The response of an idealized granular material to an incremental shear strain

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SUMMARY The incremental response of a random aggregate of identical, elastic, frictional spheres, that has been isotropically compressed, is studied. We focus on the behavior of such an aggregate when an incremental shear strain is applied with the coefficient of friction among particles assumed to be large enough to prevent any sliding; we see that, depending on the coordination number (the average number of contacts per particle), a number of local mechanisms occurs. That is, particles experience a motion not associated to the applied deformation and the aggregate can not be always considered elastic. Consequently, it is possible to identify two main regimes of deformation. In the first, we have an almost reversible behavior and a number of mechanisms negligible; the aggregate is assumed to be elastic and a theoretical model is considered by approximating the kinematic of contacting particles with an average and fluctuation deformation. The other regime is characterized by inelasticity; that is, several particles do not return to the initial configuration when a forward incremental shear strain followed by an identical reverse incremental strain is applied.

1 INTRODUCTION

The mechanical properties of confined granular materials have still several obscure points of understanding. Both elastic and inelastic behavior of such an aggregate are still poorly described by few theoretical models available that, at most, work well in particular regime of deformation. Here we restrict our attention to the first incremental response that finds considerations on wave speed problems. For example, many industrial applications, such as the optimization of well localization in an oil reservoir, crucially depend on the correct interpretation of acoustic effects in granular materials. It is exemplified by the large variation of sound speeds or elastic constants of the granular formation as a function of the initial confining pressure.

The theoretical models present in literature (e.g [1, 2, 3, 4]) introduce different hypothesis to describe the kinematic of contacting particles: their comparison with numerical simulations and experiments (e.g. [5, 6]) have shown merit and failure. Among other things, a key issue that emerges is that the response of the aggregate is strictly related to the coordination number, the average number of contacts per particle [7]. Our investigation refers to the incremental shear strain response of an idealized granular material, made by a random aggregate of identical, elastic, frictional spheres, by means of computer analysis, based on a distinct element method (DEM) [8]. We characterize the incremental behavior of the packing by the usual parameters of the initial isotropic state, confining pressure, porosity and coordination number and also, through the incremental partecipation number $\dot{\Pi}$ [9]; it represents a measure of inhomogeneity of the incremental forces and varies with the coordination number.

We show that particles can experience an irreversible behavior when small increments in strain are superimposed on the initial prestressed equilibrium configuration. We interpret this phenomenon as consequence of local lability in the packing [10]. We provide a strength of the irreversibility through a parameter ζ that measures the residual displacements of the particles in the aggregate after an incremental loading and unloading strain. We show how ζ decreases with the coordination number toward an almost constant regime, irrespective to the confining pressure. Local lability does not seem to affect the failure of the whole aggregate but it determines a weakness in the response. For high ζ the agreement between simulation and theory is quite good while for lower ζ the discrepancy increases. That is, the theory [4], based upon an elastic model in which particles move according to an average strain field and a fluctuation one, does not include particle rearrangement; therefore, for lower value of the coordination number such a theory can be seen as an upper bound for the effective moduli obtained by means of numerical simulation.

2 SIMULATIONS

We use the distinct element method [8] to prepare random assemblies of identical, frictional, elastic spheres. We deal with aggregates of 10,000 particles with radius $R = 0.1mm$ randomly generated in a periodic cubic cell. We employ material properties typical for glass spheres with shear modulus $\mu = 29$GPa and Poisson's ratio, $\nu = 0.2$. The interaction between particles is represented by a non-central contact force in which the normal component follows the non-linear Hertz's law and for the tangential component we incorporate a bilinear relationship with elastic displacement and frictional Coulomb sliding with friction coefficient $\mu_f = 0.3$ (details are given in [5]). Our protocol creates different initial isotropic states by varying the coefficient of friction among particles during the preparation. More details about the procedure followed can be found in [7]. All packings are defined as dense with the solid volume fraction ϕ close to the RCP value ($\phi \sim$0.64). As final results we have dense packings of particles with the same confining pressure p_0 but different coordination number $\bar{Z}$.

3 INCREMENTAL AVERAGE STRESS TENSOR

The general expression for the average incremental stress tensor for an aggregate of N particles is given by [11]

$$\overline{\dot{\sigma}_{ij}} = \frac{1}{V^{tot}} \sum_{c=1}^{N^C} \dot{F}_i^c d_j^c, \tag{1}$$

where N^C is the total number of contacts in the aggregate, V^{tot} is the total volume of the aggregate, $\mathbf{F}^c$ is the contact force among contacting pair of particles and $\mathbf{d}^c$ is the contact vector that goes from center to center of contacting particles. We can rewrite equation (1) by collecting the contact forces for pairs of particles whose contact vectors are close to a given direction. We take M^p to be the number of pairs with contact vectors within the p^{th} element of R equal elements $\Delta\Omega^p$ of solid angle in which the surface of the unit sphere has been partitioned such that

$$\Delta\Omega^p = \frac{4\pi}{R}, \tag{2}$$

$$\sum_{p=1}^{R} M^p = 2q. \tag{3}$$

Then

$$\overline{\dot{\sigma}_{ij}} = \frac{1}{V^{tot}} \sum_{c=1}^{q} \dot{F}_i^c d_j^c = \frac{1}{2} \frac{1}{V^{tot}} \sum_{p=1}^{R} \sum_{t=1}^{M^p} \dot{F}_i^t d_j^t. \tag{4}$$

Next, following [12], we introduce a conditional average as

$$\left\langle \dot{F}_i d_j \right\rangle_{\hat{\mathbf{d}}^p} = \frac{1}{M^p} \sum_{\mathbf{d}^{(CD)} \subset \Delta\Omega^p} \dot{F}_i^{(CD)} d_j^{(CD)}, \tag{5}$$

where $\mathbf{F}^{(CD)}$ is a contact force for a pair within the element of solid angle centered on $\hat{\mathbf{d}}^p$. Then, upon assuming that $\dot{\mathbf{F}}$ and $\mathbf{d}$ are not correlated and with $\langle \mathbf{d} \rangle_{\hat{\mathbf{d}}^p} = \mathbf{d}^p$, the incremental stress tensor becomes

$$\overline{\dot{\sigma}_{ij}} = \frac{1}{2} \frac{1}{V^{tot}} \sum_{p=1}^{R} M^p \left\langle \dot{F}_i d_j \right\rangle_{\hat{\mathbf{d}}^p} = \frac{1}{2} \frac{1}{V^{tot}} \sum_{p=1}^{R} M^p \left\langle \dot{F}_i \right\rangle_{\hat{\mathbf{d}}^p} d_j^p. \tag{6}$$

The corresponding conditional average of the incremental contact force is

$$\left\langle \dot{\mathbf{F}} \right\rangle_{\hat{\mathbf{d}}^p} = \frac{1}{M^p} \sum_{\hat{\mathbf{d}}^{(CD)} \subset \Delta\Omega^{(BA)}} \dot{\mathbf{F}}^{(CD)}; \tag{7}$$

and equation (6) becomes

$$\overline{\dot{\sigma}_{ij}} = \frac{1}{2} \frac{N}{V^{tot}} \sum_{p=1}^{R} \frac{M^p}{N} \left\langle \dot{F}_i \right\rangle_{\hat{\mathbf{d}}^p} d_j^p, \tag{8}$$

where we recall that N is the total number of particles in the aggregate, equal to twice the number of pairs.

4 INCREMENTAL RESPONSE

4.1 *Numerical calculation*

The elastic response of the aggregate has been evaluated following [5] where, after an homogeneous incremental strain, we let the aggregate relax toward a new equilibrium state. Once the deformation to apply has been fixed, we are able to measure the stress response of the material and calculate the modulus as $\overline{G} = \Delta\sigma_{12}/\Delta\epsilon_{12}$. In Figure 1 we note, as already emphasized in [5], a peak in stress associated to the homogeneous perturbation and a subsequent relaxation. Because of the random positions of the particles and their different initial contact stiffness due to the isotropic compression, the homogeneous applied strain is followed by a relaxation. This relaxation may involve a rearrangement of the particles in the aggregate; in this case the incremental response is irreversible. On the contrary, when the relaxation occurs saving a fixed geometry of the aggregate, the incremental response can be considered reversible and then elastic. In this case the relaxation is only associated to the fluctuation motion among particles.

4.2 *Theory*

The simplest theoretical approach is based upon the effective medium theories, developed by Digby and Walton [1, 13]. Contact displacement among particles is determined by the average strain; force and moment equilibrium are identically satisfied by virtue of an assumed symmetry for each particle. As result we have that the prediction of the elastic moduli is far in agreement with that obtained by numerical simulation; moreover the shear modulus scale with $p^{1/3}$ (the aggregate is seen as a simple collection of Hertian contacting spheres) in contrast with what simulation shows. Yet, as already underlined by [7], this dependence occurs if we collect aggregates with almost equal coordination number which seems to exbiht the same number of mechanisms or irreversibility. That

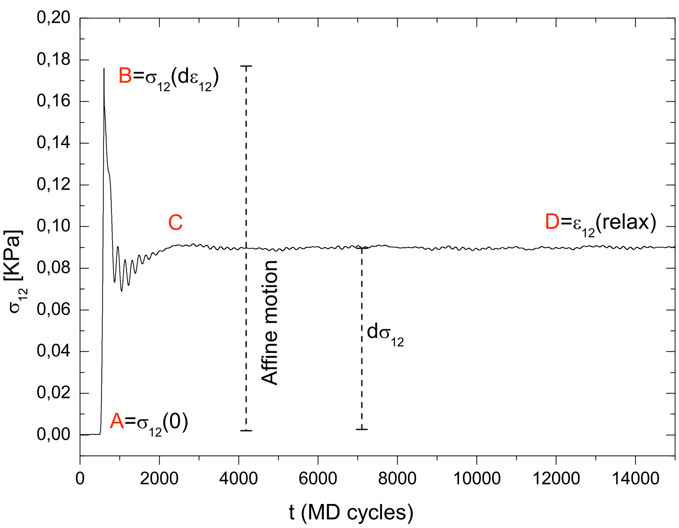

Figure 1: Numerical protocol for the calculation of the elastic response of the aggregate when an increment in shear is applied.

is, the peculiarity of the aggregates to behave as a collection of elastic spheres regards all particles except those that experience a not reversible deformation.

A better agreement between theory and simulation has been obtained by [4] where they introduce fluctuations in the kinematic of contacting particles and in their geometrical structure. Moreover force and moment equilibrium are explicitly taken in account because applied for a typical pair of particles; in this way fluctuations in kinematic are evaluated while statistical consideration are introduced to reproduce variability of the neighborhood for each pair in the aggregate. The results for the shear modulus is summarized as follows:

$$\begin{aligned} \bar{G} &= \frac{\phi\bar{Z}}{5\pi d}\left(\overline{K_N}-\overline{K_T}\right)\left[1-2\left(\rho+\rho^*\right)\right] \\ &\quad+\frac{\phi\bar{Z}}{5\pi d}\overline{K_T}\left[\frac{5}{2}-5\left(\rho+\rho^*\right)+3\left(\xi+\xi^*\right)\right] \end{aligned} \tag{9}$$

where

$$\overline{K_N}=\frac{\mu d^{1/2}}{(1-\nu)}\delta^{1/2}, \tag{10}$$

$$\overline{K_T}=\frac{2\mu d^{1/2}}{(2-\nu)}\delta^{1/2} \tag{11}$$

are the normal and tangential average contact stiffness and with the normal component δ of the contact displacement given by

$$\delta = d\left[\frac{3\pi}{2}\frac{(1-\nu)}{v\overline{Z}}\frac{p}{\mu}\right]^{2/3}; \tag{12}$$

and

$$\rho = \left(\frac{22-3\overline{Z}}{24\overline{Z}} - \frac{22-3\overline{Z}}{24\overline{Z}^2}\right) + \frac{1}{8}\chi, \tag{13}$$

$$\rho^* = \rho(1-2\rho+2\xi), \tag{14}$$

$$\xi = -\left(\frac{13\overline{Z}}{24}\right)^{-1}\left[1-\left(\frac{13\overline{Z}}{24}\right)^{-1}\right]\left(\frac{22-3\overline{Z}}{16}\right) - \frac{261}{676}\chi, \tag{15}$$

$$\xi^* = \xi(2\xi+1-2\rho). \tag{16}$$

The terms in ρ and ξ, proportional to $\overline{Z}$, are different from zero for $\overline{Z} \leq 22/3$. Moreover we also underline that Z has been treated as random variable independent and the term χ is function of $\overline{Z'^2}$ and $\bar{Z}^2$, where Z' is the fluctuation in number of contacts per particle.

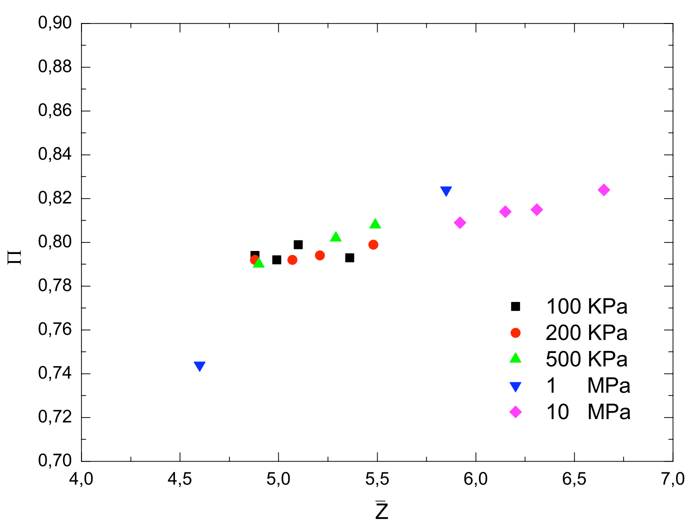

Figure 2: Variation of the incremental partecipation number with $\bar{Z}$.

4.3 *Partecipation Number*

In order to study how the distribution of contact forces vary in the aggregate and its influence on the stress tensor, we introduce a statistical parameter to quantify the degree of localization of the force during the incremental applied deformation. This parameter is the participation number $\dot{\Pi}$, introduced in [9]; for it we take the incremental form such that

$$\dot{\Pi} = \left(N^C \sum_{i=1}^{N^C} \dot{q}_i^2 \right)^{-1} \tag{17}$$

where

$$\dot{q}_i = \left| \dot{F}_i \right| / \sum_{j=1}^{N^C} \left| \dot{F}_j \right| \tag{18}$$

where $\left| \dot{F}_j \right|$ is the magnitude of the incremental total force at contact j. In particular, $\dot{\Pi} = 1$ means a spatial homogeneous force distribution $\left(\dot{q}_i = 1/N^C \forall i \right)$. On the other hand, in the limit case of complete localization, $\dot{\Pi} \approx 1/N^C - > 0$ when $N^C - > \infty$.

$\dot{\Pi}$ a simple scalar value that characterize the response of the aggregate. That is, the incremental participation number can be seen as a weight parameter for the active contacts in the aggregate. The other scalar parameter, the coordination number, has a geometric dependency on the aggregate as it does not change during the applied increments and it is only function of the pre-compressed state of equilibrium. The incremental participation number, instead, can be understood as a measure of how the incremental contact forces have been activated by the incremental loading.

In Figure 2 we plot the results of the calculation of $\dot{\Pi}$ and how it varies when an incremental shear strain is applied to each one of our packings. The variation with the coordination number is presented and we note that the behavior does not depend on the confining pressure but it is related to the coordination number alone. In particular, the incremental contact forces are distributed more equally as the coordination number increases; that is the applied strain actives a large amount of contacts. On the other hand, for low coordination number a kind of localization of the incremental contact forces seems to appear.

5 IRREVERSIBLE MOTIONS

The elastic response of the aggregate can only be associated to those deformations that are reversible. We take in account the possibility that the incremental shear strain may cause a change of configuration of the aggregate. We introduce a parameter that measures the residual displacement of the particles associated to a forward incremental shear strain and a subsequent, identical reverse deformation such that the initial configuration should be recovered for the pure elastic case. This paramenter is defined as

$$\zeta = \frac{1}{N} \sum_{i=1}^{N} \frac{\left| \mathbf{x}_i^{(2)} - \mathbf{x}_i^{(0)} \right|}{\left\langle \left| \mathbf{x}_i^{(1)} - \mathbf{x}_i^{(0)} \right| \right\rangle} \tag{19}$$

where N is the total number of particles in the aggregate, $\mathbf{x}_i^{(0)}$, $\mathbf{x}_i^{(1)}$ and $\mathbf{x}_i^{(2)}$ are the position vector of the center the $i - th$ particle, respectively in the reference state, in the relaxed state after the forward incremental strain and in the relaxed state after the reverse incremental strain.

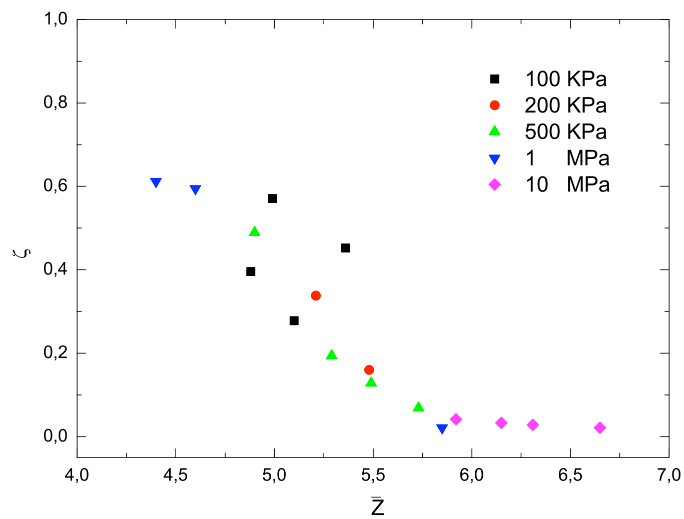

Figure 3: Variation of ζ with $\bar{Z}$ for increments in shear and compression.

Note that in the aforementioned cycle of deformation, for an ideal elastic system, $\left|\mathbf{x}_i^{(2)} - \mathbf{x}_i^{(0)}\right| = 0$ for every $i-th$ particle. We measure ζ in all our packings by applying an increment in shear that is function of the confining pressure; the ratio of each magnitude to the volume strain associated with the confining pressure is constant at about 10^{-2}. The results are plotted in Figure 3, in which ζ is shown as function of $\bar{Z}$. It is clear that ζ does not depend on the confining pressure of the aggregate, but only on the coordination number such that if we collect aggregates with similar $\bar{Z}$ they exhibit the same number of mechanisms or irreversibility. ζ increases as $\bar{Z}$ decreases and it is almost zero for $\bar{Z} \geq 6$; when $\zeta \neq 0$ irreversibility occurs for some particles and we argue that they are associated to the presence of local instability [10]. That is, there are some neighborhoods that can not sustain a load and a motion not proportional to the load occurs, in order that a new equilibrated configuration is reached. In the context of shear bands [15], such collective motion in the absence of shear stress is also seen; it occurs in a region in which particles have fewer contacts. Such a phenomenon has some kind of connection with our present experience.

For high $\bar{Z}$ the number of irreversible motions is so small that their effect is negligible and the response of the aggregate can be assumed to be elastic. On the contrary, when $\bar{Z}$ decreases, the strength of the irreversibility increases and the definition of shear modulus is questionable; that is an elastic theory is not appropriate to describe the incremental response. In Figure 4 the comparison between the prediction of the shear modulus given by the fluctuation theory (see equation 9) and the measurements of numerical simulations is proposed. In the range of high $\bar{Z}$, where it is possible to consider the behavior of the aggregate as elastic, there is a good agreement between theory and numerical data, showing that such a model is able to reproduce the variation of $\bar{G}$ with the coordination number. When $\bar{Z}$ decreases, the simulation diverges and we argue that the discrepancy that appears

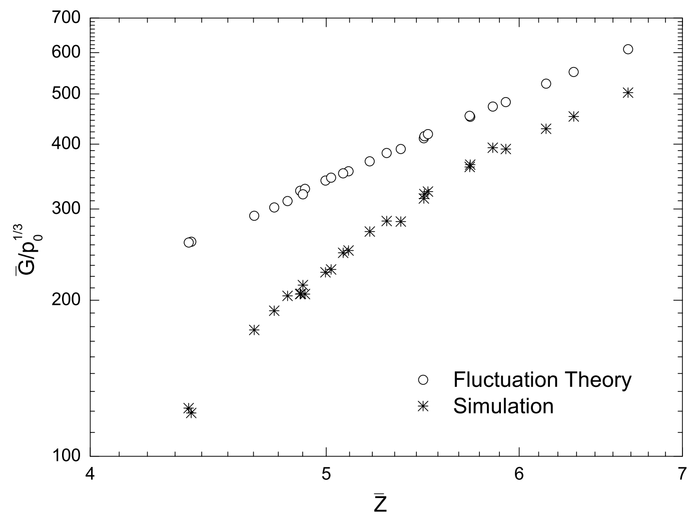

Figure 4: Comparison between theory and numerical simulation for the normalized shear modulus $\bar{G}/p_0^{1/3}$

is related with the irreversible motions seen in the simulations.

6 CONCLUSIONS

For an isotropic, confined, idealized granular material a detailed description of the response to an incremental shear strain is given. It is provided in terms of the parameter of the reference state, pressure, coordination number and porosity and the degree of localization of the contact forces, the partecipation number. Moreover we see that particles may experience irreversibility even when small perturbations are applied, those that are typically considered to measure the incremental response of the aggregate. We introduce a strength for this irreversibility by considering the possibility of mechanisms in the aggregate. This feature results to be sensitive to the coordination number. Therefore we distinguish an elastic regime where the number of mechanism is negligible from that in which mechanism become relevant (irreversible regime). In the first regime, comparison between fluctuation theory and simulations is appropriate and the results are in a good agreement.

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