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Contact radius and curvature corrections to the nonlocal contact formulation accounting for multi-particle interactions in elastic confined granular systems

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ABSTRACT

We present contact radius and curvature corrections to the nonlocal contact formulation that account for multi-particle interactions in elastic confined granular systems. The nonlocal contact formulation removes the classical assumption of independent contacts by taking into account the interplay of deformations due to multiple contact forces acting on a single particle. The contact radius correction considers the components of these deformations that contribute to the inter-particle contact area. The curvature correction improves the description of contacting surface profiles by including higher order terms in their Taylor series expansions. To validate the corrected formulation, we restrict attention to rubber spheres under different loading conditions, in the absence of gravitational forces, adhesion or friction. Specifically, we show that the predictions of contact force and radius are in remarkable agreement with finite-element simulations and experimental observations up to levels of deformation at which contact impingement occurs, which was not possible with the original elastic nonlocal contact formulation. Convergence of the curvature corrected formulation is observed at a four-term correction.

1. Introduction

The extensive applications of powder compaction, especially in manufacturing processes of critical industries like pharmaceutics, ceramic, energy, food, and metallurgy, make it a subject of intense research in the scientific community. Development of predictive and computationally efficient models that could accurately describe the behavior of granular media during compaction would directly impact optimality in manufacturing, waste reduction, and price and quality of the end product.

Macroscopic behavior of confined granular systems has been conventionally described by *continuum-based models*, which consider granular media as a continuous system and hence have a minimal emphasis on the behavior at particle scale. Many of these models were originally developed for analyzing the behavior of geological materials, such as Drucker and Prager (1952), Cam-Clay plasticity and Cap plasticity models. More recently, the Drucker-Prager Cap (DPC) plasticity model (DiMaggio & Sandler, 1971), where a cap yield surface is added to the Drucker and Prager model to allow for material

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hardening and dilatancy control during inelastic deformation, has been used for analysis of metal, ceramic and pharmaceutical powder compaction. Although requiring an elaborate mechanical testing procedure for calibration of model parameters (Cunningham, Sinka, & Zavaliangos, 2004), the DPC model is widely used due to its adaptability to finite element method (Sinka, Cunningham, & Zavaliangos, 2004). However, the accuracy of model response, especially during the decompression (unloading) phase, relies heavily on the design of calibration experiments (Sinha, Curtis, Hancock, & Wassgren, 2010) and proper elastic constitutive modeling (Han et al., 2008). In order to incorporate microstructural properties of the granular system into its global behavior, *discrete models* have been proposed, where contact behavior of individual particles is taken into account. Numerical methods in this category, such as dynamic discrete element methods (Cundall & Strack, 1979; Zhu, Zhou, Yang, & Yu, 2008) and quasi-static particle mechanics approaches (Gonzalez & Cuitiño, 2016; Gonzalez, Poorsolhjouy, Thomas, Liu, & Balakrishnan, 2018; Yohannes et al., 2016), are used in combination with a suitable contact formulation to predict the macroscopic behavior of compacted granular systems and, thus, predictability is heavily dependent on the contact law involved. The Hertz (1882) contact law for linear-elastic materials and similarity solution by Storåkers, Biwa, and Larsson (1997) for viscous-plastic power law hardening materials are fairly predictable at small deformations and low relative densities of powder compacts. However, due to the occurrence of contact interactions at higher deformations, as pointed out by Mesarovic and Fleck (2000) in their study of elasto-plastic spheres, their predictions become increasingly deviant due to the assumption of independent contacts. This was partially overcome by introducing a local relative density parameter in contact laws curve-fitted to finite element simulations of small three-dimensional packings (Harthong, Jérier, Dorémus, Imbault, & Donzé, 2009). Finally, a systematic and mechanistic connection between macroscopic and particle level behaviors, using continuum and discrete models respectively, was recently proposed (Poorsolhjouy & Gonzalez, 2018) to capture the anisotropic evolution of die-compacted systems.

Several efforts towards experimental characterization of confined granular systems have also been made to understand the deformation behavior at granular scale and to provide an efficient validation tool for the analytical contact formulations. Of particular interest is the mechanical response of single particles under confined conditions, most commonly studied using uniaxial compression experiments (Liu, Williams, & Briscoe, 1998; Lu, Tung, Hung, Shiau, & Hwang, 2001; Shima, Tatara, Iio, Shu, & Lucero, 1993; Tatara, Shima, & Lucero, 1991; Topuz & Okay, 2009; Zhang, Kristiansen, & Liu, 2007). Recently, an apparatus has been developed for triaxial testing of single particles (Jonsson, Gråsjö, Nordström, Johansson, & Frenning, 2015), providing a more realistic insight into the behavior of individual particles during powder compaction.

For elastic confined granular systems, relaxing the underlying assumptions of the Hertz contact theory that limit its applicability to small deformations could be the key to achieving predictability at moderate to large deformations. Significant efforts in this direction were made by Zhupanska (2011), who relaxed the small-strain Hertz assumption of considering contacting surfaces as elastic half spaces by proposing an analytical solution to the boundary value problem of an elastic sphere subject to contact stresses on a finite region of its surface and supported at its center. The results showed that the Hertz pressure distribution remained accurate for relatively large contact areas. Recently, Argatov, Kachanov, and Mishuris (2017) have explored the concept of far points in Hertz contact problems, emphasizing the limitations of the ”local character” of Hertz predictions. Another major contribution in this regard is the nonlocal contact formulation for confined granular systems by Gonzalez and Cuitiño (2012), which provides an accurate and mechanistic description of the force-deformation behavior at contacts of a linear-elastic spherical particle subject to multiple contact forces, a typical configuration in particulate systems compressed to high relative densities. It follows the work of Tatara (1989) and relaxes the classical contact mechanics assumption of independent contacts by invoking the principle of superposition to express the deformation at a particular contact as a sum of local (i.e., Hertzian) deformation and nonlocal deformations generated by other contact forces acting on the same particle. The nonlocal contact formulation has recently been employed successfully to study the die-compaction of large frictionless noncohesive granular systems comprising weightless elastic spherical particles (Gonzalez & Cuitiño, 2016).

A complete description of the inter-particle contact behavior in confined granular systems includes determination of both contact force and area with respect to particle deformation. While critical macroscopic quantities like compaction pressure and the reaction from die walls are directly related to inter-particle contact forces, the prediction of contact area is needed to estimate strength formation in the compacted solid (Gonzalez, 2018). In addition, the evolution of contact area is associated with contact impingement, i.e., with the merger of neighboring contacts. Since the assumption of circular contacts no longer remains valid after contact impingement, the predictions of a contact formulation may not be representative of real contact behavior beyond the occurrence of this phenomenon, making an accurate determination of contact areas ever so important.

In the context of the nonlocal contact formulation (Gonzalez & Cuitiño, 2012), nonlocal mesoscopic deformations are derived from the Boussinesq solution (Johnson, 1987; Timoshenko & Goodier, 1970) of an elastic half-space under a concentrated force. The components of these deformations normal to the contact surface constitute the nonlocal contribution to the contact displacement, for which a closed-form solution has been obtained (Gonzalez & Cuitiño, 2012). However, the derivation of an analytical solution for nonlocal components radial to the contact center, that contribute to the evolution of contact radius, remains an open problem. Therefore, part of the work presented in this paper is concerned with the development of an analytical framework for predicting nonlocal effects in the evolution of inter-particle contact area. The analysis presented is in the spirit of Tatara's (1991) work on expanded contact radius during uniaxial compression of rubber spheres.

An important aspect of this nonlocal contact formulation is that it is a direct extension of the classical Hertz contact theory. When nonlocal effects are neglected, the formulation reduces to Hertz theory. Therefore, any correction introduced in the Hertz solution should, in turn, improve the accuracy of the formulation. The second analysis presented in this paper