1]. Furthermore, fracture of sand particles was investigated in which an excellent agreement between experimental fracture and model fracture modes was observed. The fracture modes were also assessed using the powerful 3D visualization tool provided by Abaqus software. Stress and strain field estimations were also calculated to better understand particles’ fracture modes. Two different fracture modes were observed to occur in two different particles (e.g. bending versus crushing). Fracture modes were found to be dependent on particle’s boundary conditions that is induced by contacts with surrounding particles. Crushing failure mode was observed to occur under high boundary confinement while bending fracture mode occurs under less confinement and bridging action. Moreover, higher stress localization was observed to occur in bending fracture rather than crushing.

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Figure 1. Axial slice through the initial SMT scan: (a) grayscale image; (b) labeled image; and (c) 3D view of the generated surface mesh.
Figure 2. Global compressive displacement versus force calibration curve of the top end cap.
Figure 3. Specimen behavior using FE simulation in which surrounding mold is hidden for better visualization ($\varepsilon_1$ refers to the global axial strain).
Figure 4. Illustrative example of equivalent contact force calculations between particle 10 and 11 at about 7% global axial strain.
Figure 5. Evolution of (a) force chain I; (b) fracture in particle 6; (c) force chain II; and (d) fracture in particle 31. Surrounding mold is hidden for better visualization ($\varepsilon_1$ refers to the global axial strain).
Figure 6. Comparison between (a) experimental force chain I; (b) model force chain I; (c) experimental force chain II; and (d) model force chain II.
Figure 7. Visualization of interaction between force chain I and II through a common supporting particle #26 at about 7% global axial strain.
Figure 8. (a) Nodal contact forces between particle 11 and its surrounding particles and (b) stress flow in an assembly associated with force chain I and another assembly not associated with any of the detected force chains at about 7% global axial strain.
Figure 9. Visualization and comparison between experimental versus model fracture of (a) Particle 6; (b) Particle 31; (c) Particle 13; (d) Particle 27; and (e) Particle 28.
Figure 10. FE model fracture assessment for (a) Particle 6 (b) Particle 31
Figure 11. Evolution of principal stresses and strains within Particles 6 and 31.
Figure 12. Histogram of maximum tensile principal stress distribution of particles 6 and 31.