Homogenisation techniques and Cosserat Continuum modelling of materials with microstructure

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Abstract

Homogenisation schemes producing continua with additional – rotational degrees of freedom are considered. Using a simple 1D example of periodical chains of spheres connected by translational and rotational springs two techniques based on differential expansions and integral transformations are analysed. It is shown that the method of differential expansions leads to a Cosserat Continuum that provides a reasonable compromise between the accuracy and simplicity. The homogenisation strategy by integral expansions leads to a non-local Cosserat Continuum. The method of homogenisation by differential expansions is generalised for a 3D case of granular materials with random contacts between grains.

Introduction

In modelling materials and rocks with microstructure, especially in multiscale modelling, an important role is played by homogenisation methods that provide continuum description at a specified scale. The homogenisation methods are well established in the case of classical or standard continua, each point of which is characterised by three translational degrees of freedom (DOF). However, in the case when the mechanical behaviour involves additional, eg rotational DOFs, as for example in granular materials or blocky rock masses, there exist many different approaches. The present paper aims at analysing different homogenisation techniques and developing a 3D continuum model for granular material.

Simple 1D structures

In many cases generalised continuum theories provide a convenient framework for the approximate representation of an originally discrete model. For illustration we consider a material consisting of one dimensional, parallel chains of identical, spherical grains. The grains are connected by translational springs of stiffness k and rotational springs of stiffness k_φ (Figure 1). The potential energy density reads:

$$W_i = \left(2\eta a^3\right)^{-1}\left\{k\left((u_{3i}-u_{3i-1})+(a/2)(\varphi_{2i}+\varphi_{2i-1})\right)^2+k_\varphi(\varphi_{2i}-\varphi_{2i-1})^2\right\}. \quad (1)$$

Here a designates the spacing of the mass centres of neighbouring spheres, r is the sphere radius, and $a^{-2}\eta^{-1}$ is the number of chains per unit area of cross-section.

Homogenisation by differential expansion – Cosserat Continuum

We replace the finite difference expressions in (1) by corresponding differential expressions. Truncation of the Taylor expansions after the second order terms gives the following approximation

$$W(x_1) = \left(2\eta a^3\right)^{-1}\left\{k\left(\frac{\partial u_3}{\partial x_1}\right)^2 a^2 + 2k\frac{\partial u_3}{\partial x_1}\varphi_2 a^2 + k{\varphi_2}^2 a^2 + k_\varphi\left(\frac{\partial \varphi_2}{\partial x_1}\right)^2 a^2\right\}. \quad (2)$$

Differentiation of the energy density with respect to the Cosserat deformation measures (eg, Nowacki, 1970[3])

$$\gamma_{13} = \frac{\partial u_3}{\partial x_1} + \varphi_2,\ \gamma_{31} = -\varphi_2,\ \kappa_{12} = \frac{\partial \varphi_2}{\partial x_1} \quad (3)$$

gives

$$\sigma_{13} = k(\eta a)^{-1}\gamma_{13},\ \sigma_{31} = 0,\ \mu_{12} = k_\varphi(\eta a)^{-1}\kappa_{12}. \quad (4)$$

Introduction of volume forces and moments and consideration of momentum and angular momentum equilibrium yields

$$\frac{\partial \sigma_{13}}{\partial x_1} + \rho f_3 = 0,\ \frac{\partial \mu_{12}}{\partial x_1} - \sigma_{13} + \rho m_2 = 0. \quad (5)$$

Formally, equations (3-5) represent a 1D Cosserat Continuum. For suitable reinterpretation of the model parameters one obtains the governing equations of a Timoshenko beam. In this case φ_2 represents the rotation of the beam cross-section and u_3 is the displacement of its neutral fibre.

For constant volume force ρf_3 and vanishing volume moment the solution of (3-5) for the j-th sphere reads

$$u_3(ja) = u_3(0) - (a\varphi_2(0) - \frac{2k_\varphi}{ka}\overline{C}_2)j - \frac{a}{2}\overline{C}_1 j^2 - \frac{q}{2k}j^2 - \frac{a}{3}\overline{C}_2 j^3 + \frac{qa^2}{24k_\varphi}j^4, \quad (6_1)$$

$$\varphi_2(ja) = \varphi_2(0) + \overline{C}_1 j + \overline{C}_2 j^2 - \frac{aq}{6k_\varphi}j^3. \quad (6_2)$$

The exact solution of the discrete model is obtained as

$$u_j = u_0 - (a\varphi_0 + 2\frac{k(a^2/4)-3k_\varphi}{3ka}\overline{C}_2)j - \frac{a}{2}\overline{C}_1 j^2 + \left(\frac{a^2 q}{24k_\varphi} - \frac{q}{2k}\right)j^2 -$$

$$-\frac{a}{3}\overline{C}_2 j^3 + \frac{a^2 q}{24k_\varphi}j^4, \quad (7_1)$$

$$\varphi_j = \varphi_0 + \overline{C}_1 j + \overline{C}_2 j^2 - \frac{aq}{6k_\varphi} j^3 . \qquad (7_2)$$

The solutions for the rotations (6_2) and (7_2) coincide exactly, whereas the solutions for the displacements coincide only if $k_\varphi/k >> a^2$.

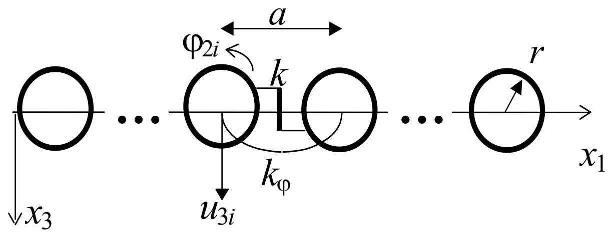

Figure 1: 1D chain of spherical grains connected by translational and rotational springs.

Homogenisation by integral transformation – non-local Cosserat Continuum

Kunin's (1982[1]) homogenisation procedure for discrete periodical structures is based on trigonometrical interpolation of discrete functions. For independent periodical chains of grains we have:

$$\begin{pmatrix} u(x) \\ \varphi(x) \end{pmatrix} = a \sum_i \begin{pmatrix} u_i \\ \varphi_i \end{pmatrix} \delta(x - ia) , \quad \begin{pmatrix} u_i \\ \varphi_i \end{pmatrix} = \int \delta(x - ia) \begin{pmatrix} u(x) \\ \varphi(x) \end{pmatrix} dx , \qquad (8_1)$$

$$\delta(x) = (\pi x)^{-1} \sin(\pi x / a) . \qquad (8_2)$$

Insertion of (8) into (1) and inclusion of volume forces and moments yields the following equations:

$$\sigma_{13}(x_1) = \left(\sqrt{\eta} a\right)^{-2} \{ E \int_{-\infty}^{+\infty} \begin{bmatrix} 2C(x_1 - y_1) - C(x_1 - y_1 - a) - \\ - C(x_1 - y_1 + a) \end{bmatrix} \gamma_{13}(y_1) dy_1 -$$

$$- E \int_{-\infty}^{+\infty} [2K(x_1 - y_1) - K(x_1 - y_1 - a) - K(x_1 - y_1 + a)] \Omega_{12}(y_1) dy_1 + \qquad (9)$$

$$+ E(a/2) \int_{-\infty}^{+\infty} [C(x_1 - y_1 - a) - C(x_1 - y_1 + a)] \Omega_{12}(y_1) dy_1 \}, \quad E = k / a$$

$$\mu_{12}(x_1) = \left(\sqrt{\eta} a\right)^{-2} \{ E(a/2) \int_{-\infty}^{+\infty} [C(x_1 - y_1 + a) - C(x_1 - y_1 - a)] \gamma_{13}(y_1) dy_1 +$$

$$+ E(a^2/4) \int_{-\infty}^{+\infty} [2C(x_1 - y_1) + C(x_1 - y_1 - a) + C(x_1 - y_1 + a)] \Omega_{12}(y_1) dy_1 +$$

$$+ E_\varphi \int_{-\infty}^{+\infty} [2C(x_1 - y_1) - C(x_1 - y_1 - a) - C(x_1 - y_1 + a)] \Omega_{12}(y_1) dy_1 +$$

$$+E\int_{-\infty}^{+\infty}[2K(x_1-y_1)-K(x_1-y_1+a)-K(x_1-y_1-a)]\gamma_{13}(y_1)dy_1+$$

$$+E\int_{-\infty}^{+\infty}[2K_1(x_1-y_1)-K_1(x_1-y_1+a)-K_1(x_1-y_1-a)]\Omega_{12}(y_1)dy_1+ \quad (10)$$

$$+Ea\int_{-\infty}^{+\infty}[K(x_1-y_1-a)-K(x_1-y_1+a)]\Omega_{12}(y_1)dy_1\}, \quad E_\varphi=k_\varphi/a$$

and

$$\frac{d\sigma_{13}(x_1)}{dx_1}+\frac{q(x_1)}{a^3\eta^2}=0,\quad \frac{d\mu_{12}(x_1)}{dx_1}-\sigma_{13}(x_1)+\frac{M(x_1)}{a^3\eta}=0\,. \quad (11)$$

The form of the angular momentum balance (11_2) is standard (cf. (5) for standard form). Equations (10, 11, 3) represent a 1D non-local Cosserat Continuum. The constitutive relationships (9), (10) reflect the non-local nature of the continuum since stress σ_{13} and moment stress μ_{12} at a point depend not only on strain and curvature at this point, but also on the corresponding deformation measures in a vicinity of this point.

This time the solution (again for vanishing volume moment) of the otherwise general 1D BVP is:

$$u(x)=u_0-(a\varphi_0+2\frac{k(a^2/4)-3k_\varphi}{3ka}\overline{C}_2)\frac{x}{a}-\frac{a}{2}\overline{C}_1\left(\frac{x}{a}\right)^2+\left(\frac{a^2q}{24k_\varphi}-\frac{q}{2k}\right)\left(\frac{x}{a}\right)^2-$$

$$-\frac{a}{3}\overline{C}_2\left(\frac{x}{a}\right)^3+\frac{a^2q}{24k_\varphi}\left(\frac{x}{a}\right)^4, \quad (12_1)$$

$$\varphi_2(x)=\varphi_2(0)+\overline{C}_1\frac{x}{a}+\overline{C}_2\left(\frac{x}{a}\right)^2-\frac{aq}{6k_\varphi}\left(\frac{x}{a}\right)^3. \quad (12_2)$$

Both (12_1) and (12_2) coincide with the solutions (7_1) and (7_2) of the discrete problem when one sets $x=ja$ in (12).

3D Cosserat Continuum model for granular material. Large deformation formulation

We describe the motion of the material points in terms of the Cartesian coordinates of their current and initial (reference) position: x_k (current) and X_k (reference) respectively; we assume $x_k(t=0)=X_k$ (k=1,2,3) and $x_i=x_i(X_j,t)$. The deformation gradient tensor and the rate of the deformation gradient tensor are $F_{iJ}=\partial x_i/\partial X_J$, $\dot{F}_{iJ}=\partial\dot{x}_i/\partial X_J=\partial v_i/\partial X_J=v_{i,J}$, ($i$, J = 1,2,3), where $v_i=\dot{x}_i$ are the components of the velocity vector and ($^\bullet$) means material derivative. We introduce the velocity gradient $\left(\dot{\mathbf{F}}\mathbf{F}^{-1}\right)_{ik}=v_{i,k}$, the symmetric part $v_{(i,k)}$ of which is the so called stretching and antisymmetric part $v_{[i,k]}$ is the spin $\boldsymbol{W}$. The rates of the Cosserat deformation measures, strains and curvature twists maybe introduced as follows

$$\gamma_{ji} = v_{i,j} - W^c_{ij},\ W^c_{ij} = \dot{R}^c_{ik} R^c_{jk},\ \kappa_{ji} = \partial \varphi_i^c \big/ \partial x_j, \tag{13}$$

where φ^c is the Cosserat rotation rate, $\boldsymbol{W}^c$ is the Cosserat spin. It can be shown that the Cosserat strain rate $\boldsymbol{\gamma}$ and curvature rate $\boldsymbol{\kappa}$ (13) are objective deformation measures.

The material time derivative of force equilibrium equation (body forces are neglected for simplicity) is obtained as

$$\rho \dot{a}_i = (\overset{\nabla}{\sigma}_{ji})_{,j} + (\sigma_{jk} W_{ik})_{,j} + (W_{jk}\sigma_{ki})_{,j} + (\sigma_{ji} v_{k,k})_{,j} - (\sigma_{ki} v_{j,k})_{,j}, \tag{14}$$

where $a_i = \dot{v}_i$, ρ is the density and the objective Jaumann- or co-rotational rate $\overset{\nabla}{\boldsymbol{\sigma}}$ and the material derivative $\dot{\boldsymbol{\sigma}}$ of the stress tensor $\boldsymbol{\sigma}$ are related through

$$\dot{\sigma}_{ji} = \overset{\nabla}{\sigma}_{ji} + \sigma_{jk} W_{ik} + W_{jk}\sigma_{ki}. \tag{15}$$

In a Cosserat Continuum the angular momentum balance of the standard continuum is extended in two respects. First, a surface moment is introduced in addition to the moment of the stress tractions (volume forces and volume moments are neglected for simplicity). Second, we have to include the angular momentum of the particles. The material derivative of the angular momentum balance for spherical grains of the diameter D reads:

$$\rho(D^2/10)\dot{\psi}_i = \varepsilon_{ikj}\overset{\nabla}{\sigma}_{kj} + \varepsilon_{ikj}\sigma_{kp}W_{jp} + \varepsilon_{ikj}W_{kp}\sigma_{pj} + \varepsilon_{ikj}\sigma_{kj}v_{q,q} +$$
$$+ (\overset{\nabla}{\mu}_{ji})_{,j} + (\mu_{jk} W_{ik})_{,j} + (W_{jk}\mu_{ki})_{,j} + (\mu_{ji} v_{k,k})_{,j} - (\mu_{ki} v_{j,k})_{,j}, \tag{16}$$

where $\psi_i = \dot{\varphi}_i$, $\boldsymbol{\mu}$ is the moment stress tensor.

To derive the constitutive equations we consider a 3D assembly of identical spherical grains. The diameter D of the grain is assumed as much smaller than typical dimensions of the problem under consideration. The particle arrangement is assumed to be statistically homogeneous. Every point of the equivalent continuum corresponds to the centroid of the reference sphere in the discrete material.

The starting point for our derivation is the equations of motion of the discrete system. Following [2] the summation over the particle contacts in the discrete system is replaced by an equivalent integral representation in which the integration is performed over the sphere's surface and a distribution function $A(\boldsymbol{x},\boldsymbol{n})$ is introduced to account for the orientational distribution of the contacts. We consider isotropic and independent of position contacts for which $A(\boldsymbol{x},\boldsymbol{n})=k/4\pi$, where $k(t)$ is the coordination number (the average number of contacts per grain). Applying the integral operation to the force and moment equations one obtains the following averaged equations of motion:

$$\rho \mathbf{a}_{sp} = \frac{6\nu_s}{\pi D^3}\int_\alpha A\mathbf{F}^n dn,\ \rho\frac{D^2}{10}\boldsymbol{\psi}_{sp} = \frac{3\nu_s}{\pi D^2}\int_\alpha A\mathbf{n}\times\mathbf{F}^n dn + \frac{6\nu_s}{\pi D^3}\int_\alpha A\mathbf{M}^n dn, \tag{17}$$

where $a_{i\,sp} = \dot{v}_{i\,sp}$, $\psi_{i\,sp} = \dot{\varphi}_{i\,sp}$, $\boldsymbol{v}_{sp}=\boldsymbol{v}_{sp}(\boldsymbol{x},t)$ and $\boldsymbol{\varphi}_{sp}=\boldsymbol{\varphi}_{sp}(\boldsymbol{x},t)$ are the expected values of the velocities and spins, ie the averages over all positions of the particles in which the reference sphere centre is originally at $\boldsymbol{x}$; $\boldsymbol{n}$ is the unit vector from the centre of a sphere to a contact on its surface.

Next we suppose that the ergodicity (as a property that every sequence or sizable sample is equally representative of the whole) is satisfied, ie the average over realisations, that is over all positions of the reference sphere, is equal to the average over large volume element. The average over realizations is given by averaging of the force equilibrium equation over all positions of contacts at the representative reference sphere. That allows us to introduce the following definitions of stress and moment stress tensors:

$$\sigma_{ji} = \frac{3\nu_s}{\pi D^2}\int_\alpha AF_i^n n_j dn,\ \mu_{ji} = \frac{3\nu_s}{\pi D^2}\int_\alpha AM_i^n n_j dn. \qquad (18)$$

Applying the considered above homogenisation by differential expansions we obtain the following objective constitutive relationships

$$\overset{\nabla}{\sigma}_{ji} = \frac{6\nu_s}{\pi D}\left[(k_n - k_s)A_{ijlm}\gamma_{lm} + k_s A_{lj}\gamma_{li}\right],\ A_{ijlm} = \frac{k}{30}\{\delta_{ij}\delta_{lm} + \delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}\},$$

$$\overset{\nabla}{\mu}_{ji} = \frac{6\nu_s}{\pi D}\left[(k_{\varphi_n} - k_{\varphi_s})A_{ijlm}\kappa_{lm} + k_{\varphi_s}A_{lj}\kappa_{li}\right],\ A_{lj} = \frac{k}{6}\delta_{lj}. \qquad (19)$$

The constitutive equations (19) are consistent with the principle of the material objectivity since the Jaumann derivatives are objective, so are the rates of the Cosserat strains and curvatures in the right hand side. The non-standard moduli in (19) are obtained from the microstructure (grain and contact distribution) and thus do not need to be calibrated from the experiments like in the phenomenological modelling.

Conclusions

Homogenisation of the governing equations by differential expansion leads to a Cosserat Continuum, while by integral transformation - to a non-local Cosserat theory. Cosserat Continuum describes the behaviour of granulates with reasonable accuracy being a long wave asymptotic approximation to the exact model. Non-local and discrete solutions for 1D granulates coincide. Homogenisation of equations of motion of separate particles based on averaging over all possible contacts leads to a Cosserat Continuum model for granular medium.

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