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Micromechanical study of elastic moduli of three-dimensional granular assemblies

N.P. Kruyt *

Department of Mechanical Engineering, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

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ABSTRACT

In micromechanics of granular materials, relationships are investigated between micro-scale characteristics of particles and contacts and macro-scale continuum characteristics. For three-dimensional isotropic assemblies the macro-scale elastic characteristics are described by the bulk and the shear modulus, which depend on the micro-scale characteristics of the coordination number (i.e. the average number of contacts per particle) and the interparticle contact stiffnesses in directions normal and tangential to the contact.

It is well-known that the uniform-strain theory (or mean-field theory) overpredicts the elastic moduli. To find improved predictions, approximations of the particle displacement and rotations fields are obtained here by solving the equilibrium equations for small subassemblies that are centred around particles. At the boundary of these subassemblies, the particle displacements and rotations are prescribed such that they conform to the mean field.

Employing this approach, improved predictions of bulk and shear moduli are obtained, in comparison with those according to the uniform-strain assumption, especially when the size is increased of the subassemblies for which equilibrium equations are solved.

The elastic moduli are evaluated from the particle displacement and rotations fields by two methods. In the first, stress-based method the micromechanical expression for the average stress tensor, in terms of the forces at contacts and the branch vectors that connect particles in contacts, is employed. In the second, energy-based method the minimum potential-energy principle is used to obtain rigorous upper bounds to the moduli. It is generally observed that the moduli obtained from the stress-based method give closer agreement with the results from Discrete Element Method simulations than those from the energy-based method.

These improvements in the predictions of the elastic moduli are observed over the range of coordination numbers and interparticle stiffnesses considered here.

1. Introduction

Knowledge of the mechanical behaviour of granular materials is important in many industrial, geotechnical and geophysical applications dealing with granular materials. This knowledge is expressed as a constitutive relation, which can be formulated heuristically or from the micromechanical viewpoint. In the micromechanical approach a granular material is modelled as an assembly of particles that interact at contacts. This approach therefore incorporates the discrete nature of granular materials. An objective of micromechanics is to investigate relationships between micro-scale characteristics and macro-scale, continuum characteristics.

The objective of this study is to study, from the micromechanical viewpoint, the elastic properties of three-dimensional, isotropic granular assemblies. At the continuum, macro-scale these elastic properties are described by the elastic moduli that link (increments of) stress to (increments of) strain. At the micro-scale of contacts the interaction between particles is modelled by springs in directions normal and tangential to the contact. Some applications of the current model are the initial elastic deformation of granular materials and certain fibrous media. Elastic (and hence reversible) deformation of cohesionless granular materials is found for very small strains, typically for strains of 10^{-3}% for stress levels encountered in engineering applications (Tatsuoka, 1999) or in dynamic problems.

In contact mechanics (see for example Johnson, 1985) the interparticle interaction at the contact is often described by nonlinear

* Tel.: +31 53 489 2528; fax: +31 53 489 3695.
E-mail address: n.p.kruyt@utwente.nl

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Hertz–Mindlin theory. The continuum elastic moduli are then dependent on the confining pressure, as studied theoretically (Digby, 1981; Walton, 1987; Goddard, 1990) and by Discrete Element Method (*DEM* for short) simulations (Makse et al., 2004; Agnolin and Roux, 2007a,b). In order to facilitate theoretical developments, here the interparticle stiffnesses are taken constant at all contacts. The values of the spring stiffnesses then depend on the confining pressure (as well as on the particle properties).

The elastic moduli of various regular packings of granular assemblies have been studied (Deresiewicz, 1958; Chang and Misra, 1989; Wang and Mora, 2009; Kruyt, 2012). Fleischmann et al. (2013a,b) used results for regular packings to obtain predictions of the Poisson ratio of fairly dense, disordered assemblies.

The uniform-strain assumption (or mean field assumption) has been frequently adopted in micromechanical studies of the elastic moduli of disordered systems (Rothenburg, 1980; Digby, 1981; Walton, 1987; Bathurst and Rothenburg, 1988a,b; Chang et al., 1990; Chang and Liao, 1994; Cambou et al., 1995). According to this assumption the relative displacement of two particles in contact is determined by the average displacement-gradient and the relative position vector of the particle centres. Corresponding predictions for the moduli are accurate for very dense assemblies, while for loose assemblies the moduli are significantly overpredicted (see for example Kruyt and Rothenburg, 1998, 2002, 2004; Makse et al., 1999; Rothenburg and Kruyt, 2001; Agnolin and Roux, 2007b; Magnanimo et al., 2008; Kruyt et al., 2010).

This limited adequacy of the uniform-strain assumption is due to the presence of *fluctuations* (relative to the deformation according to the uniform-strain assumption) that are induced by the geometrical disorder that is present in the assembly. DEM simulations have been used to study these fluctuations in two-dimensional assemblies (Kruyt and Rothenburg, 1998, 2002, 2004; Agnolin and Kruyt, 2008) and three-dimensional assemblies (Agnolin and Roux, 2008).

To find improved estimates of the elastic moduli for disordered systems, these fluctuations have been taken into account in theoretical studies that are completely analytical (Jenkins et al., 2005; Agnolin et al., 2006; La Ragione and Jenkins, 2007) or semi-numerical (Kruyt and Rothenburg, 2002, 2004; Agnolin and Kruyt, 2008; Agnolin and Roux, 2008; Kruyt et al., 2010). These theoretical approaches are based on considerations of the solutions of the equilibrium equations for small subassemblies. In the analytical, contact-based studies (Jenkins et al., 2005; Agnolin et al., 2006; La Ragione and Jenkins, 2007) the subassembly consists of a pair of particles in *contact* together with their neighbours. In the semi-numerical, particle-based studies (Kruyt and Rothenburg, 2002, 2004; Agnolin and Kruyt, 2008; Agnolin and Roux, 2008), the subassembly consists of a *particle* with its neighbours. In the analytical studies additional assumptions are employed to obtain approximate solutions to the equilibrium equations, while in the semi-numerical studies the equilibrium equations of the small subassemblies are solved numerically. These approaches are compared by Agnolin and Kruyt (2008) for the two-dimensional case and by Agnolin and Roux (2008) for the three-dimensional case. Generally, it is observed that the semi-numerical methods give more accurate predictions of the elastic moduli than the analytical methods.

Kruyt et al. (2010) extended the particle-based method to larger subassemblies for the two-dimensional case and found that this made it possible to obtain accurate predictions of the elastic moduli, even for loose assemblies with low coordination number (i.e. the average number of contacts per particle). The objective of this study is to extend this method to the three-dimensional case and to investigate its suitability for predicting the elastic moduli.

The outline of this study is as follows. Firstly, micromechanics of granular materials are summarised in Section 2. The uniform-strain assumption is described in Section 3, together with the corresponding elastic moduli. The proposed approach is detailed in Section 4. The employed isotropic assemblies and the Discrete Element Method simulations are characterised in Section 5. Results for the elastic moduli according to the various theories are presented in Section 6. Finally, findings of this study are discussed in Section 7.

2. Micromechanics

In this Section the basics of micromechanics of granular materials are described. Three-dimensional isotropic assemblies of spheres are considered. Small deformations are considered from an equilibrium configuration. Firstly, the contact geometry, statics and kinematics for the particles are described in Section 2.1. The elastic constitutive relation at the micro-scale, contact level is given in Section 2.2. The minimum potential-energy principle is summarised in Section 2.3. The uniform-strain assumption for predicting effective elastic moduli is described in Section 2.4.

2.1. Contact geometry, statics and kinematics

The interparticle contact areas are small, since the particles are stiff. The interparticle force is therefore considered as acting at the contact point. Contact moments, due to the distribution of traction over the contact region, are not considered here to keep the analysis simpler.

The vector from the centre of particle p to the contact point between particles p and q is denoted by $\boldsymbol{r}^{pq}$. The vector from the centre of particle p to the centre of particle q is denoted by $\boldsymbol{l}^{pq}$. This branch vector is given by

$$\boldsymbol{l}^{pq} = \boldsymbol{r}^{pq} - \boldsymbol{r}^{qp}. \tag{1}$$

For spherical particles where the deformation at contacts is small (i.e. the "overlap" of particles is small), we have

$$\boldsymbol{r}^{pq} = R^p \boldsymbol{n}^{pq} \text{ and } \boldsymbol{r}^{qp} = R^q \boldsymbol{n}^{qp}, \tag{2}$$

where R^p is the radius of particle p and $\boldsymbol{n}^{pq}$ is the (unit) contact normal vector directed from the centre of particle p to that of particle q. Note that $\boldsymbol{n}^{qp} = -\boldsymbol{n}^{pq}$.

The equilibrium equations for force and moment for particle p are given by

$$\sum_q \boldsymbol{f}^{pq} = \boldsymbol{0} \quad \sum_q \boldsymbol{r}^{pq} \times \boldsymbol{f}^{pq} = \boldsymbol{0}, \tag{3}$$

where $\boldsymbol{f}^{pq}$ is (the increment of) the interparticle force, exerted on particle p by particle q that is in contact with particle p, and the summation is over the particles q that are in contact with particle p.

The micromechanical expression for the average stress tensor $\boldsymbol{\sigma}$, in terms of the forces at contacts and the branch vectors, is given by (see for example Kruyt and Rothenburg, 1996)

$$\boldsymbol{\sigma} = \frac{1}{V} \sum_{c \in C} \boldsymbol{f}^c \boldsymbol{l}^c, \tag{4}$$

where the summation is over the contacts c in the set of contacts C and V is the volume (including voids) that is occupied by the assembly.

The particles have translational as well as rotational degrees of freedom. The displacement and rotation vectors of particle p are denoted by $\boldsymbol{u}^p$ and $\boldsymbol{\omega}^p$, respectively. The relative displacement vector $\boldsymbol{\Delta}^{pq}$ at the contact point between the particles p and q consists of contributions from particle displacements and rotations

$$\boldsymbol{\Delta}^{pq} = (\boldsymbol{u}^q + \boldsymbol{\omega}^q \times \boldsymbol{r}^{qp}) - (\boldsymbol{u}^p + \boldsymbol{\omega}^p \times \boldsymbol{r}^{pq}). \tag{5}$$