TWO SCALE MODEL (FEM-DEM) FOR GRANULAR MEDIA

Michał Nitka, Gaël Combe, Cristian Dascalu, Jacques Desrues

Grenoble Université, Laboratory 3S-R, BP 53-38041 Grenoble cedex 9 France

Summary. *The macroscopic behavior of granular materials, as a consequence of the interactions of individual grains at the micro scale, is studied in this paper. A two scale numerical homogenization approach is developed. At the small-scale level, a granular structure is considered. The Representative Elementary Volume (REV) consists of a set of N polydisperse rigid discs (2D), with random radii. This system is simulated using the Discrete Element Method (DEM) - molecular dynamics with a third-order predictor-corrector scheme. Grain interactions are modeled by normal and tangential contact laws with friction (Coulomb's criterion).*
At the macroscopic level, a numerical solution obtained with the Finite Element Method (FEM) is considered. For a given history of the deformation gradient, the global stress response of the REV is obtain. The macroscopic stress results from the Love (Cauchy-Poisson) average formula including contact forces and branch vectors joining the mass centers of two grains in contact.
The upscaling technique consists of using the DEM model at each Gauss point of the FEM mesh to derive numerically the constitutive response. In this process, a tangent operator is generated together with the stress increment corresponding to the given strain increment at the Gauss point. In order to get more insight into the consistency of the two-scale scheme, the determinant of the acoustic tensor associated with the tangent operator is computed. This quantity is known to be an indicator of a possible loss of uniqueness locally, at the macro scale, by strain localization in a shear band.
The results of different numerical studies are presented in the paper. Influence of number of grains in the REV cell, numerical parameters are studied. Finally, the two-scale (FEM-DEM) computations for simple samples are presented.

1 INTRODUCTION

The presented study considers a two-scale numerical scheme for the description of the behavior of granular materials. At the small-scale level, we consider that the granular structure consists of 2D round rigid grains, modeled by the discrete element method (DEM). At the macroscopic level, we consider a numerical solution obtained with the Finite Element Method (FEM). The link between scales is that of the computational homogenization, in which average REV stress response of the granular microstructure is obtained in each macroscopic Gauss point of the FEM mesh as the result of the macroscopic deformation history imposed to the

REV. We also compute the tangent stiffness matrix, at the Gauss point, and the acoustic tensor, which is an indicator of possible unstable behaviors. The influence of different parameters on the stability of the macroscopic response is presented through the results of numerical tests. At the end, some results of two-scale computations are presented.

2 MACROSCOPIC MODELLING

For a given history of the deformation gradient, we compute the global stress response of the REV. The macroscopic stress results from the average formula $\sigma_{ij} = \frac{1}{S}\sum_{c=1}^{N_c} f_i^c \cdot l_j^c;\ \ i,j \in \{x,y\}$, where S is the area of the sample, f_i^c and l_j^c are respectively the component i of the force acting in the contact c and the component j of the branch vector joining the mass centers of two grains in contact [1]. Next, we convert the Cauchy stress into the Piola-Kirhoff stress [2]. The Piola-Kirchhoff stress is depended on the history of the *gradient of deformation* **F** [3], [4]

$$\overline{\mathbf{P}}(t) = \Gamma^t\{\overline{\mathbf{F}}(\tau), \tau \in [0,t]\} \tag{1}$$

For any history of $\overline{\mathbf{F}}$, we assume that $\overline{\mathbf{P}}$ admits a right time derivative $\dot{\overline{\mathbf{P}}}$ with respect to t:

$$\dot{\overline{\mathbf{P}}} = lim_{\delta t \to 0}\frac{\overline{\mathbf{P}}(t+\delta t)\ -\ \overline{\mathbf{P}}(t)}{\delta t} \tag{2}$$

We also assume that, for given history of $\overline{\mathbf{F}}$ till time t, the right-sided derivative $\dot{\overline{\mathbf{P}}}$ depends only on the right time derivative $\dot{\overline{\mathbf{F}}}$, that is :

$$\dot{\overline{\mathbf{P}}} = \Theta(\dot{\overline{\mathbf{F}}}) \tag{3}$$

where the function Θ is generally non-linear with respect to its argument $\dot{\overline{\mathbf{F}}}$.
In what follows, we limit our study to the case when the history of $\overline{\mathbf{F}}$ is given by $\overline{\mathbf{F}} = \mathbf{I} + \alpha\mathbf{G^0}$ with $\mathbf{G^0}$ being a fixed tensor and α being time-like loading parameter which runs monotonously from 0 to 1. In this case we get: $\dot{\overline{\mathbf{P}}} = \Xi(\alpha)$ and by differentiating with respect to α, we get that $\dot{\overline{\mathbf{F}}} = \mathbf{G^0}$ along the path. According to the definition of the function Θ we can write the approximate formula [3], [4]:

$$\Theta(\mathbf{G}^0) \approx \frac{\Xi(\alpha+\Delta\alpha)\ -\ \Xi(\alpha)}{\Delta\alpha} \tag{4}$$

The loss of uniqueness for the rate-type boundary value problems is analysed through the Rice approach [5]. Following this analysis we look for the rate of deformation gradient $\dot{\overline{\mathbf{F}}}$ which is discontinuous along the boundary of a localization band. It is known that such a discontinuity can be written as [5]:

$$\dot{\overline{F^1_{kL}}} = \dot{\overline{F^0_{kL}}} + q_k N_l \tag{5}$$

where $\mathbf{N}$ is the normal ($||\mathbf{N}|| = \mathbf{1}$) to the interface, $\dot{\overline{\mathbf{F^1}}}$ is taken on the same side as $\mathbf{N}$ and $\dot{\overline{\mathbf{F^0}}}$ on the opposite side. The stress vector has to be continuous across the interface :

$$\left(\dot{\overline{P^1_{iJ}}}\ -\ \dot{\overline{P^0_{iJ}}}\right)N_J\ =\ 0 \tag{6}$$

As $\dot{\overline{P}}{}^1_{iJ}$ and $\dot{\overline{P^0_{iJ}}}$ are linked to $\dot{\overline{F^1_{iJ}}}$ and, respectively, $\dot{\overline{F^1_{iJ}}}$, by Eq. (3), the unknows $\mathbf{q}$ and $\mathbf{N}$ have to satisfy the equation

$$\left(\Theta_{iJ}\left(\dot{\overline{\mathbf{F^0}}}+\mathbf{q}\otimes\mathbf{N}\right)-\Theta_{iJ}\left(\dot{\overline{\mathbf{F^0}}}\right)\right)N_J=0 \tag{7}$$

for given $\dot{\overline{\mathbf{F^0}}}$.
In the considered macroscopic quasistatic deformation process, the question of loss of ellipticity therefore reduces to the determination of the value α for which Eq. (7) has a non-trivial solution $(\mathbf{q},\mathbf{N})$, $\mathbf{q}\neq\mathbf{0}$.

In our case we restrict the search of non-trivial solutions to the case in which the tensor $\dot{\overline{\mathbf{F^1}}}$ is closed to $\overline{\mathbf{F^0}}$. This leads to a continuous bifurcation mode in the sense of Rice [5].
So, assuming that Θ is differentiable at $\dot{\overline{\mathbf{F^0}}}$, Eq. (7) yields, after linearization:

$$B_{iJkL}\left(\dot{\overline{\mathbf{F^0}}}\right)q_kN_LN_J=0 \tag{8}$$

where $B_{iJkL}\left(\dot{\overline{\mathbf{F^0}}}\right)=\frac{\partial\Theta_{iJ}}{\partial \dot{\overline{F}}_{kl}}|_{\dot{\overline{\mathbf{F}}}=\dot{\overline{\mathbf{F^0}}}}$ It is clear that a non-trivial solution exists only if the so-called *acoustic tensor* $\mathbf{Q}$, defined by $Q_{ik}=B_{iJkL}N_LN_J$, is singular, that is only if:

$$det\,\mathbf{Q}=\mathbf{0} \tag{9}$$

For this particular process considered here and given by $\overline{\mathbf{F}}=\mathbf{I}+\alpha\mathbf{G^0}$, we have seen that $\dot{\overline{\mathbf{F}}}$ is constant and equal to $\mathbf{G^0}$ and the function $\Theta(\mathbf{G^0})$ can be approximated by Eq.(4).
As to the derivation of Θ, it can be numerically approximated by finite differences:

$$B_{iJkL}=\frac{\Theta_{iJ}(\mathbf{G}^0+\varepsilon\Delta^{kL})-\Theta_{iJ}(\mathbf{G^0})}{\varepsilon} \tag{10}$$

where Δ^{kL} is a second-order tensor such that all its components are equal to 0 except the kL one which is equal to 1. In Fig. 1 we have represented the stress at the point $\delta f\Delta\alpha$ (in the same linear direction as point n) and stresses in points with perturbations $\varepsilon\Delta^{kL}$. We also computed the tangent matrix [3], [4] as :

$$B_{iJkL}=\frac{P_{iJ}(\alpha^{n+1}+\delta f\Delta\alpha+\varepsilon\Delta^{kL})\,-\,P_{iJ}(\alpha^{n+1}+\delta f\Delta\alpha)}{\delta f\;\varepsilon\Delta^{kL}} \tag{11}$$

where $\delta f\Delta\alpha$ is a small variation step in the main direction, $\varepsilon\Delta^{kL}$ is a small perturbation of the kL component.

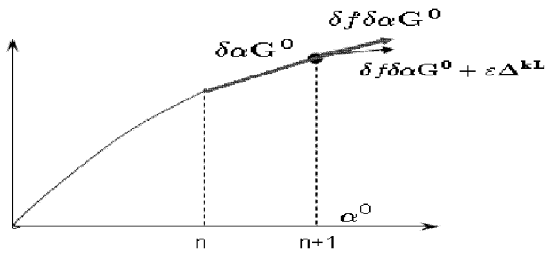

Fig. 1. Schematic representation of the computation of the tangent matrix

3 MICRO-SCALE MODELING: DEM

The system consist of a set of N polydisperse discs, with the random radii homogeneously distributed between R_{min} and $R_{max} = 2.5R_{min}$. This system is simulated using a discrete element method - molecular dynamics with a third-order predictor-corrector scheme [6]. All grains interact via a linear elastic law and Coulomb friction when they are in contact [7]. The normal contact force f_n is related to the normal apparent interpenetration δ of the contact as $f_n = k_n\delta$, where k_n is a normal stiffness coefficient ($\delta > 0$ if a contact is present, $\delta = 0$ if there is no contact). The tangential component f_t of the contact force is proportional to the tangential elastic relative displacement, with a tangential stiffness coefficient k_t. The Coulomb condition $|f_t| \leq \mu f_n$ requires an incremental evaluation of f_t in each time step, which leads to some amount of slip each time one of the equalities $f_t = \pm\mu f_n$ is imposed. A normal viscous component opposing the relative normal motion of any pair of grains in contact is also added to the elastic force f_n to obtain a critical damping of the dynamics. As the boundary condition we considered *Periodic Limit Condition* (PLC).

4 RESULTS

For the stability criterion the Rice [5] criterion was chosen, which says that if determinant of acoustic tensor is equal 0 (**det Q =0**) for some angle θ, there may exist bifurcation.
The influence of the size of the sample and the numerical parameters: small variation step δf and perturbation ε will be studied in this section. Periodic limit condition is applied for those tests. Friction between grains is assumed at $\mu = 0.5$.
The influence of the sample size for shear test for stress is presented in Fig. 2 (to be more clear, the diagrams were moved up on y-axis). Stars represent instability zones, that correspond to the $det\mathbf{Q} < \mathbf{0}$. This test was made for $\delta f = 0.1$ and perturbation $\varepsilon\Delta^{kL} = 2 \cdot 10^{-5}$. Different number of grains (400, 1024, 3025 and 4900 grains) were considered. We remark the diminution of the global number of potential instability points when the number of grains is increasing.
We have also done tests to check the influence of the small variation step $\delta f \delta\alpha$ and the small

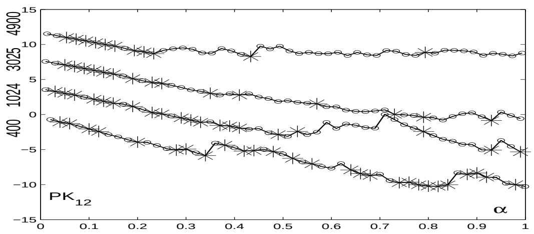

Fig. 2. Influence of the size of sample on macroscopic stability

perturbations $\varepsilon\Delta^{kL}$. In this case we have obtained larger stability zones for smaller values of small variation step $\delta f \delta\alpha$ and for smaller values of perturbation value. However, it is important to take the value of $\delta f \delta\alpha$ carefully to stay still in elasto-plasticy behaviour (not only elasticity).

To succeed in the macro-micro computations the numerical parameters should be chosen very carefully. In Discrete Element Method and also in Finite Element Method, there are different variations, which have significant influence on the convergence of the test.
For the FEM-DEM computations the open-source code 'FLagSHyP' written by J.Bonnet is used. On FEM level, the two-dimensional quadratic elements with four Gauss points were chosen.
On the micro level, in DEM calculations, according to our study of instability, the parameters: small variation step δf and small perturbation ε were chosen as 0.1 and $2 \cdot 10^{-5}$, respectively. The boundary conditions was periodic (PLC). Friction between grains $\mu = 0.5$ was chosen. Number of grains is equal 400 (only, because calculations are very time consuming).
First, the shear test was done, where incremental shear displacement is equal $\delta = 0.00025$. Results are plotted in figure 3.
Next, biaxial tests with strain control with no volume changes were done. The incremental

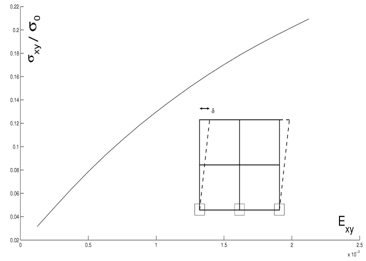

Fig. 3. DEM-FEM: Global stresses σ_{xy} for shear test with displacement $\delta = 0.00025$ imposed

deformation is $\delta E_{yy} = -\delta E_{xx} = 0.00025$. In the figure 4 (a) the stress-strain responses are presented.
The last tests were done for classical biaxial test. On the walls constant pressure is applied

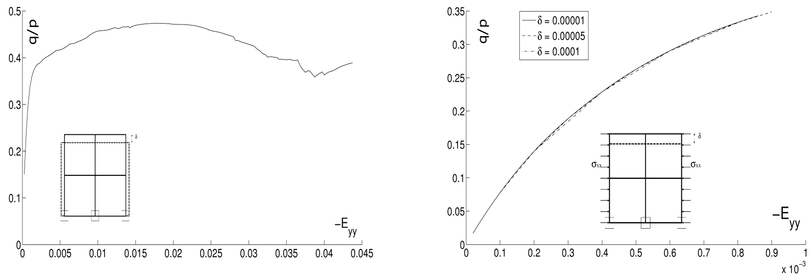

Fig. 4. DEM-FEM: Stress-strain response for (a) biaxial test (b) classical biaxial compression ($\delta = 0.00001$, $\delta = 0.00005$ or $\delta = 0.0001$).

equal to the isotropic stress. On the top displacement incremental step is imposed (three different incremental steps equal 0.00001, 0.00005 and 0.0001) 4 (b).
Those tests show that two-scale approach is possible to compute. More complicated tests as classical biaxial or shear can be simulated. It proves that even for non-linear behavior, the two scale model can work well.

5 CONCLUSIONS

A two-scale numerical approach for granular materials has been proposed, combining DEM modeling of the granular micro structure with the FEM modeling of the overall response. We focused on the consistency of the discrete-to-continuous approach, through the identification of the numerically-induced macroscopic instabilities.
The sample size plays an important role for stability zones. In order to prevent instabilities in the sense of Rice criterion, it is very important to make the correct choice for the size of the sample (not too small). It is also very important to choose the correct small variation step δf of and small perturbation ε. Both of them (as well as the number of grains in the cell) have significant influence on the number of instability points. This two parameters should be chosen in respect to the problem we want to solve. Microscopic behaviour may be a true physical behaviour, linked to instability and shear banding. As such, it should not be rejected in general. But the occurrence of such events far from the failure regime of the sample, if not limited to a few points but spread over the sample in a significant number of points, may indicate non-relevant numerical behaviour. This is a challenge to deal with, maybe by exploring more changes in the numerical parameters. However, it is still possible to compute small two-scales geotechnical problems. After study of the influence of the small variation step and perturbations coefficient, we are able to avoid numerical instabilities. Since, the computations are extremely time consuming, all tests are done for small sample with 400 grains, what causes that incremental step should be very small. For bigger incremental steps there is a problem with convergence. However this problem should disappear, when bigger REV samples will be used.

References

1. A.E.H. LOVE; ’A treatise on the mathematical theory of elasticity’; book of Cambridge University Press; 1927
2. J. BONET and R.D. WOOD; ’Nonlinear continuum mechanics for finite element analysis’; Cambridge University press, Cambridge; 1997
3. G. BILBIE, C. DASCALU, R. CHAMBON and D. CAILLERIE; ’Micro-fracture instabilities in granular solids’; In Bifurcations, Instabilities, Degradation in Geomechanics, Exadaktylos G. and Vardoulakis I. eds., pp. 231-242; 2007
4. G. BILBIE, C. DASCALU, R. CHAMBON and D. CAILLERIE; ’Micro-fracture instabilities in granular solids’; Acta Geotechnica, vol.3, pages 25-35; 2008
5. J. R. RICE; ’The localization of plastic deformation’; Theoretical and Applied Mechanics, W.T. Koiter, ed., North-Holland Publishing Company, pages 207-220; 1976
6. M.P. ALLEN and D.J. TILDESLEY; ’Computer simulations of liquids’; Clarendon Press, Oxford; 1989
7. P.A. CUNDALL and O.D.L. Strack, ’A discrete numerical model for granular assemblies’, Géotechnique 29, no. 1,47-65; 1979