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On the elastic moduli of two-dimensional assemblies of disks: Relevance and modeling of fluctuations in particle displacements and rotations

I. Agnolin[a], N.P. Kruyt[b,*]

[a] *Groupe Matière Condensée et Matériaux, University of Rennes I, Bat.11A, Campus Beaulieu, 35042 Rennes, France*
[b] *Department of Mechanical Engineering, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands*

Abstract

We determine the elastic moduli of two-dimensional assemblies of disks by computer simulations. The disks interact through elastic contact forces, which oppose the relative displacement at the contact points by means of a normal and a tangential stiffness, both taken constant. Our simulations confirm that the uniform strain assumption results in inaccurate predictions of the elastic moduli, since large fluctuations in particle displacements and rotations occur. We phrase their contribution in terms of the relative displacement they induce at the contact points. We show that the fluctuations that determine the equivalent continuum behavior depend on the average geometry of the assembly. We further separate the contributions from the center displacement and the particle rotation. The fluctuations result in a relaxation of the system, but along the tangential direction the relaxation is generally entirely due to rotations. We consider two theoretical formulations for predicting the elastic moduli that include the fluctuations, namely the "pair-fluctuation" and the "particle-fluctuation" method. They are both based on the equilibrium of a small subassembly, which is considered representative of the average structure. We investigate the corresponding predictions of the elastic moduli over a range of coordination numbers and of ratios between tangential and normal stiffness. We find a significant improvement with respect to the uniform strain theory. Furthermore, the dependence of the fluctuations on coordination number and ratio of tangential to normal stiffness is qualitatively captured.
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1. Introduction

This study investigates the elastic mechanical properties of dense random isotropic two-dimensional assemblies of disks. Our work is framed in the context of micromechanics, which focuses on the relation between macroscopic behavior and microscopic interactions. At the macroscopic scale, stress and strain are measured, whose relation is determined by the elastic moduli of the equivalent continuum. At the microscale, forces arise between contacting particles that for quasi-static deformations must satisfy the balance of force and moment for all grains.

In the context of elasticity, contact forces oppose the relative displacement between contacting grains by means of a contact stiffness. The work of Poritzky [1] about contacting thin disks reveals for its normal component a dependence on the overlap which rapidly weakens with confining pressure. We assume for our assemblies the limit case of constant normal stiffness. Since we focus on small displacements, we also consider the tangential stiffness constant [2,3]. By ignoring all inhomogeneity in the contact stiffness, we specifically focus on the effects of geometric disorder.

Given the geometry of the contact network, the constitutive law for the contact forces determines the macroscopic mechanical properties once the relative displacements at the contact points are known. Many micromechanical studies [4–12] use the so-called 'average strain hypothesis', where the relative displacements reduce to the contribution from the average strain. The resulting prediction of the elastic moduli is inaccurate [13–15], particularly for the shear modulus, as in general grains undergo additional displacements in order to attain equilibrium. More sophisticated predictions have recently been developed that incorporate such fluctuations, in [16] for three-dimensional systems and in [17,18] for two-dimensional ones. They are based on the idea that even though the deformation is not uniform, its fluctuations are strongly correlated. The study by Gaspar and Koenders [20] suggests that they occur with correlation lengths in the order of a few diameters, which implies that subassemblies of such a size already contain the essential features of the global structure.

The validity of the theoretical predictions in [17] and [18] is investigated here by comparison with the elastic moduli computed by means of Discrete Element Method (*DEM*) simulations [21]. The analysis is performed for various ratios of tangential to normal stiffness and coordination numbers. We consider assemblies with both larger and smaller coordination number than the onset of isostaticity for disordered frictionless systems. This onset equals 4 in two dimensions and is recurrent in numerical simulations, as dense assemblies are usually obtained by means of an initial frictionless compression. In experiments [19] on hard disks, coordination numbers smaller and larger than 4 are due, in turn, to the presence of friction and of ordered structures. In DEM simulations, disordered assemblies with larger coordination numbers than the onset of isostaticity can be obtained, for example by neglecting in the constitutive law for the contact force the increase in the normal stiffness with the interpenetration or by applying a large pressure. Also in three dimensions the scientific literature concentrates on samples with larger coordination numbers than the frictionless onset of isostaticity, which equals 6 in that case. However, studies concerned with the issue of numerically reproducing experimental results [22,23,35] emphasize that lower ones might be relevant to practical purposes.

The outline of the study is as follows. Firstly, the basic micromechanical quantities of interest are defined in Section 2. Then, a concise description is given in Section 3 of theoretical approaches for predicting the elastic moduli based, in turn, on the average strain assumption and on the inclusion of displacement fluctuations. The performed DEM simulations are described in Section 4. The corresponding results are analyzed in Section 5 and compared to the results of the theoretical predictions. The final section is dedicated to discussion of the results.

2. Micromechanics

We consider the contact between disks p and q of radius R^p and R^q, respectively. The contact is identified by the unit vector n_i^{pq} that points outwards from p along the line that joins the centers. The unit vector t_i^{pq} is tangent to the contact (see Fig. 1). In components,

$$\mathbf{n}^{pq} = (\cos\theta^{pq}, \sin\theta^{pq}),$$
$$\mathbf{t}^{pq} = (-\sin\theta^{pq}, \cos\theta^{pq}),$$

where θ^{pq} is the *contact orientation*, counted counterclockwise from the horizontal axis. For future reference, we also define the *branch vector* l_i^{pq}, which joins the center of particle p to that of particle q pointing outwards from p, i.e.

$$l_i^{pq} = (R^p + R^q)n_i^{pq}.$$

As in monodisperse two-dimensional assemblies crystallization occurs, a log-normal distribution for the particle radii is adopted.

Contacting particles interact by means of contact forces. We denote by f_i^{pq} the ith component of the force exerted on particle p by particle q. It has normal and tangential component to the contact f_n^{pq} and f_t^{pq}, i.e.

$$f_n^{pq} = f_i^{pq}n_i^{pq},$$
$$f_t^{pq} = f_i^{pq}t_i^{pq}.$$