Multiscale approach for granular materials including an intermediate scale

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ABSTRACT: *This paper proposes an advanced micromechanical model that introduces an intermediate scale (mesoscopic scale): elementary hexagonal patterns of adjoining particles. This is a breakthrough with respect to current micromechanical models that generally describe the material by a single distribution of contacts. In essence, such models can incorporate a variety of local physical mechanisms. In this paper, the occurrence of diffuse failure is investigated, and the existence of a broad bifurcation domain inside the plastic limit surface is verified.*

1 INTRODUCTION

Numerous materials can be regarded as granular – or quasi-granular – because a scale at which the granular micro-structure clearly appears can be defined. This scale is often denoted the microscopic scale. The micro-structure is composed of an assembly of elementary particles whose contact interactions can be described by simple laws. On the macroscopic scale, these materials behave as continuous media with an acceptable approximation; in a sample containing a sufficient number of particles, the granular structure may indeed no longer be visible, even if it continues to play a fundamental role on the macroscopic mechanical behavior. The local behavior on the contact scale can usually be simulated in a very straightforward manner by elastic–plastic laws to address the overall behavior of the assembly. In fact, the complexity of the constitutive behavior of granular assemblies does not stem only from the local properties, but also from the disordered packing. In the particular case of frictional granular materials that is considered throughout this paper, the influence of the packing is of paramount importance, since the local behavior can be roughly described by a simple elastic-plastic relation including Coulomb's solid friction law. As a result, there is a clear advantage to developing constitutive models that embed a refined description of the micro-structure of the material.

In the continuity of the micro-directional model, the hexagonal model recently developed is presented here. It is shown how incorporating an intermediate scale is advantageous.

2 A BRIEF REVIEW OF THE MICRO-DIRECTIONAL MODEL

The micro-directional model was initially developed to describe the mechanical behavior of snow (Nicot, 2003). Then, the model was generalized to any type of granular assembly, with a particular emphasis on frictional granular materials (Nicot and Darve, 2005).

The micro-directional model, which is formulated in a small-strain Eulerian formulation, allows the Cauchy stress tensor $d\sigma$ to be related to the small strain tensor $d\varepsilon$ by taking micro-mechanical characteristics into account. The reverse scheme can also be considered: starting from a given stress tensor $d\sigma$, the small strain tensor $d\varepsilon$ is deduced (Cambou *et al.*, 1995; Chang and Hicher, 2005). Fundamentally, this model is based on a homogenization/localization procedure (Fig. 1) within a representative volume element (RVE), which is assumed to contain a sufficient number of spherical grains (or contacts). The homogenization/localization procedure can be resolved in three stages that are very briefly reviewed here (For more details, see Nicot and Darve, 2005).

The stress averaging corresponds to the Love formula (Love, 1927; Mehrabadi *et al.*, 1982):

$$\sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} F_i^c \; l_j^c \tag{1}$$

where $\mathbf{l}^c$ is the branch vector joining the centers of particles in contact on contact *c*, $\overrightarrow{F^c}$ is the contact force, and the sum is extended to all the N_c contacts occurring in the RVE of volume V. The norm of the branch vector $\mathbf{l}^c$ is assumed to be a constant parameter (equal to the mean diameter of the grains) whose evolution over loading programs is ignored. This ensures that the terms $\mathbf{F}^c$ and $\mathbf{l}^c$ are uncorrelated. The discrete summation given in Eq. (2) can be replaced with a continuous integration over all the contact directions in the physical space. This scheme confers the directional character to the model:

$$\sigma_{ij} = 2r_g \iint_D \hat{F}_i \; n_j \; \omega \; d\Omega \tag{2}$$

where ω is the density of contacts along each space direction $\mathbf{n}$, r_g denotes the mean radius of the sphere-shaped grains, $\hat{\mathbf{F}}$ is the average of all contact forces $\mathbf{F}^c$ associated with contacts oriented in the direction $\mathbf{n}$, $d\Omega$ is the elementary solid angle and the integration surface D is the half sphere.

The kinematic localization is given by:

$$d\hat{u}_i(\vec{n}) = 2r_g \; d\varepsilon_{ij} \; n_j \tag{3}$$

where $\hat{\mathbf{u}}(\mathbf{n})$ is the kinematic variable linked to $\hat{\mathbf{F}}(\mathbf{n})$ along the contact direction $\mathbf{n}$. As $\hat{\mathbf{u}}(\mathbf{n})$ depends only on the direction $\mathbf{n}$, this term is also denoted the directional kinematic variable.

The local behavior is described properly using an elastic-plastic mechanical model relating both the local normal force F_n^c and the local tangential force F_t^c to both the local normal relative displacement u_n^c and the local tangential relative displacement u_t^c. This model includes a Mohr-Coulomb criterion and can be expressed under the following incremental formalism, which introduces a normal elastic stiffness k_n and a tangential elastic stiffness k_t, both constant, and a local friction angle φ_g

The micro-directional model takes into account the change in the fabric of the granular assembly by directly modeling the increase or the decrease in the number of contacts along each direction of the physical space. In this approach, the number of contacts along a given direction is not computed from any fabric tensor, but is related to the normal strain rate along this direction. Following pioneering work based on physical evidence (Oda, 1972), it is thought that the number of contacts increases along contractive directions, whereas it decreases along dilative directions. Therefore, the distribution of contacts is likely to evolve over a loading path, inducing anisotropy to the texture (see Nicot and Darve, 2005, for more details).

3 THE *H* MICRO-DIRECTIONAL MODEL

The main weakness of the micro-directional model is related to the kinematic description (Eq. 3), inducing a too large stiffness along the principal loading direction. The global stiffness of a granular assembly does not stem only from the contact stiffness, but also from the ability of the assembly for rearranging. Thus, limiting our investigation to two-dimensional conditions, an intermediate scale, made up of an hexagonal patterns of grains, is introduced.

Basically, the granular assembly is described by a distribution of regular hexagonal patterns of grains (Fig. 1). Each hexagon is assumed to deform symmetrically with respect to a given direction $\mathbf{n}$ (Fig. 2). Then, given a macroscopic incremental strain, the balance equations of each hexagon of volume $V(\mathbf{n})$ can be solved, yielding both the strained configuration and internal forces. In elastic regime, we have (see Fig. 2 for the definition of the symbols used):

$$\begin{bmatrix} 2\cos\alpha & 1 & -2d_1\sin\alpha \\ 2\sin\alpha & 0 & 2d_1\cos\alpha \\ \cos\alpha & -1 & \dfrac{(k_t\ d_1+N_1)\sin\alpha - T_1\cos\alpha}{k_n} \end{bmatrix} \begin{bmatrix} \delta d_1 \\ \delta d_2 \\ \delta\alpha \end{bmatrix} = \begin{bmatrix} \delta l_1 \\ \delta l_2 \\ 0 \end{bmatrix} \tag{4}$$

and in plastic regime,

$$\begin{bmatrix} 2\cos\alpha & 1 & -2d_1\sin\alpha \\ 2\sin\alpha & 0 & 2d_1\cos\alpha \\ \cos\alpha & -1 & \dfrac{N_1\sin\alpha - T_1\cos\alpha}{k_n} \end{bmatrix} \begin{bmatrix} \delta d_1 \\ \delta d_2 \\ \delta\alpha \end{bmatrix} = \begin{bmatrix} \delta l_1 \\ \delta l_2 \\ -\dfrac{\delta T_1\sin\alpha}{k_n} \end{bmatrix} \tag{5}$$

Averaging all incremental contact forces over the overall specimen gives the macroscopic incremental stress tensor (Love formula):

$$\underline{\underline{\sigma}} = \frac{1}{V}\int \omega_e(\vec{n})\,\underline{\underline{P}}^{-1} \begin{bmatrix} V(\vec{n})\,\tilde{\sigma}_1 & 0 \\ 0 & V(\vec{n})\,\tilde{\sigma}_2 \end{bmatrix} \underline{\underline{P}}\,d\theta \tag{6}$$

with

$$V(\vec{n})\,\tilde{\sigma}_1 = 4N_1\ d_1\cos^2\alpha - 4T_1\ d_1\cos\alpha\sin\alpha + 2N_2\ d_2 \tag{7}$$

$$V(\vec{n})\,\tilde{\sigma}_2 = 4N_1\ d_1\sin^2\alpha + 4T_1\ d_1\cos\alpha\sin\alpha \tag{8}$$

$$\underline{\underline{P}} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \tag{9}$$

A major difference with respect to the micro-directional model (Nicot and Darve, 2005), is that grains appear explicitly, giving rise to both solid and void (or, more generally, internal fluid) phases. Moreover, the compressibility of the specimen is mainly due to the relative sliding between particles, rather than to the normal stiffness at contacts. This is a great advantage, giving rise to more realistic simulations of the mechanical response of granular assemblies. A first example of simulation of the response of a dense specimen over a drained biaxial test (after an initial isotropic compression at 200 kPa) is reported in Fig. 3. For this simulation, $k_n = 1000$ kN/m, $k_t = 500$ kN/m and $\varphi_g = 20$ degree. As seen in Figs. 3 and 4, the simulated response is qualitatively satisfying. The stress peak is obtained at a small strain (2%), and then a softening regime is observed. The macroscopic friction angle is 31 degrees at the peak. This is a typical response for dense materials, as confirmed by the volumetric strain response shown in Fig. 4: after initial contractant behavior, a dilatant regime develops. It must be noted that the softening regime obtained is constitutive, as both stress and strain are considered homogeneous. It is associated with no geometrical effect that would lead to kinematical discontinuities.

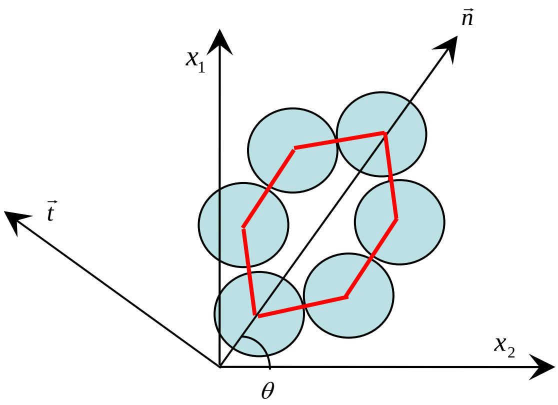

Fig. 1. Hexagonal set of contacting particles.

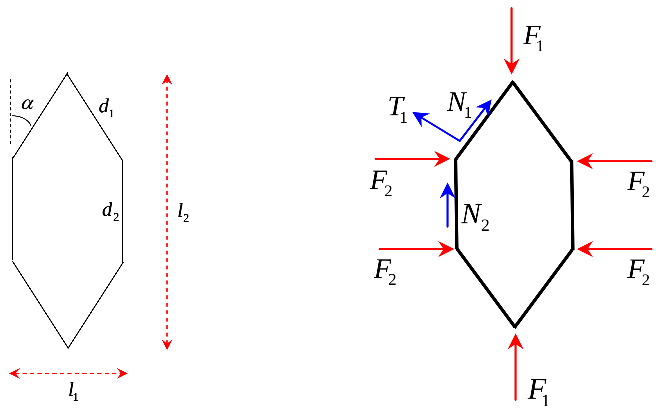

Fig. 2. Geometrical description and external forces applied to each hexagon.

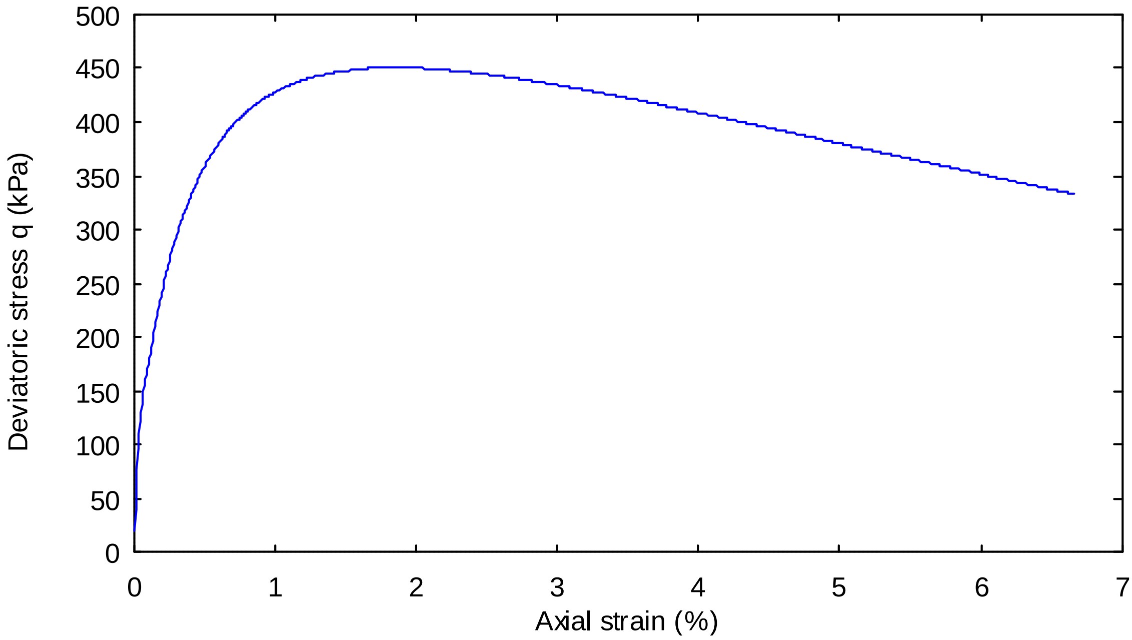

Fig. 3. Response over a drained biaxial test using the *H*-microdirectional model. Evolution of the deviatoric stress versus the axial strain.

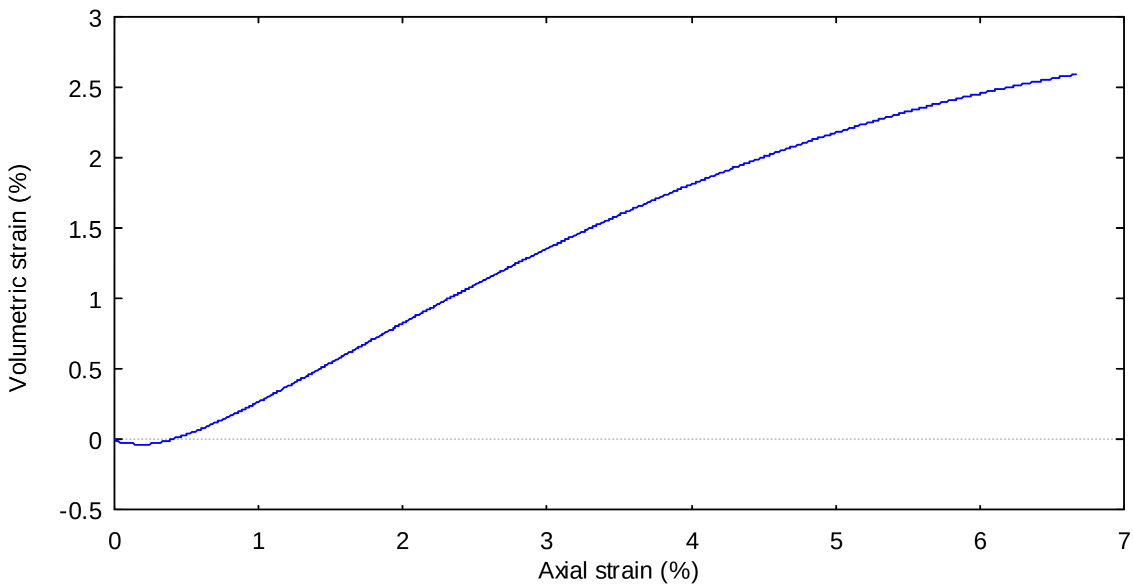

Fig. 4. Response over a drained biaxial test using the *H*-microdirectional model. Evolution of the volumetric strain versus the axial strain.

4 INSTABILITY ANALYSIS

It is of a great interest to investigate the occurrence of instability by using micromechanical models. Such enriched models can give rise to a wide set of different failure modes, such as, for example, the diffuse failure. The diffuse failure of a material is characterized by the abrupt collapse of the material, associated with a chaotic kinematic field. No localization pattern is visible. At the material point scale, such a failure mode is detected by the vanishing of determinant of the symmetric part $\mathbf{K}_s$ of the constitutive tensor $\mathbf{K}$. In two-dimensional conditions, and without rotation of the principal axes, the constitutive tensor $\mathbf{K}$ relates both the incremental stress ($\delta\sigma_1, \delta\sigma_2$) to the incremental strain ($\delta\varepsilon_1, \delta\varepsilon_2$). In fact, it can be shown that the vanishing of the determinant of $\mathbf{K}_s$ corresponds also to the existence of incremental strain directions vanishing the second-order work W_2, where $W_2 = \delta\sigma_i\ \delta\varepsilon_i$ (Darve et al., 2004). Let ($\delta\overline{\varepsilon}_1, \delta\overline{\varepsilon}_2$) be such a direction, that can be also characterized by the ratio $\overline{R} = \delta\overline{\varepsilon}_2 / \delta\overline{\varepsilon}_1$. If proportional strain paths are considered (the axial strain rate $\delta\varepsilon_1$, the proportional condition $\delta\varepsilon_2 = R\ \delta\varepsilon_1$ is prescribed where R is constant), this also means that the curve of the conjugate stress variable $\sigma_1 + R\ \sigma_2$ against the axial strain ε_1 passes through a peak for R lower than the critical value $\overline{R}$ (Nicot et al., 2009; Prunier et al., 2009).
To exemplify this, the simulation of such proportional strain loading paths was run, using the same parameters as those given in section 3. The initial confining pressure was also fixed to 200 kPa. As reported in Fig. 5, for R values lower than $R = -1.2$, the curves of $\sigma_1 + R\ \sigma_2$ against ε_1 passes through a peak. At the peak, the second order work is negative or nil, corresponding to the existence of a singular matrix $\mathbf{K}_s$. According to the theoretical background (Nova, 1994; Darve et al., 2004; Nicot and Darve, 2007), an abrupt collapse of the specimen is expected if any additional loading is applied at the peak, or along the descending branch. The ability of the micro-directional model to give rise to diffuse failure was ever discussed (Nicot and Darve, 2006). The above results show that this feature remains with the H micro-directional model. This result confirms the relevance of such micro mechanical approaches to investigate failure issues, in relation for instance with mechanical properties degradation.

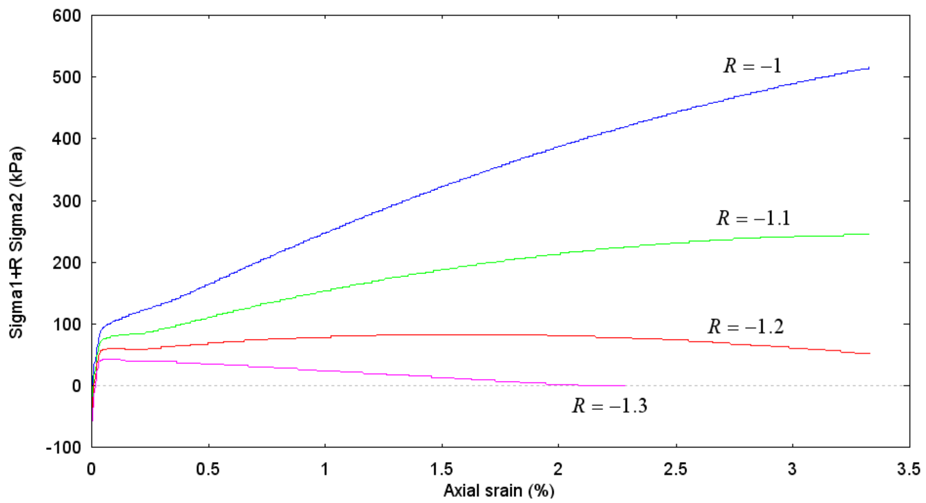

Fig. 5. Response over a proportional strain loading path using the H micro-directional model.

5 CONCLUDING REMARKS

This paper has presented the *H*-microdirectional model (Nicot and Darve, 2010), that introduces an intermediate scale between the microscopic scale and the REV scale. This multiscale model is based on a homogenization procedure that involves successively three scales: a microscopic scale, corresponding to the grain scale, a mesoscopic scale related to a hexagonal pattern of grains, and the whole assembly macroscopic scale. As such, the model allows relating the different scales, by expressing macroscopic terms from microscopic variables. The main advantage of this model, with respect to standard micromechanical approaches (Nicot and Darve, 2005) is that elementary grains patters are introduced. The deformation of such patterns results from the relative sliding between grains, rather that the deformation of grains. This leads to a more realistic kinematic description of grain assemblies, leaving aside the classical affine kinematic localization relation.

The capability of the model to exhibit a wide bifurcation domain was shown. By simulating proportional strain paths, it was shown that limit states could be obtained well before the plastic limit is reached.

This investigation draws new perspectives in the understanding of the key mechanisms leading to the failure of granular specimens. Numerical simulations based on a discrete element method are now in progress in order to examine the influence of the internal inertial mechanisms in the macroscopic destabilization of granular specimens.

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