The stress transmission universality classes of periodic granular arrays

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Abstract

The transmission of stress is analysed for static periodic arrays of rigid grains, with perfect and zero friction. For minimal coordination number (which is sensitive to friction, sphericity and dimensionality), the stress distribution is soluble without reference to the corresponding displacement fields. In non-degenerate cases, the constitutive equations are found to be simple linear in the stress components. The corresponding coefficients depend crucially upon geometrical disorder of the grain contacts.

1 Introduction

Granular media present a fascinating array of physical problems [1] and are key to a number of important technologies [2]. Distribution of stress and statistics of force fluctuations in static granular arrays show puzzling properties [3]. For instance, photoelastic visualization experiments [4] show that stresses in granular media concentrate along "stress paths" or "force chains". These are filamentary configurations of grains which carry disproportionately large amount of the total force and give rise to the phenomenon of jamming [5]. The intergranular contact forces determine the bulk properties (e.g. the load bearing capability) of granular materials [6]. Recent experiments [7] and computer simulations [8] show that the distribution of forces where forces above the mean decay exponentially is a robust property of static granular media. Despite recent theoretical attempts [9, 10, 11] and a vast engineering literature [12, 13], the transmission of stress and statistical properties of contact force distribution in granular media are still poorly understood at a fundamental level. This paper is concerned with a static granular material idealised as an assembly of rigid grains, not in general spherical and with either zero or perfect (in the sense of infinite) friction. Whilst practical applications in soil mechanics and powder technology evidently depend on much greater levels of detail considered in the engineering literature, the rigid grain paradigm provides a crucial starting point from which to appreciate the theoretical physics of the problem. We show below that for minimal coordination number there exists an analysis of stress which is independent of the analysis of strain which would be implied by slight relaxation of the rigid grain assumption. In consequence our results may also have bearing on many computer simulations of quasi-static interacting particles,
such as applied to colloids \[15\] or soils \[16\], and suggest that the detail of conservative repulsive force laws used may not always be significant.

2 The Model

Consider a static assembly of rigid grains of average coordination number \(z\), in dimension \(d\). The microscopic version of stress analysis consists of determining all of the intergranular forces, given the geometrical arrangement of grains and their contacts and the applied force and torque loadings on each grain. The number of unknowns per grain is \(zd' / 2\), where \(d' = d\) for grains with friction and \(d' = 1\) for grains without, and the required force and torque give \(d + (d^2 - d) / 2\) constraints. The minimal coordination number, at which the equations of force balance are directly soluble, is thus given by \(z_m = \frac{d^2 + d}{d'}\). Without friction this gives \(z_m = 6, 12\) in \(d = 2, 3\) respectively. With friction it gives rather low values \(z_m = 3, 4\) respectively. If we admit that grains have some compliance then the intergranular forces calculated from Newton’s equations must also be consistent with being calculated from the displacements of grains. This implies \(zd'\) constraints on the particle displacements, which at minimal coordination is precisely consistent with determining the center displacement and rotation of each particle. This situation is analogous to linear elasticity in two dimensions, where stress can be analysed independent of the elastic moduli for an isotropic material; subsequently the displacement field can be recovered (using the moduli) and of course this may be relevant for boundary conditions \[17\]. For the granular material, no assumption of linearity or isotropy is involved. Equivalent arguments, without consideration of torques and rotations, go through for frictionless spherical grains. They exhibit minimal coordination number equal to twice the dimension of space.

In this paper we will elaborate in detail the constraint equations satisfied by the stress tensor supported by simple periodic granular arrays. Here we argue how the key result, of simple linear equations of constraint, can be anticipated on quite general grounds. We consider a periodic array with \(M\) grains per unit cell and correspondingly \(Mz_m / 2\) intergranular contacts. The number of strictly periodic \((k = 0)\) solutions for the intergranular forces dictates how many linearly independent stress components the powder can support macroscopically. The general stress field of our periodic array will be decomposable over Bloch wave solutions \(\propto e^{ik \cdot r}\), and within these it is the periodic solutions with wavevector \(k = 0\) which correspond to macroscopically uniform stress. For a periodic solution the intergranular forces will be constrained by \((M - 1)d\) equations of force balance rather than \(Md\), because no intergranular force can apply a net force to the whole assembly. Unless there is accidental degeneracy (see end of this section) there will be no such mitigation of the number of torque constraints at \(M(d + (d^2 - d) / 2)\). The general result is then that at minimal coordination we have precisely \(d\) degrees of freedom corresponding to macroscopically uniform stress, to be determined macroscopically by the \(d\) macroscopic (continuum) equations of force balance \(\nabla \cdot \sigma = 0\), where \(\sigma\) is the stress tensor. The number of equations restricting the form of macroscopic stress supported, equivalent to a constitutive equation, is \((d^2 - d) / 2\), equivalent to one in \(d = 2\) and three in \(d = 3\). These equations will be developed explicitly for special cases below. The anomalous case is, unfortunately, the one case previously considered \[14\]: minimal periodic lattices of spherical grains with friction. These are the honeycomb and diamond lattices in \(d = 2, 3\) dimensions respectively, which have two grains per unit cell related to each other by a reflection symmetry. The reflection symmetry means that if the torque on one particle is balanced, then so it must also be on the other. As there is no corresponding reduction in the number of independent inter-particle forces, the number of degrees of freedom for solutions corresponding to
macroscopic stress is increased to \((d^2+d)/2\), corresponding to a full set of symmetric stress tensors. As shown in Ref.\[14\], the constitutive equation then takes differential form and has to be found from leading \(k\)-dependent behaviour. In three dimensions (and higher) the existence of intermediate classes of behaviour can be conjectured, where some but not all of the constitutive equations are differential in form. Candidate geometries include simple arrays of ellipsoids, but will not be presented here.

### 3 Frictionless aspherical grains in \(d = 2\)

Consider a periodic triangular array of smooth grains with the geometry of the contacts and their normals as shown in Figure 1. Contact 1 is at position \(u_1\) relative to the grain center, with surface outward normal \(n_1\) subject to a force \(\phi_1 n_1\). Note that periodicity requires what would be contact 4 to have normal \(-n_1\), to which end we have labelled it \(1’\), and similarly for the other opposed pairs of contacts. Balance of force around the grain, subject to external force \(F\), requires:

\[
F + (\phi_1 - \phi_1')n_1 + (\phi_2 - \phi_2')n_2 + (\phi_3 - \phi_3')n_3 = 0 \tag{1}
\]

and the (tensorial) force moment around the grain is given by:

\[
S = (\phi_1 u_1 - \phi_1'u_1')n_1 + (\phi_2 u_2 - \phi_2'u_2')n_2 + (\phi_3 u_3 - \phi_3'u_3')n_3 \tag{2}
\]

In terms of \(S\), the balance of torque on the grain requires that \(S\) be symmetric, and the macroscopic stress tensor is given by:

\[
\sigma = \frac{1}{V} \sum_{g \in V} S_g \tag{3}
\]

For Bloch wave solutions of wavevector \(k\) we have \(\phi_1' = \phi_1 e^{i k \cdot (u_1' - u_1)}\) and similarly for \(\phi_2'\) and \(\phi_3'\). Then to leading order in \(k\) we obtain:

\[
S = \phi_1 a_1 n_1 + \phi_2 a_2 n_2 + \phi_3 a_3 n_3 + \text{order } k \tag{4}
\]
where \( \mathbf{a}_1 = \mathbf{u}_1 - \mathbf{u}'_1 \) etc. are the lattice vectors, and:

\[
\mathbf{F} + i \mathbf{k} \cdot \mathbf{S} + \text{order } k^2 = 0
\]  

(5)

This last equation is just macroscopic force balance, equivalent to \( \nabla \cdot \mathbf{\sigma} + \mathbf{f} = 0 \), where \( \mathbf{f} \) is the external force per unit volume. The expression for \( \mathbf{S} \) together with the constraint that it be symmetric restricts the form of the stress tensor. It is readily verified that the lattice vectors satisfy a triangle equality \( \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 = 0 \), and we can without loss of generality rescale the lengths of the normals to obtain a further triangle of vectors \( \mathbf{m}_1 + \mathbf{m}_2 + \mathbf{m}_3 = 0 \), where \( \mathbf{m}_1 \propto \mathbf{n}_1 \) etc. Then it is not difficult to check that \( \mathbf{a}_1 \times \mathbf{S} \times \mathbf{m}_2 = \mathbf{a}_2 \times \mathbf{S} \times \mathbf{m}_1 \); the two further identities that this appears to offer by changing numerical labels are easily shown to be equivalent to it. Thus the constitutive equation restricting the stress tensor can be written explicitly as:

\[
\text{Trace } (\mathbf{P}, \mathbf{S}) = 0
\]  

(6)

governed by an order parameter \( \mathbf{P} \) given by:

\[
\mathbf{P} = R \cdot \mathbf{m}_2 R \cdot \mathbf{a}_1 - R \cdot \mathbf{m}_1 R \cdot \mathbf{a}_2
\]  

(7)

where \( R \) is a rotation through \( \pi/2 \). It is interesting that the order parameter \( \mathbf{P} \) is intrinsically chiral, with its sign sensitive to how we index contacts round the grain. If the isotropic part of \( \mathbf{P} \) happens to vanish, then our constitutive equation reduces to Fixed Principal Axes (FPA) ansatz \([9]\). However as all the vectors \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{m}_1, \mathbf{m}_2 \) are in principle independent of each other, there is no reason to expect:

\[
\text{Trace} \mathbf{P} = \mathbf{m}_2 \cdot \mathbf{a}_1 - \mathbf{m}_1 \cdot \mathbf{a}_2 = 0
\]  

(8)

and FPA ansatz remains a special case.

4 Frictionless aspherical grains in \( d = 3 \)

The simplest regular array to consider here is (affinely distorted) face-center cubic, duly giving the minimal coordination number of 12. Opposing pairs of contacts are mutually constrained as in the two dimensional case, and as wavevector \( k \) approaches zero we find the force moment tensor given by a sum over the six pairs as:

\[
\mathbf{S} = \sum_{i=1}^{6} \phi_i \mathbf{a}_i \mathbf{n}_i
\]  

(9)

Making \( \mathbf{S} \) symmetric determines three of the \( \phi_i \), so that we are left with just three degrees of freedom for the symmetric stress, as expected. The connectivity of the lattice ensures that the six lattice vectors span the edges of a tetrahedron, and there is one normal vector corresponding to each edge. Although it is not in general possible to scale the normals to fit the edges of a tetrahedron, we can scale them in usefully analogous way. The three lattice vectors meeting at any vertex have, given appropriate ordering conventions, the
property that \( \mathbf{a} \cdot \mathbf{a}' \times \mathbf{a}'' = 6V \), where the constant \( V \) is the volume of the tetrahedron. The six normal vectors can be rescaled as \( \mathbf{m}_i \propto \mathbf{n}_i \) so that any corresponding set of three obeys the analogous result \( \mathbf{m} \cdot \mathbf{m}' \times \mathbf{m}'' = 1 \). Given the above conventions it is not difficult to see that if edges 1,2,3,4 form a circuit enclosing triangles 1,2,5 and 3,4,5 then 
\[
(\mathbf{a}_1 \times \mathbf{a}_2) \cdot (\mathbf{m}_3 \times \mathbf{m}_4) = (\mathbf{a}_3 \times \mathbf{a}_4) \cdot (\mathbf{m}_1 \times \mathbf{m}_2)
\]
both sides are equal to \( 6V \phi_0 \) with appropriate scale factor. In this way we can obtain six constraint equations of the form:

\[
(\mathbf{a}_1 \times \mathbf{a}_2 \mathbf{m}_3 \times \mathbf{m}_4 - \mathbf{a}_3 \times \mathbf{a}_4 \mathbf{m}_1 \times \mathbf{m}_2) : S = 0
\]

of which only three are linearly independent of each other. For frictionless spheres the simplest periodic lattice of minimal coordination number, 2\(d\), is a cubic array, sheared over in the general case. For this arrangement it is obvious that the system can support only normal stresses along the symmetry axes. When these are at right angles this corresponds to Fixed Principle Axis behaviour, but not otherwise.

## 5 Grains with friction

For grains with friction, the simplest periodic arrays require at least two grains per unit cell because of the relatively low minimal coordination number. The honeycomb and diamond lattices (for two and three dimensions respectively) have already been discussed in [14], but with an assumption of symmetry between the two grains of the unit cell: this is that the intracell grain contact lies at the centroid of the intercell grain contacts. Here we show that if the intracell contact is displaced by a vector \( \mathbf{c} \), a simple linear rather than differential constitutive equation results. Working for simplicity in two dimensions and focusing on \( k = 0 \) solutions, the force moment (proportional to stress tensor) of the unit cell can be written as:

\[
S = a_1 f_1 + a_2 f_2
\]

where \( f_i \) is the force across the intercell contacts spanned by lattice vector \( \mathbf{a}_i \). From this we can find the \( f_i \) in terms of \( S \) and hence expressions for the torque applied to each grain in the unit cell. The sum of these torques vanishes when \( S \) is symmetric, but the difference between them is given (at \( k = 0 \)) by:

\[
\Delta G = \frac{\mathbf{c} \times S \times (\mathbf{a}_1 - \mathbf{a}_2)}{\mathbf{a}_1 \times \mathbf{a}_2}
\]

resulting in a constitutive equation

\[
\mathbf{c} \times \sigma \times (\mathbf{a}_1 - \mathbf{a}_2) = 0
\]

In three dimensions the diamond lattice calculation is analogous, with three intercell grain contacts spanning three lattice vectors, and the resulting constitutive equation is:

\[
\mathbf{c} \times \sigma.(\mathbf{a}_1 \times \mathbf{a}_2 + \mathbf{a}_2 \times \mathbf{a}_3 + \mathbf{a}_3 \times \mathbf{a}_1) = 0
\]

In both cases, when the grains become equivalent and \( \mathbf{c} = 0 \) one must work to higher order in the wavevector \( k \), leading to a differential constitutive equation as shown in [14].
6 Discussion

In this paper we have shown how the geometrical arrangement of grains and their contacts, assumed known, directly restricts the form of stress tensor that the material can support. In principle one can only apply forces to a sample, and the restrictions found on the stress tensor are no more than that required to solve for the resulting stress distribution. Independent of friction, dimensionality or even whether the particles are spheres, we find a general universality class $GL$ of mechanical constitutive equation which is simple linear in the stress components. The coefficients of this are sensitive to the intergranular geometry to a much finer level than simple objects such as the fabric tensor. Two further universality classes have been found. The first is where by symmetry of the granular array there is no coupling (of the constitutive equations) to Trace $\sigma$, equivalent to FPA ansatz behaviour \[9\]. The second class, DL, is where by internal symmetry of the granular array some of the constitutive equations become differential\[14\]. All of the above behaviour is summed up by the general form:

$$N : \sigma + \nabla.T : \sigma + ... = 0 \quad (15)$$

The nul space of $N$ acting on $\sigma$ corresponds to allowed macroscopic stress fields; when this includes pure isotropic stress we have the special class FPA. When the nul space is degenerately large, $T$ becomes crucial and we have DL behaviour: the only instances of this which we explicitly calculated had $N = 0$, but the existence of mixed cases in three dimensions (and higher) is conjectured. In practice detail of intergranular contacts is not known in advance, but should be deduced from the deposition history of the system. Truly history dependent problems are outside the scope of this paper, but for granular systems which have consolidated or sheared under the applied loading, and for pseudo-elastic assemblies which have undergone significant deformation and rearrangement under stress and/or flow, we can consider the approximation that the current stress itself influences the contact geometry. In two dimensions we then require to make one scalar equation out of the stress tensor alone, and assuming it to be independent of the magnitude of the stress this must reduce to a condition on the ratio of the principal stress components, $\sigma_1/\sigma_2 = \text{constant}$ . This is of precisely the same form as classical considerations of limiting internal friction:

$$\mu = \frac{\sigma_{\text{shear}}}{\sigma_{\text{normal}}} = \frac{\sigma_1 - \sigma_2}{2\sqrt{\sigma_1\sigma_2}} \quad (16)$$

where $\mu$ is the coefficient of shearing friction. In three dimensions we require three equations, which cannot be imposed on the only two principle stress ratios available. In this case, therefore, it appears that we must have inescapably history-dependent behaviour. There might remain the possibility that the system selects degenerate case configurations for which at least one of the constitutive equations becomes differential in form, but to achieve this appears to place conditions on the sample history or, leading to contradiction, the present stress tensor. Work on disordered arrays of rigid grains is in progress \[18\].

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