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Particle spin in anisotropic granular materials

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Abstract

We adopt the simplest theory for the description of the mechanical behavior of a random array of elastic spheres and show that it is necessary that the average rotation of the spheres about their centers be distinguished from the average rotation of the aggregate. Without such a distinction, the stress in an anisotropic aggregate, subjected to a deformation that involves an average rotation, would not be symmetric. We illustrate this by calculating the incremental stress–strain relation for an orthotropic aggregate. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The static equilibrium of an aggregate of grains subjected to a known distribution of surface and body forces involves the balance of force and moment on each of the grains of the aggregate. If there are N grains, the $6N$ degrees of freedom corresponding to the translations of the centers of mass and the rotations about the centers are determined by the appropriate forms of these balance equations. The forces of interaction between the grains are, typically, nonlinear in the relative displacements and rotations of neighboring grains, inelastic, and path dependent. In addition, during an increment of an overall deformation of the aggregate, particles initially in contact may lose contact and particles initially not in contact may be brought into contact. Also, in such an increment, points of contact on a given particle change as the contacting neighbors of the particle slide and roll over its surface.

Attempts to model the mechanical behavior of such an aggregate naturally attempt to relate measures of its average deformation to an average stress. Because of the path dependence of the contact forces and the evolution of the contact geometry, the relation between stress and strain is naturally phrased in an incremental way. Often, the stress–strain relation involves internal variables that incorporate information on the internal degrees of freedom and the geometry of the packing in an averaged or otherwise limited way. Then, because these variables evolve as the internal state of the material changes, equations of evolution for

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the state variables are required to complete the description of the material. Recent work involving these aspects of the modeling include Jenkins and Strack (1993), Koenders (1994), Mehrabadi et al. (1993), and Misra and Chang (1993).

In this paper, we will work in the context of a theory that is based on an extremely simple assumption. We assume that in a random aggregate of identical spheres, the displacements of the centers of two contacting spheres is given in terms of the average strain and rotation of the aggregate by the same expression as for a continuum. However, in order that a stress tensor defined in a relatively natural way for the granular material always be symmetric, it is necessary to retain additional degrees of freedom in the description of two contacting particles, or, equivalently, to introduce an additional internal variable in the description of the continuum. The additional variable is the average rotation of the grains about their centers.

The structure of the resulting theory is that of a Cosserat continuum in which the gradients of the rotation are identically zero (e.g. Toupin, 1964). In this event, the rotation is determined not as a solution to a boundary-value problem, but by the algebraic condition that the stress be symmetric.

The idea that the average rotations of the grains should be distinguished from the average rotation of the aggregate is rotations is not new (e.g. Chang and Misra, 1990; Jenkins, 1991); however, it seems to us to have not been sufficiently emphasized or placed in the appropriate theoretical context.

2. Theory

We focus our attention on an idealized material consisting of a random packing of identical spherical grains. We suppose that the diameter of a sphere is D and that there are n spheres per unit volume. We take $\boldsymbol{\alpha}$ to be the unit vector from the center of a sphere to a contact point on its surface and introduce the orientational distribution of contacts $A(\boldsymbol{\alpha})$, defined so that $A(\boldsymbol{\alpha})\,\mathrm{d}\boldsymbol{\alpha}$ is the probable number of contacts in the element $\mathrm{d}\boldsymbol{\alpha}$ of solid angle centered at $\boldsymbol{\alpha}$.

For a material with three orthogonal planes of symmetry, an orthotropic material, we can write $A(\boldsymbol{\alpha})$ as

$$A(\boldsymbol{\alpha}) = \frac{k}{4\pi}(1 + B_{ij}\alpha_i\alpha_j), \tag{1}$$

where $\mathbf{B}$ is a symmetric and traceless second rank tensor and k, called the coordination number, is the average number of contacts per sphere (Kanatani, 1984; Cowin, 1985).

The force $\mathbf{F}(\boldsymbol{\alpha})$ exerted by the sphere at a contact with orientation $\boldsymbol{\alpha}$ has components parallel and perpendicular to $\boldsymbol{\alpha}$:

$$F_i = P\alpha_i - T_i, \tag{2}$$

where $\mathbf{T} \cdot \boldsymbol{\alpha} = \mathbf{0}$. Following Hertz's theory of contact between elastic bodies, the component P of the contact force normal to the plane of contact is

$$P = M\left(\frac{6\delta}{D}\right)^{3/2}, \tag{3}$$

where $M \equiv 2GD^2/9\sqrt{3}(1-\nu)$, δ is the normal component of displacement, and G and ν are, respectively, the shear modulus and the Poisson ratio of the material. Here, we take the tangential component of contact force to be

$$T = Ks, \tag{4}$$

where s is the tangential displacement and K is the initial elastic stiffness of the contact, given by Mindlin (1949) as

$$K = \frac{2^{5/3}G^{2/3}}{(2-\nu)}[3(1-\nu)DP]^{1/3}. \tag{5}$$

There is the possibility of sliding contacts, but we focus on the incremental elastic behavior that would govern the propagation of long waves through the aggregate. In this case, contacts may first slide on initial loading, but then behave elastically during the cycles of unloading and loading that follow.

As indicated by Cauchy (Love (1927), Note B), an expression for the average stress tensor $\boldsymbol{\sigma}$ associated with a homogeneous deformation of the aggregate is

$$\sigma_{ij} = -\frac{Dn}{2}\int\int_{\Omega} A(\boldsymbol{\alpha})F_i\alpha_j\,\mathrm{d}\boldsymbol{\alpha}. \tag{6}$$

In general, given two spheres A and B in contact, the displacement $\mathbf{u}^{(BA)}$ of the point of contact of sphere A with respect to its center is given in terms of the displacements $\mathbf{c}^{(A)}$ and $\mathbf{c}^{(B)}$ of the centers of the two spheres, the rotations $\boldsymbol{\omega}^{(A)}$ and $\boldsymbol{\omega}^{(B)}$ of the spheres about their centers, and the unit vector $\boldsymbol{\alpha}$ directed from the center of A by

$$u_i^{(B)} - u_i^{(A)} = c_i^{(B)} - c_i^{(A)} - \frac{D}{2}\varepsilon_{ijk}\left(\omega_j^{(A)} + \omega_j^{(B)}\right)\alpha_k. \tag{7}$$

We assume that the relative displacement of the centers of the spheres is equal to the sum of the average strain $\mathbf{E}$ and the average rotation $\mathbf{W}$ of the aggregate:

$$c_i^{(B)} - c_i^{(A)} = \frac{D}{2}(E_{ij} + W_{ij})\alpha_j, \tag{8}$$

and that the rotation of the spheres about their centers is equal to the average rotation $\boldsymbol{\Omega}$ of the spheres:

$$\omega_j^{(A)} = \omega_j^{(B)} = \Omega_j. \tag{9}$$

In order to retain the freedom to insure that the stress be symmetric, we do not equate the average rotation of the aggregate with the average rotations of the spheres. Then, with these assumptions, we have

$$\mathbf{u}^{(BA)} = \frac{D}{2}(E_{ij} + W_{ij} - \Omega_{ij})\alpha_j. \tag{10}$$

A theory based upon these kinematic assumptions, called mean field theory by Jenkins (1988, 1991) and Jenkins and Strack (1993), is likely to describe the behavior of the material under rather general conditions of loading, provided that the ratio of deviatoric stress to isotropic stress is sufficiently small. In this case, Norris and Johnson (1997), for example, show good agreement between the predictions of such a theory and experiments (Domenico, 1977), provided that they assume that the coordination number is so large as 9.

We consider an aggregate that possesses orthotropic anisotropy after it has been isotropically compressed to an initial average volume strain $\varDelta$. In this initial compression, $\mathbf{W} = \mathbf{0}$ and we assume that $\boldsymbol{\Omega} = \mathbf{0}$. Small increments of homogeneous strain $\mathbf{e}$ and uniform rotation $\mathbf{w}$ are then superposed on this. So

$$u_i = \frac{D}{2}(\Delta\delta_{ij} + e_{ij} + w_{ij} - \Omega_{ij})\alpha_j. \tag{11}$$

With the displacement defined, we may calculate the normal and tangential components of the contact forces:

$$P = M\varDelta^{1/2}\left\{\left[\Delta\delta_{ij} - \tfrac{9}{2}e_{ij}\right]\alpha_i\alpha_j\right\}, \tag{12}$$

$$T_i = 9M\frac{(1-\nu)}{(2-\nu)}\varDelta^{1/2}(\delta_{ij} - \alpha_i\alpha_j)(e_{jk} + w_{jk} - \Omega_{jk})\alpha_k. \tag{13}$$

Now, we use Eqs. (1), (12), and (13) in Eq. (6) and obtain

$$\sigma_{ij} = -\frac{Dnk}{8\pi}\int\!\!\int (1 + B_{kl}\alpha_k\alpha_l)\left\{\left[M\Delta^{1/2}\left(\Delta\delta_{mn} - \frac{9}{2}e_{mn}\right)\alpha_m\alpha_n\right]\alpha_i - 9M\frac{(1-\nu)}{(2-\nu)}\Delta^{1/2}(\delta_{ip} - \alpha_i\alpha_p)(e_{pq} + w_{pq} - \Omega_{pq})\alpha_q\right\}\alpha_j\,\mathrm{d}\boldsymbol{\alpha}, \tag{14}$$

where the integration is over the surface of the unit sphere. To evaluate the integral in Eq. (14), we consider the sphere of unit radius centered at the origin and apply the divergence theorem to tensor products of the position vector $\mathbf{r}$:

$$\int\!\!\int \alpha_i\alpha_j\,\mathrm{d}\boldsymbol{\alpha} = \int\!\!\int\!\!\int r_{i,j}\,\mathrm{d}v = \frac{4}{3}\pi\delta_{ij}, \tag{15}$$

$$I_{ijkl} \equiv \int\!\!\int \alpha_i\alpha_j\alpha_k\alpha_l\,\mathrm{d}\boldsymbol{\alpha} = \int\!\!\int\!\!\int (r_ir_jr_k)_{,l}\,\mathrm{d}v = \frac{4}{15}\pi(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{16}$$

$$\int\!\!\int \alpha_i\alpha_j\alpha_k\alpha_l\alpha_p\alpha_q\,\mathrm{d}\boldsymbol{\alpha} = \int\!\!\int\!\!\int (r_ir_jr_kr_lr_p)_{,q}\,\mathrm{d}v = \frac{1}{7}(\delta_{iq},I_{jklp} + \delta_{jq}I_{klpi} + \delta_{kq}I_{lpij} + \delta_{lq}I_{pijk} + \delta_{pq}I_{ijkl}). \tag{17}$$

After carrying out the integration, Eq. (14) becomes

$$\begin{aligned}\sigma_{ij} = -\frac{Dnk}{2}M\Delta^{1/2}\Bigg\{&\frac{1}{3}\Delta\delta_{ij} + \frac{2}{15}\Delta B_{ij} - \frac{3}{10}(e_{kk}\delta_{ij} + 2e_{ij}) - \frac{3}{35}[e_{kk}B_{ij} + e_{kl}B_{kl}\delta_{ij} + 2(e_{ik}B_{kj} + B_{ik}e_{kj})]\\ &- 3\frac{(1-\nu)}{(2-\nu)}\left[e_{ij} - \frac{1}{5}(2e_{ij} + e_{kk}\delta_{ij})\right] - 3\frac{(1-\nu)}{(2-\nu)}\left[(w_{ij} - \Omega_{ij}) + \frac{2}{5}(w_{ik}B_{kj} - \Omega_{ik}B_{kj})\right]\\ &- \frac{6}{5}\frac{(1-\nu)}{(2-\nu)}e_{ik}B_{kj} + \frac{6}{35}\frac{(1-\nu)}{(2-\nu)}[e_{kk}B_{ij} + e_{kl}B_{kl}\delta_{ij} + 2(e_{ik}B_{kj} + B_{ik}e_{kj})]\Bigg\}.\end{aligned} \tag{18}$$

To insure that the stress is symmetric, we must determine $\boldsymbol{\Omega}$ in terms of $\mathbf{w}$ and $\mathbf{e}$ such that

$$(w_{ij} - \Omega_{ij}) + \tfrac{2}{5}(w_{ik}B_{kj} - \Omega_{ik}B_{kj}) + \tfrac{2}{5}e_{ik}B_{kj} = (w_{ji} - \Omega_{ji}) + \tfrac{2}{5}(w_{jk}B_{ki} - \Omega_{jk}B_{ki}) + \tfrac{2}{5}e_{jk}B_{ki} \tag{19}$$

or

$$5w_{ij} + (w_{ik}B_{kj} + B_{ik}w_{kj}) + (e_{ik}B_{kj} - B_{ik}e_{kj}) = 5\Omega_{ij} + (\Omega_{ik}B_{kj} + B_{ik}\Omega_{kj}). \tag{20}$$

Our aim is to solve Eq. (20) for $\boldsymbol{\Omega}$. To do this, we first introduce $\mathbf{C} \equiv \boldsymbol{\Omega} - \mathbf{w}$ and write it as

$$A_{ikpq}C_{pq} = e_{ij}B_{jk} - B_{ij}e_{jk}, \tag{21}$$

where

$$A_{ijpq} \equiv \tfrac{5}{2}(\delta_{ip}\delta_{jq} - \delta_{iq}\delta_{jp}) + \tfrac{1}{2}(\delta_{ip}B_{jq} - \delta_{iq}B_{jp}) + \tfrac{1}{2}(B_{ip}\delta_{jq} - B_{iq}\delta_{jp}). \tag{22}$$

If we introduce the quantities

$$a_{vw} \equiv \varepsilon_{vji}\varepsilon_{wqp}A_{ijpq} = 10\delta_{vw} - 2B_{vw}, \tag{23}$$

$$x_w \equiv \tfrac{1}{2}\varepsilon_{wqp}C_{pq}, \tag{24}$$

$$b_v \equiv \varepsilon_{vji}(e_{ik}B_{kj} - B_{ik}e_{kj}) = 2\varepsilon_{vji}e_{ik}B_{kj}; \tag{25}$$

then Eq. (21) may be written as

$$a_{vw}x_w = b_v. \tag{26}$$

When det $\mathbf{a} \neq 0$, the unique solution of Eq. (26) is

$$x_w = a_{wv}^{-1} b_v \tag{27}$$

or

$$C_{pq} = \varepsilon_{qpw}(5\delta_{wv} - B_{wv})^{-1}\varepsilon_{vji}e_{ik}B_{kj}. \tag{28}$$

Thus,

$$\Omega_{qp} = w_{qp} + \varepsilon_{qpw}(5\delta_{wv} - B_{wv})^{-1}\varepsilon_{vji}e_{ik}B_{kj}. \tag{29}$$

Eq. (29) is the relation between the average spin of the particles, the average strain and rotation of the deformation, and the anisotropy of the packing that must obtain if the stress is to be symmetric.

We recall that the trace of $\mathbf{B}$ is zero and, because $A(\boldsymbol{\alpha})$ must be nonnegative,

$$1 + B_{ij}\alpha_i\alpha_i \geqslant 0. \tag{30}$$

When these are used with definition (23) of $\mathbf{a}$ expressed diagonal form, it is easy to show that det $\mathbf{a} \neq 0$. Also, we note that when $\mathbf{e}$ and $\mathbf{B}$ have the same eigenvectors, then $\mathbf{eB} = \mathbf{Be}$; and, in this case, from Eq. (28), $\mathbf{C} = \mathbf{0}$ and $\boldsymbol{\Omega} = \mathbf{w}$.

If we now employ the general solution (28) in Eq. (18) for the stress, we obtain an explicit form for the symmetric stress given in terms of the average strain of the aggregate alone:

$$\begin{aligned}\sigma_{ij} = {} & -\frac{Dnk}{6}M\Delta^{3/2}\left(\delta_{ij} + \frac{2}{5}B_{ij}\right) + \frac{3Dnk}{10}M\Delta^{1/2}\left\{\frac{1}{2}\left(e_{kk}\delta_{ij} + 2e_{ij}\right) + \frac{1}{7}\left[e_{kk}B_{ij} + e_{kl}B_{kl}\delta_{ij}\right.\right.\\ & \left.\left. + 2\left(e_{ik}B_{kj} + e_{jk}B_{ki}\right)\right]\right\} + \frac{3Dnk}{2}M\Delta^{1/2}\frac{(1-v)}{(2-v)}\left\{\frac{3}{5}e_{ij} - \frac{1}{5}e_{kk}\delta_{ij} - \varepsilon_{jiw}(5\delta_{wv} - B_{wv})^{-1}\varepsilon_{vqp}e_{pk}B_{qk}\right.\\ & \left. + \frac{2}{5}e_{ik}B_{kj} - \frac{2}{35}\left[e_{kk}B_{ij} + e_{kl}B_{kl}\delta_{ij} + 2\left(e_{ik}B_{kj} + B_{ik}e_{kj}\right)\right] - \frac{2}{5}\varepsilon_{kiw}(5\delta_{wv} - B_{wv})^{-1}\varepsilon_{vmp}e_{pq}B_{qm}B_{kj}\right\}.\end{aligned} \tag{31}$$

The first term of Eq. (31) is the stress associated with the isotropic compression of an orthotropic material. The second term is the increment of stress associated with the normal component of the contact force. The remaining part is the increment in stress associated with the tangential component of the contact force.

When the material is transversely isotropic with its axis of symmetry in the direction of the unit vector $\mathbf{h}$, then $\mathbf{B}$ may be written as

$$B_{ij} = -\varepsilon(\delta_{ij} - 3h_ih_j). \tag{32}$$

In this case,

$$(5\delta_{wv} - B_{wv})^{-1} = \frac{1}{5+\varepsilon}\left(\delta_{wv} + \frac{3\varepsilon}{5-2\varepsilon}h_wh_v\right), \tag{33}$$

and the form of the symmetric stress appropriate for a transversely isotropic material found by Jenkins (1991) and Mühlhause and Oka (1996) may be obtained by substitution in Eq. (31).

When the material is isotropic, $\mathbf{B} = \mathbf{0}$, and

$$\sigma_{ij} = -\frac{Dnk}{8}M\Delta^{1/2}\left[\frac{4}{3}\Delta - \frac{6v}{5(2-v)}e_{kk}\right]\delta_{ij} + \frac{3Dnk}{2}M\Delta^{1/2}\left[\frac{(5-4v)}{5(2-v)}\right]e_{ij}. \tag{34}$$

It is easy to verify that the shear modulus and the bulk modulus are the same as those obtained by Digby (1981) and Walton (1987).

3. Conclusion

Working in the context of the simplest theory for a random orthotropic aggregate of identical spheres, we have shown that symmetry of the stress requires that the average spin of the particles be different from the average rotation of the aggregate. That is, the idealized material, when subjected to a homogeneous deformation, has the structure of a Cosserat continuum. This naturally raises the question of the possible role that couple stresses might play in strongly inhomogeneous deformations such as those that occur in shear bands.

Largely as the result of a paper by Mühlhaus and Vardoulakis (1987), it has become commonplace to regard the mechanics within shear bands as that of a Cosserat material. That is, a material in which the average particle rotations and their spatial gradients are required for a complete description, and for which the balance of moment must be employed to determine the rotations. The bifurcation predicted in the context of the classical theory is regularized by the introduction of the spatial gradients and the width of the shear band depends on the additional length scale associated with these.

However, the micromechanical basis for the applicability of such a theory has not yet been established and there is not yet general agreement that an antisymmetric stress can arise from point contacts between frictional spheres. For example, the micromechanical formula for the stress employed by Mühlhaus and Vardoulakis (1987) and is obviously symmetric, while the continuum theory that is meant to be motivated by the micromechanics involves a stress with an antisymmetric part. However, Jenkins (1991) and later Mühlhause and Oka (1996) do calculate couple stress tensors in an extension to strongly inhomogeneous deformations of the kinematics employed in this paper. The indications are that asymmetric stresses can be defined on the length scale of several particle diameters in situations in which the deformations are strongly inhomogeneous.

Unfortunately, no attempts have been made to measure the antisymmetric part of such a stress in numerical simulations of shear bands and to relate it to similar measurements of the rotation gradients. Instead, attempts have been made to incorporate contact couples. However, the small size of the contact region seems to insure that contact couples play an unimportant role in all but the most special of systems.

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