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Towards a new approach for modeling the behavior of granular materials: A mesoscopic-macroscopic change of scale

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ABSTRACT

This paper constitutes a preliminary demonstration of the feasibility of a multi-scale approach for the definition of a constitutive law for granular materials. The case of two-dimensional granular materials was considered and the reasoning was built on 2D Discrete Element Method (DEM) simulations of 2D biaxial tests performed on sample made of disks. The change of scale relied on an intermediary local scale called the *meso-scale* which was based on the existence of meso-domains defined as closed loops of particles in contact. At the meso-scale, six sets of meso-domains or *phases*, with different properties in terms of local texture, have been defined. Then, an elastic–hardening–plastic model was designed at the phase scale and the identification of the model parameters was performed on a stress path denoted compression stress path. The model parameters defined for each phase were found correlated with the initial meso-texture of the considered phase and with the orientation of the loading path with respect to the phase orientation. The change of scale allowed us to obtain a modeling at the sample scale in good agreement with the DEM results on the compression stress path. Finally, the relevance of the model and of the approach were tested on a different stress path denoted unloading stress path. This was performed both at the level of the six phases and at the sample scale. The results were found to be in good agreement with the DEM simulations, which tends to validate the general approach presented in this paper, including the definition of the phases at the meso-scale, the design of a constitutive model at this scale, and the change of scale process to obtain the behavior of the material at the sample scale.

1. Introduction

So far, a straightforward and reliable modeling of granular materials remained an open issue. If rather simple models can give rather good answers for the design of common geotechnical works, predictions of the behavior of granular soils submitted to complex loadings such as cyclic loadings or loadings with rotation of principal axes of stresses require significant improvements. These difficulties are essentially linked to the discrete nature of granular materials which are composed of individual grains in contact. These materials, discontinuous and highly heterogeneous, show a very specific evolution of their internal texture essentially due to the interactions between grains. Classic phenomenological models used for the modeling of granular materials are not able to take into account the evolution of this texture for complex loadings in a rational and precise way. It is therefore of great interest to explore their behavior at the macroscopic scale (scale greater than the Representative Elementary Volume) from characteristics defined at a local scale. This kind of approach has been widely developed for heterogeneous materials (fluids or solids) and is known as *the change of scale approach* which consists of building constitutive models from local constitutive laws in which the evolution of the material texture can be taken into account more easily. These models, based on local information, are thus expected to better reflect the phenomena at stake within the granular materials than those that just take into account phenomena measured at the macroscopic scale.

Another method can be used to overcome the difficulty to model the behavior of granular material at REV scale. This method couples the Finite Element Method (FEM) where the stress increment within each element is derived from a representation of the granular medium using a Discrete Element Method (DEM). A homogenization approach (various techniques can be found) allows to get the stress and strain field at the macro-scale from local information (Guo and Zhao, 2014; Miehe and Dettmar, 2004; Nguyen et al., 2014b; Nitka et al., 2011). A different reasoning is proposed in this paper.

In the last few years, two change of scale approaches have been proposed in the literature concerning granular materials. The first

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approach (Cambou et al., 1995; 2015; Emeriault et al., 1996; Emeriault and Chang, 1997; Liao et al., 1997; Walton, 1987) considers a local scale, called micro-scale, defined at the level of contacts between particles. At this scale, the local static variables are the contact forces, which can easily be related to the stress tensor defined at the Representative Elementary Volume (REV) scale. However, it is more difficult to establish a direct relationship between the kinematic variables defined at contacts (relative displacements at contacts) and the macroscopic kinematic variable, the strain tensor, as proved by various authors (Bagi, 2006; Cambou et al., 2000). In order to overcome these difficulties when considering the micro-scale, other multi-scale approaches have introduced an intermediate scale between the micro-scale and macro-scale, which is defined at the level of clusters of particles (Cambou et al., 2015; Durán et al., 2010a; 2010b; Kruyt and Rothenburg, 1996; Kuhn, 1997; 1999; Liao et al., 1997; Nicot and Darve, 2011; Sab, 1997; Satake, 1992). Such an intermediate local scale is expected to allow the local structure of granular materials to be more precisely described and the local static and kinematic variables to be more consistently defined. In previous works (Chaze and Cambou, 2014; Nguyen et al., 2011; 2014a; 2009; Nguyen, 2014), different numerical simulations of 2D granular samples were carried out and an in-depth analysis of the evolution of physical and mechanical properties at an intermediate local scale, called *the meso-scale*, was provided. At this scale, the meso-domains are formed by closed loops of particles in contact. Therefore, a 2D sample of granular material can entirely be subdivided in such local domains. Following Nguyen et al. (2011); 2014a); 2009), six sets of meso-domains with different properties in terms of local texture called *phases*, can be defined.

The work presented herein is dedicated to the analysis of the behavior of these six phases through simulations of 2D DEM biaxial tests involving disks. The behavior of the material at the sample scale is derived from constitutive models designed at the phases' scale using a change of scale process. To reach this goal:

- In Section 2, DEM biaxial tests (loading stage and unloading stage) are presented and different properties at the meso-scale are deduced;
- In Section 3, the mechanical behavior of the phases are analyzed;
- In Section 4, we propose a phenomenological modeling of the mechanical behavior of the phases; the related parameters are identified on the loading stage. We establish some relationships between the model parameters defined for each phase and two intrinsic properties of these phases: their orientation with respect to the loading direction ***1′*** and the induced anisotropy defined by the tensor component $X_{1'}$ considered in the phenomenological model;
- In Section 5, a prediction of the mechanical behavior of the phases on a stress path different from the stress path used for the identification of the parameters is carried out. It constitutes a first validation of the model;
- In Section 6, a simple model to define the evolution of the volumetric amount of each phase related to the loading is proposed. Finally, we show that we can predict the mechanical behavior of the global sample on a stress path very different from the stress path used for identification of the parameters at the meso-scale. This is performed using a change of scale process.

2. Numerical simulation of a 2D biaxial test

The numerical simulation of a biaxial compression test involving a loading and an unloading was carried out using the commercial software PFC2D (Particle Flow, ITASCA Code) based on the initial work by Cundall (1971). The numerical sample is composed of 25,000 disks which are randomly generated in a rectangular box. The box is 1.35 m high and 0.9 m wide. The diameters of particles are uniformly distributed from 4.6 mm to 9.2 mm. The normal and tangential stiffnesses at particle contacts are equal to 10^9 N/m which is 20 times greater than the ones chosen in previous works (Chaze and Cambou, 2014; Nguyen et al., 2011; 2014a; 2009) in order to limit an over-represented elasticity in the behavior of the material. The inter-particle friction angle is equal to 30° which corresponds to an inter-particle friction ratio equal to 0.57. For the contacts between a particle and any wall of the box, the friction coefficient is set to 0. The specific mass of particles is equal to 3000 kg/m^2. Further dissipation in the system is introduced by means of a damping α proportional to the acceleration forces and equal to 0.3.

Table 1
Characteristics and parameters of the numerical sample.

Parameter	Value
Number of particles	25,000
Initial number of interparticle contacts	34,594
Initial number of rattlers	4178
Dimension of sample	1.35 m × 0.9 m
Diameters of particles	4.6–9.2 mm
Specific mass of particles	3000 kg/m^2
Inter-particle friction	0.57
Initial porosity	0.167
Normal and tangential stiffnesses of particles	10^9 N/m (2D)

To create the sample, the particles are randomly positioned on a grid and their sizes are increased to provide a final isotropic state for the sample with a confining stress of 100 kPa. The gravity is not considered in the simulations. As a consequence, a significant number of particles in the assembly does not have any contact or has only one or two contacts. These particles are called *rattlers* and they do not participate in supporting the external loading. At the final isotropic state, the sample porosity is equal to 0.167 (this porosity is estimated accounting for the rattlers, as usual with the software PFC2D). The parameters of the numerical sample are given in Table 1.

The sample is compressed with a strain velocity of the upper and lower walls equal to 2.2×10^{-3} s^{-1} in the vertical direction while the lateral confining pressure in the horizontal direction is maintained at 100 kPa. The loading is performed until it reaches the critical state (Poulos, 1981; Roscoe et al., 1958), obtained for an axial deformation of 10%. Then, the sample is unloaded until it reaches a new critical state for this new loading direction. At the beginning of the unloading stage, the vertical strain velocity is reduced to 7.4×10^{-4} s^{-1} to ensure that the contacts with the walls box are maintained at all times. The evolution of both the axial stress Σ_1 and the volumetric strain E_v throughout the test is shown in Fig. 1. According to the convention in soil mechanics, compressive stresses are positive and in Fig. 1 (*b*), positive volumetric strains stand for compression starting from the initial state.

Throughout the compression path (loading), the typical behavior of a 2D dense granular material is observed, with the existence of a peak of shearing resistance followed by a softening until the critical state. When shearing, contractancy is followed by important dilative volumetric deformations whose rate decreases towards zero when reaching the critical state. For the unloading path, the classic behavior of a 2D loose granular material is observed, with a stress-strain curve reaching the critical state monotonously. As expected, a large contractancy stage followed by a dilatancy stage is observed. The critical state of volumetric deformations when unloading has not been reached when the computation was stopped.