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SECOND-GRADIENT CONSTITUTIVE THEORY FOR GRANULAR MATERIAL WITH RANDOM PACKING STRUCTURE

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Abstract—A second-gradient constitutive law for granular media is derived, in which stress is a function of the second order of strain gradient. The constitutive coefficients for granular materials with an isotropic packing structure are derived in explicit terms of inter-particle stiffness and particle size. In the present constitutive theory, the total number of elastic constants for the isotropic granular material is four: two of them are the usual Lame constants; the other two are associated with the second gradient of strain. The derived constitutive relationships illustrate the important role of micro-scale properties in the macro-scale behavior. The influence of inter-particle stiffness and particle size on the response of material due to the second gradient of strain is discussed. This paper also discusses the connection between the second-gradient theory and non-local theory. The second-gradient theory can be regarded as the first-order approximation of non-local theory.

1. INTRODUCTION

Granular material, such as soil, powder, ceramic material, etc., can be perceived as a collection of particles. The overall mechanical properties for granular materials depend significantly on the micro-scale geometric arrangement and on the contact stiffness between two interacting particles. It is desirable to derive the macro-scale constitutive law for granular materials by using suitable macro-scale continuum variables that are capable of reflecting the discrete nature at micro-scale level. A number of studies have been attempted along this line of approach. For example, the mechanical behavior of regular packings of elastic spheres was modelled by Duffy and Mindlin (1957), Deresiewicz (1958), and Duffy (1959). More recently, micromechanical models for randomly packed granular materials, considering the effect of the microstructure and discrete nature of the material, have been suggested by many investigators. For example, models without consideration of particle rotation can be found in the work by Walton (1987), Bathurst and Rothenberg (1988), Chang (1988), Jenkins (1988), etc. Models with consideration of particle rotation can be found in the work by Chang and Liao (1990), Chang and Ma (1991, 1992), and Chang (1993). With the effect of particle rotation, the macro-scale continuum for granular material is of a micro-polar or Cosserat type. It is noted that Chang and Liao (1990) suggested a method of transforming a discrete particle system into an equivalent continuum system. The continuum system is characterized by continuum fields constructed from particle displacement and particle rotation. Utilizing the method, this paper aims to develop a high-gradient constitutive theory for granular materials on the physical basis that micro-scale interaction between particles controls the macro-scale response of granular assembly.

Early high-gradient models for metals were proposed by Toupin and Gazis (1964), Mindlin (1965), and Beran and McCoy (1970b). Recently, high-gradient models considering plastic deformation have been used in the study of localized deformation (Coleman and Hodgdon, 1985; Triantafyllidis and Aifantis, 1986; Bazant and Pijandier-Cabot, 1987; Bardenhagen and Triantafyllidis, 1994). Unlike the aforementioned high-gradient models, the present model is specifically derived for granular material, and the derived moduli are in explicit terms of inter-particle contact properties. The present model is limited to the elastic condition. No plastic deformation such as particle sliding or localized shear band is considered. The micro-structure effects become important for dynamic problems involving short wavelengths.

In this paper, we first represent the displacement and rotation fields by continuous polynomial functions. The gradients of displacement and rotation fields are selected as macro-scale kinematic continuum variables for the equivalent continuum. Thus the constitutive equations include terms of gradients of displacement and rotation. Since the particle movement can be retrieved from the continuum variables, we derive the constitutive equations by considering the inter-particle properties of granular materials. In this paper, we use up to the second-order gradients of strain.

To understand better the relationship between micro and macro properties, we further derive closed-form expressions of the constitutive constants (or elastic moduli) for isotropic granular materials. Discussion is given on the relations between the derived elastic constants and micro-scale properties, such as the internal length of granular material and inter-particle stiffness. Finally, we discuss the links between the derived second-gradient theory and non-local theory. The second-gradient theory can be regarded as the first-order approximation of non-local theory.

2. MICROMECHANICAL DESCRIPTION OF GRANULAR MATERIALS

2.1. *Kinematic description in granular assembly*

A simple conceptual model for granular material is to treat it as a collection of particles. When a representative volume element of particles is subjected to an increment of load, particles undergo translations u_i^n and rotations ω_i^n, resulting in the relative deformation between particles. Considering the kinematics of two particles of convex shape, the inter-particle displacement δ_i^{nm} and relative rotation θ_i^{nm} of particle m relative to particle n at the contact point c are given by

$$\left.\begin{aligned} \delta_i^c &= \delta_i^{nm} = u_i^m - u_i^n + e_{ijk}(\omega_j^m r_k^{mc} - \omega_j^n r_k^{nc}) \\ \theta_i^c &= \theta_i^{nm} = \omega_i^m - \omega_i^n \end{aligned}\right\} \tag{1}$$

where the quantity e_{ijk} = the permutation symbols used in tensor representation for the cross product of vectors, and r_k^{nc} is the vector joining the centroid of the nth particle to the contact point as shown in Fig. 1.

Whereas the inter-particle displacements generate inter-particle forces, the inter-particle rotations generate inter-particle moments in granular materials. For two particles in contact, the relations between the contact force f_i^c and inter-particle displacement δ_i^c and between the contact moment m_i^c and inter-particle rotation θ_i^c can be expressed, respectively, as

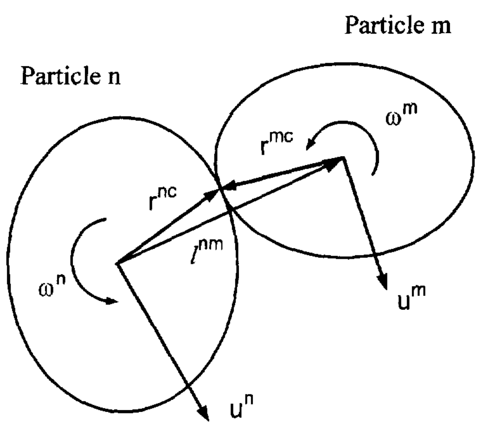

Fig. 1. Kinematics of two interacting particles.

$$\left.\begin{aligned} f_i^c &= K_{ij}^c \delta_j^c \\ m_i^c &= G_{ij}^c \theta_j^c \end{aligned}\right\}. \tag{2}$$

In eqn (2), K_{ij}, G_{ij} are the contact stiffness tensors given by

$$\left.\begin{aligned} K_{ij} &= K_n n_i n_j + K_s s_i s_j + K_t t_i t_j \\ G_{ij} &= G_n n_i n_j + G_s s_i s_j + G_t t_i t_j \end{aligned}\right\} \tag{3}$$

where **n**, **s**, and **t** are the basic unit vectors of the local co-ordinate system constructed at each contact as shown in Fig. 2. The vector **n** is normal to the contact plane. The other two orthogonal vectors, **s** and **t**, are on the contact plane, given by

$$\left.\begin{aligned} \mathbf{n} &= \cos\gamma\mathbf{e}_1 + \sin\gamma\cos\beta\mathbf{e}_2 + \sin\gamma\sin\beta\mathbf{e}_3 \\ \mathbf{s} &= \frac{\mathrm{d}\mathbf{n}}{\mathrm{d}\gamma} = -\sin\gamma\mathbf{e}_1 + \cos\gamma\cos\beta\mathbf{e}_2 + \cos\gamma\sin\beta\mathbf{e}_3 \\ \mathbf{t} &= \mathbf{n}\times\mathbf{s} = -\sin\beta\mathbf{e}_2 + \cos\beta\mathbf{e}_3 \end{aligned}\right\} \tag{4}$$

In eqn (3), the variable K_n is the contact stiffness in the direction normal to the contact plane. The variables K_s and K_t are the contact stiffnesses in the tangential directions of **s** and **t**, respectively, on the contact plane. For two identical elastic spherical particles in contact, the contact area is of circular shape, and the variables K_s and K_t are expected to be the same. In this situation, values of contact stiffness can be obtained from Hertz–Mindlin contact theory as a function of particle properties and contact force. Similarly, the variables G_n, G_s, and G_t are the contact stiffness for rotation in the directions of n, s, and t, respectively, on the contact plane. Whereas the contact stiffnesses K_n, K_s and K_t are responsible for transmitting forces through inter-particle contacts, the contact stiffnesses G_n, G_s, and G_t are responsible for transmitting moments through inter-particle contacts in a granular medium.

To develop a continuum mechanics model for the behavior of a particle assembly, it is desirable to view the discrete system as an equivalent continuum system. To this end, we define the displacement and rotation of discrete particles as macro-scale continuum fields, denoted as: displacement $u_i(x)$ *and rotation* $\omega_i(x)$. When x is located at the centroid of the nth particle, the functions represent the displacement and rotation of the nth particle:

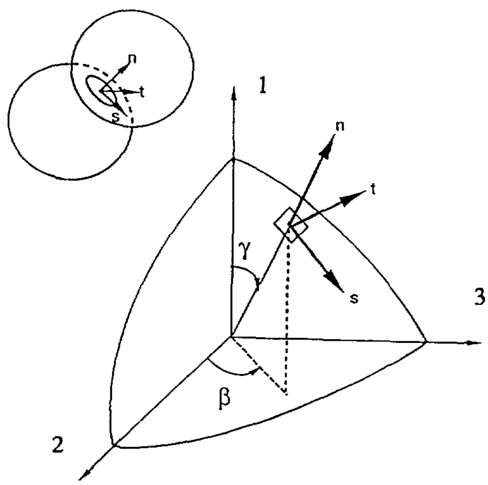

Fig. 2. Local co-ordinate system at an inter-particle contact.

$$\left.\begin{aligned} u_i(x_i^n) &= u_i^n \\ \omega_i(x_i^n) &= \omega_i^n \end{aligned}\right\}. \tag{5}$$

Following the approach by Chang and Liao (1990), using a polynomial expansion for the displacement and rotation fields, the displacement and rotation of the mth particle can be estimated from the deformation gradients at the neighboring nth particle, given by

$$\left.\begin{aligned} u_i^m &= u_i^n + u_{i,j}^n L_j^{nm} + \tfrac{1}{2} u_{i,jk}^n L_j^{nm} L_k^{nm} + \dots \\ \omega_i^m &= \omega_i^n + \omega_{i,j}^n L_j^{nm} + \tfrac{1}{2} \omega_{j,jk}^n L_j^{nm} L_k^{nm} + \dots \end{aligned}\right\} \tag{6}$$

where the branch vector $L_i^{nm} = r_i^{nc} - r_i^{mc}$; the displacement and rotation gradients of the nth particle are treated to be the continuum kinematic variables, defined as follows:

$$\left.\begin{aligned} u_{i,j}^n &= \left.\frac{\partial u_i(x_i)}{\partial x_j}\right|_{x_i = x_i^n} & \omega_{i,j}^n &= \left.\frac{\partial \omega_i(x_i)}{\partial x_j}\right|_{x_i = x_i^n} \\ u_{i,jk}^n &= \left.\frac{\partial^2 u_i(x_i)}{\partial x_j \partial x_k}\right|_{x_i = x_i^n} & \omega_{i,jk}^n &= \left.\frac{\partial^2 \omega_i(x_i)}{\partial x_j \partial x_k}\right|_{x_i = x_i^n} \end{aligned}\right\}. \tag{7}$$

It is noted that the rotation and displacement are not two independent variables. During deformation of a granular material, the rotation of a particle consists of two components: the rigid body rotation Γ_i^n and the particle spin ψ_i^n, i.e.

$$\omega_i^n = \psi_i^n + \Gamma_i^n. \tag{8}$$

Whereas the particle spin is independent of the displacement field, the rigid body rotation is solely induced by the displacement field, given by

$$\Gamma_i^n = -\tfrac{1}{2} e_{ijk} u_{[j,k]}^n ; \quad u_{[i,j]}^n = -e_{ijk} \Gamma_k^n \tag{9}$$

where $u_{[i,j]}^n$ is defined as the skew-symmetric part of displacement gradients as opposed to the strain ε_{ij}^n defined as the symmetric part of the displacement gradient, given by

$$\left.\begin{aligned} \varepsilon_{ij}^n &= \tfrac{1}{2}(u_{j,i}^n + u_{i,j}^n) \\ u_{[i,j]}^n &= \tfrac{1}{2}(u_{i,j}^n - u_{j,i}^n) \end{aligned}\right\}. \tag{10}$$

2.2. *Different classes of continua*

In the last section, we represented the discrete system as an equivalent continuum system that is characterized by the two continuous fields of displacement and rotation. The discrete variables and the continuum variables are linked through the series expression of eqn (6). When the number of terms in this series is large enough, the continuum system can capture as many details as the discrete system. The advantage of the continuum system is that one can treat the problem at desirable levels by taking different degrees of approximation of eqn (6). The ultimate goal is to have a simple model while still capturing the essential features of granular materials.

Different degrees of approximation of eqn (6) lead to different classes of 'continua'. We discuss the various degrees of approximation under two categories: (1) high-gradient continua—including higher orders of deformation gradients, and (2) first-gradient continua—including only the first order of deformation gradients.

(1) *High-gradient continua*

Class 1 : *High-gradient micro-polar continua.* On substituting eqn (6) into eqn (1), the inter-particle displacement and the inter-particle rotation between the nth particle and the mth particle can be expressed by a series, given by:

$$\left.\begin{aligned}\delta_k^{nm} &= u_{k,l}^n L_l^{nm} + \tfrac{1}{2} u_{k,lm}^n L_l^{nm} L_m^{nm} + \tfrac{1}{6} u_{k,lmn}^n L_l^{nm} L_m^{nm} L_n^{nm} \\ &\quad + e_{klm}[r_m^{mc}(\omega_{l,p}^n L_p^{nm} + \tfrac{1}{2}\omega_{l,pq}^n L_p^{nm} L_q^{nm}) + \omega_l^n L_m^{nm}] + \dots \\ \theta_k^{nm} &= \omega_{k,l}^n L_l^{nm} + \tfrac{1}{2}\omega_{k,lm}^n L_l^{nm} L_m^{nm} + \tfrac{1}{6}\omega_{k,lmn}^n L_l^{nm} L_m^{nm} L_n^{nm} + \dots .\end{aligned}\right\} \tag{11}$$

Equation (11) is a general form. Particle spin and moment transmitting through the continua are considered.

Class 2 : *High-gradient couple stress/Cosserat continua.* In the situation in which particle spin is neglected, the particle rotation is equal to the rigid body rotation given in eqn (9). The inter-particle displacement and the inter-particle rotation between the nth particle and the mth particle in eqn (11) reduce to

$$\left.\begin{aligned}\delta_k^{nm} &= \varepsilon_{lk}^n L_l^{nm} + \tfrac{1}{2}\varepsilon_{kl,m}^n L_l^{nm} L_m^{nm} + \tfrac{1}{6}\varepsilon_{kl,pq}^n L_l^{nm} L_p^{nm} L_q^{nm} \\ &\quad + u_{[k,l],m}^n L_m^{nm}\left(\frac{L_l^{nm}}{2} - r_l^{cm}\right) + \tfrac{1}{2} u_{[k,l],mn}^n (\tfrac{1}{3} L_l^c - r_l^{cm}) L_m^{nm} L_n^{nm} + \dots \\ \theta_k^{nm} &= \tfrac{1}{2} e_{kpq} u_{q,pl}^n L_l^{nm}.\end{aligned}\right\} \tag{12}$$

It is noted that, even though the particle spin is neglected, the gradients of rigid body rotation can still contribute to inter-particle rotation and cause the transmission of contact moments through granular material. This mechanism resembles that proposed in couple stress theory and Cosserat theory (Cosserat and Cosserat, 1909; Truesdell and Toupin, 1960; Toupin, 1962; Mindlin and Tiersten, 1962).

Class 3: *High-gradient non-polar continua.* In the same situation as class 2, where particle spin is neglected, the particle rotation is equal to the rigid body rotation given in eqn (9). We further neglect the moment transmission caused by inter-particle rotation θ_i^{nm}. On ignoring inter-particle rotation, eqn (12) reduces to

$$\begin{aligned}\delta_k^{nm} &= \varepsilon_{lk}^n L_l^{nm} + \tfrac{1}{2}\varepsilon_{kl,m}^n L_l^{nm} L_m^{nm} + \tfrac{1}{6}\varepsilon_{kl,pq}^n L_l^{nm} L_p^{nm} L_q^{nm} \\ &\quad + u_{[k,l],m}^n L_m^{nm}\left(\frac{L_l^{nm}}{2} - r_l^{cm}\right) + \tfrac{1}{2} u_{[k,l],mn}^n (\tfrac{1}{3} L_l^c - r_l^{cm}) L_m^{nm} L_n^{nm} + \dots .\end{aligned} \tag{13}$$

The continuum variables still involve high gradients of displacement.

(2) *First-gradient continua*

Class 4 : *Micro-polar continua.* By using up to the first-order gradients of displacement and rotation, eqn (11) is simplified. The inter-particle displacement and the inter-particle rotation can be expressed as

$$\begin{aligned}\delta_i^{nm} &= (u_{[i,j]}^n - e_{ijk}\omega_k^n) L_j^{nm} + e_{ijk}\omega_{j,l}^n (r_k^{nm} L_l^{nm} - r_k^{nm} L_l^{nm}) \\ \theta_i^{nm} &= \omega_{i,j}^n L_j^{nm}.\end{aligned} \tag{14}$$

The first gradient of rotation, $\omega_{i,j}^n$, is termed the micro-polar strain (Eringen, 1968). To study the influence of inter-particle stiffness on macro-behavior, Chang and Ma (1991,

1992) derived a constitutive law for granular material based on eqn (14). The form of the derived constitutive law resembles that of the micro-polar continua in which particle spin and moments transmission are considered.

Class 5—Quasi-micro-polar continua. On neglecting the particle rotation gradient in eqn (14), the inter-particle rotation θ_i^{nm} vanishes and eqn (14) becomes

$$\delta_i^{nm} = (u_{i,j}^n - e_{ijk}\omega_k^n)L_j^{nm}. \tag{15}$$

With the absence of particle rotation gradient and of moment transmitting, the granular medium is no longer a micro-polar medium. Note that, in eqn (15), the particle rotation ω_i^n (including particle spin) is considered even though the rotation gradient $\omega_{i,j}^n$ is neglected. Since the effect of particle spin ψ_i^n is considered, the granular medium is of a quasi-micropolar type. Using the expression of eqn (15), Chang and Misra (1989) and Chang (1993) derived constitutive models for granular materials.

Class 6: Classic continua. On neglecting the particle spin in eqn (15), the particle rotation is equal to the rigid body rotation given in eqn (9). Equation (15) becomes

$$\delta_i^{nm} = \varepsilon_{i,j}^n L_j^{nm}. \tag{16}$$

This simple linear approximation provides a link between strain and inter-particle displacement. The constitutive law for a granular medium derived on the basis of eqn (16) resembles that of classic continua in solid mechanics. Under the assumption of eqn (16), constitutive models for granular material can be found in the work by Walton (1987), Bathurst and Rothenberg (1988), Chang (1988), Jenkins (1988), etc.

Most work in the literature on micro–macro properties of granular material treat granular material as first-gradient continua in classes 4–6. However, very little attention has been paid to the representation of granular material as high-gradient continua in classes 1–3. This is primarily due to the difficulties of dealing with the high-rank tensors. In the present paper, we aim to develop a constitutive model of the simple high-gradient continua (i.e. class 3).

2.3. *Stress in an assembly*

The equilibrium equations for an infinitesimal element within a particle is given by

$$\tau_{ij,i} = 0 \tag{17}$$

where τ_{ij} is the Cauchy stress for the infinitesimal element. We define the mean stress σ_{ij}^n for a particle as the average of the stress τ_{ij} over the volume of the particle:

$$\sigma_{ij}^n = \frac{1}{V^n}\int_{V^n} \tau_{ij}\,\mathrm{d}v. \tag{18}$$

By using the equilibrium condition and divergence theorem, the volume integral in eqn (14) can be converted into a surface integral, which can in turn be expressed by a summation over the discrete boundary forces, given by (Chang and Liao, 1989)

$$\sigma_{ij}^n = \frac{1}{V^n}\sum_{c=1}^{N^n} f_j^c r_i^{nc} \tag{19}$$

where N^n is the total number of contacts of the nth particle.

Now, we envisage a representative volume of granular material that is sufficiently small when compared with the scale of the boundary value problem, yet consists of a sufficiently large number of particles to be statistically representative of the behavior of the material. The stresses for such a representative unit can be defined on the basis of the volume average of stresses at particle level as

$$\sigma_{ij} = \frac{1}{V}\sum_{n=1}^{M} \sigma_{ij}^{n} V^{n} = \frac{1}{V}\sum_{n=1}^{M}\sum_{c=1}^{N^{n}} f_j^c r_i^{nc} \tag{20}$$

where M is the total number of particles in the representative volume V.

It is noted that the double summation in eqn (16) can be expressed by a single summation over the total number of contacts N in the representative volume, given by

$$\sigma_{ij} = \frac{1}{V}\sum_{c=1}^{N} f_j^c L_i^c \tag{21}$$

where L^c is the branch vector, the same as that defined in eqn (6). The expression of mean stress in eqn (21) is similar to that derived by Christoffersen *et al.* (1981) and Rothenberg and Selvadurai (1981) from the principle of virtual work.

2.4. *Constitutive relationship for an assembly*

On the basis of the mean stress defined in eqn (21), we now seek to derive the stress–strain relationship. We first use the inter-particle contact law of eqn (2) to express the inter-particle force in eqn (21) in terms of inter-particle displacement and then use the kinematic relationship [eqn (13)] to express the inter-particle displacement in terms of strain and higher gradients of strain, thus

$$\sigma_{ij} = \frac{1}{V}\sum_{c=1}^{N} L_i^c K_{jk}^c \left(\varepsilon_{lk}^{n} L_l^c + \tfrac{1}{6}\varepsilon_{kl,mn}^{n} L_l^{nm} L_m^c L_n^c + \tfrac{1}{2}\varepsilon_{kl,m}^{n} L_l^c L_m^c \right.$$
$$\left. + u_{[k,l],m}^{n}\left(\frac{L_l^c}{2} - r_l^{cm}\right) L_m^c + \tfrac{1}{2} u_{[k,l],mn}^{n}\left(\frac{L_l^{nm}}{3} - r_l^{cm}\right) L_m^c L_n^c \right). \tag{22}$$

We adopt the kinematic hypothesis that the geometric deformation is the same for all particles (i.e. the particle strain, ε_{ij}^{n}, equals the overall strain, ε_{ij}). The constitutive equations can be expressed in the following form:

$$\sigma_{ij} = A_{ijkl}\varepsilon_{kl} + B_{ijklmn}\varepsilon_{kl,mn} + C_{ijklm}\varepsilon_{kl,m} + D_{ijklm}u_{[k,l],m} + E_{ijklmn}u_{[k,l],mn} \tag{23}$$

where

$$A_{ijkl} = \frac{1}{V}\sum_{c=1}^{N} L_i^c K_{jk}^c L_l^c$$

$$B_{ijklmn} = \frac{1}{6V}\sum_{c=1}^{N} L_i^c K_{jk}^c L_l^c L_m^c L_n^c$$

$$C_{ijklm} = \frac{1}{2V}\sum_{c=1}^{N} L_i^c K_{jk}^c L_l^c L_m^c$$

$$D_{ijklm} = \frac{1}{V}\sum_{c=1}^{N} L_i^c K_{jk}^c \left(\frac{L_l^c}{2} - r_l^{cm}\right) L_m^c$$

$$E_{ijklmn} = \frac{1}{2V}\sum_{c=1}^{N} L_i^c K_{jk}^c \left(\frac{L_l^{nc}}{3} - r_l^{cm}\right) L_m^c L_n^c.$$

The constitutive constants are functions of the branch length, inter-particle stiffness, and number of contacts in the representative volume.

Compared with the conventional stress–strain law, stress in this constitutive equation is a function not only of strain but also of higher gradients of strain. For a representative volume of the granular material, the medium can be treated as statistically homogeneous and can thus be regarded as possessing central symmetry. In this situation, $C_{ijklm} = 0$, $D_{ijklm} = 0$. The effects of the first gradient of strain and rotation can be neglected.

The constitutive equation for the granular assembly becomes

$$\sigma_{ij} = A_{ijkl}\varepsilon_{kl} + B_{ijklmn}\varepsilon_{kl,mn} + E_{ijklmn}u_{[k,l],mn}. \tag{24}$$

The derived second-gradient constitutive law for granular material is in the same class of constitutive law as that proposed by Toupin and Gazis (1964), Mindlin (1965), Coleman and Hodgdon (1985), etc. The present constitutive theory is interesting in that the constitutive coefficients are derived directly from the inter-particle contact stiffness. Thus the present constitutive theory provides a link between micro-scale properties and macro-scale behavior.

3. CONSTITUTIVE CONSTANTS FOR AN ISOTROPIC GRANULAR ASSEMBLY

3.1. *Constitutive coefficient tensors in integration form*

It is of interest to evaluate the role of inter-particle properties and particle size (internal length) in the constitutive behavior. To this end, we select an idealized packing structure and derive closed-form expressions for the constitutive constants explicitly in terms of inter-particle stiffness. The idealized granular material is made of equal-size spheres and has an isotropic packing structure. The packing has the same inter-particle properties for all contacts. The contact stiffness is constant and independent of the contact force.

Since the representative volume consists of a large number of particles, a summation of any quantity over all particle contacts can be expressed in an integral form by introducing a density function $\xi(\gamma,\phi)$. Let F^c be the quantity, dependent on the orientation of contact, to be summed over all contacts. The summation of F^c can be written in an integral form, given by

$$\sum_{c=1}^{M} F^c(\gamma,\phi) = \frac{1}{2}\int_0^{\pi}\int_0^{2\pi} F^c(\gamma,\phi)\xi(\gamma,\phi)\sin\gamma\, d\gamma\, d\phi. \tag{25}$$

For a packing structure with an isotropic orientational distribution of inter-particle contacts,

$$\xi(\gamma,\phi) = \frac{M}{2\pi}.$$

The summation becomes

$$\sum_{c=1}^{N} F^c(\gamma,\phi) = \frac{M}{4\pi}\int_0^{\pi}\int_0^{2\pi} F^c(\gamma,\phi)\sin\gamma\, d\gamma\, d\phi. \tag{26}$$

For packing with equal spheres of radius r, the branch vector $L_i^c = 2rn_i^c$. The unit contact normal vector n_i^c is a function of γ,ϕ as given in eqn (4). The constitutive coefficients in a summation form as in eqn (17) can now be expressed in an integral form as follows:

$$\left.\begin{aligned} A_{ijkl} &= \frac{r^2 M}{\pi V}\int_0^{\pi}\int_0^{2\pi} n_i[k_n n_j n_k + k_s s_j s_k + k_t t_j t_k]n_l \sin\gamma \,\mathrm{d}\gamma\,\mathrm{d}\phi \\ B_{ijklmn} &= \frac{2Mr^4}{3\pi V}\int_0^{\pi}\int_0^{2\pi} n_i n_m n_n[k_n n_j n_k + k_s s_j s_k + k_t t_j t_k]n_l \sin\gamma\,\mathrm{d}\gamma\,\mathrm{d}\phi \\ E_{ijklmn} &= -\frac{Mr^4}{3\pi V}\int_0^{\pi}\int_0^{2\pi} n_i n_m n_n[K_n n_j n_k + K_s s_j s_k + K_t t_j t_k]n_l \sin\gamma\,\mathrm{d}\gamma\,\mathrm{d}\phi \end{aligned}\right\}. \tag{27}$$

3.2. *Isotropic conditions for constitutive tensors*

A tensor is termed an isotropic tensor if the components of the tensor remain invariant under all orthogonal transformations. Examining the tensors A_{ijkl}, B_{ijklmn}, E_{ijklmn} in eqn (27) shows that these constitutive tensors are all isotropic. This condition of isotropy is expected because the coefficient tensors are derived for granular materials with an isotropic contact orientational distribution, which is independent of the rotation of cartesian co-ordinates.

On the basis of Weyl's theory (1944) for an isotropic tensor, the coefficient tensors hold certain properties. Owing to the condition of isotropy, the 81 constants in the fourth-rank tensor A_{ijkl} are reduced to three non-zero constants. The fourth-rank tensor can be expressed as:

$$A_{ijkl} = a_1\delta_{ij}\delta_{kl} + a_2\delta_{ik}\delta_{jl} + a_3\delta_{il}\delta_{jk} \tag{28}$$

where a_1, a_2, and a_3 are the three constitutive constants, and δ_{ij} is the Kronecker delta.

For the same reason, the 729 constants in the sixth-rank tensor B_{ijklmn} are reduced to 15 non-zero constants, given by:

$$\left.\begin{aligned} B_{ijklmn} = {} & B_1\delta_{ij}\delta_{kl}\delta_{mn} + B_2\delta_{ij}\delta_{km}\delta_{ln} + B_3\delta_{ij}\delta_{kn}\delta_{lm} B_4\delta_{ik}\delta_{jl}\delta_{mn} \\ & + B_5\delta_{ik}\delta_{jm}\delta_{ln} + B_6\delta_{ik}\delta_{jn}\delta_{lm} + B_7\delta_{il}\delta_{jk}\delta_{mn} + B_8\delta_{il}\delta_{jm}\delta_{ln} \\ & + B_9\delta_{il}\delta_{jn}\delta_{km} + B_{10}\delta_{im}\delta_{jk}\delta_{ln} + B_{11}\delta_{im}\delta_{jl}\delta_{kn} + B_{12}\delta_{im}\delta_{jn}\delta_{kl} \\ & + B_{13}\delta_{ni}\delta_{jk}\delta_{lm} + B_{14}\delta_{ni}\delta_{jl}\delta_{km} + B_{15}\delta_{ni}\delta_{jm}\delta_{kl} \end{aligned}\right\} \tag{29}$$

where $B_i (i = 1, \ldots, 15)$ are the 15 constitutive constants. Similarly, the sixth-rank tensor E_{ijklmn} can be represented by another 15 constitutive constants.

3.3. *Symmetric conditions*

From the objectiveness requirement of the constitutive equations, we note the following conditions of suffixes: (1) the symmetric condition of strain [i.e. mutation of (k, l)], (ii) the antisymmetric condition of the rotation (i.e. alternation of $[k, l]$), and (iii) the symmetrical condition of the differentiation sequence for second-order gradients of strain and rotation [i.e. mutation of (m, n)].

On the basis of these conditions, we can rewrite the constitutive equation in the following form:

$$\sigma_{ij} = A_{ij(kl)}\varepsilon_{kl} + B_{ij(kl)(mn)}\varepsilon_{kl,mn} + E_{ij[kl](mn)}u_{[k,l],mn} \tag{30}$$

where indices contained in parentheses (or square brackets) are assumed to be subject to the operation of symmetrization (or alternation).

We now decompose the stress tensor into symmetric and anti-symmetric parts, and eqn (30) becomes

$$\sigma_{(ij)} = A_{(ij)(kl)}\varepsilon_{kl} + B_{(ij)(kl)(mn)}\varepsilon_{kl,mn} + E_{(ij)[kl](mn)}u_{[k,l],mn} \tag{31}$$

$$\sigma_{[ij]} = A_{[ij](kl)}\varepsilon_{kl} + B_{[ij](kl)(mn)}\varepsilon_{kl,mn} + E_{[ij][kl](mn)}u_{[k,l],mn}. \tag{32}$$

After the operation of symmetrization (or alternation) to the coefficient tensors, corresponding to the symmetric stress, the isotropic tensor $A_{(ij)(kl)}$ has two constants; $B_{(ij)(kl)(mn)}$ has five constants, and $E_{(ij)[kl](mn)}$ has one constant, given in the following form:

$$\left.\begin{aligned} A_{(ij)(kl)} &= \lambda\delta_{ij}\delta_{kl}+2\mu\delta_{ik}\delta_{jl} \\ B_{(ij)(kl)(mn)} &= b_1\delta_{ij}\delta_{kl}\delta_{mn}+b_2\delta_{ij}(\delta_{km}\delta_{ln}+\delta_{kn}\delta_{lm}) \\ &\quad +b_3\delta_{mn}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})+b_4\delta_{kl}(\delta_{jm}\delta_{ni}+\delta_{jn}\delta_{im}) \\ &\quad +b_5[\delta_{ik}(\delta_{jm}\delta_{ln}+\delta_{jn}\delta_{lm})+\delta_{il}(\delta_{jm}\delta_{kn}+\delta_{jn}\delta_{km}) \\ &\quad +\delta_{jk}(\delta_{im}\delta_{ln}+\delta_{ni}\delta_{lm})+\delta_{jl}(\delta_{im}\delta_{kn}+\delta_{ni}\delta_{km})] \\ E_{(ij)[kl](mn)} &= e_1[\delta_{ik}(\delta_{jm}\delta_{ln}+\delta_{jn}\delta_{lm})-\delta_{il}(\delta_{jm}\delta_{kn}+\delta_{jn}\delta_{km}) \\ &\quad +\delta_{jk}(\delta_{im}\delta_{ln}+\delta_{ni}\delta_{lm})-\delta_{jl}(\delta_{im}\delta_{kn}+\delta_{ni}\delta_{km})] \end{aligned}\right\} . \tag{33}$$

Similarly, for anti-symmetric stress, the isotropic tensor $A_{[ij](kl)}$ vanishes; $B_{[ij](kl)(mn)}$ has one constant, and $E_{[ij][kl](mn)}$ has two constants, given in the following form:

$$\left.\begin{aligned} A_{[ij](kl)} &= 0 \\ B_{[ij](kl)(mn)} &= b_6[\delta_{ik}(\delta_{jm}\delta_{ln}+\delta_{jn}\delta_{lm})+\delta_{il}(\delta_{jm}\delta_{kn}+\delta_{jn}\delta_{km}) \\ &\quad -\delta_{jk}(\delta_{im}\delta_{ln}+\delta_{ni}\delta_{lm})-\delta_{jl}(\delta_{im}\delta_{kn}+\delta_{ni}\delta_{km})] \\ E_{[ij][kl](mn)} &= e_2\delta_{mn}(\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}) \\ &\quad +e_3[\delta_{ik}(\delta_{jm}\delta_{ln}+\delta_{jn}\delta_{lm})-\delta_{il}(\delta_{jm}\delta_{kn}+\delta_{jn}\delta_{km}) \\ &\quad -\delta_{jk}(\delta_{im}\delta_{ln}+\delta_{ni}\delta_{lm})+\delta_{jl}(\delta_{im}\delta_{kn}+\delta_{ni}\delta_{km})] \end{aligned}\right\} . \tag{34}$$

The 11 constants in eqns (33) and (34), as a result of the integration of eqn (27), are given as follows:

$$\left.\begin{aligned} &\lambda = 4\alpha(K_n-K_s);\quad \mu = 2\alpha(2K_n+3K_s) \\ &b_1 = b_2 = b_4 = \tfrac{8}{21}\alpha r^2(K_n-K_s);\quad e_1 = -\tfrac{1}{3}K_s\alpha r^2 \\ &b_3 = \tfrac{8}{21}\alpha r^2(K_n+\tfrac{5}{2}K_s);\quad b_5 = \tfrac{8}{21}\alpha r^2(K_n+\tfrac{3}{4}K_s) \\ &e_2 = \tfrac{2}{3}K_s\alpha r^2;\quad e_3 = \tfrac{1}{3}K_s\alpha r^2;\quad b_6 = -\tfrac{2}{3}K_s\alpha r^2 \end{aligned}\right\} \tag{35}$$

where $\alpha = Mr^2/15V$, representing the density of the packing structure, M is the total number of inter-particle contacts in the representative volume V, and r is the radius of particles.

It is noted that, in eqn (35), the 11 constants are interrelated. Out of the 11 constants, there exist only four independent variables, namely, K_n, K_s, α, r. The interrelations among the 11 constants are caused by other additional restrictions of suffixes, for example, the mutations of (j, k), (i, l) and (m, l).

3.4. *Derived constitutive equation*

It is noted that the following relationships exist between the gradients of strain and rotation, given by

$$u_{[i,n]nj}+u_{[j,n]ni} = \nabla^2\varepsilon_{ij}-\varepsilon_{kk,ij} \tag{36}$$

$$\varepsilon_{kn,nl}-\varepsilon_{ln,nk} = \nabla^2 u_{[k,l]}. \tag{37}$$

The relationships in eqns (36) and (37) can be proved by using the mutation property of suffixes associated with the differentiation sequence.

On substituting the expressions for the constitutive tensors $A_{(ij)(kl)}$, $B_{(ij)(kl)(mn)}$, and $E_{(ij)[kl](mn)}$ given in eqns (33) into eqn (31), and using the relationship given in eqn (36), the symmetrical stress becomes

$$\sigma_{(ij)} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} + C_1\delta_{ij}\nabla^2\varepsilon_{kk} + C_2\nabla^2\varepsilon_{ij} + C_3\varepsilon_{kk,ij} \tag{38}$$

where

$$\left.\begin{aligned} C_1 &= b_1 + 2b_2 \\ C_2 &= 2(b_3 + 2b_5 + 2e_1) \\ C_3 &= 2(b_4 + 2b_5 - 2e_1) \end{aligned}\right\}. \tag{39}$$

On substituting the expressions for constitutive tensors $A_{[ij](kl)}$, $B_{[ij](kl)(mn)}$, and $E_{[ij][kl](mn)}$ given in eqns (34) into eqn (32), and using the relationship given in eqn (37), the skew-symmetrical stress becomes

$$\sigma_{[ij]} = C_4\nabla^2 u_{[i,j]} \tag{40}$$

where

$$C_4 = 2(e_2 + 2e_3 + 2b_6). \tag{41}$$

By substituting the constants in eqn (35) into eqn (41), it follows that $C_4 = 0$. This leads to a null skew-symmetric stress. The result is expected, since the moment transmitting through inter-particle contacts is neglected. On substituting the constants in eqn (35) into eqn (39), the final expression of the constitutive relation is given by

$$\sigma_{(ij)} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} + C_1\delta_{ij}\nabla^2\varepsilon_{kk} + C_2(\nabla^2\varepsilon_{ij} + \varepsilon_{kk,ij}) \tag{42}$$

where λ and μ in terms of inter-particle stiffness are given in eqn (35). The other two constants are as follows:

$$\begin{aligned} C_1 &= \tfrac{8}{7}\alpha r^2(K_n - K_s) \\ C_2 &= \tfrac{16}{7}\alpha r^2(K_n + \tfrac{3}{4}K_s). \end{aligned}$$

3.5 *Micro–macro properties*

On comparing the derived stress–strain law in eqn (42) with the generalized Hooke's law, the constants λ and μ are the usual Lame constants. The corresponding Young's modulus and Poisson's ratio, from eqn (35), are derived as:

$$\left.\begin{aligned} E &= \frac{4Mr^2}{3V}\left(\frac{2K_n + 3K_s}{4K_n + K_s}\right) \\ v &= \frac{K_n - K_s}{4K_n + K_s} \end{aligned}\right\}. \tag{43}$$

Equation (43) provides a method for estimating elastic moduli based on the values of inter-particle stiffness.

Equation (35) can also be rearranged to give:

$$\left.\begin{aligned} K_n &= \frac{3\lambda+2\mu}{20\alpha} \\ K_s &= \frac{\mu-\lambda}{10\alpha} \end{aligned}\right\}. \tag{44}$$

Equation (44) provides a means for estimating inter-particle stiffness based on the measured value of elastic moduli.

The values of the high-gradient constitutive coefficients C_1 and C_2 are expressed in terms of contact stiffness as given in eqn (42). By substituting eqn (44) into eqn (42), the values of C_1 and C_2 can be expressed in terms of Lame constants as follows:

$$\left.\begin{aligned} C_1 &= \tfrac{2}{7}\lambda r^2 \\ C_2 &= \tfrac{4}{7}\mu r^2\left(1+\frac{3(\lambda-\mu)}{10\mu}\right); \quad \text{or} \quad C_2 = \tfrac{2}{35}\mu r^2\left(\frac{7-8v}{1-2v}\right) \end{aligned}\right\}. \tag{45}$$

Equation (44) provides a useful method for estimating the high-gradient constitutive constants, C_1 and C_2, directly from the Lame constants and particle size. This relationship is practical, since the high-gradient constitutive coefficients are difficult to evaluate from a laboratory test.

3.6. *Role of internal length and inter-particle stiffness*

The high-gradient constitutive constants, C_1 and C_2 are functions of the internal length r of the granular assembly that represents the particle size. When the particle size of a granular material is very small compared with the representative volume of the material, the effect of the strain gradient in the constitutive equation can be neglected. Thus the constitutive equation reduces to the generalized Hooke's law for granular materials. On the other hand, the effect of the strain gradient becomes pronounced as the particle size increases.

Inter-particle stiffness has a significant effect on the second-gradient constitutive coefficients. Three cases are noted, as detailed below.

(1) K_s/K_n is less than 1: this corresponds to particles with a smooth surface. Such a ratio of inter-particle stiffness leads to a positive Poisson's ratio and thus a positive λ and a positive C_1. As the ratio of K_s/K_n decreases (i.e. a smoother surface), values of C_1 and λ increase whereas the value of C_2 decreases. The limiting value physically possible for K_s/K_n is zero. Corresponding to this limiting condition, it is noted that, under the present formulations for granular assemblies with spherical particles, the predicted Poisson's ratio cannot be greater than 0.25 and the Lame constant λ cannot be greater than μ.

(2) K_n/K_s is equal to 1: this corresponds to particles with a rough surface. Such a ratio of inter-particle stiffness leads to a zero Poisson's ratio and thus a zero λ and a zero C_1. Under these conditions C_2 is a positive number.

(3) K_s/K_n is greater than 1: this corresponds to particles with a very rough surface, which is an unusual situation. Such a ratio of inter-particle stiffness leads to a negative Poisson's ratio and thus a negative λ and a negative C_1.

4. COMPARISON WITH OTHER MODELS

4.1. *Simplified form of second-gradient theory*

A convenient simple form based on the second-gradient theory can be arrived at by neglecting the effects of the volume strain gradient $\varepsilon_{kk,ij}$ in eqn (42), and by assuming the condition of $K_s = 0$.

The simplified version of eqn (42) takes the following form of constitutive equation

$$\sigma_{ij} = (1+c\nabla^2)(\lambda\delta_{ij}\varepsilon_{kk}+2\mu\varepsilon_{ij}) \tag{46}$$

where c is a positive constant, given by $c = 2r^2/7$.

It is noted that the simplified model of second-gradient theory (with $K_s = 0$) given in eqn (46) is similar to the form given by Bazant and Pijaudier-Cabot (1989), based on non-local continuum theory, and the linear model of Mindlin's second-gradient theory (Mindlin, 1965; Beran and McCoy, 1970b).

4.2. *Second-gradient theory and non-local theory*

Comparison between a non-local model and a higher-gradient model for composite media can be found in the work by Beran and McCoy (1970a, b) and Levin (1971). Here we discuss the relations between non-local theory and the present second-gradient theory for granular material. On the basis of Taylor's expansion [eqn (6)], the high gradients of displacement at the local point n contribute to the displacement at another local point m in the neighboring distance. Second-order gradient terms in the present model therefore reflect the effect of the neighboring medium on a local point. It is thus deduced that the second-gradient theory is equivalent to the non-local theory under certain conditions.

In the Eringen–Kroener model of non-local elasticity, the constitutive equation is

$$\sigma_{ij}(x) = \int_V \alpha(|x-x'|)(\lambda\delta_{ij}\varepsilon_{kk}(x')+2\mu\varepsilon_{ij}(x'))\,\mathrm{d}v(x') \tag{47}$$

where α ($|x-x'|$) is the non-local function [see Kroener, 1967; Eringen and Edelen, 1972; Eringen, 1973]. Expand the strain in the integrand at point x, i.e.

$$\varepsilon_{ij}(x') = \varepsilon_{ij}(x)+(x'_k-x_k)\frac{\partial\varepsilon_{ij}(x)}{\partial x_k}+\tfrac{1}{2}(x'_k-x_k)(x'_l-x_l)\frac{\partial^2\varepsilon_{ij}(x)}{\partial x_k\partial x_l}+\ldots \tag{48}$$

and substitute the series of the strain in eqn (49) into eqn (47) of the non-local model. After neglecting higher terms, we obtain the first-order approximation of the nonlocal model, given by:

$$\left.\begin{aligned}\sigma_{ij} &= (1+c\nabla^2)(\lambda\delta_{ij}\varepsilon_{kk}+2\mu\varepsilon_{ij})\\ c &= \int_V \tfrac{1}{2}\alpha(|x'-x|)(x'_k-x_k)^2\,\mathrm{d}v(x')\end{aligned}\right\} \tag{49}$$

in which the integrand of eqn (49b) and the resultant c are positive. The value of c depends on the non-local function. Note that the first-order approximation of the non-local model given in eqn (49) is the same as the simplified form of the present second-gradient model in eqn (46). According to the second-gradient theory, the constant in eqn (49), $c = 2r^2/7$.

4.3. *Shear stress and gradient of volume strain*

The second-order gradient of volume strain in eqn (42) represents the inhomogeneous distribution of volume strain along two perpendicular directions. The inhomogeneous volume deformation results in symmetric shear stress along the two directions. This interaction of shear stress and volume strain is an interesting aspect of the second-gradient theory.

5. CONCLUSIONS

In this paper, a second-gradient constitutive theory is developed for granular materials, in which the effect of the second order of the strain gradient is considered. For granular material with an isotropic packing structure, the constitutive coefficients are derived in closed-form expressions, in terms of inter-particle properties. For isotropic material, there are four elastic constitutive constants, including two Lame constants and two constants associated with the strain gradient. The relationship in eqn (44) provides a useful method for obtaining the second-gradient constitutive coefficients directly from the Lame constants. This relationship is useful, since the values of the second-gradient constitutive coefficient are difficult to evaluate from a laboratory test.

The second-gradient constitutive coefficients are functions of internal length r (particle size) of the granular assembly. When the particle size in a granular material is very small, the effect of the strain gradient in the constitutive equation can be neglected. On the other hand, the effect of the strain gradient becomes pronounced for materials with large-size particles. Inter-particle stiffness has a significant effect on the second-gradient constitutive constants. The values of Poisson's ratio, λ and C_1, are positive for particles with a smooth surface (K_s/K_n less than 1), but they become negative for particles with a very rough surface (K_s/K_n greater than 1).

A simplified form of the present second-gradient theory resembles other second-gradient models proposed by Mindlin (1965), Bazant and Pijaudier-Cabot (1989), and Beran and McCoy (1970). The simplified model of the present second-gradient theory also resembles the first-order approximation of the Eringen–Kroner model in non-local elasticity.

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