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A numerical homogenized law using discrete element method for continuum modelling of boundary value problems

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Abstract. This paper presents a new way to define constitutive laws based on particles interactions within the Discrete Element Method (DEM). The concept is based on Volume Element (VE) for which the constitutive law is constructed through a numerical homogenization process. The new law fully accounts for the discrete nature of granular materials. By using the response envelope diagrams proposed by Gudehus [1], a graphical representation of the constitutive law is obtained. The results suggest that the current law can fully capture the main features of granular materials such as anisotropy, path dependence and non-linearity.

Keywords: FEMxDEM Modelling, Granular materials, Homogenization.

1 Introduction

Granular materials are a special class of materials: some authors consider their behavior as intermediate between solid and fluid (see for instance [2]). Their behavior is heterogeneous and anisotropic by nature. In the context of continuum modeling of boundary value problems (BVP) by Finite Element Method (FEM), seeking after a constitutive model that can reproduce all the relevant properties of these materials, or a significant part of them, has a long story. Many works have been dedicated to this subject, attempting to model as much as possible the complex behavior of granular materials. They are often based on the theory of plasticity. Only a few of them allow representing an anisotropic behavior, e.g. [3,4]. Taking into account anisotropy in the plastic part in elastoplasticity response requires complex mathematical descriptions which can be difficult to implement, and to calibrate as well. In view of these persistent difficulties, a new trend was introduced in the geomechanical constitutive modelling landscape since the early 2000' years; it consists in building constitutive models directly based on discrete modeling, using a step by step computational homogenization [5,6,7].

Discrete Element Method (DEM) has been well known as an effective method for modeling granular material at the grain scale. Nevertheless, despite the advantages of the DEM approach, it seems to be impossible in most cases to model boundary value

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problems involving both real-size grains and real-size structures. Thus, building a constitutive law based on this method (i.e. DEM) and then implementing this homogenized law (NHL) into a FEM framework is of real interest. Such a model is expected to naturally describe specific features of granular materials. By using this new class of constitutive laws, real-size grain micro-structure on real-size macroscopic problems can be performed, without facing the intractable problem of dealing with trillions of grains in a full DEM model.

In the present paper, we focus on the response characteristics of this new constitutive law. The paper is thus structured as follows: Section 2 presents the DEM based constitutive law. A graphical representation of this constitutive law by response envelopes is studied and discussed in section 3. Some conclusions are given in section 4.

2 Numerical law based on DEM

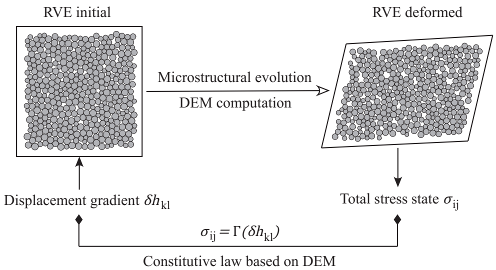

Fig. 1. Numerical constitutive law based on DEM

The constitutive law is a key ingredient of a Boundary Value Problem (BVP). This law expresses the local stress as a function of the history of the local deformation gradient. Constitutive models can be categorized into phenomenological models and micromechanical models (or macro- versus micro-scale models). Micromechanical constitutive models require a thorough understanding and models for each constituent which is not given for all materials. However, we believe that this is definitely the case for granular materials which can reliably be modelled using DEM (and a Volume Element). The latter can be considered to be similar to a constitutive law with a large (but delimited) number of internal variables such as: grain geometries, contact network and contact forces. The procedure to build this law was detailed in [5,7].

The overall picture of this law is illustrated in Fig. 1. A Volume Element (RVE) is used to define the constitutive law. At any state, this RVE is characterized by the size and interaction of the grains of which it is made. By applying a deformation gradient δh_{kl}, the system is simulated by DEM computation. The Cauchy stress σ_{ij} results from microscopic forces between grains [8]:

$$\sigma_{ij} = \frac{1}{S} \sum_{(p,q)\in C} f_i^{q/p} \, . \, r_j^{pq} \tag{1}$$

where S in two dimensional problem is the area of the microstructure; $f_i^{q/p}$, r_j^{pq} are respectively the contact forces acting in contact $c = (p, q)$, and the branch vector joining the mass center of two grains (p, q) in contact; C is the set of all contacts in the granular assembly. The VE is a granular assembly of polydisperse circular 2D particles. All grains interact via linear elastic laws and Coulomb friction when they are in contact. The normal repulsive contact force f_{el} is related to the normal apparent interpenetration δ by normal stiffness coefficient k_n ($\delta < 0$ if a contact is present, $\delta = 0$ if there is no contact). In order to model cohesive-frictional materials, a local cohesion is introduced for each contact by adding an attractive force f_c to f_{el}. Thus, the overall normal contact force is written as:

$$f_n = f_{el} + f_c = -k_n\delta + f_c \tag{2}$$

A degradation of the cohesion is taken into account by considering that f_c can vanish when a contact separation occurs. The tangential contact force f_t results from an accumulation of increments $\Delta f_t = k_t \Delta u_t$ computed at each time. Δu_t is the tangential relative displacement in the contact and k_t is the corresponding tangential stiffness. The Coulomb friction is considered as follow [9].

$$|f_t| \leq \mu f_{el} \tag{3}$$

3 Characterizing the response of the NHL: Gudehus' response envelopes

Gudehus 1979 proposed the concept of response envelopes as a powerful tool for the graphical representation of an incremental constitutive law [1]. By applying a deformation increment $\Delta\varepsilon$ in different directions in the deformation increment space, different stress increments $\Delta\sigma$ are obtained, that can be plotted in the stress increment space. The response envelopes are polar diagrams in the stress increment space of the stress increments resulting from different unit deformation increments in the deformation increment space. Their shapes and sizes depend upon the behavior of the constitutive law, and the way it takes into account the history of previous deformation, which can be very complex (e.g. cycles).

In the present paper, we use the response envelopes concept to analyze the incremental response of our DEM-based Numerical Homogenized law (NHL), which is expected to naturally describe the properties of granular materials.

Incremental strain $\underline{\Delta\varepsilon}$ defined as $\Delta\varepsilon_1 = \|\Delta\varepsilon\|.sin\alpha$ and $\Delta\varepsilon_2 = \|\Delta\varepsilon\|.cos\alpha$ ($0 \leq \alpha \leq 360°$) with $\|\Delta\varepsilon\| = \sqrt{(\Delta\varepsilon_1)^2 + (\Delta\varepsilon_2)^2} = 1$ is applied to the VE to compute numerically the incremental stress responses $\Delta\sigma$. Five initial stress states issued from a biaxial loading are used, labelled A, B, C, I, L. They correspond to the cases of the VE in the following states (Fig. 2): isotropic, intermediate anisotropic, failure (peak strength) and so called "critical state" – i.e. post failure stationary behavior.

The VE used for the study presented here is a 2D assembly made of 400 circular grains, with distribution of size between r_{min} and r_{max} such that $r_{max}/r_{min} = 5/3$. The initial coordination number and void ratio are respectively 4.2 and 0.18. The material is cohesive-frictional. The normal stiffness of contact k_n is such that $\kappa = k_n/\sigma_0 = 1000$, where σ_0 is the 2D confining pressure. The stiffness ratio $k_n/k_t = 1$. The cohesion force is defined regarding to the confining pressure by cohesion level $p^* = f_c/(a\,\sigma_0) = 1$ with a the typical diameter of grain in VE. The intergranular angle of friction is set $\mu = 0.5$. When sliding or disjunction occurs at one contact, the cohesion is considered as destroyed, so p^* vanishes for this contact.

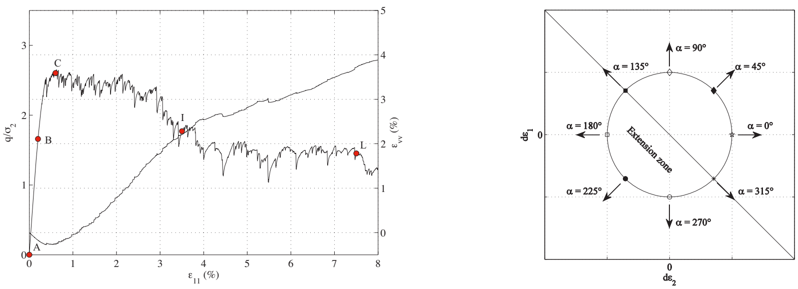

Fig. 2. DEM responses subjected to biaxial loading. Studied points (A, B, C, I, L) are marked in red (left); and direction of strain increment applied (right).

It is worth recalling that for each of these stress states –naturally associated with a VE state – a full characterization of the stress increment response has been performed over a 0-360° range of the deformation increment orientation, by 5° steps. Moreover, for each orientation, various magnitude of the incremental strain $\|\Delta\varepsilon\|$ is applied, from 0.05% to 0.5% in five steps.

Response envelopes of the different initial stress state (A, B, C, I, L) are plotted in Fig. 3. It is found that, at initial stress state (A – isotropic) (Fig. 3.a), with $\|\Delta\varepsilon\| = 0.05\%$ and $\|\Delta\varepsilon\| = 0.1\%$, response envelopes are close to an ellipse centered at the origin of stress plan. This shape corresponds to a linear behavior [1,10]. Any significant deviation of this kind of response indicates a non-linear behavior (e.g. changes of envelope center from origin point, or shape deformed); hence, if $\|\Delta\varepsilon\| > 0.1\%$ the behavior becomes non-linear.

For B, C, I and L configurations, stress states are anisotropic. The response envelopes show non-linear behavior and irreversible even with a very small incremental strain applied. As seen in Fig. 3.(b,c), response envelopes become flat on one side, and decentered, even for the smallest incremental strain magnitudes (0.05%, 0.1%) . These results suggest that at an anisotropic state, the behavior of the NHL law is always strongly non-linear. By considering the evolutions of responses envelopes at different states, it is observed that the rigidity of VE is decreased due to changes in microscopic properties. It is interesting to note that we obtain these effects naturally, while in classic continuum modeling, it is necessary to define and manage a set of variables to describe history loading dependency.

From the isotropic elasticity equation, we can easily obtain that an ellipse centered at the initial stress characterizes the envelope response and its major axis direction is 45°. It is because the horizontal and vertical stiffness are equal. In our results, as shown in Fig. 3.a, at small strain increment ($\|\Delta\varepsilon\| < 0.1\%$) the stress response is elastic. The highest absolute values of the stress responses also occur in the direction 45°. This means that, the preparation procedure of the specimen gives a quasi-isotropic response at the initial state (isotropic stress state). However, the limit of elastic behavior is very slight and it means that an anisotropic initial state can be obtained by changing some parameters in the preparation procedure of the sample. Obviously, it can be seen on Fig. 3.a that the extension part of response envelopes tends towards a limit (clearly from $\|\Delta\varepsilon\| > 0.2\%$). This corresponds to extension limit of VE characterized by the cohesion of intergranular contact. Meanwhile, the size of response envelopes in compression part increase with strain increment $\|\Delta\varepsilon\|$, especially in the 45° direction, corresponding to an isotropic compression loading $d\varepsilon_1 = d\varepsilon_2 > 0$.Induced anisotropy is an important property of granular materials. However, describing induced anisotropy in usual constitutive law is a difficult task. This property can naturally be described in our DEM model. By considering 3 VE at different states, corresponding to a VE subjected to biaxial loading: A – isotropic, B – intermediate and C – peak state, we observe that the anisotropy is induced throughout the loading. Rotations and size of response envelopes at small and large increment strain as well indicate clearly the changes in anisotropic properties.

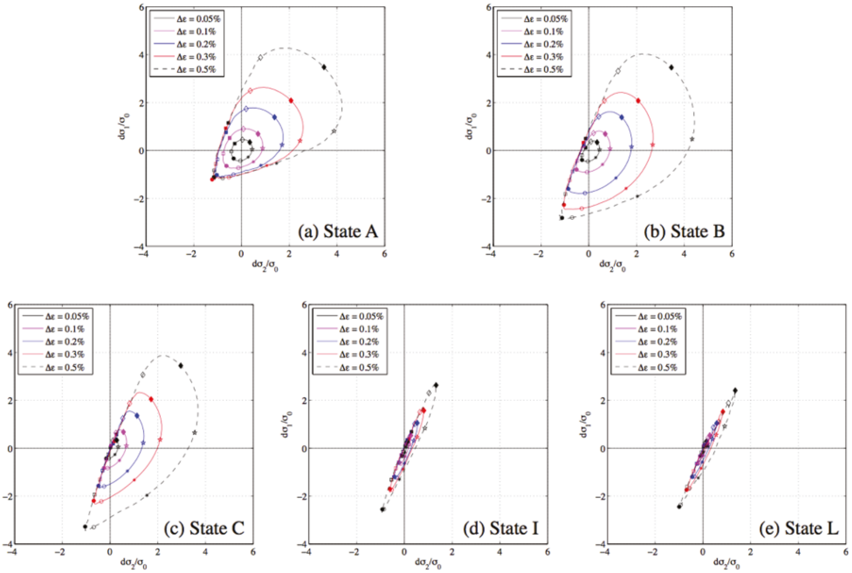

Fig. 3. Incremental response envelopes

Obviously, at the same strain increment, response envelopes at different states show history loading dependency of material behavior. As shown in Fig. 3, the size of response envelopes decreases with increasing of mean stress from initial state. This means that the stiffness decrease. This latter is due to the fact that increasing loading cause failure in contact cohesion, and thus reduces the stiffness of material.

At critical state (L), we can consider the response envelope is composed of two sections: elastic unloading and elasto-plastic loading. The section representing elasto-plastic loading is reduced, tending to a straight line. This means that the model predicts a very small stress rate for elasto-plastic loading at critical state. Two reasons that explain why we cannot obtain a perfect straight line: firstly, state L is not absolutely critical state because of the scattering of DEM responses; secondly, usual elas-to-plastic model predicts zero stress state due to consistency condition.

4 Conclusion

A numerical law based on Discrete Element Modeling has been presented. This is accomplished in the framework of numerical homogenization method applied to granular media. A conventional way to study constitutive law by using response envelopes is then applied. By performing a series of numerical test on VE, the overall picture of the constitutive relation is captured. The results show the ability to take into account many natural features of granular materials such as induced anisotropy, non-linear, stress path dependent or reduction in stiffness according to mechanical loading. This highlights a great advantage of this new model compared to conventional model employed in geomechanical modeling.

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