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Extended Abstract+

Statistical Distributions of the Elastic Moduli of Particle Aggregates at the Mesoscale

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1. Introduction

The current work is part of an ongoing effort to couple the Discrete Element Method (DEM), used as a mesoscale method, with Statistical Mechanics in order to construct a framework for the modeling, homogenization, and uncertainty quantification of particulate geomaterials. The aspect of the framework tackled in this work, is the quantification of stress and deformation of heterogenous DE models. Such quantification is necessary to allow DEM to "speak continuum". DEM is a discrete particle method, wherein the concept of "stress" does not fit naturally, but where each particle pair is considered to interact through discrete forces. Additionally, DEM is an explicit method, and equivalent continuum deformation must be defined in the context of particle kinematics.

2. Computational Approach

2.1. Surface Reconstruction of Particle Aggregate Boundaries with Alpha Shapes

The definition of a boundary for free-floating particles in space, also known as a "point cloud", requires some sort of surface reconstruction algorithm. Serendipitously, surface reconstruction from point clouds has been an area of intensive research and progress in recent years. This has been spurred by rapid developments in 3D scanning and photogrammetry. There are several approaches used to extract an exterior surface from a point cloud.

Discrete Element Models do pose an additional challenge for surface reconstruction algorithms, the discrete particles are actually spheres with radii, surface area, and volume. This complication can be resolved by using "weighted" alpha shapes, that account for the radii of the DEM particles. The alpha-shape associated with a set of points is a generalization of the concept of the convex hull [1].

For each real number α, define the concept of a generalized disk of radius 1/α as follows:

- If $\alpha = 0$, it is a closed half-plane (convex hull)
- If $\alpha > 0$, it is closed disk of radius $1/\alpha$
- If $\alpha < 0$, it is the closure of the complement of a disk of radius $-1/\alpha$

Weighted alpha shapes on a regular triangulation of the DEM particles can be used to construct a Laguerre-Voronoi Diagram (a.k.a. Power Diagram) of the boundary [2]. The LV Diagram essentially is a map on the DE model boundary of the boundary areas belonging to each particle determined by the weighted alpha shape algorithm to be a boundary particle

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2.2. Surface Reconstruction for Stress and Deformation Quantification

A highlight of this micromechanical boundary implementation is that the boundary particles may become interior particles and vice-versa. While this makes micromechanical boundaries more versatile, it does increase computation complexity for original-to-deformed mapping schemes such as the deformation gradient. This complexity is herein resolved by introducing into the computation a fixed rectangular grid which is “fitted” to the particle aggregate boundary at either configuration. The interpolated regular surface grid makes it possible to compute stress and deformation by providing matching reference points for the current as well as the reference configuration.

The fitting of this regular grid is done by 1) translating the coordinates of the LV Diagram into spherical coordinates, 2) translating the coordinates of a surface grid from a tessellation of a unit cube into spherical coordinates, 3) linear interpolation of the radii of the unit cube from the LV Diagram, 4) conversion of the interpolated spherical coordinates back to Cartesian coordinates.

2.3. Deformation Gradient from Particle Kinematics

The macroscopic deformation gradient is defined by the volume average of the macro-scale deformation:

$$\overline{\mathbf{F}} = \frac{1}{V}\int_{V} \mathbf{F} dv \tag{1}$$

where the deformation gradient is defined as:

$$\mathbf{F} = \nabla \mathbf{x} \tag{2}$$

Application of the divergence theorem, gives:

$$\overline{\mathbf{F}} = \frac{1}{V}\int_{\partial V} \mathbf{x} \otimes \mathbf{N} ds \tag{3}$$

where $\mathbf{N}$ is the unit normal vector at the outer boundary for the reference configuration. Defining the area vector as

$$\mathbf{A_q} = \int_{\partial V} \mathbf{N} ds \tag{4}$$

then for a discrete setting Equation (4) is equivalent to:

$$\overline{\mathbf{F}} = \frac{1}{V}\sum_{q=1}^{Q} \mathbf{x}_q \otimes \mathbf{A_q} \tag{5}$$

which may be described as the volume average of the tensor products of the area vectors in the reference configuration and the particle position vectors in the current configuration.

2.4. Love-Weber Average of the Cauchy Stress Tensor

The volume average of the Cauchy stress tensor may be defined as:

$$\overline{\boldsymbol{\sigma}}_{ij} = \frac{1}{V}\int_V \boldsymbol{\sigma}_{\mathbf{ik}} \frac{\partial \mathbf{x}_\mathbf{k}}{\partial \mathbf{x}_\mathbf{j}} dv \tag{6}$$

Using the chain rule and applying the divergence theorem, Equation (6) becomes

$$\overline{\boldsymbol{\sigma}}_{ij} = \frac{1}{V}\int_{\partial V} \boldsymbol{\sigma}_{ik} \mathbf{x}_j \mathbf{N}_k dS - \frac{1}{V}\int_V \frac{\partial \boldsymbol{\sigma}_{ik}}{\partial \mathbf{x}_k} \mathbf{x}_j dv \tag{7}$$

Incorporating the balance of momentum equation into the second term of Equation (7), gives:

$$\overline{\boldsymbol{\sigma}}_{ij} = \frac{1}{V}\int_{\partial V} \boldsymbol{\sigma}_{ik} \mathbf{x}_j \mathbf{N}_k dS - \frac{1}{V}\int_V \left(\rho \dot{\mathbf{v}}_i - \boldsymbol{\gamma}_i\right) \mathbf{x}_j dv \tag{8}$$

If $\mathbf{f}_i^{ext}$ is the exterior force for all points on the boundary, then:

$$\overline{\boldsymbol{\sigma}}_{ij} = \frac{1}{V}\int_{\partial V} \mathbf{f}_i^{ext} \mathbf{x}_j dS - \frac{1}{V}\int_V \left(\rho \dot{\mathbf{v}}_i - \boldsymbol{\gamma}_i\right) \mathbf{x}_j dv \tag{9}$$

From Equation (9), it is obvious that the average Cauchy stress tensor is composed of two parts. The first integral on the right side of Equation (9) represents the static component of the stress, involving the forces applied at the boundary. The second integral is an inertial term, representing the acceleration of each material point. For static and quasi-static analyses, the second term may be ignored.

For the case of a particle aggregate with P interior particles and Q boundary particles, Equation (9) may be written as:

$$\overline{\boldsymbol{\sigma}}_{ij} = \frac{1}{V}\sum_{q=1}^{Q} \mathbf{f}_i^{ext,q} \mathbf{x}_j^q - \frac{1}{V}\sum_{q=1}^{P+Q} \int_{V_q} \left(\rho \dot{\mathbf{v}}_i - \boldsymbol{\gamma}_i\right) \mathbf{x}_j dV \tag{10}$$

For a particle aggregate in equilibrium when subjected to external forces the second term vanishes, giving the classical Love-Weber formula of the average Cauchy stress tensor [3, 4]:

$$\overline{\boldsymbol{\sigma}}_{ij}^{LW} = \frac{1}{V}\sum_{q=1}^{Q} \mathbf{f}_i^{ext,q} \mathbf{x}_j^q \tag{11}$$

2.5. Simulating Eglin Sand

In this work, a well-graded fine sand known in various settings as either Eglin sand, or Quikrete sand 1961, is used to illustrate the approach and utility of the methodology developed. Eglin sand is chosen for one important reason, it is a sand that has been tested micro-experimentally and had its micro-mechanical characteristics described statistically [5-10]. This, along with triaxial test data [11], makes it possible to evaluate the quality of both the mesoscale as well as the macroscale model. This is perhaps not essential to the current effort, which is mostly geometric and analytical in nature, however it is crucial to the evaluation of the overall framework the current effort is part of.

The Particle Size Distribution (PSD) of Eglin sand is used to build a DEM packing of $1\text{x}10^8$ particles, hereafter referred to as the "source" model. The source model is then sampled thousands of times to build mesoscale DEMs of a set size. All simulations in the current work were carried out on DEMs of 1000 particles each, sampled from the source particle model.The ensemble used here consists of 22000 DEMs. Each realization is confined to three different mean stress targets of 5MPa, 20MPa, and 50MPa.

Each of these models is then loaded along three different paths using both the uniform displacement as well as the uniform traction boundary conditions. The loading paths used are:

1) Isotropic Compression – the forces/velocities on the boundary particles are increased until a volumetric strain of about 0.5% is achieved. The slope of the mean stress vs. volumetric strain curve is equal to the bulk modulus.
2) Uniaxial Stress – the forces/velocities on the boundaries are adjusted to achieve an axial strain of about 0.8%, with a constant lateral stress. The slope of the principal stress difference vs. axial strain is equal to the Young's modulus.
3) Deviatoric Stress – the forces/velocities on the boundaries are adjusted to achieve a principal stress difference increase while maintaining a constant mean stress with a target deviatoric strain of about 0.6%. The slope of the deviatoric stress vs. deviatoric strain curve is equal to twice the shear modulus.

The stresses and strains are computed from the Love-Weber averages of the Cauchy stress and the averaged deformation gradient as indicated in the preceding sections. Each of the three moduli: the bulk modulus, the Young's modulus, and the shear modulus, were evaluated for each realization in the ensemble at confinements of 5MPa, 20 MPa, 50 MPa, 100MPa, 200MPa, and 400 MPa.

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