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Connecting discrete particle mechanics to continuum granular micromechanics: Anisotropic continuum properties under compaction

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ABSTRACT

A systematic and mechanistic connection between granular materials' macroscopic and grain level behaviors is developed for monodisperse systems of spherical elastic particles under die compaction. The Granular Micromechanics Approach (GMA) with static assumption is used to derive the stiffness tensor of transversely isotropic materials, from the average behavior of particle-particle interactions in all different directions at the microscale. Two particle-scale directional density distribution functions, namely the directional distribution of a combined mechano-geometrical property and the directional distribution of a purely geometrical property, are proposed and parametrized by five independent parameters. Five independent components of the symmetrized tangent stiffness tensor are also determined from discrete particle mechanics (PMA) calculations of nine perturbations around points of the loading path. Finally, optimal values for these five GMA parameters were obtained by minimizing the error between PMA calculations and GMA closed-form predictions of stiffness tensor during the compaction process. The results show that GMA with static assumption is effective at capturing the anisotropic evolution of microstructure during loading, even without describing contacts independently but rather accounting for them in an average sense.

1. Introduction

The macroscopic, or global, mechanical behavior of materials is a direct function of their microstructure and associated micromechanical characteristics [1]. This is most clear when dealing with granular materials where the microstructure is composed of grains and, therefore, their arrangement clearly affects the macroscopic behavior. Modeling the behavior of these materials using macroscopic tensorial continuum mechanics results in an obvious neglect of the effects of the granular microstructure and its evolution, as well as of micro-mechanical phenomena taking place at grain scale, on the macroscopic mechanical response.

In order to incorporate microstructural properties of the material into its global behavior, many different schemes working in different spatial scales are available. In the broadest sense, all models can be categorized into two distinct groups, namely (i) *discrete models* where, according to the length scale being resolved, grains/particles/molecules/atoms are regarded as material's building blocks (e.g., atomic models [2,3], molecular-dynamics [4,5], bead-spring models [6], dynamic discrete element methods [7,8] and quasi-static particle mechanics approaches [9–13]); (ii) *continuum models* where the material point is assumed to be a homogeneous continuum body whose behavior is interpreted in terms of tensorial quantities such as stress, strain, and stiffness [14–16].

Discrete models in principle can be used to derive highly accurate results with high fidelity. Moreover, discrete analysis has been shown to be an effective approach for modeling material systems with a discrete nature [17], even with imperfections [18], and even result in reduced computational demand. These models, however, rely upon correctly attainable details of material microstructure and of micro-mechanical phenomena. Continuum models, on the other hand, derive material response without exact consideration of microstructure and therefore, lack a connection between macroscopic observable behavior and its microscopic roots.

The Granular Micromechanics Approach (GMA) provides a robust framework for connecting these two groups of models and bridges the gap between them. This is achieved by deriving such continuum macroscopic response from the study of average behavior of particle-particle interactions in all different directions at the microscale [19–22]. In doing so, GMA delivers the most cru-

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cial advantages of discrete models, i.e., it incorporates material's micromechanical features, microstructural effects, and load-path dependent anisotropic evolution of microstructure, while avoiding the comparatively large computational cost associated with identifying and following each and every particle as well as their contacts. It is worth noting that grain-pair interactions in GMA do not represent the behavior of two isolated grains, but rather, that of a grain-pair embedded in the granular microstructure. The global anisotropic continuum behavior of the granular material is then derived from the effective and directional behavior of grain-pair interactions. Therefore, the most critical element in deriving a predictive GMA model of any given material is formulating force-displacement relationships for grain-pair interactions.

In this communication, we address the issue of formulating particle-particle interactions, and their anisotropic evolution, during die compaction of a monodisperse system of spherical elastic particles. We focus on developing a systematic and mechanistic approach for identifying these relationships from discrete particle mechanics simulations of the granular system. The proposed methodology, therefore, effectively connects discrete particle mechanics to continuum granular micromechanics. Next, we briefly describe the GMA with static assumption adopted in this work.

2. GMA with static assumption

The GMA can take two general approaches, namely the method with a kinematic constraint and that with a static constraint. The approach with a kinematic constraint is based on the assumption that inter-particle displacements $\delta_i \in \mathcal{V}$ can be derived as the projection of macroscopic strain tensor $\epsilon_{ij} \in \mathcal{V}^2$ on the particle-particle relative position $l_i \in \mathcal{V}$, i.e., $\delta_i = \epsilon_{ij} l_j$. On the other hand, the approach with static constraint assumes a relationship between macroscopic stress tensor $\sigma_{ij} \in \mathcal{V}^2$ and inter-particle force vectors $f_i \in \mathcal{V}$. Here $\mathcal{V}$ is a three-dimensional real vector space.

The GMA with static assumption enforces the kinematic constraint in a weak sense, that is

$$\epsilon_{pq} = \arg \min_{\epsilon_{pq} \in \mathcal{V}^2} \sum_{\alpha=1}^{N_c} \left\| \delta_i^\alpha - \epsilon_{ij} l_j^\alpha \right\| \tag{1}$$

where N_c denotes the total number of contacts α in the representative volume element. Therefore, GMA with static constraint minimizes the sum, over all contacts, of the residual differences between the inter-particle displacement and the projection of macroscopic strain tensor on the vector joining centroids of the particles forming pair-contacts. Furthermore, the Principle of Virtual Work stating the equality of macroscopic strain energy density and the volume average of inter-particle energies of all contacts is enforced

$$W = \sigma_{ij}\epsilon_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N_c} f_i^\alpha \delta_i^\alpha \tag{2}$$

where V is the volume of the representative volume element. Substituting (1) into (2) yields the following relationship between macroscopic stress tensor and microscopic inter-particle forces

$$f_i = \sigma_{ij} N_{jq}^{-1} l_q; \qquad \text{with} \qquad N_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N_c} l_i^\alpha l_j^\alpha \tag{3}$$

where $N_{ij} \in \mathcal{V}^2$ is the second rank fabric tensor. The above relationship is commonly known as the static constraint, hence the name of the method. With some algebraic manipulation, the following expressions for macroscopic compliance, $S_{ijkl} \in \mathcal{V}^4$, and strain, $\epsilon_{ij} \in \mathcal{V}^2$, tensors are obtained

$$S_{ijkl} = \frac{\partial \epsilon_{ij}}{\partial \sigma_{kl}} = N_{jp}^{-1} N_{lq}^{-1} \frac{1}{V} \sum_{\alpha=1}^{N_c} s_{ik}^\alpha l_p^\alpha l_q^\alpha \tag{4a}$$

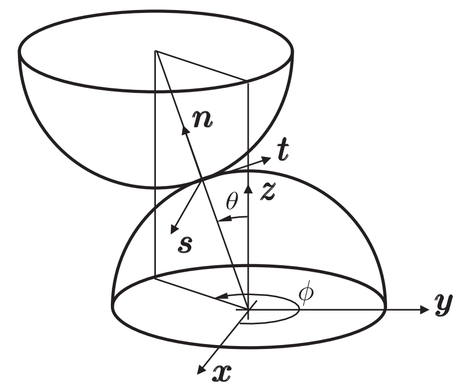

Fig. 1. Two grains in contact and the local coordinate system along with the global Cartesian and spherical coordinate systems.

$$d\epsilon_{ij} = S_{ijkl} d\sigma_{kl} \tag{4b}$$

where $s_{ij}^\alpha \in \mathcal{V}^2$ is the local compliance tensor connecting inter-particle force and displacement of contact α, that is $\delta_i^\alpha = s_{ij}^\alpha f_j^\alpha$. For a more detailed description of the above formulation see [23].

For convenience, the inter-particle force-displacement relationship $f_i^\alpha(\delta_j^\alpha)$ can be formulated in a local coordinate system defined by the following three mutually orthogonal axes: one normal axis n_i^α in the direction of the vector joining the centroids of the particles, and two tangential axes s_i^α and t_i^α (see Fig. 1). Therefore, the microscopic constitutive relationship can be expressed on the local coordinate systems as follows

$$\begin{Bmatrix} \delta_n^\alpha \\ \delta_s^\alpha \\ \delta_t^\alpha \end{Bmatrix} = \begin{bmatrix} s_n^\alpha & 0 & 0 \\ 0 & s_s^\alpha & 0 \\ 0 & 0 & s_t^\alpha \end{bmatrix} \begin{Bmatrix} f_n^\alpha \\ f_s^\alpha \\ f_t^\alpha \end{Bmatrix} \tag{5}$$

where the local compliance tensor is assumed to be symmetric by neglecting cross-coupling terms and thus $s_n^\alpha = 1/k_n^\alpha$, $s_s^\alpha = 1/k_s^\alpha$, and $s_t^\alpha = 1/k_t^\alpha$ are the reciprocals of the local stiffness coefficients.

2.1. Integral form of the formulation

It bears emphasis that the relationships given in Eqs. (1)–(4) are in summation form over all pair-interactions within the granular system that constitutes the representative volume element of interest. However, both the inter-particle force-displacement relationships and geometrical properties, such as the relative distance between interacting particles, depend strongly on direction with respect to a reference frame. It is then convenient to derive an integral form of the constitutive relationship by defining two particle-scale directional density distribution functions, namely the directional distribution of a combined mechano-geometrical property and the directional distribution of a purely geometrical property [24]. In this formulation, for convenience, a global spherical coordinate system is utilized wherein θ, ϕ, and ρ denote the polar zenith angle, the azimuth angle, and the radial coordinate, respectively (see Fig. 1). Specifically, for defining the fabric tensor N_{ij} in integral form, a directional distribution $\xi'(\theta, \phi)$ of the particle-particle relative distance squared, i.e., of $||\boldsymbol{l}||^2$, is proposed