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# ${\rm FEM} \times {\rm DEM}$ modelling of cohesive granular materials: numerical homogenisation and multi-scale simulation

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#### Abstract

This article presents a multi-scale modelling approach of cohesive granular materials, its numerical implementation and its results. At microscopic level, a Discrete Element Method (DEM) is used to model dense grains packing. At the macroscopic level, the numerical solution is obtained by a Finite Element Method (FEM). In order to bridge the micro and macro scales, the concept of Representative Elementary Volume (REV) is applied, in which the average REV stress and the consistent tangent operators are obtained in each macroscopic integration point as the results of DEM's simulation. In this way, the numerical constitutive law is determined through the detailed modelling of the microstructure, therefore taking into account the nature of granular materials. We first elaborate the principle of the computation homogenisation (FEM  $\times$  DEM), then demonstrate the features of our multi-scale computation in terms of a biaxial compression test. Macroscopic strain localization is observed and discussed.

**Key words:** Multi-scale, FEM, DEM, homogenisation, cohesive granular materials.

# 1. INTRODUCTION

The paper is organized as follows. Section 2 presents the homogenisation methods to bridge the scale between micro- and macro- level. Section 3 describes the numerical model by DEM. Some numerical results obtained with the multiscale computation (FEM × DEM) is demonstrated in section 4.

#### 2. HOMOGENISATION METHOD

$$\sigma_{ij}(t) = \Gamma^t \{ h_{kl}(\tau), \tau \in (0, t) \}$$

$$\tag{1}$$



Fig.1 Computational homogenisation scheme (Nguyen et al. 2013)

In order to capture the main effects of granular materials, a numerical homogenisation method by DEM computation is used to build the constitutive law.
 In this way, for a given history of macroscopic displacement gradient hkl, the macroscopic Cauchy stress \$\sigma\_{ij}\$ results from microscopic forces between grains through a well etablished homogenisation formula (Weber 1966):

$$\sigma_{ij} = \frac{1}{S} \cdot \sum_{(n,m)\in C} \vec{f}^{m/n} \otimes \vec{r}^{nm}$$
<sup>(2)</sup>

$$C_{ijkl} = \frac{d\sigma_{ij}}{dh_{kl}} \tag{3}$$

The consistent tangent operators can be found analytically for simple laws, butThe consistent tangent operators can be found analytically for simple laws, butThe consistent tangent tangent operators can be found analytically for simple laws, butThe consistent tangent tangent

For an increment of displacement gradient displacement gradient displacement of displacement gradient displacement gradient displacement ar first step in which we compute the stress at the end of this increment, noted  $\sigma_{ij}(\delta h_{kl})$ . Then we consider potter between the end of displacement gradient displacement displacement gradient displacement disp

$$\Delta_{kl}^{mn} = \delta_{mk} \cdot \delta_{nl} \tag{4}$$

Finally, the results of these two steps allow for the determination of consistent tangent operator:

$$C_{ijkl} = \frac{\sigma_{ij}(\delta h_{kl} + \epsilon \cdot \Delta_{kl}^{mn}) - \sigma_{ij}(\delta h_{kl})}{\epsilon}$$
(5)

This procedure is performed in every time step and in every Gauss point of themacroscopic finite element discretization. At the beginning and the end of eachstep, the REV is in a state of equilibrium.

#### 3. MICROSCOPIC DEM MODEL

The numerical approach used to model the REV of granular material is the Discrete Element Method (DEM) using bi-Periodic Boundary Conditions (PBC) (for details see Radjai and Dubois 2011). The REV of grains is a dense packing of 400 polydisperse circular 2D particles in which grains radii are uniformly distributed between  $R_{min}$  and  $R_{max}$  such that  $R_{max}/R_{min} = 5/2$ , Fig. 2(a). All grains interact via linear elastic laws and Coulomb friction when they are in <br/> contact. The normal repulsive contact force f<sub>el</sub> is related to the normal apparent interpenetration  $\delta$  (Fig. 2(b)) in the contact as  $f_{el} = -k_n \cdot \delta$ , where  $k_n$  is a normal stiffness coefficient ( $\delta < 0$  if a contact is present,  $\delta = 0$  if there is no contact). In order to model a cohesive material, a local cohesion is introduced for each contact by adding an attractive force  $f_c$  to  $f_{el}$ ;  $f_c < 0$  is here chosen constant for each pair of particles in contact. Thus, the overall normal force in a contact is f<sub>n</sub> = f<sub>el</sub> + f<sub>c</sub>. A degradation of the cohesion is taken into account by considering a vanishing of  $f_c$  when a contact separation occurs. If a new contact is created during the deformation process of the REV, then the local cohesion remains nil (un-recoverable cohesion). That give "fragility property" to the assembly of grains such that it models brittle materials.



Τa	a b l	e 1	Microscopie	c parameters
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	Parameter	Value
$\kappa = k_n / \sigma_0$	Stiffness number	1000
$k_n/k_t$	Stiffness ratio	1
$\mu$	Intergranular friction coefficient	0.5
$p^*$	Cohesion number	1



The Mohr – Coulomb failure criterion is widely applied for cohesive granular materials. With this criterion, the maximum strength is ruled by the Coulomb equation  $\tau = \sigma_n \tan \varphi + C$ , with two phenomenological intrinsic parame-



Fig.4 Mohr – Coulomb analysis of two biaxial tests. Circles I and III correspond to two stress states for biaxial test in compression. Circles II and IV show two stress states during the biaxial test in extension. Circles I and II correspond to the stress state for the maximum strength, for the two biaxial tests. Circles III and IV show the stress state for large strains, in the two biaxial tests. Bold lines shows the Coulomb criterion failure, with friction and cohesion on the left and only friction on the right, the one on the left recalled the one on the right figure with a dashed line.

### 4. MULTISCALE FEM $\times$ DEM SIMULATION

The FEM  $\times$  DEM approach was implemented in the FEM code Lagamine (Charlier 1987) which is able to manage finite strains. The implementation involved significant modification in the original code, but it essentially consisted in adding the DEM modelling as a constitutive numerical law.

To highlight the capabilities of this new FEM $\times$ DEM approach, we present hereafter a two-scale modeling of a Biaxial vertical compression test. The granular



## 4.1. Macroscopic results



with 64 Q8 elements

o. FD128: FEM×DEM with 128 Q8 elements

c. FD106: FEM×DEM with 106 Q8 elements







#### 4.2. Microscopic analysis

In order to highlight the advantage of our methods and to understand the origin of macroscopic phenomena, which comes from the microscopic evolution, in this section, we propose to analyze the stress evolution in various Gauss points at different location in the mesh. The mesh of 128 elements Q8 is chosen for this analysis. The focus is on the Gauss points into Q8  $n^{o}$  46 and Q8  $n^{o}$  52 (see Fig.8b). The element 52 is located in the shear band whereas the element 46 is far from the shear band, in a homogeneous zone.

Fig.10 shows the evolution of principal stresses (PS hereafter) (minor and major) in the two elements. As for the major PS, we observe that their respective evolutions diverge once the maximum shear strength is reached. The stress variations are rather smooth in element 46 and noisy in 52. Both 46 and 52



Fig.10 Microscopic analysis: Principal stress in elements 46 and 52 ( $\varepsilon_{11}$  is the equivalent overall axial strain for the specimen).



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show stress reduction, which is consistent with the softening of the specimen as a structure: despite the degradation of the material's properties is concentrated in the shear between the degradation of the material's properties as a structure: despite the degradation of the material's properties as a structure: despite the degradation of the material's properties as a structure: despite the degradation of the material's properties as a structure: despite the degradation of the material's properties as a structure: despite the degradation of the material's properties as a structure: despite the degradation of the material's properties as a structure: despite the degradation of the structure as a structure as a structure as a structure: despite the degradation of the structure as a structure as a structure as a structure; despite the structure as a structure as a structure; despite the structur



Fig.12 REV deformed at Gauss point of element 46 at global specimen strain  $\varepsilon_{11} = 3\%$ . (See Fig.3(b) for color convention).



Fig.13 REV deformed at Gauss point of element 52 at global specimen strain  $\varepsilon_{11} = 3\%$ . (See Fig.3(b) for color convention).

#### 5. CONCLUSION

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