EFFECTIVE ELASTIC MODULI OF HETEROGENEOUS GRANULAR SOLIDS

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Abstract—A micro-mechanical model is employed to study the elastic stress–strain behavior of heterogeneous granular solids. The granular material is idealized as a collection of spherical particles interacting through inter-particle contacts. Based on this idealized model an equivalent continuum description of the granular solid is envisaged and the overall stiffness tensor of the granular solid is determined in terms of the stiffness of the inter-particle deformation. To facilitate the derivation of overall stiffness tensor, the granular solid is considered to be composed of continuum cells made of a single particle and the associated void space. A local stiffness tensor is defined for each cell. The local stiffness tensor is obtained in terms of the inter-particle stiffness, the number of contacts and the relative position of the neighboring particles. The local stiffness tensor is utilized to obtain the overall behavior of a representative volume of granular solid through the "self consistent" averaging technique. The overall stress and strain for the representative volume are determined as a volume average of the corresponding local quantities. To account for the heterogeneity of deformation in the granular medium, a "concentration" factor is defined for each cell. Based on the concept of volume averaging and the "concentration" tensor an overall stiffness tensor is derived for the granular solid. The applicability of the derived micro-mechanical model is evaluated by comparing its results with those obtained from the computer simulation method.

INTRODUCTION

The effective stiffness of a granular solid is significantly dependent upon the inter-particle contact stiffness and the geometric arrangement of particles. Recently, based upon micro-mechanical considerations of inter-particle interactions, a number of efforts have been made to obtain the effective moduli of granular materials accounting for the contact stiffness and packing structure. Some of these consider regular packing arrangements (Chang *et al.*, 1989), others consider random packing structure, however, with some simplifying assumptions (Digby, 1981; Walton, 1987; Jenkins, 1987; Bathurst and Rothenburg, 1988; Chang, 1987). The primary assumption made in the above analyses is that granular solids deform in accordance with a uniform strain field. Although these micro-mechanical based models effectively account for inter-particle interactions and packing arrangement, their applicability is limited due to the uniform strain assumption (Chang and Misra, 1990).

In all the aforementioned analyses, little effort has been made to model the stress–strain behavior of granular solids accounting for the heterogeneity at a particle level. Efforts have been made to characterize the fluctuations from uniform strain fields [such as Koenders (1987) and Chang (1989)]. By considering the equilibrium of particle clusters consisting of a particle and its neighbors, Koenders (1987) has presented an analysis of two-dimensional granular systems to derive expressions for corrections to the uniform strain stiffness. In Koenders analysis as well, a uniform average strain field governs the deformation of all the clusters in the granular assembly while fluctuations are admitted within each cluster. Most importantly, the interactions between the clusters are neglected. By considering higher order strain tensors to represent the heterogeneity of deformation fields, a stress–strain relationship was derived for granular packings (Chang, 1989; Chang and Liao, 1990). In this approach the order of strain tensors required to best represent the heterogeneity is difficult to specify.

On the other hand, the "self consistent" method, which has been successfully employed in modelling the effective properties of heterogeneous materials such as polycrystals and composites [see for example Hill (1967) and Hutchinson (1970)], offers a powerful technique to account for heterogeneity. In this paper, the general framework of the "self consistent" method is used in conjunction with the micro-mechanics based modeling scheme to develop an effective stress–strain relationship of granular solids accounting for heterogeneity. The micro-mechanics scheme is useful for describing constitutive law at a local level for a micro-element, while the "self consistent" method provides a tool for describing the effect of interactions among the micro-elements.

A key requirement for modelling the effective properties based on the "self consistent" method is the description of local behavior. In contrast to polycrystals and composites, the description of local stress–strain behavior, for granular solids, poses a unique problem since it must account for the inter-particle interaction. In this paper, the local stress–strain relationship is established at a particle level based upon the methodology developed in micro-mechanical studies [such as Chang and Misra (1990)]. The local constitutive law is derived by considering the interaction of a particle with its neighbors. The local stiffness tensor is obtained as a function of the relative position of the neighboring particles in contact, the number of contacts and the inter-particle contact stiffness. Note that due to the random nature of granular solids, the local stiffness tensor is different at each particle location.

By defining the local constitutive law, a granular solid can be conceptually viewed as a continuum material composed of cells (local volumes) with a local stiffness tensor assigned to each cell. Such a continuum system is analogous to a material with randomly varying stiffness. The overall stress–strain relationship of a representative volume of such a continuum system, consisting of a large number of particles, can be determined in terms of the local constitutive law through the "self consistent" averaging process. This is achieved by employing Hill's averaging principle (1967) and a "concentration" tensor. The "concentration" tensor acts as a weighting function which accounts for the heterogeneity of granular system. It is noted that the "concentration" tensor is, in general, different for each cell. The "concentration" tensor is obtained by considering an analogous problem to the Eshelby's classical boundary value problem of a single inclusion in an infinitely extending homogeneous material. In this regard, the method followed here is similar to that used for modelling effective properties of polycrystals [such as Hutchinson (1970)]. It is also noteworthy that the uniform strain assumption used in previous micro-mechanics based studies is equivalent to assuming the "concentration" tensor to be an identity tensor.

In what follows, we first discuss an equivalent continuum description and a discrete description of the idealized granular system. Further developments are focussed on the equivalent continuum approach. We first describe the kinematics of granular media with the purpose of defining strain in granular media. We then proceed to derive a local stress–strain relationship at a continuum cell and an overall stress–strain law for a representative volume of the granular solid. Finally, some examples are presented to demonstrate the capability of the model as well as to verify some of assumptions made in this model.

PROBLEM DESCRIPTION

Idealized granular system

We consider an idealized granular material consisting of circular particles arranged randomly in space which support imposed loads at the boundary through resistance at inter-particle contacts. It is assumed that all the particles have same stiffness properties. The particles are also assumed to be bonded together such that there is no loss or gain of contacts. With the intent of keeping the discussions simple, the attention of this paper is focussed on the elastic portion of granular deformation.

Under an arbitrary deformation of the granular assembly, the relative displacement δ_i^{nm} between two particles, m and n, is given by

$$\delta_i^{nm} = u_i^m - u_i^n + e_{ijk}(\omega_j^m r_k^m - \omega_j^n r_k^n),$$ (1)

where u_i = the particle displacement, ω_k = the particle rotation, r_j is the vector joining the centroid of a particle to the contact point, the superscripts, n and m, refer to the particles and e_{ijk} is the permutation symbol. The tensor summation convention is used for the subscripts throughout this paper.

The relative movement between particles in contact leads to development of contact forces which are modeled using the Hertz–Mindlin model of two non-conforming elastic bodies in contact (Mindlin and Deresiewicz, 1953). The contact force f_i and the relative displacement δ_i^{nm} are related via the stiffness K_{ij} as follows:

$$f_i = K_{ij}\delta_j,$$ (2)

where K_{ij} is also referred to as the contact stiffness tensor. For the numerical examples in this paper, the contact stiffness tensor is represented by the following simple form

$$K_{ij} = K_n n_i n_j + K_s(s_i s_j + t_i t_j),$$ (3)

where K_n and K_s are the contact stiffnesses along the normal and tangential direction of the contact surface respectively. The unit vector $\mathbf{n}$ is normal to the contact surface and vectors $\mathbf{s}$ and $\mathbf{t}$ are arbitrarily chosen such that $\mathbf{nst}$ forms a local Cartesian coodinate system. Also, for simplicity, the contact stiffnesses are taken to be independent of the contact force unlike the Hertz–Mindlin contact stiffnesses. It is noted that the present analysis assumes that there is no resistance to relative rotation between particles, hence no moments are transmitted at the inter-particle contacts.

For the idealized granular system considered here, two alternative mathematical representations may be envisaged, namely: (1) an equivalent continuum description; and (2) a completely discrete description. The focus, herein, is on the equivalent continuum representation of the discrete granular system.

Equivalent continuum system

For the purposes of continuum description, the granular media is conceptually viewed to be composed of continuum cells. To preserve the discrete nature, however, the local stiffness tensor is derived in terms of the inter-particle interaction and relative locations of neighboring particles in accordance with the micro-mechanical modelling scheme [see Chang and Misra (1990)]. For convenience, the continuum cells are considered to be "Voronoi" polyhedra constructed of a single particle and associated void space. The size of these cells is given by $V^n = V_s^n(1+e)$ where V^n is the volume of the nth cell, V_s^n is the volume of the particle in the cell and e is the void ratio of the granular media. The "Voronoi" polyhedron is found to be specifically useful in capturing the heterogeneity at each location of the granular system.

For the equivalent continuum system, the governing equations are obtained by considering the condition of static equilibrium at each point, such that for the nth cell

$$\sigma_{ij,i}^n = 0$$ (4)

and

$$e_{jpq}\sigma_{pq}^n = 0,$$ (5)

where σ_{ij}^n is the Cauchy stress tensor and (,) comma represents differentiation. It is assumed that couple stresses are not transmitted in the idealized granular system considered here. This implies the symmetry of the Cauchy stresses [see eqn (5)].

The boundary conditions are specified as either displacement or traction boundary conditions as in the usual continuum mechanics. The boundary conditions may be written

as

$$\hat{u}_j = X_i \bar{\varepsilon}_{ij} \tag{6}$$

for the displacement boundary conditions, where $\bar{\varepsilon}_{ij}$ is the symmetric applied strain, X_i is the position vector of the boundary point, and $\hat{u}_j$ is the displacement of the boundary. Alternatively,

$$\hat{f}_i = \bar{\sigma}_{ij} n_j \tag{7}$$

for the traction boundary condition, where $\bar{\sigma}_{ij}$ is the symmetric applied stress, n_j is the normal at the boundary surface, and $\hat{f}_i$ is the force acting at the boundary.

The governing equations, that is eqns (4), (5), (6) and (7), along with the local stiffness tensor completely define the equivalent continuum system. However, it is more desirable to describe the average or overall behavior of an element of granular media containing several particles. The "self consistent" averaging method offers a powerful approach for obtaining the overall stress–strain behavior of a collection of particles. In this regard, the "self consistent" method similar to that used for polycrystals, albeit in a more generalized setting, is utilized here to obtain the overall stiffness tensor for the granular media.

Discrete system

Although the focus of this work is on continuum modeling, for the sake of completeness and contrast we digress briefly to discuss a discrete representation of granular media. In contrast to the equivalent continuum representation, the governing equations of discrete representation are obtained by considering the particle equilibrium in terms of the contact forces and moments generated from interaction with neighbors and any externally imposed force or moment acting at the particle centroid. Thus, for the mth particle in the assembly, equilibrium equations are written as

$$F_i^m - \sum_\alpha f_j^{m\alpha} = 0 \tag{8}$$

and

$$M_i^m - \sum_\alpha e_{ijk} f_j^{m\alpha} r_k^{m\alpha} = 0, \tag{9}$$

where F_i^m and M_i^m are the externally imposed force and the moment acting at the centroid of the mth particle, $f_j^{m\alpha}$ is the force acting at the αth contact of the mth particle and the summation is carried out over all the contacts of the mth particle. Note that contact moment is neglected. For the particles within the granular assembly which are not located at the boundary no external load is acting therefore $F_i^m = 0$ and $M_i^m = 0$. For the particles at the boundary the particle force and moment may be non-zero.

The boundary conditions, in the discrete representation, are specified in terms of either the displacement and rotation or the force and moment on the centroid of the boundary particle. Since, in the laboratory experiments it is difficult to apply rotations and moments on the boundary particles, the boundary conditions may be written as

$$\hat{u}_j = X_i \bar{\varepsilon}_{ij} \tag{10}$$

for the displacement boundary conditions, where $\bar{\varepsilon}_{ij}$ is the symmetric applied strain, X_i is the position vector of the particle centroid, and $\hat{u}_j$ is the displacement of the boundary particle. Alternatively, for the force boundary conditions,

$$\hat{f}_i = \hat{A} \bar{\sigma}_{ij} n_j, \tag{11}$$

where $\bar{\sigma}_{ij}$ is the symmetric applied stress, $\hat{A}$ is the surface area associated with the particle, n_j is the normal at the boundary surface, and $\hat{f}_i$ is the force acting at the centroid of the boundary particle.

Equations (8) and (9) with (10) or (11) define the governing equations and the boundary conditions for the discrete system. Based on these, the problem can be formulated in terms of simultaneous equations connecting the particle displacements and rotations to the particle forces and moments. The solution of these simultaneous equations forms the numerical or computer simulation method developed by Serrano and Rodriguez-Ortiz (1973) and discussed in Chang and Misra (1989). A dynamical form of the discrete representation of the granular system considering inertial forces has been developed by Cundall and Strack (1979).

KINEMATICS OF PARTICLE ASSEMBLY

For the purposes of continuum modeling, we express the displacement and rotation of a particle as a part compatible with the overall average strain of a packing and a fluctuation part that varies from particle to particle. Thus, the relative displacement from eqn (1) becomes:

$$\delta_i^{nm} = \bar{u}_{ij} l_j^{nm} + e_{ijk} \bar{\omega}_k l_j^{nm} + \tilde{u}_i^m - \tilde{u}_i^n + e_{ijk}(\tilde{\omega}_j^m r_k^m - \tilde{\omega}_j^n r_k^n) \tag{12a}$$

or

$$\delta_i^{nm} = \bar{\varepsilon}_{ji} l_j^{nm} - \tilde{\phi}_i^n + \tilde{\phi}_i^m, \tag{12b}$$

where, $l_i^{nm} = X_i^m - X_i^n$ is the branch vector joining the centroid of the nth particle with its mth neighbor. In eqn (12), the terms with bar ($^-$) represent the averages, the terms with tilde ($^\sim$) represent the fluctuations, and the displacement function ϕ_i, introduced for convenience, is given, for say the nth particle, by

$$\phi_i^n = u_i^n + e_{ijk}\omega_j^n r_k^{nm}. \tag{13}$$

In eqn (12), the average strain tensor, $\bar{\varepsilon}_{ji}$, defined to include the effect of particle rotation, is expressed as (Chang and Liao, 1990)

$$\bar{\varepsilon}_{ji} = \bar{\phi}_{i,j} = \bar{u}_{i,j} + e_{ijk}\bar{\omega}_k, \tag{14}$$

where $\bar{u}_{i,j}$ is the overall or average displacement gradient, and $\bar{\omega}_k$ is the average particle rotation. The strain tensor defined in eqn (14) is, in general, non-symmetric. The conventional definition of strain tensor is recovered by taking the symmetric part of the distortion, $\varepsilon_{(kl)}$, which is identical to the symmetric part of the displacement gradient $u_{(l,k)}$. The non-symmetric part represents the net particle rotation in excess of rigid body rotation [see Chang and Misra (1990)].

To characterize the fluctuation terms in eqn (12), the equilibrium of the particles in the assembly is considered. From force equilibrium of the nth particle, we get

$$\bar{\varepsilon}_{mj} \sum_m K_{ij}^{nm} l_m^{nm} - \tilde{\phi}_j^n \sum_m K_{ij}^{nm} + \sum_m K_{ij}^{nm} \tilde{\phi}_j^m = 0 \tag{15a}$$

and for its mth neighbor, we get

$$\bar{\varepsilon}_{mj} \sum_p K_{ij}^{mp} l_m^{mp} - \tilde{\phi}_j^m \sum_p K_{ij}^{mp} + \sum_p K_{ij}^{mp} \tilde{\phi}_j^p = 0. \tag{15b}$$

Similar equilibrium conditions may be written for the neighbors of the mth neighboring particles, and so on. Since, for the present discussion, the particle rotations need not be determined explicitly, only force equilibrium is considered. The fluctuations of particle rotations may be determined explicitly by considering the moment equilibrium of the particles as well. For example, moment equilibrium of the nth particle yields

$$\bar{\varepsilon}_{qp}\sum_{m}e_{ijk}K^{nm}_{jp}l^{nm}_{q}r^{nm}_{k} - \tilde{\phi}^{n}_{p}\sum_{m}e_{ijk}K^{nm}_{jp}r^{nm}_{k} + \sum_{m}e_{ijk}K^{nm}_{jp}r^{nm}_{k}\tilde{\phi}^{m}_{p} = 0. \tag{16}$$

Similar equations may be written for other particles in the assembly. The rotations may now be obtained by simultaneously considering eqns (15) along with eqn (16).

For further discussions, it is convenient to rewrite the force equilibrium condition for the nth particle [eqn (15a)] as

$$\tilde{\phi}^{n}_{j} - \left(\sum_{m}K^{nm}_{ij}\right)^{-1}\sum_{m}K^{nm}_{il}\tilde{\phi}^{m}_{l} = \Gamma^{n}_{jkl}\bar{\varepsilon}_{kl}, \tag{17}$$

where

$$\Gamma^{n}_{jkl} = \left(\sum_{m}K^{nm}_{ij}\right)^{-1}\sum_{m}K^{nm}_{il}l^{nm}_{k}. \tag{18}$$

Similarly, the force equilibrium of the mth particle [eqn (15b)] is rewritten as

$$\tilde{\phi}^{m}_{j} - \left(\sum_{p}K^{mp}_{ij}\right)^{-1}\sum_{p}K^{mp}_{il}\tilde{\phi}^{p}_{l} = \Gamma^{m}_{jkl}\bar{\varepsilon}_{kl} \tag{19}$$

and so on for other particles in the assembly. Equations (17) and (19) along with similar equilibrium equations for other particles in the assembly yield a set of $3N$ equations for N particles in terms of the fluctuations, $\tilde{\phi}^{n}_{j}$, etc. From the solution of this set of simultaneous equations, the fluctuations, $\tilde{\phi}^{n}_{j}$ and $\tilde{\phi}^{m}_{j}$, are conveniently written in terms of the average strain tensor, $\bar{\varepsilon}_{ji}$, as

$$\tilde{\phi}^{n}_{j} = (\Gamma^{n}_{jkl} + \hat{\Gamma}^{n}_{jkl})\bar{\varepsilon}_{kl} \tag{20a}$$

and

$$\tilde{\phi}^{m}_{j} = (\Gamma^{m}_{jkl} + \hat{\Gamma}^{m}_{jkl})\bar{\varepsilon}_{kl}. \tag{20b}$$

The first term on the right-hand side of eqns (20) involves only the nearest neighbor as seen from eqn (18), while the second term involves terms associated with all the other particles in the assembly.

Thus, from eqn (12b), the relative displacement δ^{nm}_{j} can be written in terms of the average strain tensor, $\bar{\varepsilon}_{kl}$, as

$$\delta^{nm}_{j} = (\delta_{jl}l^{nm}_{k} - \Gamma^{n}_{jkl} - R^{n}_{jkl})\bar{\varepsilon}_{kl}, \tag{21}$$

where δ_{jl} is the Kronecker delta. In eqn (21), Γ^{n}_{jkl} denotes the term describing the influence of the nearest neighbors on the nth particle and R^{n}_{jkl} denotes the remainder terms describing the influence of other particles in the assembly on nth particle, where

$$R^{n}_{jkl} = \hat{\Gamma}^{n}_{jkl} - \Gamma^{m}_{jkl} - \hat{\Gamma}^{m}_{jkl}. \tag{22}$$

In order to evaluate the remainder term [eqn (22)], a knowledge of the complete connectivity of the particles in an assembly is required. Consequently, it is desirable to simplify the analysis. To this end, we define a local average strain in the neighborhood of nth particle denoted by ε^{n}_{kl}, such that the relative displacement δ^{nm}_{j} can be written in terms of the nearest neighbors only, as follows:

$$\delta^{nm}_{j} = (\delta_{jl}l^{nm}_{k} - \Gamma^{n}_{jkl})\varepsilon^{n}_{kl}, \tag{23}$$

where the local average strain ε^{n}_{kl} is given by

$$\varepsilon^n_{kl} = \bar{\varepsilon}_{kl} + \Delta\varepsilon^n_{kl}. \tag{24}$$

In eqn (24), $\Delta\varepsilon^n_{kl}$ is defined as the fluctuation strain in the neighborhood of the nth particle.

For the equivalence of relative displacements given in eqns (21) and (23), the fluctuation strain $\Delta\varepsilon^n_{kl}$ is related to the overall average strain $\bar{\varepsilon}_{kl}$ via

$$(\delta_{jl} l^{nm}_k - \Gamma^n_{jkl})\Delta\varepsilon^n_{kl} + R^n_{jkl}\bar{\varepsilon}_{kl} = 0. \tag{25}$$

Equation (25) represents three equations for each contact of the nth particle while nine components of the fluctuation strain $\Delta\varepsilon^n_{kl}$ need to be determined. Thus, for a particle with three contacts explicit solutions of fluctuation strains are possible and eqn (23) is exact. However, for particles with other than three contacts, the system of equations based on eqn (25) is either over determined or under determined, that is explicit solutions of fluctuation strains are not possible. Moreover solving eqn (25) is undesirable since it still requires the complete connectivity of particles in the assembly. Therefore, we need an alternative estimate of the fluctuation strain $\Delta\varepsilon^n_{kl}$ in terms of the overall average strain $\bar{\varepsilon}_{kl}$. Clearly, the accuracy of eqn (23) will depend upon this estimate of the fluctuation strain $\Delta\varepsilon^n_{kl}$.

For estimating fluctuation strain $\Delta\varepsilon^n_{kl}$ in terms of the overall average strain $\bar{\varepsilon}_{kl}$, we note that the problem at hand is analogous to one from continuum mechanics regarding strain distributions in an inhomogeneous material with randomly varying local stiffness tensor. In this paper, we adopt the powerful "self consistent" technique for the determination of local strains. Although the "self consistent" method is expected to yield an approximate relative displacement at a contact, it provides considerable simplification in the derivation of the overall stress–strain relationship. In a later section, we examine the capability of the "self consistent" technique via comparison with results of the discrete approach. These numerical examples show a close agreement between the relative displacements obtained from the discrete method using eqn (1) and those from eqn (23) based upon the "self consistent" scheme.

Since a key requirement of the "self consistent" method is the local stiffness tensor, our immediate task is to establish a local stress–strain relationship which we describe in the next section. The "self consistent" method will be discussed in the section thereafter.

LOCAL STRESS–STRAIN RELATIONSHIP

The local stress–strain relationship is defined at each particle of the granular media or cell of the equivalent continuum media, such that for the nth cell

$$\sigma^n_{ij} = C^n_{ijkl}\varepsilon^n_{kl}, \tag{26}$$

where the superscript n refers to the cell and C^n_{ijkl} is the local stiffness tensor. The local stiffness tensor C^n_{ijkl} is derived in terms of the contact stiffness and the relative position of the neighboring particles. The derivation is facilitated by considering: (a) the relationship between local strain and relative movement of the particle in the cell with respect to neighboring particles [given in eqn (23)]; (b) the interaction of two particles [given in eqn (2)]; and (c) the relationship of local stress and contact forces. The local stress σ^n_{ij} for the nth cell is given in terms of the contact forces f^{nm}_j as (Christoffersen et al., 1981)

$$\sigma^n_{ij} = \frac{1}{2V^n}\sum_m l^{nm}_i f^{nm}_j, \tag{27}$$

where V^n is the volume associated with the nth particle.

Thus, using eqns (2), (23) and (27), the local stiffness tensor C^n_{ijkl} is found to be

$$C_{ijkl}^n = \frac{1}{2V^n} \sum_m l_i^{nm} K_{jl}^{nm} l_k^{nm} - \frac{1}{2V^n} \sum_m l_i^{nm} K_{jr}^{nm} \Gamma_{rkl}^n. \tag{28}$$

The stiffness tensor thus obtained is a function of the packing structure measures l_i and V^n, and contact stiffnesses K_n and K_s. The local stiffness tensor C_{ijkl}^n is, in general, asymmetric with respect to the interchange of leading as well as terminal pairs of indices. However, due to the symmetry of the contact stiffness tensor K_{ij}, the local stiffness tensor has the following symmetry:

$$C_{ijkl}^n = C_{ilkj}^n, \tag{29a}$$

$$C_{ijkl}^n = C_{klij}^n. \tag{29b}$$

STRESS–STRAIN RELATIONSHIP FOR GRANULAR SOLID

To obtain the overall constitutive law, we consider a given volume of the granular solid. This given volume is assumed to contain enough particles in order to be representative of the material behavior of the granular solid. The representative volume is conceptually equivalent to a point in the conventional continuum media. Thus by defining the overall stress, strain and stiffness tensors for this representative volume, we seek to homogenize the granular media. Note that the stress and strain fields (i.e. local stresses and strains) are highly heterogeneous within the representative volume. In the subsequent discussion, the overall quantities are defined for a representative volume as average of the heterogeneous local quantities. Additionally, we define a relationship between the local strain and the global strain via a "concentration tensor". The "concentration tensor" is determined using Eshelby's analysis commonly employed in the "self consistent" method.

Volume averaging

We employ the method of volume averaging to relate the local field quantities to the corresponding overall quantities. The volume averages are written as

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_n V^n \sigma_{ij}^n, \tag{30}$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V} \sum_n V^n \varepsilon_{ij}^n, \tag{31}$$

where $\bar{\sigma}_{ij}$ and $\bar{\varepsilon}_{ij}$ are the overall stress and strain tensors defined for a representative volume, σ_{ij}^n and ε_{ij}^n are the local stress and strain tensors defined at a cell level, V is the volume of the representative volume given by $\sum_n V^n$ where summation is carried over all the particles in the volume. This definition of overall stress and strain has been shown to hold under both displacement and traction boundary conditions provided the displacements or tractions are compatible with a uniform overall strain or stress (Hill, 1967).

The field quantities within the representative volume may themselves be written as the summation of the average term uniform everywhere and a fluctuation term for each cell such that for stresses

$$\sigma_{ij}^n = \bar{\sigma}_{ij} + \Delta\sigma_{ij}^n \tag{32}$$

and for strains, from eqn (24),

$$\varepsilon_{ij}^n = \bar{\varepsilon}_{ij} + \Delta\varepsilon_{ij}^n. \tag{33}$$

We also define a volume average stiffness tensor $\bar{C}_{ijkl}$ in terms of the cell stiffness C_{ijkl}^n as

$$\bar{C}_{ijkl} = \frac{1}{V} \sum_n V^n C^n_{ijkl}. \tag{34}$$

In the selfsame manner of eqns (32) and (33), the stiffness within the volume may also be written as the summation of a quantity uniform everywhere and a fluctuation term

$$C^n_{ijkl} = \bar{C}_{ijkl} + \Delta C^n_{ijkl}. \tag{35}$$

Clearly, by definition the volume average of fluctuation terms will vanish, that is

$$\frac{1}{V} \sum_n V^n \Delta \sigma^n_{ij} = \frac{1}{V} \sum_n V^n \Delta \varepsilon^n_{ij} = \frac{1}{V} \sum_n V^n \Delta C^n_{ijkl} = 0. \tag{36}$$

The aim of the paper is to relate the overall stress and strain tensors through an effective stiffness tensor, such that

$$\bar{\sigma}_{ij} = C_{ijkl} \bar{\varepsilon}_{kl}, \tag{37}$$

where C_{ijkl} is the effective stiffness tensor of the homogenized equivalent continuum. It is remarked that the effective stiffness tensor C_{ijkl} is, in general, different from the volume average stiffness tensor $\bar{C}_{ijkl}$. The volume average stiffness tensor $\bar{C}_{ijkl}$, defined in eqn (34), is the effective stiffness of the representative volume if and only if the strain field within the volume is uniform (Chang and Misra, 1990).

Concentration tensor

To proceed with our objective of deriving the effective stiffness tensor we recall our discussion regarding eqns (23) and (25) in view of eqns (26), (30) and (37). In light of this, it is expedient to relate the local strain ε^n_{ij} to the overall strain $\bar{\varepsilon}_{ij}$ through a, as yet unknown, "concentration" tensor H^n_{mnkl} such that

$$\varepsilon^n_{mn} = H^n_{mnkl} \bar{\varepsilon}_{kl}. \tag{38}$$

From eqn (31), it can be seen that volume averaging requires

$$\frac{1}{V} \sum_n V^n H^n_{ijkl} = I_{ijkl}, \tag{39}$$

where I_{ijkl} is a fourth rank identity tensor defined in terms of the Kronecker delta δ_{ij} (where $\delta_{ij} = 1$ for $i = j$; $= 0$ for $i \neq j$) as

$$I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{40}$$

Thus the effective stiffness tensor C_{ijkl} can be written in terms of cell stiffness tensor C^n_{ijkl} as [from eqns (30), (31), (37) and (38)]

$$C_{ijkl} = \frac{1}{V} \sum_n V^n C^n_{ijmn} H^n_{mnkl}. \tag{41}$$

It now remains to obtain the unknown "concentration" tensor H^n_{mnkl} to completely define the overall stiffness tensor in terms of known quantities. To this end we consider the continuum cell to be an inhomogeneity with stiffness C^n_{ijkl} embedded in an infinite medium of stiffness C_{ijk}. We employ the method of obtaining the stress disturbance due to the presence of an inhomogeneity in an infinite media first discussed by Eshelby (1957) for isotropic elastic materials.

In this discussion hereafter, we consider, for conceptual simplicity, the representative volume to be an infinitely continuum media. This assumption is reasonable in the view that

the volume occupied by each cell is infinitesimally small compared to the size of the representative volume itself. From the condition of static equilibrium within the representative volume, denoted by V, of effective stiffness C_{ijkl}, we get

$$\sigma_{ij,i} = 0 \quad \text{in} \quad V. \tag{42}$$

Let this representative volume be subjected at the boundary, S, to displacements compatible with a uniform overall strain $\bar{\varepsilon}_{kl}$, that is

$$\bar{\varepsilon}_{ij}X_i \to \hat{u}_j \quad \text{as} \quad |X_i| \to \infty \quad \text{at} \quad S. \tag{43}$$

Consider embedded within this media a single inhomogeneity, V^n, of stiffness C^n_{ijkl}. The stress within this media is now given by

$$\sigma_{ij}(x_p) = C_{ijkl}\varepsilon_{kl}(x_p) \quad \text{in} \quad V - V^n, \tag{44}$$

$$\sigma_{ij}(x_p) = C^n_{ijkl}\varepsilon_{kl}(x_p) \quad \text{in} \quad V^n, \tag{45}$$

where $V - V^n$ is the region outside the inhomogeneity. Following the essence of the method by Eshelby, the stress within the inhomogeneity, V^n, can be expressed in terms of the stiffness of the outer media by

$$\sigma_{ij}(x_p) = C_{ijkl}(\varepsilon_{kl}(x_p) - \varepsilon^*_{kl}) \quad \text{in} \quad V^n, \tag{46}$$

where ε^*_{kl} is an "equivalent transformation strain". The "equivalent transformation strain" can in turn be related to the strain in the inhomogeneity. Note that though the "equivalent transformation strain" is conceptually similar to the so called Eshelby's "stress free transformation strain" (Eshelby, 1957) or Mura's "equivalent eigenstrain" (Mura, 1985), it is distinctive in the present setting since it is defined to include the effect of particle rotation in accord with the definition of strain given in eqn (14).

By subtracting the uniform part of the stress, $\bar{\sigma}_{ij}(= C_{ijkl}\bar{\varepsilon}_{kl})$, at all points in the media, the fluctuation term, $\Delta\sigma_{ij}(x_p)$, is found to be [from eqns (32), (33), (44) and (46)]

$$\Delta\sigma_{ij}(x_p) = C_{ijkl}\Delta\varepsilon_{kl}(x_p) \quad \text{in} \quad V - V^n, \tag{47}$$

$$\Delta\sigma_{ij}(x_p) = C_{ijkl}(\Delta\varepsilon_{kl}(x_p) - \varepsilon^*_{kl}) \quad \text{in} \quad V^n. \tag{48}$$

Correspondingly, subtracting the uniform part of strain $\bar{\varepsilon}_{kl}$ from all points in the media leads to a strain free boundary. Thus the boundary value problem defined by eqns (42), (43), (44) and (45), for an inhomogeneity embedded in a homogeneous media, is reduced to the following "auxiliary" problem for a homogeneous media with an "equivalent transformation strain" in V^n

$$\Delta\sigma_{ij,i} = 0 \quad \text{in} \quad V \tag{49}$$

and

$$\Delta u_j \to 0 \quad \text{as} \quad |X_i| \to \infty \quad \text{at} \quad S, \tag{50}$$

where the fluctuation term of the stress field, $\Delta\sigma_{ij}(x_p)$, is given by eqns (47) and (48). The solution of the above auxiliary problem leads to a relationship between the "equivalent transformation strain" ε^*_{kl} and the fluctuation term of the strain $\Delta\varepsilon^n_{ij}(x_p)$ in the inhomogeneity of the form given by

$$\Delta\varepsilon^n_{ij} = E_{ijkl}\varepsilon^*_{kl} \quad \text{in} \quad V^n, \tag{51}$$

where E_{ijkl} is an Eshelby type transformation tensor and superscript n refers to the strain

field within the inhomogeneity (that is the strain field at a cell level). To keep the present discussion focussed on the derivation of an effective tensor C_{ijkl}, we shall postpone the discussion of the "auxiliary" problem to the next section.

Overall stiffness tensor

We can now proceed to derive the expression for the overall stiffness tensor C_{ijkl}. Equating the stress tensors at a cell, σ_{ij}^n, obtained from eqns (26) and (32) using eqns (33) and (46), we get

$$C_{ijkl}^n(\bar{\varepsilon}_{kl} + \Delta\varepsilon_{kl}^n) = C_{ijkl}(\bar{\varepsilon}_{kl} + \Delta\varepsilon_{kl}^n - \varepsilon_{kl}^*). \tag{52}$$

Note, again, that we denote the fluctuation stress and strain at a cell level, that is within V^n, with a superscript n. Now, substituting for ε_{kl}^* from eqn (51) and rearranging, the fluctuation term $\Delta\varepsilon_{mn}^n$ is found to be

$$\Delta\varepsilon_{mn}^n = (C_{mnpq} - C_{mnpq}^n - C_{mnrs}E_{rspq}^{-1})^{-1}(C_{pqkl}^n - C_{pqkl})\bar{\varepsilon}_{kl}. \tag{53}$$

Thus, from eqns (33) and (38), the "concentration" tensor H_{mnkl} is given by

$$H_{mnkl}^n = I_{mnkl} + (C_{mnpq} - C_{mnpq}^n - C_{mnrs}E_{rspq}^{-1})^{-1}(C_{pqkl}^n - C_{pqkl}), \tag{54}$$

where I_{mnkl} is a fourth rank identity tensor defined in eqn (40). Substituting the "concentration" tensor in eqn (41), the fluctuation term of the stiffness tensor is found to be

$$\Delta C_{ijkl}^n = C_{ijmn}^n(C_{mnpq} - C_{mnpq}^n - C_{mnrs}E_{rspq}^{-1})^{-1}(C_{pqkl}^n - C_{pqkl}). \tag{55}$$

After some manipulation the effective stiffness tensor can be simplified to

$$C_{ijkl} = \frac{1}{V}\sum_n V^n C_{ijmn}^n [E_{mnpq}(C_{pqrs}^{-1}C_{rskl}^n - I_{pqkl}) + I_{mnkl}]^{-1}. \tag{56}$$

Note that the unknown effective stiffness tensor C_{ijkl} occurs on both sides of eqn (56). Even for the simplest cases, a numerical effort is required in order to evaluate the effective stiffness tensor.

Auxiliary problem

Though the method used here to solve the boundary value problem, stated in eqns (49) and (50), is conceptually similar to the one used by Eshelby, the problem addressed here is unique in that the definition of strain incorporates the effect of particle rotation, which departs from the conventional analysis. However, by employing the "generalized" displacement function $\phi_j(x_p)$ defined by eqn (13) such that

$$\Delta\varepsilon_{ij} = \Delta\phi_{j,i} = \Delta u_{j,i} - e_{mij}\Delta\omega_m \tag{57}$$

the form of the equations and solutions are, fortunately, reduced to those of the conventional analysis. In the subsequent discussion, therefore, we shall confine ourselves to basic equations necessary for completeness of the presentation and such details which are not presented elsewhere. For further details one may refer to literature such as Mura (1985).

Rewriting eqn (49) in terms of displacements, we obtain [from eqns (48), (49) and (57)]

$$C_{pqrs}\Delta\phi_{s,rp}(x) - C_{pqrs}\varepsilon_{rs,p}^* = 0 \quad \text{in } V^n. \tag{58}$$

It can be seen that the contribution $C_{pqrs}\varepsilon_{rs,p}^*$ in eqn (58) is equivalent to a body force acting

in the x_q direction. Problems of the type given in eqn (58) are often solved by employing the so-called Green's function or the fundamental solution.

Let $\Psi_{st}(x-x')$ be the Green's function, satisfying

$$C_{pqrs}\Psi_{st,rp}(x-x') = \delta_{qt}\delta(x-x'),$$ (59)

where C_{pqrs} is the effective stiffness tensor and $\delta(x-x')$ is the Dirac delta function with the property

$$\int_{-\infty}^{\infty} F(x')\delta(x-x')\,dx' = F(x).$$ (60)

In eqn (59), the tensor $\Psi_{st}(x-x')$ represents the fundamental value of the "generalized displacement" $\Delta\phi_s(x)$ in the infinite homogeneous media of stiffness C_{pqrs} subjected to a concentrated force of unit magnitude acting at x' along the x_t direction. From the Fourier transform of eqn (59), the Green's function Ψ_{ij} is found to be

$$\Psi_{ij}(x_k-x'_k) = (2\pi)^{-3}\int_{-\infty}^{\infty} N_{ij}(\xi_k)D^{-1}(\xi_k)\exp\{i\xi_k(x_k-x'_k)\}\,d\xi_1\,d\xi_2\,d\xi_3$$ (61)

or

$$\Psi_{ij}(x-x') = (2\pi)^{-3}\int_{-\infty}^{\infty} N_{ij}(\xi)D^{-1}(\xi)\exp\{i\xi\cdot(x-x')\}\,d\xi,$$ (62)

where

$$D(\xi) = e_{pqr}B_{p1}B_{q2}B_{r3},$$ (63)

$$N_{pq}(\xi) = B_{pm}B_{mq} - B_{mm}B_{pq} + \delta_{pq}(e_{mn1}B_{m2}B_{n3} + e_{mn2}B_{m3}B_{n1} + e_{mn3}B_{m1}B_{m2}),$$ (64)

$$B_{pr} = C_{pqrs}\xi_q\xi_s.$$ (65)

The "generalized displacement field" $\Delta\phi_i(x)$ due to "equivalent transformation strain" ε^*_{kl} can be obtained by integrating the product of force $C_{pqrs}\varepsilon^*_{rs,p}$ and the Green's function Ψ_{iq} over the domain as

$$\Delta\phi_i(x) = C_{pqrs}\int_{-\infty}^{\infty}\varepsilon^*_{rs,p}\Psi_{iq}(x-x')\,dx'.$$ (66)

Since ε^*_{kl} is zero everywhere outside the inhomogeneity, the displacement field within an inhomogeneity of elliptical shape, after integrating eqn (66) by parts, is obtained as (Mura, 1985)

$$\Delta\phi_i(x) = C_{pqrs}\int_{V^n}\varepsilon^*_{rs}\Psi_{iq,p}(x-x')\,dx',$$ (67)

where V^n is the domain of the inhomogeneity. For a uniform "equivalent transformation strain" ε^*_{kl}, the strain defined as $\Delta\phi_{j,i}$ ($=\Delta\varepsilon_{ij}$) is uniform within the inhomogeneity, given by

$$\Delta\varepsilon_{ij} = \Delta\phi_{j,i} = C_{pqrs}\varepsilon^*_{rs}\int_{V^n}\Psi_{jq,pi}(x-x')\,dx',$$ (68)

where $\Psi_{jq,pi}(x-x')$ can be obtained from eqn (62). Thus, the solution of the boundary

value problem [eqns (49) and (50)] is obtained in the form given in eqn (51), where E_{ijkl} is given by

$$E_{ijkl} = C_{pqkl} G_{ipjq} \tag{69}$$

and

$$G_{ipjq} = \int_{V^n} \Psi_{jq,pi}(x-x')\,dx' = \frac{1}{4\pi}\int_{-1}^{1}\int_{0}^{2\pi} \xi_j \xi_q N_{ip}(\xi) D^{-1}(\xi)\,d\theta\,d\zeta_3, \tag{70}$$

where

$$\xi_i = \frac{\zeta_i \zeta}{a_i} \quad \text{(no sum on } i\text{)}, \tag{71}$$

$$\zeta_1 = (1-\zeta_3^2)^{1/2}\cos\theta, \tag{72}$$

$$\zeta_2 = (1-\zeta_3^2)^{1/2}\sin\theta, \tag{73}$$

$$\zeta = (\zeta_1^2 + \zeta_2^2 + \zeta_3^2)^{1/2} \tag{74}$$

and a_i are the half principal axes of the elliptical inhomogeneity.

For the two-dimensional case, the procedure to evaluate the tensor E_{ijkl} is outlined in the Appendix.

RESULTS AND COMPARISON

To demonstrate the applicability of the derived stress–strain law [eqn (37)], we study the elastic stress–strain behavior of random packings of planar disks. The results of the equivalent continuum model are compared with those obtained from computer simulation method based on the discrete description discussed earlier in the paper. The details of the computer simulation method are discussed elsewhere in Chang and Misra (1989).

The random packing of particles used in this study are shown in Fig. 1. The packings are formed such that they represent a periodic space. It is seen that the two X as well as the two Y boundaries are images of each other. Such a periodic space is a representative volume of the granular solid, since the granular media can be constructed by repetitively stacking this space. The packing parameters for the two packings are given in Table 1. It is noted that for calculations based on the present model, the inhomogeneity shape is taken to be circular, i.e. $a_1 = a_2$.

Effective modulus

The effective modulus computed from eqn (56) is compared with that obtained from the computer simulation method to evaluate the accuracy of the "self consistent" averaging method. In Figs 2 and 3, the ratio of effective modulus M_r is plotted versus the ratio of contact stiffnesses K_s/K_n. The modulus ratio M_r is taken to be the ratio of the modulus based on eqn (56) and the modulus obtained from computer simulation. Also plotted in Figs 2 and 3 is the ratio of modulus based on uniform strain theory and that obtained from computer simulation. The modulus based on uniform strain theory is obtained from eqn (34) and the first term in eqn (28).

The effective moduli based on eqn (56) exhibit an encouraging agreement with moduli obtained from computer simulation. In contrast to the uniform strain theory, the present method provides a better estimate of moduli over a wider range of contact stiffness ratios. It is observed that the number of particles in the packing has little effect on the trends displayed by the results, although the agreement with computer simulation results is slightly improved.

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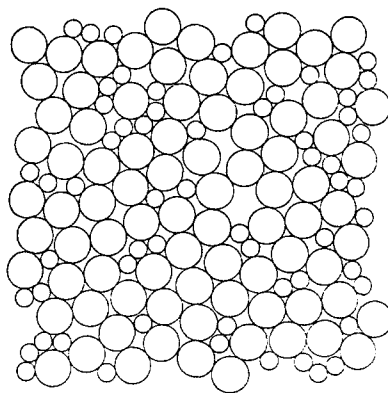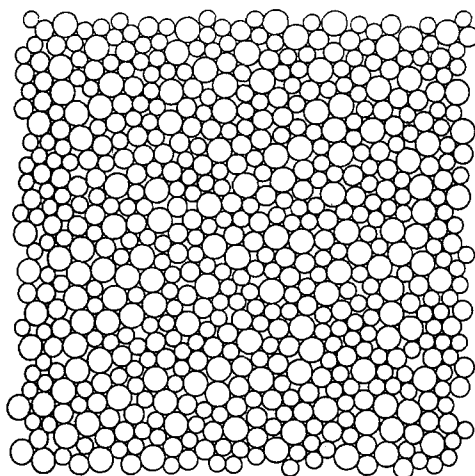
PACKING A

PACKING B

Fig. 1. Packing of circular disks.

Heterogeneity

The variations of local stress and strain are investigated to illustrate the heterogeneous nature of these field quantities in granular solids and the ability of the present model to capture the effect of heterogeneity. In Fig. 4 we plot the frequency distribution of the three components of cell stress versus the percentage of cells obtained from the computer simulation and the present methods for packing A. The cell stresses are computed based on eqn (27). While the mean stress [based on a definition in eqn (30)] is the same for the two methods, the computer simulation method shows greater inhomogeneity compared to the present method. These results are for the loading condition: $\varepsilon_{yy} = 0.01\%$ and $\varepsilon_{xx} = \varepsilon_{xy} = \varepsilon_{yx} = 0$, and contact stiffnesses: $K_n = 1750$ kN m^{-1} and $K_s = 175$ kN m^{-1}.

Table 1. Packing parameters for the packings in Fig. 1

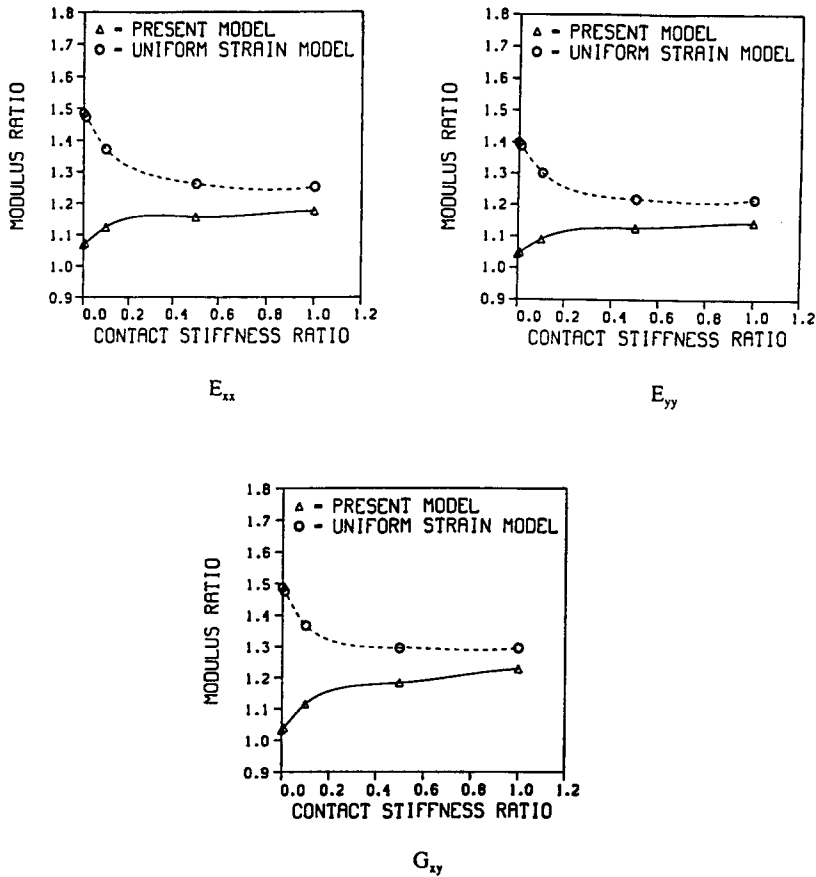| Parameter	Packing A	Packing B
Particle diameter (number of particles)	0.105 mm (60)	0.10 mm (301)
	0.210 mm (84)	0.12 mm (150)
		0.15 mm (125)
Number of contacts	327	1384
Coordination number	4.54	4.80
Area	16.5 mm^2	28.9 mm^2
Void ratio	0.202	0.153

Fig. 2. Modulus ratio M_r versus the contact stiffness ratio K_s/K_n for packing A.

In Fig. 5 the frequency distribution of the three components of strain at cell level obtained from the present method are plotted versus the percentage of cells. The strains at cell level are computed from eqn (38) for the above mentioned loading condition. The figures show that the strain field is inhomogeneous within the media. Moreover, the normal strain, ε_{xx}^n, and shear strain, $\gamma_{xy}^n = (\varepsilon_{xy}^n + \varepsilon_{yx}^n)$, do not vanish at the cell level, even though the applied values of these components are zero. Similar results are obtained from the computer simulation method.
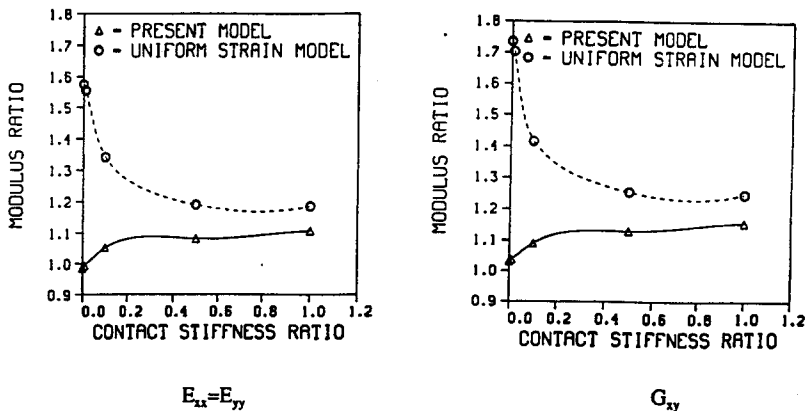

Fig. 3. Modulus ratio M_r versus the contact stiffness ratio K_s/K_n for packing B.
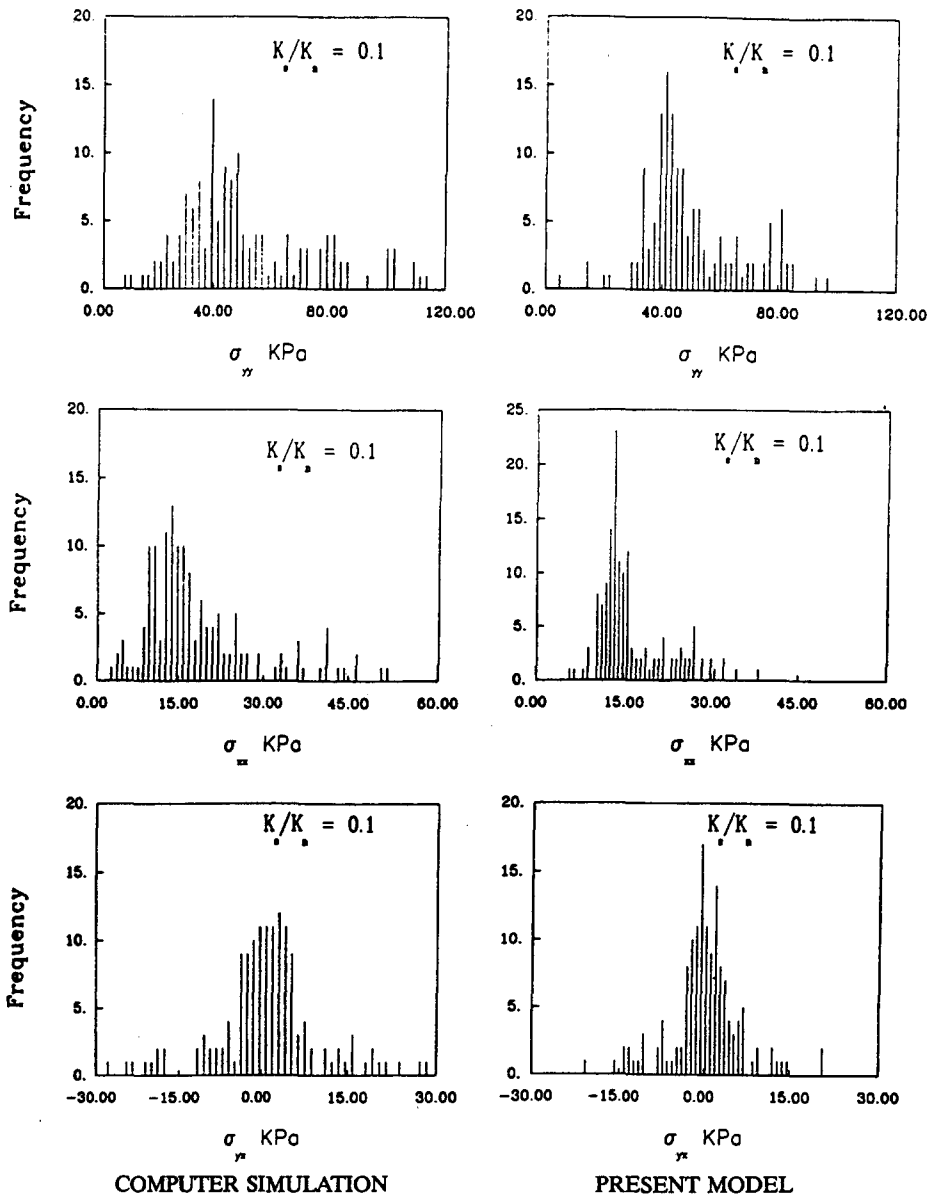
Fig. 4. Frequency distribution of the three components of local stress in the packing under uniaxial loading based on : (a) computer simulation method, and (b) present model.

Variation of micro-mechanical quantities

We next investigate the applicability of the present method in predicting the micro-mechanical quantities in the packing. In this context, the directional distributions of relative displacements at the contacts in packing A are studied for the loading condition and contact stiffnesses used above.

The directional distributions of relative displacements normal to and tangential to the contact plane, obtained from the computer simulation method, the present method and the uniform strain method, are plotted in Fig. 6. For a quantitative comparison of the relative displacement distributions, Fourier approximations of the distributions were obtained as

$$\delta(\theta) = \frac{C}{2\pi}(1 + a_2\cos 2\theta + b_2\sin 2\theta + a_4\cos 4\theta + b_4\sin 4\theta). \tag{75}$$

The coefficients C, a_2, b_2, a_4 and b_4 are given in Table 2 for the three methods. From the
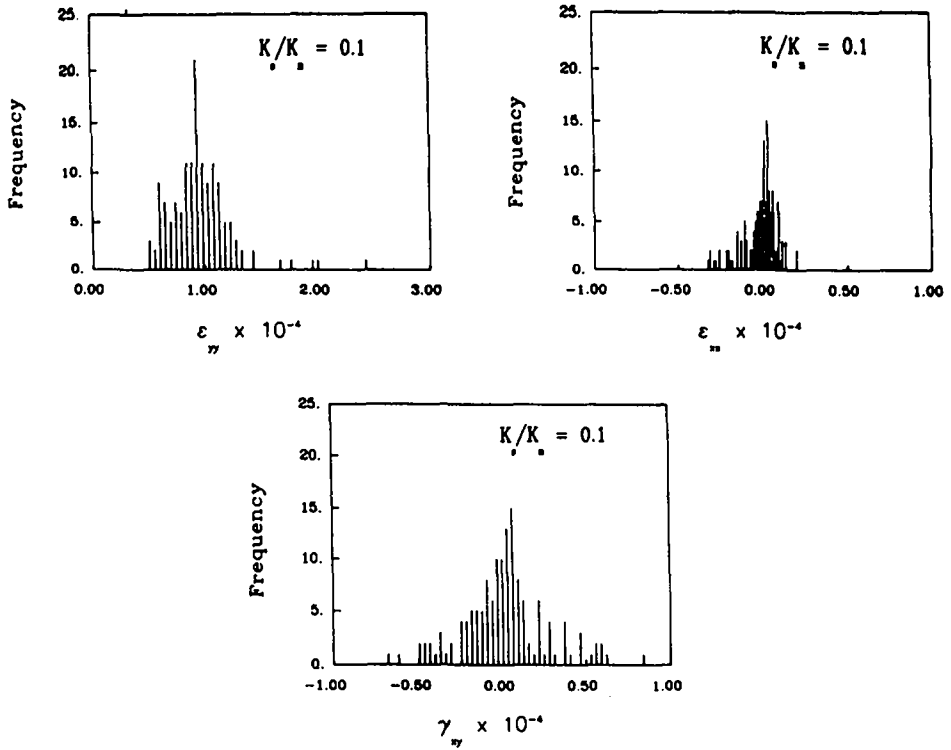
Fig. 5. Frequency distribution of the three components of local strain in the packing under uniaxial loading based on the present model.
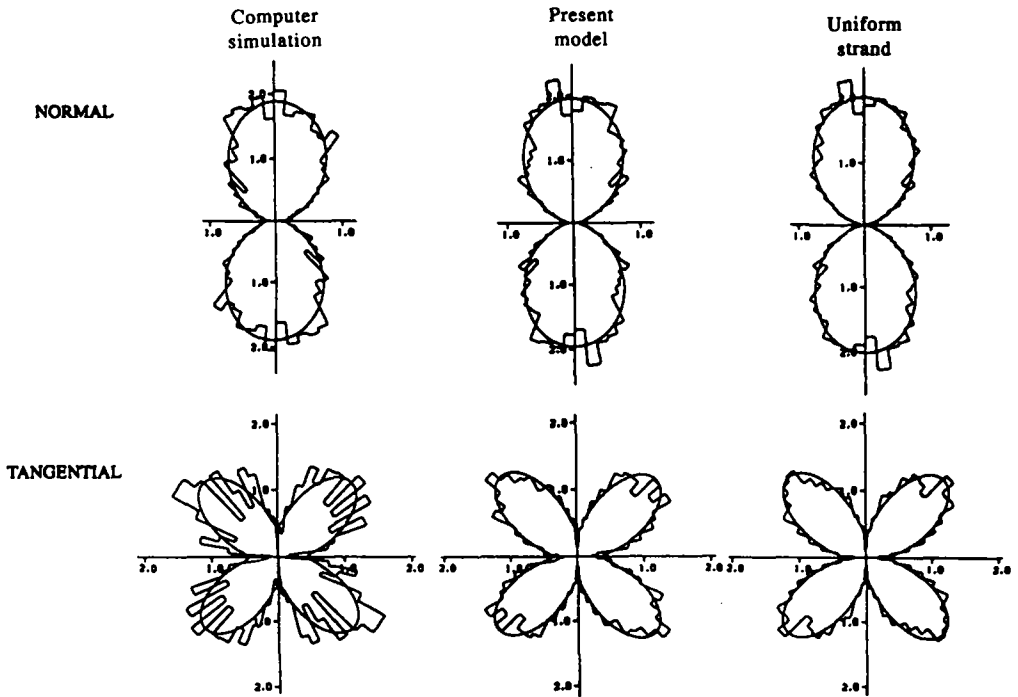

Fig. 6. Directional distribution of the normal and tangential components of relative displacements at contacts.

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Table 2. Coefficients for Fourier approximation of relative displacement distributions

	Method	$C \times 10^{-3}$	a_2	b_2	a_4	b_4
	Computer simulation	1.6	−0.924	0.05	0.02	0.0
Normal displacement	Present	1.6	−0.931	0.01	0.02	0.0
	Uniform strain	1.6	−1.115	0.01	0.02	0.0
	Computer simulation	1.1	0.0	0.02	−0.627	0.0
Shear displacement	Present	1.1	0.0	0.02	−0.642	0.06
	Uniform strain	1.1	0.0	0.02	−0.667	0.05

Fourier approximation it is seen that the relative displacements in the normal direction to the contact are larger for the uniform strain theory *vis à vis* the present method and the computer simulation method. These relative displacements show close agreement for the present method and the computer simulation method. The relative displacements in the tangential direction show little variation for the three methods, although they tend to be higher for the present and computer simulation methods. This implies that the uniform strain method will give a stiffer response in comparison with the other two methods as seen in Figs 2 and 3.

CONCLUSIONS

An effective stress–strain relationship is derived for a representative volume of granular solids based upon the micro-mechanical methodology and "self consistent" averaging technique. The primary aim of this paper is to account for the effect of heterogeneity of granular media in the stress–strain model. To facilitate this, the granular solid is considered to be composed of continuum cells made of a single particle and the associated void space. For each cell a local constitutive law is established by considering the interaction of particle in the cell and its neighbors. The local stiffness tensor depends on the number of inter-particle contacts, the relative positions of the neighboring particles and the inter-particle contact stiffnesses. The local constitutive law is then utilized to obtain the overall stress–strain relationship of a representative volume containing several particles based upon the "self consistent" averaging method. In the "self consistent" method, the heterogeneity of the granular material is accounted by employing a "concentration" tensor which relates the overall strain to the local strain for each cell. The "concentration" tensor is obtained by treating each cell in the granular assembly to be an inhomogeneity embedded in an equivalent homogeneous media.

In the equivalent continuum model, based upon the "self consistent" method, the requirement of exactly satisfying the equilibrium and continuity conditions at each location in the granular media is relaxed. In spite of these simplifying assumptions, the model provides a viable method of accounting for heterogeneous nature of granular media. The advantage of the approach presented in this paper is that heterogeneity of deformation is captured without resorting to a discrete computer simulation approach in which each particle is tracked during the deformation process and therefore a much larger computational effort is required.

Applicability of the derived overall stress-strain relationship is investigated by comparing results with the computer simulation method. Results of the derived micro-mechanical model show that the model provides an improved prediction of the moduli and micromechanical variables in comparison to a model without the consideration of heterogeneity. Frictional granular materials have shown evidence of a large amount of heterogeneity before failure or strain localization. It is believed that this model can be potentially extended to non-linear granular systems.

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APPENDIX

For the two-dimensional case the tensor E_{ijkl} is evaluated for $\zeta_3 \to 0$. Thus the components of vector ζ are reduced to [from eqns (71)–(74)]

$$\xi_1 = \frac{\cos\theta}{a_1} \quad \text{and} \quad \xi_2 = \frac{\sin\theta}{a_2}. \tag{A1}$$

Furthermore the integral in eqn (60) is reduced to the form $\int_0^{2\pi} R(\cos\theta, \sin\theta)\, d\theta$, where $R(\cos\theta, \sin\theta)$ is a rational function of $\cos\theta$ and $\sin\theta$. This integral over θ can be converted into a contour integral in the complex plane by setting $Z = e^{i\theta}$, and substituting

$$d\theta = \frac{dZ}{iZ}, \tag{A2}$$

$$\cos\theta = \frac{1}{2}\left(Z + \frac{1}{Z}\right), \tag{A3}$$

$$\sin\theta = \frac{1}{2i}\left(Z - \frac{1}{Z}\right). \tag{A4}$$

Thus

$$G_{ipjq} = \frac{1}{4\pi} J_{ipjq}, \tag{A5}$$

where

$$J_{ipjq} = \frac{1}{i}\int_C \frac{P_{ipjq}(Z)}{Q(Z)}\, dZ = 2\pi\, \text{Res}\left[\frac{P_{ipjq}(Z)}{Q(Z)}\right], \tag{A6}$$

$i = \sqrt{-1}$, $P_{ipjq}(Z)$ and $Q(Z)$ are polynomial functions of Z, and Res [·] denotes the sum of the residues of function $P_{ipjq}(Z)/Q(Z)$ existing within the unit circle $|Z| = 1$.

The polynomial $Q(Z)$ is given by

$$Q(Z) = q_1 Z^9 + q_2 Z^7 + q_3 Z^5 + \mathbf{q}_2 Z^3 + \mathbf{q}_1 Z, \tag{A7}$$

where

$$q_1 = (C_{33} - \alpha^2 C_{44} - 2i\alpha C_{34})(C_{11} - \alpha^2 C_{22} - 2i\alpha C_{12})$$

$$+ (C_{23} - i\alpha C_{24})(2i\alpha C_{13} + 2\alpha^2 C_{14} + \alpha^2 C_{23} - i\alpha^3 C_{24}) + (\alpha C_{14} + iC_{13})^2, \quad \text{(A8)}$$

$$q_2 = -4\alpha^3 C_{44}(\alpha C_{22} + iC_{12}) - 4i\alpha C_{34}(\alpha^2 C_{22} + C_{11}) - 4C_{33}(i\alpha C_{12} - C_{11}) + 4\alpha^3 C_{24}(\alpha C_{24} + i(C_{23} + C_{14}))$$

$$- 4C_{13}(i\alpha(C_{23} + C_{14}) - C_{13}), \quad \text{(A9)}$$

$$q_3 = 2\alpha^2 C_{44}(3\alpha^2 C_{22} + C_{11}) + 8\alpha^2 C_{12} C_{34} + 2C_{33}(\alpha^2 C_{22} + 3C_{11})$$

$$- 2(\alpha^2 C_{24} + C_{13})^2 - 4(\alpha^4 C_{24}^2 + C_{13}^2) + 2\alpha^2(C_{23} + C_{14})^2, \quad \text{(A10)}$$

$$\bar{q}_1 = \text{conjugate}\,(q_1), \quad \bar{q}_2 = \text{conjugate}\,(q_2) \quad \text{(A11)}$$

and

$$\alpha = \frac{a_1}{a_2}, \quad \text{(A12)}$$

where a_1 and a_2 are the major and minor principal axes of the ellipsoidal inhomogeneity.

The polynomials $P_{ijkl}(Z)$ are given by

$$P_{ijkl}(Z) = r_{ijkl}Z^8 + s_{ijkl}Z^6 + t_{ijkl}Z^4 + \bar{s}_{ijkl}Z^2 + \bar{r}_{ijkl}, \quad \text{(A13)}$$

where coefficients $\bar{r}_{ijkl}$ and $\bar{s}_{ijkl}$ are complex conjugates of r_{ijkl} and s_{ijkl}, respectively. The polynomials $P_{ijkl}(Z)$ possess the following symmetry $P_{ijkl} = P_{ijlk} = P_{jikl}$. Thus there are only nine independent $P_{ijkl}(Z)$ given by

$$r_{1111} = C_{33} - \alpha^2 C_{44} - 2i\alpha C_{34}, \quad s_{1111} = 4(C_{33} - i\alpha C_{34}), \quad t_{1111} = 2(\alpha^2 C_{44} + 3C_{33}), \quad \text{(A14)}$$

$$r_{1212} = \alpha^2 C_{24} + i\alpha(C_{23} + C_{14}) - C_{13}, \quad s_{1212} = 2i\alpha(C_{24} + C_{14}) - 4C_{13}, \quad t_{1212} = -2(\alpha^2 C_{24} + 3C_{13}), \quad \text{(A15)}$$

$$r_{1222} = C_{11} - \alpha^2 C_{22} - 2i\alpha C_{12}, \quad s_{1222} = 4(C_{11} - i\alpha C_{12}), \quad t_{1222} = 2(\alpha^2 C_{22} + 3C_{11}), \quad \text{(A16)}$$

$$r_{2211} = -\alpha^2(C_{33} - \alpha^2 C_{44} - 2i\alpha C_{34}), \quad s_{2211} = -4\alpha^3(C_{44} - i\alpha C_{34}), \quad t_{2211} = 2\alpha^2(C_{33} + 3\alpha^2 C_{11}), \quad \text{(A17)}$$

$$r_{1211} = i\alpha(\alpha^2 C_{44} - C_{33}) - 2\alpha^2 C_{34}, \quad s_{1211} = -2i\alpha(\alpha^2 C_{44} - C_{33}), \quad t_{1211} = 4\alpha^2 C_{34}, \quad \text{(A18)}$$

$$r_{1212} = i\alpha(C_{13} - \alpha^2 C_{24}) + \alpha^2(C_{23} - C_{14}), \quad s_{1212} = 2i\alpha(\alpha^2 C_{24} - C_{13}), \quad t_{1212} = -2\alpha^2(C_{23} + C_{14}), \quad \text{(A19)}$$

$$r_{1222} = i\alpha(\alpha^2 C_{22} - C_{11}) - 2\alpha^2 C_{12}, \quad s_{1222} = -2i\alpha(\alpha^2 C_{22} - C_{11}), \quad t_{1222} = 4\alpha^2 C_{12}, \quad \text{(A20)}$$

$$r_{2212} = \alpha^2 C_{13} - \alpha^4 C_{24} - i\alpha^3(C_{23} - C_{14}), \quad s_{2212} = 2\alpha^3(2\alpha C_{24} + i(C_{23} + C_{14})), \quad t_{2212} = -2\alpha^2(C_{13} + 3\alpha^2 C_{24}), \quad \text{(A21)}$$

$$r_{2222} = -\alpha^2(C_{11} - \alpha^2 C_{22} - 2i\alpha C_{12}), \quad s_{2222} = -4\alpha^3(\alpha C_{22} + iC_{12}), \quad t_{2222} = 2\alpha^2(C_{11} + 3\alpha^2 C_{22}). \quad \text{(A22)}$$

Here,

$$C_{11} = C_{1111}, \quad C_{12} = C_{1112}, \quad C_{13} = C_{1121}, \quad C_{14} = C_{1122}, \quad \text{(A23)}$$

$$C_{21} = C_{1211}, \quad C_{22} = C_{1212}, \quad C_{23} = C_{1221}, \quad C_{24} = C_{1222}, \quad \text{(A24)}$$

$$C_{31} = C_{2111}, \quad C_{32} = C_{2112}, \quad C_{33} = C_{2121}, \quad C_{34} = C_{2122}, \quad \text{(A25)}$$

$$C_{41} = C_{2211}, \quad C_{42} = C_{2212}, \quad C_{43} = C_{2221}, \quad C_{44} = C_{2222}. \quad \text{(A26)}$$

Since the $Q(Z)$ is a polynomial of degree 9 with unknown coefficients, a numerical effort is needed to evaluate J_{ijkl}.