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DISCRETE ELEMENT METHODS FOR THE MICRO-MECHANICAL INVESTIGATION OF GRANULAR RATCHETING

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Abstract. *Discrete element methods have been extensively used for simulating a wide range of granular systems because they correspond to the discrete nature of the granulates. Historically, Molecular Dynamics (MD) and Event-Driven algorithms had been used for many years when M.Jean and J.J.Moreau developed the Contact Dynamics (CD) method some fifteen years ago. The differences between these three methods stem from the way interactions between the particles are treated. Both ED and MD are numerical resolutions of the equations of motion of the system. In CD, the contact forces are calculated through an iterative scheme that takes into account some physical constraints such as perfect volume exclusion and Coulomb friction. In this contribution the applicability of the MD and CD schemes will be investigated for the study of the micro-mechanics of a simple model of a granular soil. Results of MD and CD simulations of a dense system of spheres under biaxial test conditions will be presented. We will focus in particular on the study of the granular ratcheting [1] that has been recently reported in MD simulations in the quasi-static regime.*

1 INTRODUCTION

Molecular Dynamics (MD) has been extensively used for more than fifty years in the numerical solution of a wide variety of problems. Although molecular fluids were the original application of the method [2], it has been also applied successfully in the field of soil mechanics [3]. In this context, the term discrete element method is often used to emphasize the differences with finite element methods. These differences also reflect different approaches to soil mechanics. On the one hand, a continuum description of the material is possible based on constitutive equations, whose parameters are usually measured experimentally. On the other hand, a discrete description will take into account that the material is composed of distinct grains or particles that interact with each other. The final aim of this micro-structural approach is, however, to find macroscopic state variables in terms of micro-variables such as contact forces, grain displacements, local interactions, ..., etc, in the same way that hydrodynamic fields can be connected with motion of molecules in a fluid. There is however no analogous to Kinetic Theory in soil mechanics, although some useful results are available connecting macroscopic mechanical variables with a local, microscopic description of the material [4, 5].

Contact Dynamics (CD) is also a discrete element method, in the sense that the evolution of the system is solved reproducing the dynamics of the particles in terms of their inter-particle interactions [6]. It has been profusely used in the investigation of force networks and contact forces [7, 8, 9, 10].

In this contribution, the applicability of both MD and CD discrete schemes to the study of the micro-mechanics of a simple granular soil model will be investigated. Results from MD and CD simulations of a dense system of spheres under the conditions of a biaxial test will be presented. In a cyclic loading above the shakedown limit, there is a plastic response of the system characterized by a constant strain-rate and a cyclic behavior of the sliding contacts (ratcheting) [1, 11]. In order to investigate these phenomena, we reproduce the first loading cycle and analyze the differences found using both simulational methods. This will lead us to the investigation of the response of the system to a gradual increase of pressure up to the point where deformation starts.

This paper is organized as follows. In Section 2 some basic features of MD and CD methods are presented. In Section 3, we present the results of the simulation of rigid and deformable particles under biaxial test conditions. We use Contact Dynamics for rigid particles and Molecular Dynamics for deformable ones. We conclude, in Section 4, with the discussion of the results.

2 DISCRETE ELEMENT SIMULATION

A granular medium is a physical system composed by distinct basic units (grains) of a macroscopic size (typically bigger that $1\mu m$). If the material is dry and non-cohesive, the only interactions between grains are friction and repulsion. How these interactions are modeled is an interesting subject itself [12]. We will stick to the usual case of Mohr-

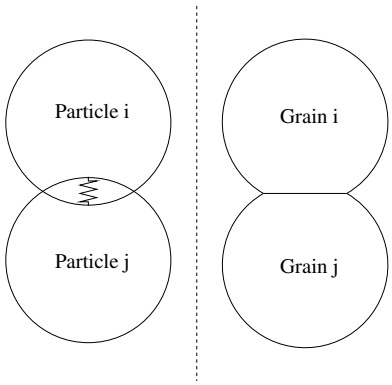

Figure 1: Model of the deformation of the grains in the collision. The particles (idealized grains on the left side of the figure) are allowed to overlap, but they are subjected then to an elastic force proportional to the overlapping that pull them apart. The collision of two grains is represented on the right side of the figure, where their deformation is explicitly shown.

Coulomb friction. The discrete character of the medium results in a complex behavior during loading and unloading that cannot be described properly by any constitutive equation. Given the nature of the system, it is possible, however, to solve numerically the evolution of the grains once a valid model has been established. The most simple model reproducing most of the key features of granular material is an assembly of disks (or spheres, in 3D). In the MD method, the disks can overlap, and the interaction between them is visco-elastic and proportional to the overlap. This idealization mimics the deformation that two real grains experience in their collision (see Figure 1). In CD, the grains are rigid and an implicit algorithm is used, which has the significant advantage that the implementation of friction is straightforward. We will describe the algorithms used for the MD and CD simulations presented in this paper, after dealing with the boundary conditions used in the simulations.

2.1 Boundary conditions: biaxial test

The biaxial test is often used in engineering to characterize the stress-strain behavior of materials. A sample is closed in a rectangular test chamber, and subjected to a confining pressure. Then a force is applied to the upper and lower plates of the cylinder, so that $\sigma_1 \neq \sigma_2$, as shown in Figure 2. In this paper, we put a granular material in the biaxial test chamber, and start with $\sigma_1 = \sigma_2$. The walls compress the originally dilute material into a dense packing. Then, σ_2 increases gradually until the sample starts to deform, i.e., σ_1 and σ_2 obey

$$\sigma_1 = P_0,\ \sigma_2 = P_0(1 + \alpha t), \tag{1}$$

where the constant α controls the rate of loading. We choose α small enough so that the system is loaded quasi-statically, that is, it passes through a series of stationary states, up to the value of αt where the sample yields. The response of the system will be characterized

by the adimensional quantity γ, which is be defined in terms of the deviatoric permanent strain. This, analogously to the deviatoric stress, is the difference of the strains in the principal directions. Let the permanent strains in the principal directions be:

$$\epsilon_1(t) = \frac{L_x(t)}{L_x^0}, \tag{2}$$

$$\epsilon_2(t) = \frac{L_y(t)}{L_y^0}. \tag{3}$$

Where $L_{x/y}(t)$ are the dimensions of the system at the time t, whereas $L_{x/y}^0$ are the dimension at the beginning of the loading. Then, γ is defined as:

$$\gamma = \epsilon_2 - \epsilon_1. \tag{4}$$

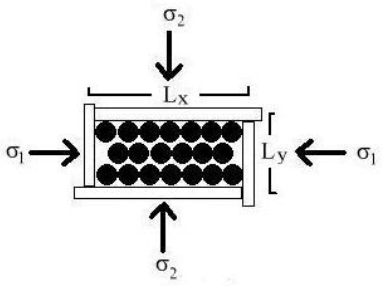

Figure 2: Hambly's principle for biaxial test. The degrees of freedom of the walls allows to impose any pair of stresses σ_1,σ_2 to the system.

2.2 Molecular Dynamics

In MD, the contact forces are calculated by considering that the overlap between two touching particles represents the deformation that generates the collision. The algorithm originally proposed by Cundall and Strack [13] for granular materials will be used. Let us suppose that two particles i and j first touch at time t_*. Two imaginary springs are then created, one pointing along the normal direction, and the other along the tangential direction. The two springs have different properties to account for the difference between normal and tangential forces. The normal spring simply oppose to further overlapping (as shown in Figure 1). The constant of the spring, k_n, controls the stiffness of the contact (i.e. the typical depth of the overlapping). Besides this elastic force exert in each contact, a viscous damping is also imposed, assuring some dissipation during the collision. Thus the normal force is

$$R = k_n\delta_n - \gamma\dot{\delta}_n, \tag{5}$$

where δ_n is the length of the normal spring.

The calculation of the tangential forces T is slightly more complicated, because they must obey the Coulomb condition $|T| \leq \mu R$, where μ is the static friction coefficient. We suppose that a tangential spring is created at time t_* and it is related to the tangential force via a second spring constant k_t and a damping constant γ_t. One must first calculate a candidate tangential force

$$\tilde{T} = k_t \delta_t - \gamma \dot{\delta}_t, \tag{6}$$

where δ_t is the length of the tangential spring. Then, the Coulomb condition is enforced:

$$T = \begin{cases} \tilde{T}, & |\tilde{T}| \leq \mu R, \\ sgn(\tilde{T})\mu R, & \text{otherwise.} \end{cases}$$

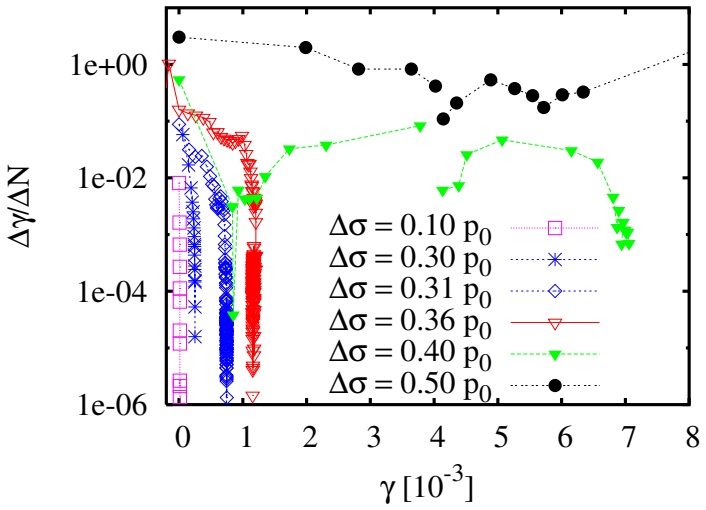

Figure 3: Strain rate versus the accumulated permanent strain for different values of the loading $\Delta\sigma$. All the curves correspond to MD simulations of 400 disks, whose parameters are $k_n = 2$ MPa (k_n is the normal stiffness of the contacts), $\mu = 0.1$ and $P_0 = 6 \cdot 10^{-4} k_n$.

2.3 Contact Dynamics

In Contact Dynamics, there is no overlapping of disks, for they are considered as perfectly rigid and interacting with each other only at the contact point. The algorithm is basically an iterative procedure after which a force network is calculated down to some precision satisfying certain physical restrictions [14]. Each contact force depends on the adjacent contact forces, which means that the problem cannot be solved locally for each contact. The main constrain to be fulfilled is impenetrability. The normal force is chosen to be the smallest value R needed to avoid interpenetration. The proper tangential force is

chosen that prevents the contact from sliding. If Coulomb's condition cannot be satisfied, the contact will slide with $T = \mu R$ against the relative velocity. The main drawback of CD is the indeterminacy of the forces. The important question arises: what makes the CD method choose one of these possible solution among the others? or, is the selected solution somehow special among the other admissible, or are they all equivalent [15, 16]?

We conclude by noting one important difference between the CD and MD approach. In CD, the granular packing has access to any possible force network, whereas in MD, its choice is restricted, because the forces can only be modified by small motions of the grains.

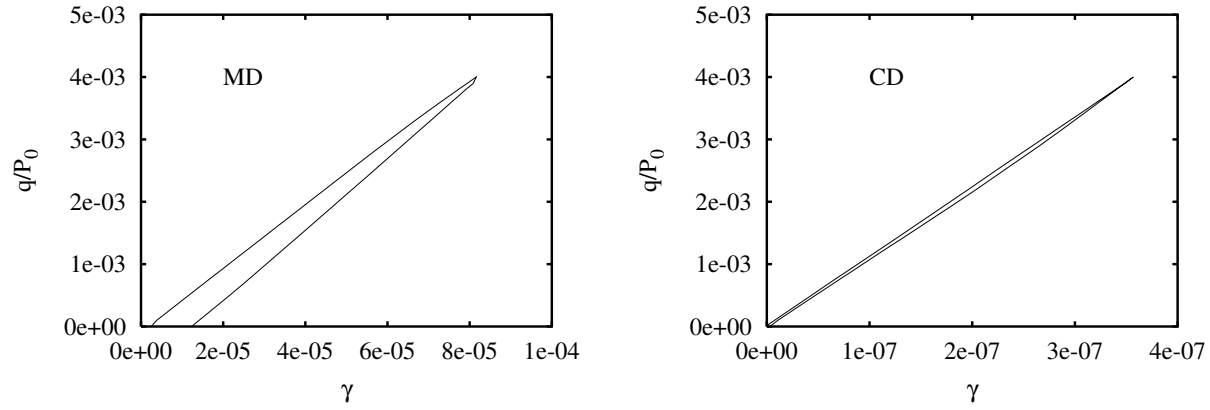

Figure 4: Stress-strain curve obtained after the loading and unloading of a compressed sample in a MD (left) and CD (right) simulation. The initial condition was the same in both experiments. The system was compressed at a linear rate and the decompressed at the same rate until the original stress state was reached. Note the difference in horizontal axes (γ).

3 RESULTS

The existence of granular ratcheting has been reported in MD simulations of a dense packing of polygons [1] and disks [11]. The response of a given compressed system of disks subjected to cyclic loading varies according to the imposed loading as it is shown in Figure 3. Here, all the samples have the same initial condition: the system is homogeneously compressed under a certain pressure $P_0 = \frac{\sigma_1+\sigma_2}{2}$, until a compacted state is reached. This first stage is carried out with the MD algorithm. After this preparation of the sample, two different simulations (MD and CD) are run in which the axial component of the stress, σ_2, is periodically changed,

$$\sigma_2(t) = P_0 \left[1 + \frac{\Delta\sigma}{2}\left(1 - \cos\left(\frac{2\pi t}{t_0}\right)\right)\right], \tag{7}$$

where t is the time and t_0 is the period of the cyclic loading. The changes in the loading are characterized by the parameter $\Delta\sigma$, which is directly related to the maximum value

of the deviatoric stress.

Three ranges of response can be differentiated in the figure. If the loadings are low enough, the excitations shakedown in the material. This implies the adaptation of the system to the imposed loads, after which there will be practically no accumulation of permanent strain. This is related to the disappearance of sliding contacts in the sample. On the opposite limit, for very high loadings, the strain rate does not apparently diminish, leading to a fast failure of the material. This incremental collapse can be seen in cases $\Delta\sigma = 0.40$ and $\Delta\sigma = 0.50$ of the figure. For loads above the shakedown limit but far from collapse, the material accumulates permanent strain at a constant but very small rate. This behavior is associated to a quasi-periodic response of the sliding contacts and is the so called granular-ratcheting.

Figure 4 shows the strain-stress curve after on cycle obtained with the MD algorithm (left) and with the CD algorithm (right). The differences in the range of values are already obvious for this first cycle. The perturbation that the loading exerts on the system is much weaker in the CD simulation, and related to the precision of the method. But note also that the energy dissipated is bigger in the MD cycle, and so is the remanent strain at the end of the process.

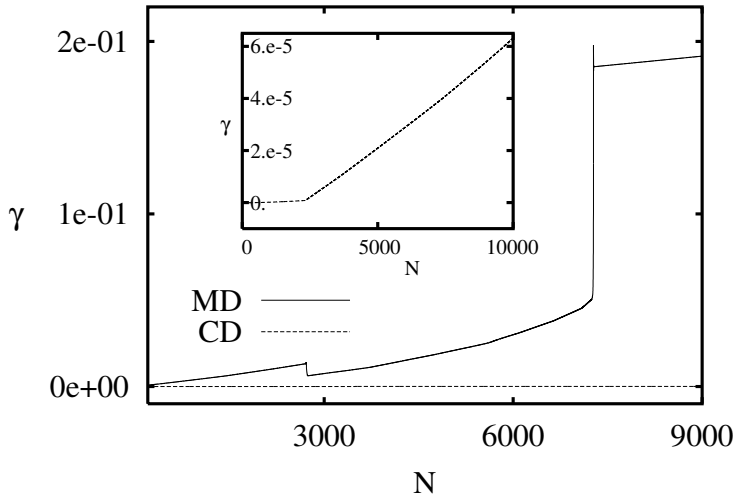

Figure 5: Evolution of the permanent strain γ in the Molecular Dynamics and in the Contact Dynamics simulations. The inset shows, in a more appropriate scale, the behavior of γ in the CD simulation.

The higher *inertia* of the CD method is even more clearly observed in Figure 5, where the evolution of the strain γ is plotted for both methods in the experiment indicated in equation (1). In the MD simulation, the system starts expanding slowly. A sudden compression is perceived $N = 2700$, after which the deformation rate seems to grow in each cycle. This leads to a collapse of the sample at the end of the simulation. In this

range of values, however, the CD simulated sample seems to remain unaltered. A closer look to its behavior is presented in the inset of the figure. In the CD simulation, the response is smoother than in the MD case. At a first stage, the system seems not to be affected by the imposed loading. There is however a critical load, beyond which, the system expands. In contrast to the MD experiment, this expansion is carried out without any collapse or breakage of the physical structure of the grains.

4 CONCLUSIONS

A different behavior of the plastic response of a system simulated by a MD algorithm and a CD algorithm has been shown. The response of the material is more apparent in the MD simulation, while CD is much more resistant to collapse. This behavior is probably related to the indeterminacy of the forces in the CD method [15, 16]. In the Contact Dynamics method, the system has many possible force configurations that are compatible with the stress conditions. The system can jump from one force configuration to another without any movement of the particles. This is not the case in the Molecular Dynamics scheme, were the forces can only be changed by small motions of the grains.

MD results have been compared with experimental triaxial tests data and a good correlation has been found [11]. No similar validation of the CD method for the repetitive loading case has been reported yet, although CD method has been successfully applied by different authors to the description of the contact forces of a static packing [7, 8, 9, 10]. Further investigation is therefore needed in order to delimit the exact physical implications of the divergences between methods reported here.

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