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Microstructure evolution of compressible granular systems under large deformations

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ABSTRACT

We report three-dimensional particle mechanics static calculations that predict the microstructure evolution during die-compaction of elastic spherical particles up to relative densities close to one. We employ a nonlocal contact formulation that remains predictive at high levels of confinement by removing the classical assumption that contacts between particles are formulated locally as independent pair-interactions. The approach demonstrates that the coordination number depends on the level of compressibility, i.e., on Poisson's ratio, of the particles. Results also reveal that distributions of contact forces between particles and between particles and walls, although similar at jamming onset, are very different at full compaction. Particle–wall forces are in remarkable agreement with experimental measurements reported in the literature, providing a unifying framework for bridging experimental boundary observations with bulk behavior.

1. Introduction

The microstructure of confined granular media is typically inhomogeneous, anisotropic and disordered. Under external loading, these systems exhibit a non-equilibrium jamming transition from a liquid-like to a solid-like state (Liu and Nagel, 1998; Jin and Makse, 2010; Trappe et al., 2001; O'Hern et al., 2003; Song et al., 2008). Under increasing confinement, these amorphous solids support stress by spatial rearrangement and deformation of particles and by the development of inhomogeneous force networks (Majmudar and Behringer, 2005; Durian, 1995; Makse et al., 2000; Blair et al., 2001; Liu et al., 1995; Radjai et al., 1996; Chan and Ngan, 2005). Understanding and predicting the formation and evolution of such microstructure under finite macroscopic deformations and at high levels of confinement remains a fundamental goal of granular mechanics (Edwards and Oakeshott, 1989; Cates et al., 1998; Richard et al., 2005; Blumenfeld and Edwards, 2009; Ciamarra et al., 2012; Ostojic et al., 2006).

In this paper, we report three-dimensional particle mechanics static calculations that enable us to predict microstructure evolution during die-compaction of elastic spherical particles up to relative densities close to one. We employ a nonlocal contact formulation (Gonzalez and Cuitiño, 2012) that remains predictive at high levels of confinement by removing the classical assumption that contacts between particles are formulated locally as independent pair-interactions. We specifically study a noncohesive frictionless granular system composed of 40,000 weightless elastic spherical particles with radius

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$R=0.125$ mm, Young's modulus $E=7.0$ GPa, and Poisson's ratio ν. The granular bed, which is numerically generated by means of a ballistic deposition technique (Jullien and Meakin, 1989), is constrained by a rigid cylindrical container of diameter 10 mm. The systems are deformed under die-compaction up to a relative density ρ of 1. Assuming a sufficiently small compaction speed, we consider rate-independent material behavior and we neglect traveling waves, or any other dynamic effect (Richard et al., 2005). The deformation process is therefore described by a sequence of static equilibrium configurations. In this work we employ 125 quasi-static load steps and we consider two materials that only differ in their level of compressibility, namely $\nu=0.35$ and $\nu=0.45$.

The paper is organized as follows. The particle mechanics approach used to generate a sequence of static equilibrium configurations of granular systems at high levels of confinement is presented in Section 2. The evolution of microstructural statistical features of these equilibrium configurations is investigated in Section 3. Specifically, we study the evolution of the mechanical coordination number (number of non-zero contact forces between a particle and its neighbors) in Section 3.1, punch and die-wall pressures in Section 3.2, the network of contact forces in Section 3.3, and the network of contact radiuses in Section 3.4. Finally, a summary and concluding remarks are collected in Section 4.

2. Particle mechanics approach to granular systems at high levels of confinement

Due to the high level of confinement experienced by the particles in the system, we adopt a nonlocal contact formulation (Gonzalez and Cuitiño, 2012) that accounts for the interplay of deformations due to multiple contact forces acting on each single particle. This nonlocal formulation removes the classical assumption that contacts between particles are formulated locally as independent pair-interactions. Its predictions are in remarkable agreement with detailed finite-element simulations of a neo-Hookean solid extended to the compressible range and with experimental observations of a rubber sphere that exhibits no permanent deformations. This good agreement at moderate to large levels of confinement, however, is not obtained with Hertz theory (see Fig. 1 and Gonzalez and Cuitiño, 2012 for further details). It bears emphasis that the nonlocal contact formulation is not an extension of Hertz theory to finite deformations but rather a systematic approach for accounting the interaction between contact interfaces. In a manner analogous to interacting cracks or dislocations in elastic media, the nonlinear behavior is confined to small regions and the interaction between these regions is through an elastic field of deformations.

An equilibrium configuration is defined by the solution of two sets of coupled nonlinear equations. The first set of equations corresponds to static equilibrium of the granular system, that is sum of all elastic contact forces acting on each particle equals zero. The second set of equations accounts for the contribution to each contact interface of the nonlocal mesoscopic deformations induced by all other contact forces acting on the particles, that is for the nonlocal terms γ^{NL} (Gonzalez and Cuitiño, 2012). Thus, the nonlinear system of equations is given by

$$\sum_{j\in\mathcal{N}_i} n_{ij}^{\mathrm{H}}(R_i+R_j-\|\mathbf{x}_i-\mathbf{x}_j\|+\gamma_{ij}^{\mathrm{NL}})_+^{3/2}\frac{\mathbf{x}_i-\mathbf{x}_j}{\|\mathbf{x}_i-\mathbf{x}_j\|}=\mathbf{0}$$

$$\gamma_{ij}^{\mathrm{NL}}-\sum_{k\in\mathcal{N}_i,k\neq j}\frac{n_{ik}^{\mathrm{H}}(R_i+R_k-\|\mathbf{x}_i-\mathbf{x}_k\|+\gamma_{ik}^{\mathrm{NL}})_+^{3/2}}{n_{jik}^{\mathrm{NL}}(\mathbf{x}_j,\mathbf{x}_i,\mathbf{x}_k)}-\sum_{k\in\mathcal{N}_j,k\neq i}\frac{n_{jk}^{\mathrm{H}}(R_j+R_k-\|\mathbf{x}_j-\mathbf{x}_k\|+\gamma_{jk}^{\mathrm{NL}})_+^{3/2}}{n_{ijk}^{\mathrm{NL}}(\mathbf{x}_i,\mathbf{x}_j,\mathbf{x}_k)}=0 \tag{1}$$

where $\mathbf{x}_i$ and $\mathcal{N}_i$ are the position and all the neighbors of particle i, respectively, $\gamma_{ij}^{\mathrm{NL}}=\gamma_{ji}^{\mathrm{NL}}$ by definition, and $(\cdot)_+=\max\{\cdot,0\}$.

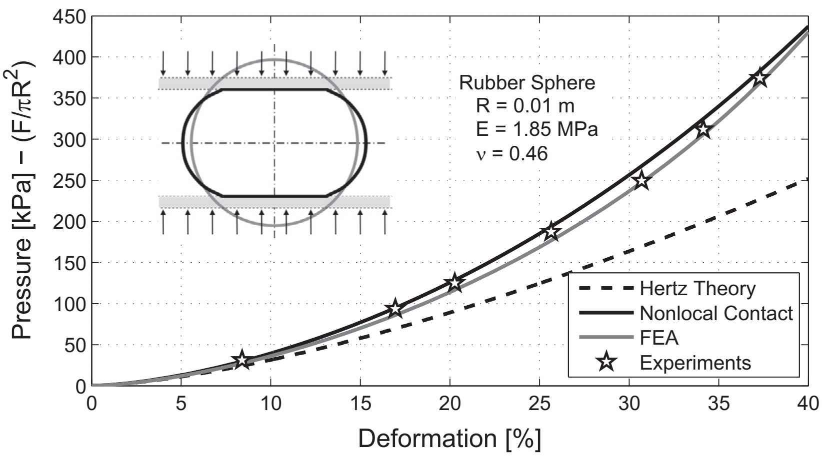

Fig. 1. Validation of the nonlocal contact formulation with experimental measurements obtained for a rubber sphere compressed between two rigid plates (Tatara, 1989) and with detailed finite-element simulations (Gonzalez and Cuitiño, 2012).