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Nonlinear elasticity of granular media

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Abstract

The linear and nonlinear elastic properties of granular media are analyzed within the context of effective medium theories, as well as with numerical molecular dynamic simulations, assuming the validity of the Hertz–Mindlin theory at the single contact level. There is a crucial distinction between force laws which are path independent, leading to a hyper-elastic effective medium theory, and those which are path dependent, for which the deformation history must be followed explicitly. The effective medium theories provide a reasonable description of existing experimental data, considered as a function of applied stress, but there are significant discrepancies. Numerical simulations resolve the question as to whether the problem lies with the treatment of the individual grain–grain contact or with the effective medium approximation (ema). We find that the problem lies principally with the latter: The bulk modulus is well described by the ema but the shear modulus is not, principally because the ema does not correctly allow for the grains to relax from the affine motion assumed by the ema.

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1. Introduction

The elastic properties of granular aggregates, such as sedimentary rocks, can be enormously nonlinear as compared with the properties of nonporous materials [1]. The end member of such systems may be taken to be a loose/unconsolidated aggregate of glass beads which acquire a stiffness solely as a result of applied stress. This is because if two grains are just touching, the force, considered as a function of displacement, does not initially grow linearly, as with most systems, but it has a power law behavior (Eqs. (1) and (2) below). Aside from posing an interesting problem in the physics of disordered systems, these systems are unusually nonlinear in their response and they can exhibit path dependence. By this we mean that the work done in deforming the system can depend upon whether one first compresses the system, then shears it, or first shears then compresses, or compresses and shears simultaneously, etc. The result depends upon the path taken in $\{\varepsilon_{ij}\}$ space and not just on the final state of strain $\{\varepsilon_{ij}\ (\text{final})\}$.

Here, we review some recent theoretical research we have undertaken in an attempt to understand these systems. We first discuss effective medium theories of the elastic properties, then we present our molecular dynamic simulations, and we end with a brief summary.

2. Effective medium theories

The starting point is the behavior of a single grain–grain contact, which we assume to be describable by the Hertz–Mindlin theory and variations thereof. Two touching grains are displaced in compression along a line joining their centers by an amount $2w$. They may also suffer a transverse relative displacement of their centers

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by an amount $2s$, holding their rotational orientation fixed for the moment. The normal and transverse forces, $\boldsymbol{f}_n$ and $\boldsymbol{f}_t$ may be written in terms of w and s. The idea is that as two spheres are pressed together the circle of contact continuously grows; the result is that the contact becomes increasingly stiffer with respect to further compression. Similarly, it may be assumed, for example, that the contact circle is a no-slip zone. The more the spheres are pressed together, the stiffer the contact becomes with respect to transverse relative displacement of the sphere centers (assuming the spheres are not allowed to rotate). The relevant expressions relating the forces to the displacements may be written as

$$f_n = \tfrac{2}{3} C_n R^{1/2} w^{3/2}, \tag{1}$$

$$\Delta f_t = C_t (Rw)^{1/2} \Delta s. \tag{2}$$

The prefactors $C_n = 4G/(1-\nu)$ and $C_t = 8G/(2-\nu)$ are defined in terms of the shear modulus G and the Poisson's ratio ν of the individual particles. R is the harmonic mean of the radii of the two spheres.

Eq. (2) is written in differential form to emphasize the fact that the actual value of the transverse force, f_t, depends upon the deformation path taken in $\{w, s\}$ space and not simply on the final values of w and s. Thus f_t depends upon the entire history of the trajectory: $f_t = f_t[\{w(\xi)\}, \{s(\xi)\}]$ where ξ is some conveniently chosen parameter (see Refs. [2,3] and references therein). Along a given trajectory there is no hysteresis, meaning the grain–grain contact is exactly reversible along that trajectory. But one does different amounts of work depending upon the trajectory taken; if one releases the forces along a trajectory different than the one in which they were established, there will be a net loss of energy. This behavior of a single grain–grain contact leads directly to the path dependence of the macroscopic ensemble, considered as a function of applied strain, $\{\varepsilon_{ij}\}$.

The basic idea of the effective medium theories relevant to these problems is that the macroscopic work done in deforming the system is set equal to the sum of the work done on each grain–grain contact and that the latter is replaced by a suitable average. There are two assumptions: (1) The center of each grain displaces according to the dictates of the macroscopic strain tensor, ε_{ij}:

$$u_i = \varepsilon_{ij} X_j, \tag{3}$$

where $\boldsymbol{X}$ is the initial position of the center of the grain. When the deformation is describable by a symmetric deformation, $\nabla \times \boldsymbol{u} = 0$, none of the grains rotate. This is called the "assumption of affine motion". (2) Each grain experiences essentially the same environment as any other grain. On average, the distribution of contacts is spherically symmetric. Under these assumptions, the total work done on the system may be written in terms of angular averages of the work done on a single contact. This sort of "effective medium theory" is simpler than the conventional Bruggeman type of ema [4] (see also Ref. [5]) in that it is more analogous to a simple average of the non-linear spring constants.

As written, the transverse force, Eq. (2), was derived under the assumption that once the grains are pressed together, there is perfect sticking of the contact circles. This force is path dependent, meaning that whether the grains are first pressed and then sheared, or vice versa, makes a difference in the work done on the contact. The numerical value of f_t depends upon the path taken in (w, s) space. Were we to assume, on the other hand, that there is perfect slippage of the particles, $\boldsymbol{f}_t \equiv 0$ instead of Eq. (2), then the resulting forces are path independent. The practical result of this path independent assumption is that the resulting work done in deforming the system is now a function of the state of strain and is not dependent upon the way in which the strain is applied. The path independent forces lend themselves to the development of a macroscopic strain energy density, and thus to a well-defined theory of hyper-elasticity, whereas the path dependent forces need to be treated specially. We consider these two cases in turn. A cautionary note: In reality the contact may slip over an annular ring if the coefficient of friction is finite [6]. In the limit of infinitesimal Δs we either neglect the slippage altogether or we assume complete slip, as the case may be. In any case, the forces are conservative in the sense that if the deformation path, whatever it may be, is reversed exactly, the total work done is zero.

2.1. Path independent forces

If the work done on a single contact is independent of the order in which the normal and transverse forces are applied, i.e. they are path independent, then the system as a whole is said to be hyper-elastic. An energy density, $U(\{\varepsilon_{ij}\})$, can be defined in terms of the macroscopic strain tensor, ε_{ij}, and it can usefully be expanded in powers thereof. For any isotropic system this expansion takes the form [7]:

$$U(\{\varepsilon_{ij}\}) = U_0 - p\varepsilon_{ii} + \tfrac{1}{2}[K - \tfrac{2}{3}\mu]\varepsilon_{ii}^2 + \mu\varepsilon_{ij}^2 + \tfrac{1}{3}A\varepsilon_{ij}\varepsilon_{jk}\varepsilon_{ki} + B\varepsilon_{ik}^2\varepsilon_{ll} + \tfrac{1}{3}C\varepsilon_{ll}^3 + \cdots. \tag{4}$$

Here, p is the static pressure and the strain tensor, ε_{ij}, is measured relative to the system in its reference state at pressure p. The second-order elastic constants are K, the bulk modulus, and μ, the shear modulus; they determine the speeds of small amplitude sound:

$$V_p = \sqrt{[K + (4/3)\mu]/\rho} \tag{5}$$

is the compressional sound speed and

$$V_s = \sqrt{\mu/\rho} \tag{6}$$

is the shear speed. (ρ is the density.) The third-order elastic constants, A, B, C describe how the speeds of sound change to first order in an additional applied stress, $\Delta\sigma_{ij}$, and they also describe such nonlinear effects as second harmonic generation, shock wave formation, etc. For the path-independent model described above (i.e. when we set $\boldsymbol{f}_t \equiv 0$), it is straightforward to carry out this expansion to derive analytic expressions for the various moduli [2]. Indeed, the path-independent models can be generalized slightly to include those in which the beads are first welded together over a radius $b > 0$ [8].

Theoretical predictions of the speeds of sound from this path-independent model for different values of b are plotted in Fig. 1, taken from Ref. [2]. One of the third-order constants from this model is plotted in Fig. 2. (Here, the third order constants are in the ratio $A:B:C::8:4:1$ so it is necessary to plot only one of them.)

For the case in which $b = 0$ (i.e. unconsolidated beads) the ema predictions can be simply expressed as functions of the pressure:

$$K = \frac{C_n}{12\pi}[(1-\phi)Z]^{2/3}\left[\frac{6\pi p}{C_n}\right]^{1/3}, \tag{7}$$

$$\mu = \frac{C_n}{20\pi}[(1-\phi)Z]^{2/3}\left[\frac{6\pi p}{C_n}\right]^{1/3}, \tag{8}$$

$$A = -\frac{C_n}{70\pi}[(1-\phi)Z]^{4/3}\left[\frac{6\pi p}{C_n}\right]^{-1/3}. \tag{9}$$

Here, Z is the average coordination number and ϕ is the porosity.

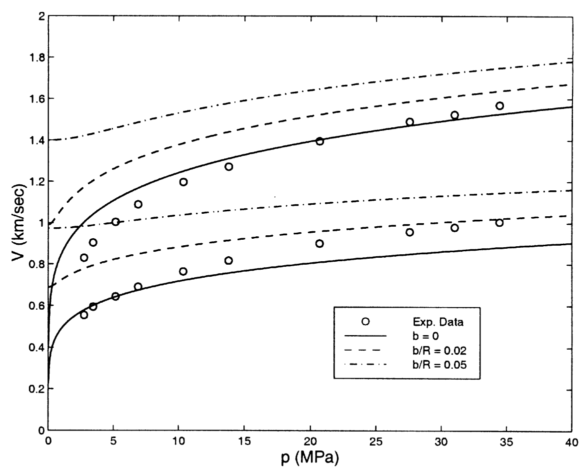

Fig. 1. Path independent ema predictions of pressure dependent sound speeds of granular media with welded contacts. The experimental data of Domenico [9] should be compared against the $b = 0$ curves. A coordination number $Z = 9$ was assumed (from Ref. [2]).

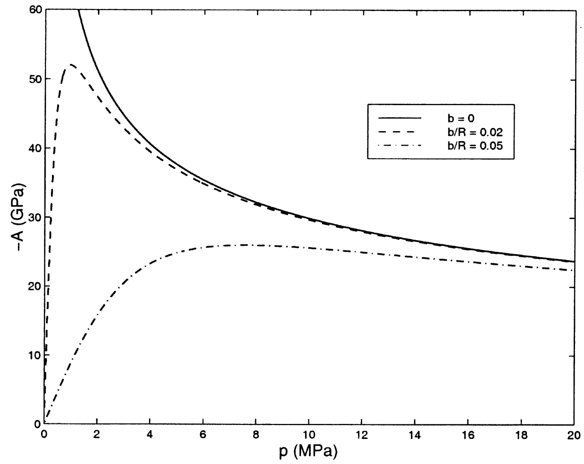

Fig. 2. Path independent ema for one of the third-order elastic constants of frictionless glass beads, as a function of confining pressure.

From Eqs. (7)–(9) as well as from Figs. 1 and 2, we see that, for unconsolidated beads, the second-order constants decrease to zero as the confining pressure decreases to zero but the third-order (and higher) elastic constants actually diverge. It is in this sense that unconsolidated granular media can be said to be extremely nonlinear. The presence of a welded contact, $b > 0$, acts to cut-off the divergence, but even so these systems can be orders of magnitude more nonlinear than ordinary, non-granular materials, such as metals, glasses, plastics, etc., for which the third-order constants are of the same order of magnitude as the second.

2.2. Path dependent forces

When the transverse force is given by Eq. (2), the work done in deforming the system is dependent upon the order (path) in which this is done. An expansion such as Eq. (4) therefore does not exist. Nonetheless, it is possible to develop an effective medium theory in which one keeps track of the order (path) in which the deformation is applied. The resulting stress tensor, σ_{ij}, depends upon the path taken in arriving at the final state of strain, ε_{ij}. As it turns out, the second-order elastic constants are in fact, well-defined path-independent quantities which depend only upon the final state of strain. In a typical experiment, however, the sound speeds may be measured as a function of applied stress, σ_{ij}, not applied strain, ε_{ij}, and so the sound speeds, considered as a function of applied stress, depend upon the order in which those stresses are applied. If the deformation path can be parameterized by some known functions, $\{\varepsilon_{ij}(\xi)\}$ where ξ is a convenient parameter, the relationship between sound speeds and applied stress can be derived [2].

For the special case of loose beads in which the system is hydrostatically compressed to its final pressure, p, the ema expressions for K and μ are particularly simple. K is unchanged from Eq. (7) and μ is changed by virtue of the transverse forces:

$$K = \frac{C_n}{12\pi}[(1-\phi)Z]^{2/3}\left[\frac{6\pi p}{C_n}\right]^{1/3}, \tag{10}$$

$$\mu = \frac{C_n + (3/2)C_t}{20\pi}[(1-\phi)Z]^{2/3}\left[\frac{6\pi p}{C_n}\right]^{1/3}. \tag{11}$$

We see that K is predicted to be independent of C_t and μ is predicted to be linearly dependent upon C_t, a point to which we return later.

The ema can be applied to any stress protocol, not just hydrostatic stress. In Fig. 3 we show the results of measurements of sound speeds on loose glass beads confined to a rigid cylinder. This is the so-called uniaxial strain test. The speeds are plotted as a function of applied stress, σ_{zz}. We show the predictions of the effective medium theory, in which certain reasonable assumptions about some of the parameters were made. (See Ref. [10] for details.) We see that the application of non-hydrostatic stress breaks the symmetry of the system, with the result that the speed of a longitudinal wave traveling along the direction of the applied stress increases more rapidly than that propagating perpendicular to it. Additionally, a transverse wave propagating perpendicular to the direction of applied stress can have two inequivalent polarizations each of which is different than that of a transverse wave parallel to the direction of applied stress. The effective medium theory for the different sound speeds is in rough accord with the experimental data.

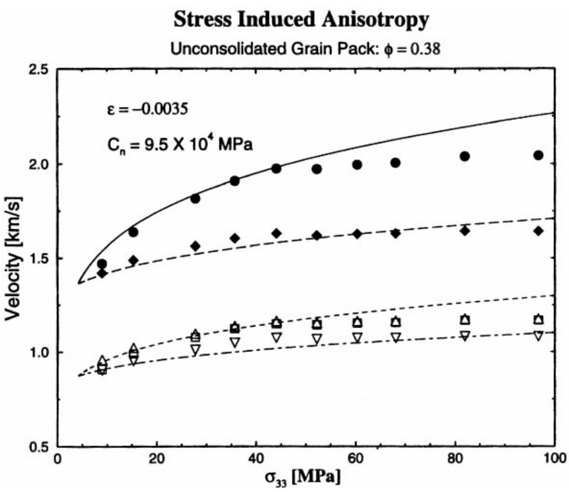

Fig. 3. A comparison of the experimentally determined speeds of sound in a uniaxial strain test, as a function of applied stress. The solid symbols are compressional speeds parallel and perpendicular to the stress direction, and the open symbols are the shear speeds, parallel to the stress direction and perpendicular to it, both polarizations. The continuous lines are the predictions of the ema (from Ref. [10]).

3. Molecular dynamics simulations

With reasonable choices of the relevant parameters, the effective medium theories described above can give a good approximate description of the acoustic properties of granular media, as in Fig. 1, but there are problems, even for the simplest case of unconsolidated beads: (1) The effective medium theory predicts that the second order moduli vary with confining pressure as $p^{1/3}$, regardless of the values of coordination number, Z, and regardless of the values of C_n or C_t. It is clear from Fig. 1 that the real data do not obey this power law. (2) Absent a molecular dynamics simulation, one does not know the appropriate value of the average coordination number, Z, to use in Eqs. (10) and (11). (3) The ratio K/μ, or, equivalently V_p/V_s, is predicted from Eqs. (10) and (11) to be independent of pressure. Experimentally the ratio K/μ is indeed roughly constant but with a value which is intermediate between the two ema predictions, Eqs. (7) and (8) on the one hand, and Eqs. (10) and (11) on the other. Thus the implication is that C_t (in Eq. (11)) is much smaller in real systems than expected from the Mindlin theory, Eq. (2), or that the ema is wrong.

These facts have motivated us to undertake molecular dynamics simulations [11]. In Fig. 4 we show the existing experimental data for K and μ on loose glass beads along with predictions of the effective medium theory (Eqs. (10) and (11)). From the simulations we find that the numerical value of the average coordination number is $Z \approx 6$ (not $Z = 9$ as in Fig. 1) for pressures less than 100 MPa, so this is the value we use in Eqs. (10) and (11). We also show the results for our simulations. Although there is

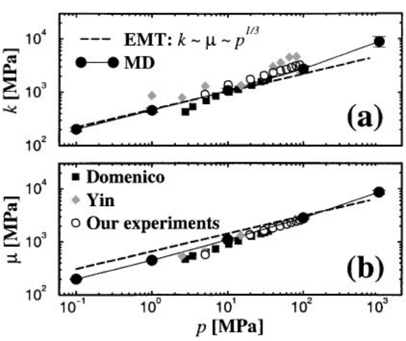

Fig. 4. Pressure dependence of the elastic moduli from MD, experiments, and path dependent ema: (a) bulk modulus, and (b) shear modulus. The data are from Refs. [9,11,12].

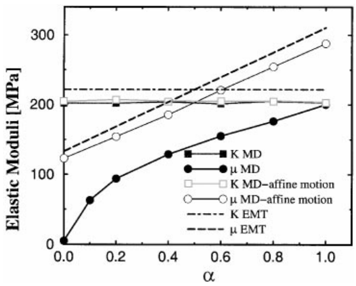

Fig. 5. Bulk modulus, K, and shear modulus, μ, vs. α for a fixed pressure, $p = 100$ kPa. The effective medium theory is compared against the unrestricted numerical simulations. For comparison, we also show the results of simulations in which the displacement of each grain is restricted to affine motion and rotation is disallowed.

scatter within and disagreement between the different data sets, we see immediately that the simulations, the effective medium theory, and the data are in reasonable agreement for the bulk modulus, K. The experimental data and the simulations are in reasonable agreement for μ. The ema, however, significantly over-predicts μ. Our conclusions are that the assumption of the Hertz–Mindlin contact law, Eqs. (1) and (2), is not seriously in error, the ema is quite accurate in predicting K, and it is quite inaccurate in predicting μ.

According to the ema, the transverse force, f_t, contributes only to the shear modulus and not to the bulk modulus. Thus, we are motivated to examine molecular dynamic simulations in which C_t in Eq. (2) is replaced by αC_t where the dimensionless parameter α is varied from 0 to 1. The results for a confining pressure of $p = 100$ kPa are shown in Fig. 5, along with the predictions of Eqs. (10) and (11). The simulations confirm that K is essentially independent of the strength of the transverse force. Astonishingly, the shear modulus is extremely sensitive in that it (nearly) vanishes as $\alpha \to 0$, in sharp contrast to the prediction of Eq. (11). What is the most serious problem with the ema? We believe it to be the "affine assumption" we discussed earlier. Thus, we redo the numerical simulations by forcing each ball to translate according to Eq. (3) and not rotate at all. Finally, these simulations, which are also shown in Fig. 5 are indeed in agreement with the ema predictions, Eq. (11). What is evidently happening in the unconstrained simulations, and in the experiments, is that the beads in the immediate neighborhood of each grain move around relative to the central grain in such a way that if there are central forces only ($C_t = 0$), there is a nearly complete relaxation of the system to an applied shear. The system is a fluid, or nearly so.

4. Conclusions

We have found that: (1) The Hertz–Mindlin contact theory is a good approximation to the actual grain-grain contact law in real glass bead systems subjected to a known stress. (2) The very simple effective medium approximation gives a reasonable, if approximate, description of the response of the system. (3) There is a big difference between systems in which the forces may be presumed to be conservative and path independent and those for which the forces are path dependent. In the former, a hyper-elastic theory of the elastic constants may be developed whereas in the latter the third-order (and higher-order) constants are undefinable. (4) The molecular dynamic simulations establish the validity of the effective medium theory for the bulk modulus and also establish that the ema for the shear modulus is in serious error. The problem lies with the inability of the ema to correctly treat the relaxation of the surrounding grains when a shear deformation is applied.

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