THE INCREMENTAL RESPONSE OF RANDOM AGGREGATES OF IDENTICAL ROUND PARTICLES

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ABSTRACT

This paper is concerned with a dense, randomly packed, granular material that consists of identical spheres or disks with elastic, frictional interactions, that is first isotropically compressed and subsequently loaded along an arbitrary stress path. An analytical relationship between the overall stress and strain increments is determined for the pre-failure regime. The purpose of the modelling is to understand how this relation depends upon the features of the packing and the particle interactions. From the outset it is recognised that the packing and interactive properties for these materials may vary substantially from grain to grain and the heterogeneity introduced in this manner is fully accounted for. Moment equilibrium equations are solved for each particle and force equilibrium equations are solved for each neighbourhood. Then, the heterogeneity of the aggregate is taken into account by introducing means and fluctuations in the description of the local deformations and the measures of the particles and interactions. The general development is illustrated with an example in two dimensions in which the packing and contact interactions are approximated by angular distributions and the heterogeneity is introduced by variations in these. For an isotropic medium with constant contact stiffnesses the theory provides predictions that compare well with results obtained from numerical simulations.

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1. INTRODUCTION

Reliable stress-strain relations for granular materials are necessary for predicting the pre-failure behavior and failure of natural aggregates of sand, gravel, or rocks. Behaviour of interest to soils and foundation engineering includes wave propagation, stress response, volume change, and localization (failure). A better understanding of the mechanics of densely packed granular media will also be of benefit to the pharmaceutical and the chemical process industries. In this paper, we develop incremental stress-strain relations for the pre-failure response of densely packed, compressed aggregates from micro-mechanical considerations.

The particles are assumed to be essentially rigid and to experience deformation only in the immediate area of contacts. Because the relationship between the contact forces and the contact displacements are strongly non-linear and path dependent, it is appropriate to use incremental forms for the contact forces and displacement measures. Then, when the equilibrium equations for force and moment on each particle are phrased in terms of the increments in contact force, they are linear in the increments of displacement and rotation.

In the past, stress–strain relations for periodic packings of identical spheres (Thornton, 1979) and discs (e.g. Chang, 1988) that interact through elastic, frictional contacts have been obtained using

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homogeneous deformations in which the equilibrium of force and moment are satisfied identically. The response of random arrays of identical spheres has also been studied, assuming that the deformation is homogeneous (Digby, 1981; Walton, 1987; Jenkins and Strack, 1993; Norris and Johnson, 1997). However, because the interactive and packing properties may vary widely from grain to grain, so do the translations and rotations of the individual particles. Therefore, the assumption of homogeneous deformation does not reflect the true physics of the random aggregate. As a consequence, a number of quantitative features of granular materials are not well described: the stiffnesses are over predicted, the volume change is under predicted, at least along certain important stress paths, and failure is not likely to be predicted correctly. The reasons for such shortcomings and methods for overcoming them have been put forward by several authors. Makse *et al.* (2000) attribute the failure of theories based on homogeneous deformations to the change in the number of contacts as the material is deformed. Misra and Chang (1993) emphasise the heterogeneity of the packing in a calculation of effective moduli based upon a self-consistent calculation for a random continuous medium. Koenders (1987, 1994) focused on the influence of the heterogeneity of both the packing and interactions on approximate solutions of the equilibrium equations that lead to calculations of effective moduli. Jenkins (1997) departed from the assumption of a homogeneous deformation and introduced pair fluctuations in an effort to solve the equilibrium equation. Cambou *et al.* (1995) introduce an assumption of a homogeneous stress rather than a homogeneous deformation in their attempts to predict the mechanical response of idealised aggregates.

The introduction of heterogeneity is, in part, motivated by the inspection of both physical experiments on photoelastic materials (Drescher and De Josselin de Jong, 1972; Konishi, 1978; Allersma, 1982) and by numerical simulations (e.g. Cundall and Strack, 1979; Thornton, 2000; Moreau, 1994; Williams and Rege, 1997; Zhuang *et al.*, 1995; Koenders and Stefanovska, 1993). In these simulations the translations and rotations of the particles are linked to the increments in the average strain and rotation of the aggregate through the equilibrium equations. The number of balance equations for force and moment on each particle is equal to the number of translational and rotational degrees of freedom. Consequently, with information regarding the translations and rotations of the bounding particles or information regarding the average strain and rotation of the aggregate, the translations and rotations of the individual particles may be determined. Then, with an appropriate definition of the stress increment, an incremental relation between the stress and strain may be obtained.

In this paper, we attempt to obtain analytical, incremental stress-strain relations based on the equilibrium equations. Because there are a great number of degrees of freedom involved in even the smallest assembly for which an increment of strain can reasonably be defined, this must inevitably include some approximations. We focus on a relatively small number of particles and express the translations and rotations of these particles in terms of a limited number of degrees of freedom. Then the equations of force and moment balance are used in an approximate way to determine the degrees of freedom in terms of the average strain and rotation of the aggregate. In such an approach, various measures of the interactive and packing properties enter into the procedure and these find their way into the incremental stress-strain relationship. We follow Koenders (1987) and call such measures structural sums; these are specific, well-defined examples of internal state variables. The state variables can only be identified in the context of an approximate analytical theory based upon the equilibrium equations. Because substantial variability of the contact orientation and the magnitude and direction of the contact forces are typical features of random close-packing with elastic, frictional interactions, the state variables involve not only averages over particles of the aggregate, but also measures of variability.

A related formulation has been put forward of late, aiming to capture and systematise the complexity of force and displacement patterns in small assemblies. In this formulation higher order measures of stress and strain are introduced. Examples of papers on this subject, relevant to granular mechanics are Suiker et al (2001), Chang et al (2002) and Kruyt (2003). Other authors have attempted to approach the assembly as a thermodynamic entity, which may possibly be correct for certain limiting cases; Edwards and Grinev (2002) advocate such an approach. Various effects relating to wall effects for finite, not too large assemblies have been treated by Zhu and Yu (2002).

We derive a stress-strain relation for an aggregate of N particles that we take to be the smallest collection over which a homogeneous strain may be defined. The derivation is based on the equilibrium of the particles in this assembly. We first express the translations and rotations of the particles in the neighborhood of a typical particle as a power series in their position from its center. We indicate the number of coefficients in this expansion that must be retained in order that a characteristic small assembly can be taken to be the central particle and its nearest neighbors. The coefficients for the rotational degrees of freedom for the particles of this assembly are then determined in terms of the translations by satisfying the individual balances of momentum (e.g. Koenders, 1994). The determination of the rotations permits the force balance of a typical particle in the small assembly to be expressed in terms of the first and second order coefficients for the displacement power series.

Incremental stress-strain relations for small neighbourhoods are then put forward. These may be deployed to give a first order mean field (volume average) estimate for the incremental response of the medium. This estimate is rather inadequate, in that it tends to over-predict the moduli. The force balances for each small neighbourhood provide a starting point for improved estimates of overall stiffnesses. The fact that small-scale incremental stress-strain relations are available implies that, in order to obtain overall incremental stiffnesses, the correlation between the strain increment fluctuations and local incremental stiffness fluctuations are required. Using the force balance and assuming moderate fluctuations in incremental stiffnesses, an adaptation of Kröner's (1967) method is developed, which yields estimates for the strain increment fluctuations. The associated deviation from the mean field stiffness estimate follows. This scheme is elaborated in some detail for an isotropic material, giving a prediction of the overall incremental bulk and shear moduli. Benefiting from reported two-dimensional numerical simulations, the special case of constant contact stiffnesses is investigated, leading to a favourable comparison between analytical prediction and (numerical) experiment.

The theory outlined in this paper may be employed to ask questions of numerical simulations that have direct mechanical relevance. For situations in which the fluctuations in the main components of the structural sums are large, more development of a suitable homogenisation methodology is required.

2. EQUILIBRIUM EQUATIONS, KINEMATICS, OBJECTIVITY AND NOTATION

Equilibrium equations

A notation is introduced similar to the one used by Koenders (1987). Particles are distinguished by a Greek superscript; they have both translational and rotational degrees of freedom. The relative displacement increment at a contact between two particles, the centers of which are connected by a vector $\mathbf{c}^{\mu\nu} = \mathbf{x}^{\nu} - \mathbf{x}^{\mu}$, is expressed in the increment of displacement $\mathbf{u}$ and the increment of rotational motion (spin increment) $\boldsymbol{\omega}$ as

$$\Delta_i^{\mu\nu} = u_i^{\mu} - u_i^{\nu} - \tfrac{1}{2}\varepsilon_{ijk} c_j^{\mu\nu}\left(\omega_k^{\mu} + \omega_k^{\nu}\right). \qquad (1)$$

The contact force increment $\mathbf{f}^{\mu\nu}$ is linear in the incremental contact displacement with proportionality tensor **K**. The actual values of the components of **K** depend on the details of the contact law for the elasto-frictional interaction (e.g., Jenkins and Strack, 1993).

The equilibrium equations for the balance of force and moment take the form

$$\sum_{\nu=1}^{N^\mu} f_p^{\mu\nu} = \sum_{\nu=1}^{N^\mu} K_{pi}^{\mu\nu}\left[u_i^\mu - u_i^\nu - \tfrac{1}{2}\varepsilon_{ijk}c_j^{\mu\nu}\left(\omega_k^\mu + \omega_k^\nu\right)\right] = 0 \tag{2}$$

and

$$\varepsilon_{pqr}\sum_{\nu=1}^{N^\mu} c_q^{\mu\nu} f_r^{\mu\nu} = \varepsilon_{pqr}\sum_{\nu=1}^{N^\mu} c_q^{\mu\nu} K_{ri}^{\mu\nu}\left[u_i^\mu - u_i^\nu - \tfrac{1}{2}\varepsilon_{ijk}c_j^{\mu\nu}\left(\omega_k^\mu + \omega_k^\nu\right)\right] = 0\,. \tag{3}$$

There are as many equations as there are unknowns: for N particles, 3N displacements and 3N particle spins, matched by 6N equilibrium equations. The latter are coupled and, as a result, it is expected that the equivalent continuum description also contains a coupling to the medium outside the small assembly for which the description is sought.

Kinematics

The displacement and spin increments in the vicinity of the particle labelled μ may be approximated with a polynomial. The approximation is fitted in a least-squares sense to the kinematic quantities of the relevant particles, labeled by the superscript κ. The polynomials have coefficients **U** and **Ω** which are arranged as follows:

$$u_i^\kappa \approx U_i^{0,\mu} + U_{ij}^{1,\mu}c_j^{\mu\kappa} + \tfrac{1}{2}U_{ijk}^{2,\mu}c_j^{\mu\kappa}c_k^{\mu\kappa} + \ldots\ldots \tag{4}$$

and

$$\omega_i^\kappa \approx \Omega_i^{0,\mu} + \Omega_{ij}^{1,\mu}c_j^{\mu\kappa} + \tfrac{1}{2}\Omega_{ijk}^{2,\mu}c_j^{\mu\kappa}c_k^{\mu\kappa} + \ldots\ldots\,. \tag{5}$$

The expansion involves a distance dependence in terms of $\left|\mathbf{c}^{\mu\nu}\right|$. In order to give more or less equal weight to distant particles the number of particles that participate in the determination of the coefficients is taken to be slightly larger than the number that is strictly necessary (the number of independent coefficients). This leads naturally to the use of a least squares method of coefficient determination, in that the coefficients **U** and **Ω** are given by the conditions in a *neighbourhood* of particle μ

$$\sum_{\kappa}\left[u_i^\kappa - \left(U_i^{0,\mu} + U_{ij}^{1,\mu}c_j^{\mu\kappa} + \tfrac{1}{2}U_{ijk}^{2,\mu}c_j^{\mu\kappa}c_k^{\mu\kappa} + \ldots\ldots\right)\right]^2 = \text{minimal} \tag{6}$$

and

$$\sum_{\kappa}\left[\omega_i^{\kappa}-\left(\Omega_i^{0,\mu}+\Omega_{ij}^{1,\mu}c_j^{\mu\kappa}+\tfrac{1}{2}\Omega_{ijk}^{2,\mu}c_j^{\mu\kappa}c_k^{\mu\kappa}+.....\right)\right]^2=\text{minimal}. \qquad (7)$$

Table 1 illustrates the number of independent coefficients for given order of approximation; the numbers in the third and fourth column are obtained by simply counting the coefficients: for example, for a first order approximation of the spin in two dimensions the gradient is required, which possesses two coefficients. For the latter case the number is equal to the dimension, but for higher orders some coefficients are not independent, as there are symmetry relations. In two dimensions, the number of independent coefficients for the spins is 1, 2 and 3 in the zero, first and second order terms, respectively. For the displacements, the numbers are 2, 4 and 6. A small assembly that is described up to a certain order is able to accommodate an exact number of particles in the description. For instance, an assembly that is described up to first order in two dimensions has for the spin zeroth and first order coefficients. The former contributes one coefficient, the latter adds two more, altogether providing for three describing coefficients. So, if an assembly contains exactly three particles, its kinetics may be captured by means of this first order description. From the table it is deduced that in two dimensions an assembly size of some six particles is fitted using the zero, first and second order approximations for an exact fit. In three dimensions, the numbers are the same for the spin and displacement approximations: 3, 9 and 18 independent numbers for zero, first and second order sets of coefficients. Thus zero and first order together would accommodate four particles exactly, while zero, first and second order approximations fits the kinematic properties of ten grains. Note, that it is not necessary that the same order of displacements and spins be used in the same application.

Table 1

	Order	**Displacements**	**Spins**	**Exact number of particles**
2 dimensions	0	2	1	1
	1	4	2	3
	2	6	3	6
3 dimensions	0	3	3	1
	1	9	9	4
	2	18	18	10

In two dimensions a small assembly consisting of one particle surrounded by five others is a very reasonable representation for a densely packed situation. In three dimensions one particle surrounded by nine others is similarly useful for a dense packing. The neighbors need not all touch the central particle; they are merely required to fill the space. The smallest useful assembly would then consist of one particle and its immediate neighbors, described by the zero, first and second order approximation.

Objectivity

The issue of objectivity is conveniently addressed using the fact that force and moment equilibrium are here formulated in terms of displacements and spins. It is shown that the anti-symmetric part of the 'distortion' $\mathbf{U}^{1,\mu}$ can be eliminated from the force equilibrium equation. To demonstrate this, the displacement difference between two adjacent particles is written as $u_i^{\mu}-u_i^{\nu}=U_{ij}^{1,\mu}c_j^{\mu\nu}+$ higher orders.

The sums of the spins that appear in the equilibrium equations for each particle are equal to some constant vector $\boldsymbol{\eta}$ plus other terms. The displacement of the contact in the equilibrium equations takes the form

$$\left\{ \tfrac{1}{2}\left(U_{ij}^{1,\mu}+U_{ji}^{1,\mu}\right)+\tfrac{1}{2}\left(U_{ij}^{1,\mu}-U_{ji}^{1,\mu}\right) \right\} \; c_j^{\mu\nu}-\tfrac{1}{2}\varepsilon_{ijk}c_j^{\mu\nu}\eta_k^{\mu}+ \text{ other terms } . \tag{8}$$

The anti-symmetric tensor can always be written as

$$\tfrac{1}{2}\left(U_{ij}^{1,\mu}-U_{ji}^{1,\mu}\right)=\varepsilon_{ijk}\varpi_k \, , \tag{9}$$

where $\boldsymbol{\varpi}$ is a vector. Therefore, only the vector difference $\varpi_k-\eta_k^{\mu}$ appears in the equilibrium equations, thus ensuring objectivity.

Thus, the anti-symmetric part of $\mathbf{U}^{1,\mu}$ is subtracted from the lowest order term in the spin approximation $\boldsymbol{\Omega}^{0,\mu}$. The spin approximation corrected in this way is called $\bar{\boldsymbol{\Omega}}^{0,\mu}$. The result is that when the displacement difference $\mathbf{u}^{\mu}-\mathbf{u}^{\nu}$ is approximated in the equilibrium equations, the symmetric part of $\mathbf{U}^{1,\mu}$, which will be denoted by $\mathbf{E}^{1,\mu}$, occurs only in combination with the objective difference in the rotations.

Structural sums

Structural sums involve sums over neighbouring particles of the product of the interactive tensor $\mathbf{K}^{\mu\nu}$ with any number of components of the connecting vectors $\mathbf{c}^{\mu\nu}$. They are called **A**

$$A_{pq}^{\mu}\equiv\sum_{\nu=1}^{N^{\mu}}K_{pq}^{\mu\nu} \, , \; A_{pqr}^{\mu}\equiv\sum_{\nu=1}^{N^{\mu}}K_{pq}^{\mu\nu}c_r^{\mu\nu} \, , \; A_{pqrs}^{\mu}\equiv\sum_{\nu=1}^{N^{\mu}}K_{pq}^{\mu\nu}c_r^{\mu\nu}c_s^{\mu\nu} \, , \; \textit{etc.} \tag{10}$$

The summation is over all the nearby particles in the small assembly; the number is of these is N^{μ}. However, for non-contacting particles the interactive tensor is zero, so that in the evaluation of the structural sums, only the number of contacting neighbours appears.

The question that needs to be addressed is, up to what rank of these tensors is reasonable to employ? In principle the tensors can be 'measured' in a numerical simulation and there is no upper limit to the order that can be determined. However, higher order structural sums contain angular variations over arcs that are far smaller than a particle diameter and add little or no useful information on the spatial distribution of the interactive tensors.

The equilibrium equations for each particle are expressed in the kinematic variables, truncated to neglect structural sums representing a moment that is higher than two:

$$A_{pij}^{\mu}\left(E_{ij}^{1,\mu}+\varepsilon_{ijk}\bar{\Omega}_k^{0,\mu}\right)+\tfrac{1}{2}A_{pijk}^{\mu}\left(E_{ijk}^{2,\mu}+\varepsilon_{ijl}\bar{\Omega}_{lk}^{1,\mu}\right)=0 \, ; \tag{11}$$

and

$$\varepsilon_{pqr}A_{rijq}^{\mu}\left(E_{ij}^{1,\mu}+\varepsilon_{ijk}\bar{\Omega}_k^{0,\mu}\right)=0 \, . \tag{12}$$

If the order of the structural sum had not have been cut off, then the force equation would remain unaltered, but the moment equation would have had two additional terms, both proportional to the third order structural sum; these terms are $\frac{1}{2}\varepsilon_{pqr}A^{\mu}_{rijqs}\left(E^{2,\mu}_{ijs}+\varepsilon_{ijk}\bar{\Omega}^{1,\mu}_{ks}\right)$. Now, both the third order structural sum and the two higher order kinematic variables have vanishing mean value and their inclusion in the rotation equation needs to be compared with the terms in equation (12). Here, we assume that this product of fluctuating terms is small compared to the terms of lowest order.

3. The incremental stress

The force equilibrium equation (11) may be recast by writing the double gradients as derivatives of the first gradients. This leads to

$$A^{\mu}_{pij}\left(E^{1,\mu}_{ij}+\varepsilon_{ijk}\bar{\Omega}^{0,\mu}_{k}\right)+\tfrac{1}{2}A^{\mu}_{pijk}\frac{\partial}{\partial x_k}\left(E^{1,\mu}_{ij}+\varepsilon_{ijl}\bar{\Omega}^{0,\mu}_{l}\right)=0\,. \tag{13}$$

This form is used to motivate the introduction of a stress increment $\boldsymbol{\sigma}$. A stress increment describes equilibrium when $\partial\sigma_{ij}/\partial x_j=0$; furthermore, the stress increment is expected to be symmetric. The one-particle equilibrium equation is modified slightly to read

$$\frac{\partial}{\partial x_k}\left[A_{pijk}\left(E^{1}_{ij}+\varepsilon_{ijl}\bar{\Omega}^{0}_{l}\right)\right]=-\left(2A^{\mu}_{pij}-\frac{\partial A_{pijk}}{\partial x_k}\right)\left(E^{1,\mu}_{ij}+\varepsilon_{ijk}\bar{\Omega}^{0,\mu}_{k}\right), \tag{14}$$

where all derivatives are evaluated at $\mathbf{x}^{\mu}$.

Because $\varepsilon_{pqr}A^{\mu}_{rijq}\left(E^{1,\mu}_{ij}+\varepsilon_{ijk}\bar{\Omega}^{0,\mu}_{k}\right)=0$, a reasonable symmetric stress increment is $\sigma_{rq}\left(\mathbf{x}^{\mu}\right)=(2v)^{-1}A^{\mu}_{rijq}\left(E^{1,\mu}_{ij}+\varepsilon_{ijk}\bar{\Omega}^{0,\mu}_{k}\right)$, where v is the volume per particle. This is a local form of the generally accepted definition of the particle stress (e.g., Love (1944), Dantu and Weber (1968), Drescher and de Josselin de Jong (1972), Lätzel *et al* (2000)), although other definitions are possible (Babic (1997), Goldhirsh and Goldenberg (2002), Zhu and Yu (2002)). However, this local form does not necessarily possess the property that $\partial\sigma_{ij}/\partial x_j=0$. The latter form of the equilibrium equation is not valid for a single particle, though there may be circumstances in which the right-hand side of (14) vanishes.

The rotational equilibrium equation is solved for $\bar{\boldsymbol{\Omega}}^{0}$

$$\bar{\Omega}^{0,\mu}_{l}=-\left(\mathbf{B}^{\mu}\right)^{-1}_{lp}\varepsilon_{pqr}A^{\mu}_{rijq}E^{1,\mu}_{ij}\,,\ \text{where}\ B^{\mu}_{pk}\equiv\varepsilon_{pqr}\varepsilon_{ijk}A^{\mu}_{rijq}\,. \tag{15}$$

The key constitutive tensor is therefore

$$Z^{\mu}_{pkst}\equiv A^{\mu}_{pstk}-\varepsilon_{nqr}\varepsilon_{ijl}A^{\mu}_{pijk}\left(\mathbf{B}^{\mu}\right)^{-1}_{ln}A^{\mu}_{rstq}\,. \tag{16}$$

In this way, the local incremental stress-strain relation takes the form

$$\sigma_{pk}\left(\mathbf{x}^{\mu}\right)=(2v)^{-1}Z^{\mu}_{pkst}E_{st}\left(\mathbf{x}^{\mu}\right). \tag{17}$$

The equilibrium equation, expressed in the local stiffness **Z** is, then,

$$\frac{\partial}{\partial x_k}\left(Z_{pkst}E^{l}_{st}\right)=-\left(2A^{\mu}_{pij}-\frac{\partial A_{pijk}}{\partial x_k}\right)\left(E^{l,\mu}_{ij}-\varepsilon_{ijl}\left(\mathbf{B}^{\mu}\right)^{-1}_{ln}\varepsilon_{nqr}A^{\mu}_{rstq}E^{l,\mu}_{st}\right)=0. \tag{18}$$

In a perfectly uniform medium, odd structural sums and spatial derivatives of structural sums vanish. In this case the stiffness of the medium is simply $(2v)^{-1}\mathbf{Z}$. When the medium is non-uniform the mean stress is found from equation (17). Denoting averages by an over bar and fluctuations by a prime, the mean stress can be written as

$$\bar{\sigma}_{pk}=(2v)^{-1}\bar{Z}_{pkst}\bar{E}_{st}+(2v)^{-1}\overline{Z'_{pkst}E'_{st}}. \tag{19}$$

The second term on the right-hand side is a vital element in the prediction of the overall stiffness for realistic granular medium. Equation (18) may be deployed to find the correlation between the fluctuations in the structural sums and the strain fluctuations, but this is not a trivial task.

4. Homogenisation

There are various methods by which the strain fluctuations can be obtained. These include the pair-fluctuation method (Jenkins (1997)), or more general inclusion methods (Torquato (2002)) and cumulant neglect methods (Beran (1968)), such as Kröner's (1967). These methods all result in predictions of overall mechanical properties from the statistical distributions of the micro-mechanical features.

In this paper, we make the rather arbitrary choice to employ an adaptation of Kröner's method. In order to do this, the discrete third rank tensor **A** in equation (14) needs to be expressed as a partial derivative of an even structural sum. This is plausible, because the asymmetry that is represented in the odd structural sum is closely associated with systematic variation of contact properties across the particle. The simplest assumption of this type that can be made is that

$$A^{\mu}_{ijk}=\tfrac{1}{2}\Lambda^{\mu}_{ijklmn}\left(\left.\frac{\partial A_{lmnp}}{\partial x_p}\right|_{\mathbf{x}^{\mu}}+\left.\frac{\partial A_{lmpn}}{\partial x_p}\right|_{\mathbf{x}^{\mu}}\right). \tag{20}$$

Below, it will be shown that only the aggregate-averaged value $\bar{\mathbf{\Lambda}}$ of the tensor $\mathbf{\Lambda}^{\mu}$ enters.

The simplest possible form for $\bar{\mathbf{\Lambda}}$ is now discussed. For elastic interactions, the tensor **K** is symmetric, implying symmetry in the subscripts (i, j) and (l, m). For an isotropic material the sixth rank tensor in equation (20) is reduced to a simple isotropic tensor. Introducing four non-dimensional coefficients $\bar{\lambda}_{1..4}$ this assumption leaves

$$\bar{\Lambda}_{ijk\mathit{l}mn} = \bar{\lambda}_1\delta_{ij}\delta_{\mathit{l}m}\delta_{kn} + \bar{\lambda}_2\delta_{ij}\left(\delta_{k\mathit{l}}\delta_{mn} + \delta_{km}\delta_{\mathit{l}n}\right) + \bar{\lambda}_3\delta_{\mathit{l}m}\left(\delta_{ik}\delta_{jn} + \delta_{jk}\delta_{in}\right) + \bar{\lambda}_4\delta_{kn}\left(\delta_{i\mathit{l}}\delta_{jm} + \delta_{im}\delta_{j\mathit{l}}\right). \qquad (21)$$

In general, the components of $\bar{\mathbf{\Lambda}}$ will evolve with the deviatoric component of the mean total strain and, in this way, isotropy is be lost.

5. An example: the isotropic, perfectly random aggregate

Formula (19) may be viewed as a two-step way to estimate the overall incremental stiffness of a granular aggregate. The first term on the right hand side gives the mean field approximation; the second term represents the correction due to fluctuations in the assembly. In order to illustrate the concepts discussed in the previous sections, an example is worked out that demonstrates the effect of the latter term. As mentioned before, the method chosen here is an adaptation of Kröner's (1967) method, which is done for an isotropic two-dimensional material. This material may be subjected either to an increment of deviatoric strain or a further increment of isotropic strain. Refinements to cope with anisotropy induced by an applied overall deviatoric strain may be implemented at the cost of significantly more algebra. The results are given in equations (33) and (34).

In Kröner's method the equilibrium equations are approximated to first order in the fluctuations. This is valid while the fluctuations in the stiffness tensor of the problem are small compared to the mean value. There is evidence (Gaspar (2001)) that in granular materials that have been subjected to a deviatoric strain that is a significant fraction of the isotropic strain, the fluctuations may be sizeable; then more sophisticated homogenisation methods than the one discussed here need to be employed. It is immediately seen that neglecting the higher order terms in the fluctuations implies that only the average of $\mathbf{\Lambda}^{\mu}$ is required.

An estimate for the fluctuation in the deformation is now obtained. The odd structural sum in the right hand side of the equilibrium equation – either equation (14) or equation (18) – is expressed as a derivative according to equation (20). The connection between the spin tensor and the local strain is given by equation (15). Introducing a tensor $\mathbf{T}^{\mu}$, defined as $T^{\mu}_{ijst} = \delta_{is}\delta_{jt} - \varepsilon_{ij\mathit{l}}\varepsilon_{pqr}\left(\mathbf{B}^{\mu}\right)^{-1}_{\mathit{l}p} A^{\mu}_{rstq}$, the equilibrium equation may be written in terms of averages and fluctuations. As noted above, only first order terms in the fluctuations are retained; averages are denoted by an overbar and fluctuations by a prime. Equation (14) is then cast in the form

$$\bar{A}_{pijk}\bar{T}_{ijst}\frac{\partial E'_{st}}{\partial x_k} = -\bar{A}_{pijk}\frac{\partial T'_{ijst}}{\partial x_k}\bar{E}_{st} - \bar{\Lambda}_{pij\mathit{l}mn}\left(\left.\frac{\partial A'_{\mathit{l}mnq}}{\partial x_q}\right|_{\mathbf{x}} + \left.\frac{\partial A'_{\mathit{l}mqn}}{\partial x_q}\right|_{\mathbf{x}}\right)\bar{T}_{ijst}\bar{E}_{st}. \qquad (22)$$

The gradient of the strain fluctuations is written as double gradients of displacement fluctuations

$$\frac{\partial E'_{st}}{\partial x_k} = \tfrac{1}{2}\left(\frac{\partial^2 u'_s}{\partial x_t \partial x_k} + \frac{\partial^2 u'_t}{\partial x_s \partial x_k}\right). \qquad (23)$$

The assumption of isotropy implies that the mean structural sum $\bar{\mathbf{A}}$ is isotropic. Thus with the introduction of two material constants $\bar{\nu}$ and $\bar{\varepsilon}$, one may write

$$\bar{A}_{pijk} = \bar{\nu}\delta_{pi}\delta_{kj} + \bar{\varepsilon}\left(\delta_{pk}\delta_{ij} + \delta_{pj}\delta_{ki}\right). \tag{24}$$

This form respects the symmetry in the subscripts j and k and also in p and i. The latter implies that the interactive tensor is symmetric and therefore represents an elastic interaction. The isotropy assumption together with the symmetry property of the strain results in $\bar{T}_{ijst}E_{st} = E_{ij}$.

A tensor $\mathbf{S}'$ is introduced as

$$S'_{pijq}(\mathbf{x}) \equiv \bar{A}_{pstq}T'_{stij}(\mathbf{x}) + \bar{\Lambda}_{pijlmn}\left[A'_{lmnq}(\mathbf{x}) + A'_{lmqn}(\mathbf{x})\right]. \tag{25}$$

Equation (22) takes the form

$$\tfrac{1}{2}\left(\bar{\nu}+\bar{\varepsilon}\right)\frac{\partial^2 u'_p}{\partial x_q^2} + \tfrac{1}{2}\left(\bar{\nu}+3\bar{\varepsilon}\right)\frac{\partial^2 u'_q}{\partial x_p \partial x_q} + \frac{\partial S'_{pijq}}{\partial x_q}\bar{E}_{ij} = 0. \tag{26}$$

Spatial Fourier transformation of the fluctuating quantities (denoted by a hat) with wave vector **k** yields the following solution for the incremental displacement gradient fluctuation

$$ik_s\hat{u}_p = 2k_q k_s\left[\frac{\delta_{pr}}{k^2\left(\bar{\varepsilon}+\bar{\nu}\right)} - \frac{k_p k_r\left(3\bar{\varepsilon}+\bar{\nu}\right)}{2k^4\left(\bar{\varepsilon}+\bar{\nu}\right)\left(2\bar{\varepsilon}+\bar{\nu}\right)}\right]\hat{S}_{rijq}\bar{E}_{ij}. \tag{27}$$

The inverse transform is

$$\frac{\partial u'_p}{\partial x_s}(\mathbf{x}) = \frac{2\bar{E}_{ij}}{(2\pi)^2}\int d^2y \int d^2k S'_{rijq}\left(\mathbf{x}+\mathbf{y}\right)k_q k_s e^{i\mathbf{k}.\mathbf{y}}\left[\frac{\delta_{pr}}{k^2\left(\bar{\varepsilon}+\bar{\nu}\right)} - \frac{k_p k_r\left(3\bar{\varepsilon}+\bar{\nu}\right)}{2k^4\left(\bar{\varepsilon}+\bar{\nu}\right)\left(2\bar{\varepsilon}+\bar{\nu}\right)}\right]. \tag{28}$$

The integrand peaks sharply for $\mathbf{y} \to 0$ and the 'local' contribution is obtained by calculating

$$\frac{2\bar{E}_{ij}}{(2\pi)^2}S'_{rijq}\left(\mathbf{x}\right)\int_R d^2y \int d^2k k_q k_s e^{i\mathbf{k}.\mathbf{y}}\left[\frac{\delta_{pr}}{k^2\left(\bar{\varepsilon}+\bar{\nu}\right)} - \frac{k_p k_r\left(3\bar{\varepsilon}+\bar{\nu}\right)}{2k^4\left(\bar{\varepsilon}+\bar{\nu}\right)\left(2\bar{\varepsilon}+\bar{\nu}\right)}\right], \tag{29}$$

where R is a small circle. The integrals are evaluated, which leaves the following estimate for the displacement gradient fluctuations

$$\left.\frac{\partial u'_a}{\partial x_b}\right|_{\mathbf{x}} = -\tfrac{1}{2}S'_{pijq}(\mathbf{x})\bar{E}_{ij}\left(\frac{2\delta_{ap}\delta_{qb}}{\bar{\varepsilon}+\bar{\nu}} - \tfrac{1}{4}\frac{\left(3\bar{\varepsilon}+\bar{\nu}\right)\left(\delta_{ap}\delta_{qb}+\delta_{aq}\delta_{pb}+\delta_{ab}\delta_{pq}\right)}{\left(\bar{\varepsilon}+\bar{\nu}\right)\left(2\bar{\varepsilon}+\bar{\nu}\right)}\right); \tag{30}$$

The non-local contributions are neglected, which is permitted when the material is perfectly random. In this respect Kröner's method resembles inclusion methods.

Bearing in mind the impact that with isotropy $\varepsilon_{nqr}\varepsilon_{ijl}A^{\mu}_{pijk}\left(\mathbf{B}^{\mu}\right)^{-1}_{ln}A^{\mu}_{rstq}\overline{E}_{st}=0,.$, a first estimate of the overall stress increment is

$$\overline{\sigma}_{rq}=(2v)^{-1}\overline{A}_{rijq}\overline{E}^{1}_{ij}+\frac{(2v)^{-1}}{2}\overline{Z^{/}_{rijq}\left(\frac{\partial u^{/}_{i}}{\partial x_{j}}+\frac{\partial u^{/}_{j}}{\partial x_{i}}\right)}. \tag{31}$$

It is seen from this formula that the overall stiffness tensor is a function of the parameters $\overline{\nu}$ and $\overline{\varepsilon}$, as well as the auto and cross correlation of the components of the tensor $\mathbf{A}^{/}$. The Kronecker deltas in formulas (21) and (30) indicate which of the possible correlation combinations are important. They are somewhat limited by the symmetry relations of $\mathbf{A}^{/}$: there is symmetry in the last two subscripts and the assumption of an elastic contact interaction implies symmetry in the first two subscripts. Furthermore, the assumption of isotropy also extends to the correlations, so that, for example, $\overline{\left(A^{/}_{1111}\right)^{2}}=\overline{\left(A^{/}_{2222}\right)^{2}}$. Taking this into account, the correlation between the following pairs of components need to be incorporated: $\overline{\left(A^{/}_{1111}\right)^{2}}$, $\overline{\left(A^{/}_{1212}\right)^{2}}$, $\overline{\left(A^{/}_{1212}A^{/}_{1111}\right)}$, $\overline{\left(A^{/}_{1211}\right)^{2}}$, $\overline{\left(A^{/}_{1112}A^{/}_{1211}\right)}$, $\overline{\left(A^{/}_{1112}\right)^{2}}$, $\overline{\left(A^{/}_{2222}A^{/}_{1111}\right)}$. Thus seven extra material parameters are to be provided to describe the effect of heterogeneity on the overall behaviour.

A further simplification is required. The approximation is introduced that the fluctuations in the structural sums are themselves generated by isotropic tensors of the form

$$A^{/}_{pijk}=\nu^{/}\delta_{pi}\delta_{kj}+\varepsilon^{/}\left(\delta_{pk}\delta_{ij}+\delta_{pj}\delta_{ki}\right). \tag{32}$$

For this isotropic case the tensor $B^{\mu}_{pk}=\varepsilon_{pqr}\varepsilon_{ijk}A^{\mu}_{rijq}$ takes a diagonal form and $T^{\mu}_{ijst}=2\delta_{is}\delta_{jt}-\delta_{it}\delta_{js}$; the latter is a constant and as a consequence the assumption causes the elimination of the first term in the definition (25) of $\mathbf{S}^{/}$. Now, the overall stiffness is expressed in the averages $\overline{\nu}$ and $\overline{\varepsilon}$, as well as the correlations $\overline{\left(\nu^{/}\right)^{2}}$, $\overline{\left(\varepsilon^{/}\right)^{2}}$ and $\overline{\left(\varepsilon^{/}\nu^{/}\right)}$. The overall bulk and shear moduli are then

$$K=\frac{(2v)^{-1}}{2}\left(3\overline{\varepsilon}+\overline{\nu}\right)+$$
$$-\frac{(2v)^{-1}}{\left(2\overline{\varepsilon}+\overline{\nu}\right)}\left[3\overline{\left(\varepsilon^{/}\right)^{2}}\left[\overline{\lambda}_{1}+3\left(\overline{\lambda}_{2}+\overline{\lambda}_{3}+\overline{\lambda}_{4}\right)\right]+2\overline{\left(\varepsilon^{/}\nu^{/}\right)}\left[2\overline{\lambda}_{1}+3\left(\overline{\lambda}_{2}+2\overline{\lambda}_{3}+\overline{\lambda}_{4}\right)\right]+\overline{\left(\nu^{/}\right)^{2}}\left(\overline{\lambda}_{1}+\overline{\lambda}_{2}+3\overline{\lambda}_{3}+\overline{\lambda}_{4}\right)\right], \tag{33}$$

$$G=\frac{(2v)^{-1}}{2}\left(\overline{\varepsilon}+\overline{\nu}\right)+$$
$$-\frac{(2v)^{-1}\left(5\overline{\varepsilon}+3\overline{\nu}\right)}{2\left(\overline{\varepsilon}+\overline{\nu}\right)\left(2\overline{\varepsilon}+\overline{\nu}\right)}\left[\overline{\left(\varepsilon^{/}\right)^{2}}\left(\overline{\lambda}_{1}+3\overline{\lambda}_{2}+\overline{\lambda}_{3}+\overline{\lambda}_{4}\right)+2\overline{\left(\varepsilon^{/}\nu^{/}\right)}\left(\overline{\lambda}_{1}+2\overline{\lambda}_{2}+\overline{\lambda}_{3}+\overline{\lambda}_{4}\right)+\overline{\left(\nu^{/}\right)^{2}}\left(\overline{\lambda}_{1}+\overline{\lambda}_{2}+\overline{\lambda}_{3}+\overline{\lambda}_{4}\right)\right]. \tag{34}$$

The material properties described by expressions (33) and (34) still require nine parameters. By making additional assumptions this number is further reduced.

6. CONSTANT CONTACT STIFFNESSES

The incremental contact stiffness tensor **K** is a key parameter in the evaluation of the structural sums. In general it will depend on the actual total contact force as well as the direction of the contact. The direction of the contact unit normal pointing from particle μ to particle ν is called $\mathbf{n}^{\mu\nu}$ and this is the principal anisotropy direction for the contact stiffness tensor. The components of $\mathbf{K}^{\mu\nu}$ are decomposed in directions parallel and normal to $\mathbf{n}^{\mu\nu}$. Bearing in mind the elastic symmetry of $\mathbf{K}^{\mu\nu}$, the general form for the tensor is

$$K_{ij}^{\mu\nu} = k^{(n)\mu\nu} n_i^{\mu\nu} n_j^{\mu\nu} + k^{(t)\mu\nu} \left(\delta_{ij} - n_i^{\mu\nu} n_j^{\mu\nu} \right). \tag{35}$$

This form takes care of the directional aspect of $\mathbf{K}^{\mu\nu}$. The coefficients $k^{(n)}$ and $k^{(t)}$ may depend on the total force across the contact.

Two limiting cases are distinguished to illustrate the physical meaning of (35). . When a contact has the property that $k^{(t)} = 0$, no tangential force increment is generated and the contact slides. The other extreme is when $k^{(t)}$ is nonzero; in this condition a tangential force increment may be generated and such contacts are here called 'sticking' contacts. Generally speaking, of course, a whole range of possibilities may occur, depending on the nature of the contact law.

Below a number of measures for contact numbers are needed. The two parameters that have already been introduced are the total number of particles in the assembly, N, and the number of not necessarily touching neighbours of μ, N^{μ}. The subscript c denotes parameters pertaining to touching particles; for example, the number of contacts of particle ν is N_c^{ν}. The assembly average of N^{μ} is denoted by $\overline{N}$. A local neighbourhood mean in the vicinity of particle μ is indicated by brackets.

The parameter $\overline{N}$ may be related to the packing properties of the aggregate through the solids volume fraction. In two dimensions the mean solids area of a particle plus its neighbours equals $\pi \overline{N} D^2 / 8$, while the total area of the enclosed assembly equals $\frac{1}{2} \overline{N} D^2 \sin\left(\pi\left(\overline{N} - 2\right)/\overline{N}\right)$; thus the solids volume fraction ϕ is related to $\overline{N}$ as $\phi = \frac{1}{4}\pi / \sin\left[\pi\left(\overline{N} - 2\right)/\overline{N}\right]$. The other parameter that appears in the theory is the volume per particle v, which is $v = \frac{1}{4}\pi D^2 / \phi$.

In this section the simplifying assumption is made that the values of $k^{(n)}$ and $k^{(t)}$ are constant throughout the medium. This situation can only be created by numerical means, as in reality a variable, total contact force dependent, contact law applies. However, by making the simplification, an impression of the order of magnitude of the various parameters in the theory is obtained. The structural sum $\overline{\mathbf{A}}$ is determined by replacing the sum with an integral, weighted with a mean angular contact number distribution $p(\theta)$:

$$\overline{A}_{pqrs} \equiv \overline{\sum_{\nu=1}^{N^{\mu}} K_{pq}^{\mu\nu} c_r^{\mu\nu} c_s^{\mu\nu}} \rightarrow \int_0^{2\pi} p(\theta) \left[k^{(n)} n_p n_q + k^{(t)} \left(\delta_{pq} - n_p n_q \right) \right] c_r c_s \, d\theta . \tag{36}$$

In isotropy, $p(\theta)$ is a constant, p, which is related to the mean number of contacts $\bar{N}_c$ through $p = \bar{N}_c/(2\pi)$. As the magnitude of **c** for small indentations approximates the diameter of the particles D, the integral in equation (36) is easily evaluated. The phenomenological coefficients $\bar{\nu}$ and $\bar{\varepsilon}$ are identified as

$$\bar{\nu} = \frac{D^2 \bar{N}_c}{8}\left(k^{(n)} + 3k^{(t)}\right) \text{ and } \bar{\varepsilon} = \frac{D^2 \bar{N}_c \left(k^{(n)} - k^{(t)}\right)}{8}. \tag{37}$$

For constant contact stiffnesses the coefficients $\bar{\lambda}_{1..4}$ can also be investigated further; this leads to the expressions for the shear and bulk moduli that are given in equations (50) and (51). To begin the investigation a volume integral over a small assembly with volume V^μ and area A^μ is taken of expression (20); Gauss' theorem is applied to give

$$A^\mu_{ijk} V^\mu = \tfrac{1}{2} \bar{\Lambda}_{ijk\,lmn} \oint_{A^\mu} \left(A_{lmnp} + A_{lmpn} \right) n_p dA. \tag{38}$$

In two dimensions the volume is approximately a circular disc with radius D. Thus, the volume V^μ may be replaced by πD^2. The integral on the right-hand side of Equation (38) is replaced by a summation over the neighbouring particles; the area dA is substituted with its approximation $2\pi D / N^\mu$. This gives

$$DA^\mu_{ijk} = \frac{1}{N^\mu} \bar{\Lambda}_{ijk\,lmn} \sum_{\nu=1}^{N^\mu} n_p^{\mu\nu} \left(A^\nu_{lmnp} + A^\nu_{lmpn} \right). \tag{39}$$

The coefficients of $\bar{\Lambda}$ follow from

$$\sum_{\mu=1}^{N} \left(DA^\mu_{ijk} - \frac{1}{N^\mu} \bar{\Lambda}_{ijk\,lmn} \sum_{\nu=1}^{N^\mu} n_p^{\mu\nu} \left(A^\nu_{lmnp} + A^\nu_{lmpn} \right) \right)^2 = \min \tag{40}$$

The intention is to insert the form (21), then differentiate with respect to the coefficients $\bar{\lambda}_{1..4}$ and solve the resulting equations. Before carrying this out, $\sum_{\nu=1}^{N^\mu} n_p^{\mu\nu} \left(A^\nu_{lmnp} + A^\nu_{lmpn} \right)$ is modelled. The structural sums $\mathbf{A}^\nu$ are approximated as in expression (24); the number of contacts for each sum is N_c^ν, which implies $p^\nu = N_c^\nu/(2\pi)$. In reality the local structural sums may be anisotropic and modelling them as isotropic ones is only true in approximation. At the same time, this approximation is analogous to the assumption introduced in (32) and therefore consistent with the other assumptions that have been made in order to arrive at an isotropic theory. It results in the following:

$$A^{\nu}_{lmnp} = \tfrac{1}{2} N_c^{\nu} D^2 \left[\tfrac{1}{4}\left(k^{(n)} - k^{(t)}\right)\left(\delta_{lm}\delta_{np} + \delta_{ln}\delta_{mp} + \delta_{lp}\delta_{mn}\right) + k^{(t)}\delta_{lm}\delta_{np} \right]. \tag{41}$$

Inspection of this form reveals that the quantity $\sum_{\nu=1}^{N^{\mu}} n_p^{\mu\nu}\left(A^{\nu}_{lmnp} + A^{\nu}_{lmpn}\right)$ is essentially dependent on the odd angular distribution around particle μ of the contact numbers of the neighbours N_c^{ν}.

A first rough approximation is introduced to obtain an impression of the odd angular distribution of the contact numbers; it is assumed that it can be represented by a simple vector relation: $V_i^{\mu} n_i(\theta)$. The quantity $\sum_{\nu=1}^{N^{\mu}} n_p^{\mu\nu}\left(A^{\nu}_{lmnp} + A^{\nu}_{lmpn}\right)$ is then approximated as

$$\sum_{\nu=1}^{N^{\mu}} n_p^{\mu\nu}\left(A^{\nu}_{lmnp} + A^{\nu}_{lmpn}\right) = D^2\left[\tfrac{1}{4}\left(k^{(n)} - k^{(t)}\right)\left(\delta_{lm}\delta_{np} + \delta_{ln}\delta_{mp} + \delta_{lp}\delta_{mn}\right) + \delta_{lm}\delta_{np}k^{(t)} \right] V_i^{\mu} \int_0^{2\pi} n_p n_i d\theta. \tag{42}$$

The remaining integral is easily performed and yields $\pi\delta_{ip}$.

The odd structural sum in equation (40) may be modelled in a similar manner. The contacts of particle μ have an odd distribution according to a vector relation of the form $W_i^{\mu} n_i(\theta)$, which leaves

$$A^{\mu}_{ijk} = \pi D W_p^{\mu}\left[\tfrac{1}{4}\left(k^{(n)} - k^{(t)}\right)\left(\delta_{ij}\delta_{kp} + \delta_{ip}\delta_{jk} + \delta_{ik}\delta_{jp}\right) + k^{(t)}\delta_{ij}\delta_{kp} \right]. \tag{43}$$

The product $\bar{\Lambda}_{ijklmn}\left(N^{\mu}\right)^{-1}\sum_{\nu=1}^{N^{\mu}} n_p^{\mu\nu}\left(A^{\nu}_{lmnp} + A^{\nu}_{lmpn}\right)$ with the isotropic expression (21) for $\bar{\mathbf{\Lambda}}$ gives a form that – insofar as its dependence on $\bar{\lambda}_{1..4}$ is concerned – depends on two quantities only; these are called X and Y

$$X \equiv k^{(n)}\left(2\bar{\lambda}_1 + 4\bar{\lambda}_2 + 4\bar{\lambda}_3 + 3\bar{\lambda}_4\right) + k^{(t)}\left(2\bar{\lambda}_1 + 4\bar{\lambda}_3 + \bar{\lambda}_4\right), \tag{44}$$

$$Y \equiv k^{(n)}\left(2\bar{\lambda}_3 + \bar{\lambda}_4\right) + k^{(t)}\left(2\bar{\lambda}_3 - \bar{\lambda}_4\right). \tag{45}$$

This does not constitute an under-representation of the problem in that four λs are represented by two coefficients X and Y. Next, $\mathbf{A}'$ is calculated using (42), that is, N_c^{ν} is replaced with N_c'. It transpires that

$$\varepsilon' = \nu' \frac{k^{(n)} - k^{(t)}}{k^{(n)} + 3k^{(t)}}, \tag{46}$$

and substituting this into the expressions for the bulk and shear modulus - (33) and (34) - the only two coefficients that remain (and that have physical significance) are $k^{(n)}\left(\bar{\lambda}_1 + 2\bar{\lambda}_2 + 3\bar{\lambda}_3 + 2\bar{\lambda}_4\right) + k^{(t)}\left(\bar{\lambda}_1 + 3\bar{\lambda}_3\right)$ for the bulk modulus and

$k^{(n)}\left(\bar{\lambda}_1+2\bar{\lambda}_2+\bar{\lambda}_3+\bar{\lambda}_4\right)+k^{(t)}\left(\bar{\lambda}_1+\bar{\lambda}_3+\bar{\lambda}_4\right)$ for the shear modulus. These two parameters are easily expressed in terms of X and Y as $\frac{1}{2}\left(X+Y\right)$ and $\frac{1}{2}\left(X-Y\right)$, respectively.

The determination of X and Y in terms of the vectors **V** and **W** is elementary. The approximations (42) and (43) are introduced into the functional (40), as is (21); then, the number of neighbours, N^{μ}, is approximated by its average value $\bar{N}$ and differentiation with respect to X and Y is carried out, which results in the following two equations

$$\left(X-Y\right)\sum_{\mu=1}^{N}\left(V_i^{\mu}\right)^2-\bar{N}\left(k^{(n)}+k^{(t)}\right)\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right)=0\,, \tag{47}$$

$$\left(X-3Y\right)\sum_{\mu=1}^{N}\left(V_i^{\mu}\right)^2-2\bar{N}k^{(t)}\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right)=0\,. \tag{48}$$

The solution is

$$X=\frac{\left(3k^{(n)}+k^{(t)}\right)\bar{N}}{2\sum_{\mu=1}^{N}\left(V_i^{\mu}\right)^2}\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right)\ \text{and}\ Y=\frac{\left(k^{(n)}-k^{(t)}\right)\bar{N}}{2\sum_{\mu=1}^{N}\left(V_i^{\mu}\right)^2}\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right). \tag{49}$$

The bulk and shear moduli - expressions (33) and (34) – are also expressed in the parameters of the contact stiffness tensor; they become

$$K=\frac{(2v)^{-1}}{4}D^2\bar{N}_c k^{(n)}-\frac{(2v)^{-1}D^2\overline{\left(N_c^{/}\right)^2}k^{(n)}\left(X+Y\right)}{2\bar{N}_c\left(3k^{(n)}+k^{(t)}\right)}, \tag{50}$$

$$G=\frac{(2v)^{-1}}{8}D^2\bar{N}_c\left(k^{(n)}+k^{(t)}\right)-\frac{(2v)^{-1}D^2\overline{\left(N_c^{/}\right)^2}\left(2k^{(n)}+k^{(t)}\right)\left(X-Y\right)}{4\bar{N}_c\left(3k^{(n)}+k^{(t)}\right)}. \tag{51}$$

Finally, estimates for the correlations $\overline{\left(N_c^{/}\right)^2}/\bar{N}_c^2$ and $\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right)/\sum_{\mu=1}^{N}\left(V_i^{\mu}\right)^2$ are required. The vector $\mathbf{V}^{\mu}$ describes the asymmetry in the number of contacts of particles that neighbour particle μ. This number is correlated with the asymmetry of the number of contacts of particle μ itself. The neighbouring particles ν possess three kinds of contacts (not necessarily touching): (1) contacts with particle μ, (2) contacts with other neighbours ν and (3) contacts with particles that are neither μ nor neighbours of μ. A deterministic correlation between the asymmetry of contacts of μ and the number of contacts of the neighbours ν can only be established through contacts of category (1). The latter represents one contact per neighbour, that is, a fraction of the number of contacting particles of the neighbours ν of $1/\left\langle N_c^{\nu}\right\rangle_{\mu}$. Thus, if the correlation were perfect and the two vectors $\mathbf{V}^{\mu}$ and $\mathbf{W}^{\mu}$ were

perfectly aligned, their magnitudes would be related by the form $\left|\bar{\mathbf{V}}\right| = \left(\left\langle N_c^{\nu}\right\rangle_{\mu}\right)^{-1}\left|\bar{\mathbf{W}}\right|$. However, the alignment of the vectors $\mathbf{V}^{\mu}$ and $\mathbf{W}^{\mu}$ need not be perfect; *on average* they will lie in the same direction, but there is a probability that they do not.

Let χ be the angle that $\mathbf{V}^{\mu}$ makes with the '1' axis and ψ the corresponding angle of the vector $\mathbf{W}^{\mu}$. There is a probability $p(\psi)d\psi$ that the angle ψ lies between ψ and $\psi + d\psi$. This probability has a maximum for $\psi = \chi$ and tails off to zero when ψ deviates much from χ. The probability is here supposed to have an easily integrable form, for example

$$p(\psi)d\psi = p_0 \cos\left(\frac{\psi - \chi}{\alpha}\right)d\psi. \tag{52}$$

The width of the distribution is such that all the angles ψ lie in the interval $\chi \pm \alpha\pi/2$. Thus, $p_0 = 1/(2\alpha)$. The correlation $\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right)$ becomes

$$\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right) \to \frac{V^2}{2\alpha\overline{\left\langle N_c^{\nu}\right\rangle_{\mu}}}\int_{\chi-\alpha\pi/2}^{\chi+\alpha\pi/2}\left(\cos\chi\cos\psi + \sin\chi\sin\psi\right)\cos\left(\frac{\psi-\chi}{\alpha}\right)d\psi = \frac{V^2}{\left(1-\alpha^2\right)\overline{\left\langle N_c^{\nu}\right\rangle_{\mu}}}\cos\left(\tfrac{1}{2}\pi\alpha\right). \tag{53}$$

Therefore, using the fact that $\overline{\left\langle N_c^{\nu}\right\rangle_{\mu}} = \bar{N}_c$

$$\frac{\sum_{\mu=1}^{N}\left(V_i^{\mu}W_i^{\mu}\right)}{\sum_{\mu=1}^{N}\left(V_i^{\mu}\right)^2} = \frac{\cos\left(\tfrac{1}{2}\pi\alpha\right)}{\bar{N}_c\left(1-\alpha^2\right)}. \tag{54}$$

The expectation is that α will be such that there is an excluded region; this region points in the negative $\mathbf{V}^{\mu}$ direction, which essentially indicates that the vector $\mathbf{W}^{\mu}$ never opposes $\mathbf{V}^{\mu}$. The order of magnitude of this region is roughly the equivalent angular region of one particle $2\pi/\bar{N}$; in other words, α is of the order of $2\left(1-1/\bar{N}\right)$.

The correlation $\overline{\left(N_c^{/}\right)^2}/\bar{N}_c^2$ is a material parameter, which depends on the packing characteristics of the material. Simulations by Kuhn (1999, 2000) on disks with an elasto-frictional interaction it was found that the isotropic state had a co-ordination number $\bar{N}_c = 4.1$ and 92% of the contacts were sticking; he examined the special case for which $k^{(t)} = k^{(n)}$ and an interparticle friction angle of 26^0. Kuhn reports $\overline{\left(N_c^{/}\right)^2}/\bar{N}_c^2 \approx 0.35$ and also the mean field and overall shear and bulk moduli; these are given in the table below

Modulus	Mean value (Nm^{-1})	Effective value (Nm^{-1})	Fraction change
bulk	2.8e7	2.3e7	0.18
shear	2.6e7	1.9e7	0.28

Using expressions (50), (51) and (54) the theoretical estimates for these quantities are determined in the limit $k^{(t)} = k^{(n)}$

$$K = \frac{1}{8v} D^2 \bar{N}_c k^{(n)} \left[1 - \frac{\overline{\left(N_c'\right)^2}}{\left(\bar{N}_c\right)^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)} \right] \text{ and } G = \frac{1}{8v} D^2 \bar{N}_c k^{(n)} \left[1 - \frac{3\overline{\left(N_c'\right)^2}}{2\left(\bar{N}_c\right)^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)} \right], \quad (55)$$

where both v and $\bar{N}$ may be related to the solids volume fraction ϕ. A comparison with the theoretical prediction and the numerical experiment shows good agreement for $\alpha = 1.76$ with $\bar{N} = 5$. This is the right order of magnitude, as $2\left(1 - 1/\bar{N}\right) = 1.6$. The value $\bar{N} = 5$ is obtained from the solids volume fraction, which is reported as 0.82. Note that the ratio of the differences between mean and overall shear and bulk moduli is exactly correct; from (55) it is seen that it is $3/2$, which is also the experimental value.

A parameter that describes the biaxial volume change is Δ, the ratio of the minor principal strain increment to the major principal strain increment under loading in which the minor principal stress increment is zero. For the isotropic medium Δ is $\left(G - K\right)/\left(G + K\right)$. In the special case for which $k^{(t)} = k^{(n)}$, the effect of heterogeneity is to change this value from zero in the mean field estimate to

$$\Delta = -\frac{\frac{\overline{\left(N_c'\right)^2}}{\left(\bar{N}_c\right)^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)}}{2\left[1 - \frac{5}{2} \frac{\overline{\left(N_c'\right)^2}}{\left(\bar{N}_c\right)^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)} \right]} \approx -\frac{\overline{\left(N_c'\right)^2}}{2\left(\bar{N}_c\right)^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)}. \quad (56)$$

In this case, any volume change observed for the sticking contact limit is entirely due to heterogeneity.The mean field parts of expressions (55) have also been obtained by Kruyt and Rothenburg (1998, 2002) for assemblies of bonded granulates.

For frictionless contacts, $k^{(t)} = 0$, the bulk and shear moduli are

$$K = \frac{1}{8v} D^2 \bar{N}_c k^{(n)} \left[1 - \frac{4\overline{\left(N_c'\right)^2}}{3\bar{N}_c^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)} \right] \text{ and } G = \frac{1}{16v} D^2 \bar{N}_c k^{(n)} \left[1 - \frac{4\overline{\left(N_c'\right)^2}}{3\bar{N}_c^2} \frac{\bar{N}}{\bar{N}_c} \frac{\cos\left(\frac{1}{2}\pi\alpha\right)}{\left(1-\alpha^2\right)} \right]. \quad (57)$$

While no two-dimensional data are available for this limit, the general observation that follows from these formulae is that the difference between overall and mean moduli should be of the same order of magnitude as that for the all-stick case. Recently, numerical experiments in three dimensions have

become available, Makse *et al*. (2000). These do not conform to the requirement that the interactive tensor is a constant throughout the medium, because a Hertzian contact law has been used, the incremental value of which depends on the total contact force (Landau and Lifschitz (1982)). These numerical experiments demonstrate that the mean field shear modulus is very substantially reduced while the mean field bulk modulus is only slightly affected by the heterogeneity. The general point is that heterogeneity is a vital ingredient in the understanding of the overall response of a granular assembly. A three dimensional analysis that can also accommodate a variable contact law is required and will be published in the future.

6. CONCLUSIONS

An analytical relationship between the overall stress and strain increments has been determined in the pre-failure regime of a dense, random aggregate of round grains interacting through elastic, frictional contacts. The analytical relationship depends upon the means and fluctuations of structural sums. In order to arrive at this expression, a kinematic description has been explored that describes the displacement and spin variables in a small neighbourhood by means of tensors that are the coefficients of a Taylor expansion. Care has been taken not to over-specify the kinematics in terms of the tensor components. The result is that the first order spin and second order deformation variables are the smallest set sufficient to describe of the motion of a small neighbourhood of particles.

Neglecting products of fluctuations compared to means of both the kinematic parameters and the structural sums, the spin variables have been eliminated from the expression for the contact force. The heterogeneity of the small assemblies is then incorporated using a suitable homogenisation technique. This heterogeneity is an essential ingredient in the description of granular aggregates.

In an example for a two-dimensional, isotropic aggregate, the mean and variance in the packing characteristics are used to arrive at first order expressions for the incremental stiffness components. A favourable comparison with numerical experiments is found.

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REFERENCES

Allersma, H.G.B. (1982) Photo-elastic stress analysis and strains in simple shear. In Deformation and failure of granular materials (IUTAM Symposium, ed. Vermeer, P.A. and Luger, H.J.) pp 345-354. Balkema, Rotterdam.

Babic, M. (1997) Average balance equations for granular materials *Int. J. Engng. Sci.* **35** (5), 523-548.

Beran, M.J. (1968) Statistical continuum mechanics. Wiley, New York.

Cambou, B., Dubujet, Ph., Emeriault, F. and Sidoroff, F. (1995) Homogenization for granular materials. *Eur. J. Mech. A/Solids* **14**, 225-276.

Chang, C.S. (1988) Micromechanical modelling of constitutive relations for granular material. In *Micromechanics of Granular Materials* (ed.Satake, M. and Jenkins, J.T.) pp 271-278. Elsevier, Amsterdam.

Chang, C.S., Askes, H. and Sluys, L.J. (2002) Higher-order strain/higher-order stress gradient models derived from a discrete microstructure, with application to fracture. *Engineering Fracture Mechanics* **69**, 1907-1924.

Cundall, P.A. and Strack, O.D.L. (1979) A discrete numerical method for granular assemblies. *Géotechnique* **29**, 47-65.

Dantu, P. and Weber, J. (1968) Etudes statistique des forces intergranulaire dans un milieu pulverulent. *Géotechnique* **18**, 50-55.

Digby, P.J. (1981) The effective elastic moduli of porous granular rocks. *J. Appl. Mech* **48**, 803-808.

Drescher, A., de Josselin de Jong, G. (1972) Photoelastic verification of a mechanical model for the flow of a granular material. *J. Mech. Phys. Solids* **20**, 337-351.

Edwards, S.F. and Grinev, D.V. (2002) Granular materials: towards the statistical mechanics of jammed configurations. *Advances in Physics* **51** (8), 1669-1684.

Gaspar, N. (2001) Structures and heterogeneity in deforming, densely packed granular materials. PhD thesis: Kingston University UK.

Goldhirsch, I. and Goldenberg, C. (2002) On the microscopic foundations of elasticity. *Eur. Phys. J. E* **9**, 245-251.

Jenkins, J.T., Strack, O.D.L, (1993) Mean-field inelastic behavior of random arrays of identical spheres. *Mech. of Materials* **16**, 25-33.

Jenkins, J.T. (1997) Inelastic behavior of random arrays of identical spheres. In *Mechanics of Granular and Porous Materials* (ed. Fleck, N.A., Cocks, A.C.F.) pp. 11-22. Kluwer, Amsterdam.

Johnson, K.L. (1985) *Contact Mechanics*. Cambridge University Press.

Koenders, M.A. (1987) The incremental stiffness of an assembly of particles. *Acta Mechanica* **70**, 31-49.

Koenders, M.A. and Stefanovska, E. (1993) The numerical simulation of a dense assembly of particles with elasto-frictional interaction. *Powder Technology* **77**, 115-122.

Koenders, M.A. (1994) Least squares methods for the mechanics of nonhomogeneous granular assemblies. *Acta Mechanica* **106**, 23-40.

Konishi, J. (1978) Microscopic model studies on the mechanical behaviour of granular mechanics. In Continuum mechanical and statistical approaches in the mechanics of granular materials (US-Japan Seminar, Sendai Japan, ed. Cowin, S.C. and Satake, M.) pp27-46. Gakujutsu Bunken Fukyu-Kai, Tokyo.

Kröner, E. (1967) Elastic moduli of a perfectly disordered material. *J. Mech Phys Solids* **15**, 319-329.

Kruyt, N.P. and Rothenburg, L. (1998) Statistical theories for the elastic moduli of two-dimensional assemblies of granular materials. *Int. J. Engng. Sci* **36**, 1127-1142.

Kruyt, N.P. and Rothenburg, L. (2002) Micromechanical bounds for the effective elastic moduli of granular materials. *Int. J. of Solids and Structures* **39**, 311-324.

Kruyt, N.P. (2003) Statics and kinematics of discrete Cosserat-type granular materials. *Int. J. of Solids and Structures* **40** (3), 511-534.

Kuhn, M. R. (1999) Structured deformation in granular materials. *Mech. of Mater.* **31**, 407-429.

Kuhn, M.R. (2000) Private communication.

Lätzel, M., Luding, S. and Herrmann, H.J. (2000) Macroscopic material properties from quasi-static, microscopic simulations of a two-dimensional shear-cell. *Granular Matter* **2**, 123-135.

Landau L.D., Lifshitz, E.M., Pitaevskii, L.P. and Kosevich, A.M. (1982) Theory of Elasticity: Course of Theoretical Physics. Pergamon, Oxford.

Love, A.E.H (1944) A Treatise on the Mathematical Theory of Elasticity. New York: Dover Publications.

Makse, H., Gland, N., Johnson, D., Schwartz, M. (2000) Why effective medium theory fails in granular materials. *Phys. Rev. Letters* **83**, 5070-5073.

Misra, A. and Chang, C.S. (1993) Effective elastic moduli of heterogeneous granular solids. *Int. J. Solids Structures* **30**, 2547-2566.

Moreau J.J. (1994) Some numerical methods in multi-body dynamics: application to granular materials. *Eur. J. Mech. A/Solids* **13** (*4*), 93-114.

Norris, A.N., Johnson, D.L. (1997) Nonlinear elasticity of granular media. *J. Appl. Mech.* **64**, 39-49.

Suiker, A.S.J., de Borst, R. and Chang, C.S. (2001) Micro-mechanical modelling of granular material. Part 1: Derivation of a second-gradient micro-polar constitutive theory. *Acta Mechanica* **149**, 161-180.

Torquato, S. (2002) Random heterogeneous materials. Springer-Verlag, New York.

Thornton, C. (1979) The conditions for failure of a face-centred cubic array of uniform rigid spheres. *Géotechnique* **29**, 441-459.

Thornton, C. (2000) Numerical simulation of deviatoric shear deformation of granular media. *Géotechnique* **50**, 43-53.

Walton, K. (1987) The effective elastic moduli of a random packing of spheres. *J. Mech. Phys. Solids* **35**, 213-226.

Williams, J.R. and Rege, N. (1997) Coherent vortex structures in deforming granular materials. *J. Mechanics of Cohesive-Frictional Materials* **2**, 223-236.

Zhuang, X., Didwania, A.K. and Goddard, J.D. (1995) Simulation of the quasi-static mechanics and scalar transport properties of ideal granular assemblages. *J. Comp. Physics* **121** *2*, 331-346.

Zhu, H.P. and Yu, A.B. (2002) Averaging methods of granular materials. *Phys Rev E* **66**, 021302.