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Enhanced micropolar model for wave propagation in ordered granular materials

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ABSTRACT

The vibrational properties of a face-centered cubic granular crystal of monodisperse particles are predicted using a discrete model as well as two micropolar models, first the classical Cosserat and second an enhanced Cosserat-type model, that properly takes into account all degrees of freedom at the contacts between the particles. The continuum models are derived from the discrete model via a micro–macro transition of the discrete relative displacements and particle rotations to the respective continuum field variables. Next, only the long wavelength approximations of the models are compared and, considering the discrete model as reference, the Cosserat model shows inconsistent predictions of the bulk wave dispersion relations. This can be explained by an insufficient modeling of sliding mode of particle interactions in the Cosserat model. An enhanced micropolar model is proposed including only one new elastic tensor from the more complete second–order gradient micropolar theory. This enhanced micropolar model then involves the minimum number of elastic constants to consistently predict the dispersion relations in the long wavelength limit.

1. Introduction

The classical theory of elasticity consists of a macroscopic material description. The material is not described at the micro-level by considering the displacement of the different particles in interaction, but is described as a continuum by considering macroscopic quantities as stress and strain. The classical elasticity theory can be viewed as a first gradient of the displacement field approximation of solid state theory (Ashcroft and Mermin, 1976) and is thus valid in the long wavelength limit only. Granular media, due to their micro-inhomogeneous character, are not well described by the standard continuum theory of elasticity. In contrast to classical continua, where the sizes of the vibrating atoms can be assumed to be negligible compared to the macroscale, the sizes of the particles in a granular assembly are comparable to it (Schwartz et al., 1984). In addition, considering the sliding, twisting and rolling resistances at the level of the contacts between the particles, a consistent description of the elasticity of a granular medium needs to take into account all the rotational degrees of freedom of each individual particle and thus all the relative degrees of each pair.

By including the rotational degrees of freedom into the analysis, the evaluation of the different elastic constants in the quasistatic behavior of granular assemblies becomes complex (Jenkins, 1990; Jenkins and Ragione, 2001; 2003; Ragione and Jenkins, 2009; Ragione and Magnanimo, 2012). The elastic behaviors of crystalline structures of monodisperse beads can be efficiently described by a discrete model, where the displacement and rotation of each individual bead are taken into account. One of the major differences with classical elasticity is the existence of optical-type rotational-related modes of wave propagation. Especially, the dispersion relations given by the discrete model of the bulk waves propagating in crystalline structures of contacting monodisperse beads, without solid bridges between them, is consistent with experimental results (Merkel et al., 2010; 2011) in a hexagonal close-packed structure, and with numeric simulation results in a face-centered cubic structure (Mouraille et al., 2006; 2009; Mouraille, 2008). Nevertheless, the discrete model can be solved analytically only for well-known regular crystalline structures, the case of a random assembly of beads can be done (Kruyt, 2010; 2012) but is too complex for large systems. Moreover, due to diffraction scattering and attenuation effects, even for a small level of randomness, only long wavelength waves will propagate in a granular assembly (Mouraille and Luding, 2008; Dazel and Tournat, 2010). More specifically, only the long wavelength waves can propagate as a coherent ballistic wave (Jia et al., 1999; Jia, 2004; Langlois and Jia, 2014). Considering that only the long wavelength waves will propagate in random assemblies, which differs from the ideal crystalline case, and that their discrete modeling is too complex, a continuum formulation seems

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more suitable. A continuum model is also relevant when considering the wave propagation in a granular assembly in contact with an elastic solid (Wallen et al., 2015).

The generalization of the classical elasticity theory accounting for the rotational degrees of freedom of bodies is known as the Cosserat theory (Cosserat and Cosserat, 1909; Eringen, 1999). For instance, a Cosserat model can explain the strain localization in a sheared fault gauge (Pasternak et al., 2003; 2004; 2006). But, from a direct comparison between the dispersion relations predicted with a discrete model and with the ones of a Cosserat model, the latter does not predict correctly the dispersion relations of the modes of propagation related to the rotational motion of the beads (Merkel et al., 2011). Similarly, the simulation results of a Couette shear cell differ from the predictions of a Cosserat model (Mohan et al., 1999; Lätzel et al., 2001; Mohan et al., 2002; Latzël, 2003). Despite many theoretical efforts, the comparison between experimental results and predictions from the Cosserat theory remains inconclusive; a consistent continuum description of granular assemblies is still challenging, see Maugin and Metrikine (2010) and Goddard (2014) and the references therein. As it will be shown below, one of the interactions, or relative degrees of freedom, between the beads involving the rotational degrees of freedom is not modeled properly leading to inconsistent results. A reconstruction of the Cosserat moduli (Pasternak and Dyskin, 2014) can lead to misleading results. The drawback of the Cosserat theory can be overcome using a second-order gradient theory (Mühlhaus and Oka, 1996; Suiker et al., 2001a; 2001b; Suiker and de Borst, 2005), where the homogenization is performed by differential expansions (Pasternak and Mühlhaus, 2002b; Pasternak and Mühlhaus., 2005). Nevertheless, the second-order gradient micropolar theory introduces three new elastic tensors, which involve too many new elastic constants to represent a feasible alternative to the discrete modeling. A homogenization by integral transformation resulting into a non-local Cosserat continuum theory gives the same results as the discrete model, but this approach does not provide any simplification compared to the discrete model, see Pasternak and Mühlhaus (2002a) and Pasternak and Mühlhaus. (2005) and the references therein, and it is not considered here.

In this work, after an identification of the drawbacks of the Cosserat model, we propose a model based on a continuum formulation that correctly describes the wave propagation in granular media in the long wavelength limit. In Section 2 and in order to get a reference for the comparison of the continuum models, the general theoretical evaluation of the bulk wave propagation in a granular assembly using a discrete model, which follows the derivation in Merkel et al. (2010), is presented. The different interactions between the beads due to contact forces and torques are discussed. In Section 3, the dispersion relations of the bulk eigenmodes propagating in a Face-Centered Cubic (FCC) structure along the x-axis are derived using the discrete model. The long wavelength approximations of the dispersion relations, which can be directly compared with the predictions of the continuum models, are then derived. Two cases of contacts between the beads are considered. In the first one, the contacts are considered without solid bridges between the beads and the surface roughness is negligible; this case is called the *frictional case* corresponding to normal and sliding resistant contacts. In the second one, the contacts between the beads are considered with solid bridges and this case is called the *rolling and twisting resistant case*. In Section 4, the dispersion relations of the discrete model are compared to those obtained trough numerical simulations of wave propagation in a FCC structure. In Section 5, the macroscopic continuum models are derived from the microscopic relations of the discrete model following the homogenization techniques proposed in Suiker et al. (2001a; 2001b). In Section 6, the dispersion relations of the bulk eigenmodes in a FCC structure are derived with the Cosserat model. The problems and drawbacks of this model are then discussed. Finally in Section 7, the enhanced micropolar model is presented and it is shown that its approximations for small wavenumber are exactly equal to those of the discrete model in both frictional, rolling and twisting resistant cases.

2. Description of the problem, starting from the discrete theory

An assembly of monodisperse beads is considered, all of them being composed by the same material. The diameter of the beads is a, the mass density of the material constituting the beads is ρ_b, its Poisson's ratio is ν. The mass of one bead with homogeneous density is $m_b = \pi\rho_b a^3/6$, its moment of inertia is $I_b = m_b a^2/10$. The problem is considered in Cartesian coordinates with unit vectors $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$. The position of a bead α is defined by the vector $\mathbf{R}^\alpha$. A local coordinate system (**n, s, t**) at the level of the surface of contact between two beads is defined: The unit vector **n**, normal to the surface of contact between two beads α and β, is defined as Merkel et al. (2010) and Chang and Gao (1995a); 1995b)

$$\mathbf{n} = (\mathbf{R}^\beta - \mathbf{R}^\alpha)/|\mathbf{R}^\beta - \mathbf{R}^\alpha| \\ = \cos\phi\hat{\mathbf{x}} + \sin\phi\cos\theta\hat{\mathbf{y}} + \sin\phi\sin\theta\hat{\mathbf{z}} \simeq (\mathbf{R}^\beta - \mathbf{R}^\alpha)/a, \quad (1)$$

where it is assumed that the static and dynamic overlaps between the particles are negligible compared to their diameter, $\phi = \arccos(\mathbf{n}\cdot\hat{\mathbf{x}})$, $\theta = \arccos(\mathbf{n}\cdot\hat{\mathbf{y}}/\sin\phi)$ if $\phi \neq 0$ and $\theta = \phi$ if $\phi = 0$ or π (Chang and Gao, 1995a). The two unit vectors **s** and **t**, which are in the contact plane, are defined as

$$\mathbf{s} = \partial\mathbf{n}/\partial\phi = -\sin\phi\hat{\mathbf{x}} + \cos\phi\cos\theta\hat{\mathbf{y}} + \cos\phi\sin\theta\hat{\mathbf{z}}, \\ \mathbf{t} = \mathbf{n}\times\mathbf{s} = -\sin\theta\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}. \quad (2)$$

The infinitesimal displacement of bead α is $\mathbf{u}^\alpha$, its infinitesimal angular rotation is $\mathbf{w}^\alpha$. The dispersion relations are deduced below from the equations of motion for translation

$$m_b \frac{\partial^2\mathbf{u}^\alpha}{\partial t^2} = \sum_\beta \mathbf{F}^{\beta\alpha}, \quad (3)$$

and rotation

$$I_b \frac{\partial^2\mathbf{w}^\alpha}{\partial t^2} = \sum_\beta \mathbf{M}^{\beta\alpha} + \frac{1}{2}\sum_\beta \mathbf{D}^{\beta\alpha}\times\mathbf{F}^{\beta\alpha}, \quad (4)$$

where the summation is over all the beads β in contact with the bead α and the branch vector is

$$\mathbf{D}^{\beta\alpha} = \mathbf{R}^\beta - \mathbf{R}^\alpha. \quad (5)$$

The direct use of the branch vector in Eq. (5) in the equation of motion for rotation in Eq. (4) is only valid in the case of monodisperse beads, i.e., $|\mathbf{R}^\beta| = |\mathbf{R}^\alpha|$, see Suiker et al. (2001a), Chang and Gao (1995a), Chang and Gao (1995b) and Luding (2008) for more general formulations. From the linearization of the Hertz-Mindlin contact model between two beads, the contact interactions can be modeled by using a normal and a shear stiffness K_N and K_S, respectively (Duffy and Mindlin, 1956; Johnson, 1985; Thornton and Yin, 1991; Gilles and Coste, 2003). It should be noticed that this excludes all the nonlinear effects from the analysis (Nesterenko, 2001; Tournat and Gusev, 2010). In the case where all the monodisperse beads are composed by the same material, the ratio of shear to normal stiffness is given by $\Delta_K = K_S/K_N = 2(1-\nu)/(2-\nu)$. Since the overlap of the beads in contact is small, also the diameter of the surface of contact d is assumed to be small compared the diameter of the beads, e.g. $d \ll a$. Considering the projections on the x, y, z axis of the force applied by bead β on bead α as Merkel et al. (2010) and Suiker et al. (2001a)

$$F_i^{\beta\alpha} = K_N n_i n_j (u_j^\beta - u_j^\alpha) + K_S(s_i s_j + t_i t_j)$$