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2008 EPL 81 34006

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Characterizing the shear and bulk moduli of an idealized granular material

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received 2 October 2007; accepted in final form 30 November 2007
published online 3 January 2008

PACS 45.70.-n – Granular systems

PACS 45.70.Cc – Static sandpiles; granular compaction

PACS 46.40.-f – Vibrations and mechanical waves

Abstract – Physical experiments on wave propagation on granular material control two macroscopic parameters that are assumed to characterize the response of a given assembly: the isotropic pressure p_0 and the solid volume fraction ϕ . Here, by means of numerical simulation, we investigate the effect of the coordination number \bar{Z} (the average number of contacts per particle) and the fluctuation of the number of contacts per particle Z' . We adopt a numerical protocol to create several initial packings characterized by the same volume fraction and, for a given isotropic pressure, we are able to obtain different coordination numbers. That is, pressure and coordination number, for a given volume fraction, are independent. The result is that packings with fixed volume fraction and isotropic pressure exhibit a different elastic response. We attribute this behavior only to the coordination number as we find, surprisingly, that \bar{Z} is linked to Z' .

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Introduction. – Understanding the elastic response of granular materials is important due to the large number of applications as well as for elucidating fundamental aspects of the behavior of particulate systems [1–3]. However, a basic understanding of the physics of granular elasticity is currently lacking. For instance, basic issues such as the determination of the proper state variables to describe the average shear \bar{G} and bulk \bar{K} moduli of the assembly are still unsolved. Furthermore, a previous analysis (see [2] for a review) raises serious questions about the validity of the generally accepted theoretical elastic formulations. Conventional approaches in the framework of solid-state elasticity [4] consider a uniform strain at all scales, and that the displacement field of the grains is affine with the macroscopic deformation (affine approximation). These average strain theories developed by Digby and Walton [5,6] in the 1980s predict the moduli in terms of the external pressure, the volume fraction and average coordination number (p_0, ϕ, \bar{Z}). In particular, the pressure dependency is $\bar{G} \sim \bar{K} \sim p_0^{1/3}$, a direct consequence of the Hertz interaction between the particles. The difficulty in describing theoretically the shear modulus of an aggregate of grains is due to the complex relaxation of the particles

from the initial uniform strain approximation related to the structural disorder in the packing [7]. Going beyond these theoretical frameworks requires a more sophisticated theory in which we explicitly account for collective fluctuations and relaxation of the particles. Recent attempts in this direction are developed in [8–10] where statistical parameters from a fluctuation analysis are introduced to describe the scaling of the moduli. In particular, the role of the fluctuation of the number of contacts per particles $Z' = \bar{Z} - \bar{Z}$ seems to be relevant. In these theoretical models, fluctuations are introduced in the kinematics of contacting particles. They are determined as functions of “fabric tensors” that describe, on average, the packing geometry and the variation of the number of contacts per particle. The proposed theories are able to predict an elastic resistance of the aggregate comparable to numerical simulation.

Physical experiments [11–16] carried out on sand and glass beads show that wave propagation in the aggregate depends upon the confining pressure and the volume fraction. Recently Agnolin *et al.* [16], in physical experiments on glass beads, show that packings with a fixed confining pressure and different solid volume fraction exhibit

different elastic moduli. They also provide numerical simulation to show that different elastic responses correspond to different coordination number.

Motivated by the need for a general theoretical framework for the elasticity of granular matter, we study a granular assembly made by a random packing of Hertz-Mindlin frictional spheres [5,6]. Our goal is to analyze the role of \bar{Z} and Z' on the elastic behavior of the aggregate. We employ a numerical protocol that is able to generate packings with constant pressure and volume fraction but different coordination number. We investigate the relation among the parameters p_0 , \bar{Z} and Z' , in the case of dense packings ($\phi \simeq 0.64$), and how they affect the elastic properties of the system.

We find that pressure and coordination number are independent, as also underlined by Agnolin *et al.* [16], although they realize packings with different volume fractions. As underlined before, theoretical predictions of the elastic moduli [8,10] have emphasized the role of a parameter, $\chi = \frac{(Z - \bar{Z})^2}{\bar{Z}^2}$, which is a measure of the fluctuation of the contact number per particle. The presence of this parameter in the theory has motivated the investigation of it in our packings. We find, surprisingly, that χ is related to \bar{Z} and the structure of packings can be defined, therefore, by \bar{Z} alone. That is, packings with the same coordination number, created in a different way and under different confining pressure, exhibit almost identical contact distributions. Finally, we obtain a unique curve for the ratio of the overall elastic moduli of the aggregate, $\eta = \bar{G}/\bar{K}$, as a function of coordination number, independent of the confining pressure. This is a direct consequence of the dependence of both elastic moduli on $p_0^{1/3}$ for packings with the same \bar{Z} . Measurements of \bar{G} and \bar{K} from physical experiments might provide, therefore, information about the internal structure of the packing such as the coordination number.

Numerical simulation. –

Reference state. We use the distinct element method [17] and prepare random assemblies of identical, frictional, elastic spheres. We deal with aggregates of 10000 particles with radius $R = 0.1$ mm randomly generated in a periodic cubic cell. We employ material properties typical for glass spheres: a shear modulus $G_g = 29$ GPa and Poisson's ratio, $\nu = 0.2$. The interaction between particles is a non-central contact force in which the normal component follows the non-linear Hertz's law. For the tangential component we incorporate a bilinear relationship with elastic displacement followed by Coulomb sliding with friction coefficient μ (details are given in [7]).

Because we are interested in dense aggregates of frictional particles, we require that ϕ be close to its value at random close packing ($\phi_{RCP} \simeq 0.64$ for monodisperse aggregates [18]). It is well known experimentally that different packing structures are realizable according to the preparation protocol [19–21]. Our approach is to generate

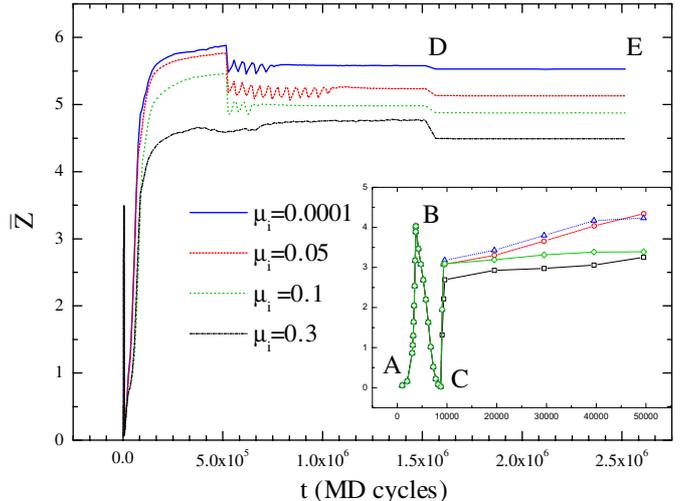


Fig. 1: Variation of the coordination number during the preparation of four packings having the same pressure $p_0 = 500$ kPa and different friction coefficients μ_i . The inset shows the variation of \bar{Z} in the first steps of the preparation protocol.

numerically packings of different structure and determine the relevant variables needed to characterize the elastic response. Independently of the preparation used, we are interested in the final structure of the packings which in turn determines the moduli. Here we employ a protocol [7] where ϕ and p_0 are set in two different phases of the compression, as depicted in fig. 1.

After random generation, frictionless particles are isotropically compressed from an initial gas (point A in the inset of fig. 1) to the desired volume fraction (point B in the inset of fig. 1). The compression is stopped just before the RCP volume fraction to obtain a dense but non-equilibrated packing. Then, the sample is relaxed, reaching zero-pressure and zero-coordination number, with constant volume fraction for all packings, at point C in the inset of fig. 1. Then follows a second isotropic compression with friction to reach the desired pressure using a servo-mechanism. In this step, for a fixed pressure, we use four different coefficients of friction, $\mu_i = 0.0001, 0.05, 0.1$ and 0.3 , to create four different packings, respectively. When the coordination number becomes constant with variation of number of cycles, at point D in fig. 1, we impose the same final friction coefficient $\mu_f = 0.3$ for all packings and, with further servo-control adjustment, we create an equilibrated condition for the system, until the system is fully equilibrated at point E in fig. 1.

All packings are now characterized by the same friction coefficient. However, their structure depends on different preparations during the compaction loading. We apply this procedure for five different values of confining pressure, $p_0 = 100$ kPa, 200 kPa, 500 kPa (shown in fig. 1), 1 MPa, 10 MPa, and for each of them we have four different packings related to the coefficients of friction adopted during the preparation. The result is that, for a given

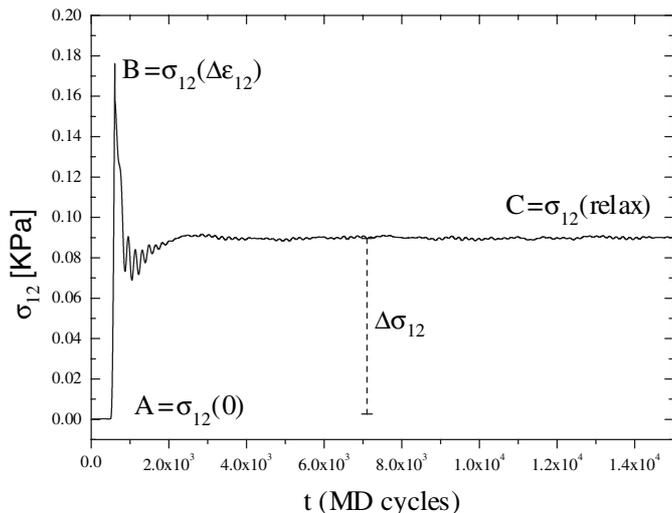


Fig. 2: Numerical protocol for the calculation of the shear modulus \bar{G} , showing the variation of the shear stress σ_{12} after the application of a shear strain $\Delta\epsilon_{12}$ from A to B and the subsequent relaxation until C.

pressure and volume fraction, we have packings with different coordination number, ranging from $\bar{Z} = 4.88$ at the lowest pressure to $\bar{Z} = 6.65$ at the highest.

All our packings are generated to have the same solid volume fraction, $\phi \simeq 0.64$ and friction coefficient $\mu_f = 0.3$, when they reach the final reference state. We underline that for most of the packings there is a small volume fraction variation; for example, for $p_0 = 100$ kPa, $\phi = 0.6355 \pm 0.0002$. This small change cannot be the cause of significant differences in the coordination number. We also note that for pressure higher than 1 MPa the volume fraction exceeds the RCP value. The packings obtained differ from those studied in [7,22] that were prepared with $\mu_i = 0$, in order to reach a high coordination number $\bar{Z} \geq 6$.

Elastic moduli. The elastic moduli of the aggregate are calculated applying an incremental strain to the sample and then allowing it to relax, as reported in fig. 2 [22]. The friction coefficient is set on a very high value to prevent sliding among grains; that is, we refer to the elastic resistance of the aggregate.

We apply a shear strain, $\Delta\epsilon_{12}$ (from A to B in fig. 2) and measure the stress response σ_{12} until the full relaxation (point C in fig. 2), to obtain \bar{G} . We also apply an isotropic strain, $\Delta v = \Delta\epsilon_{11} + \Delta\epsilon_{22} + \Delta\epsilon_{33}$, to measure \bar{K} . Furthermore we calculate the bulk modulus indirectly using the measured values of the Young modulus \bar{E} and \bar{G} through $\bar{K} = \bar{E} - 4/3\bar{G}$ and obtain the same result. The data are reported in table 1. For each calculation, we verify that the applied strain is small enough to be in the linear response regime. We note that the coordination number does not vary during the applied increment of deformation and the subsequent relaxation toward the equilibrium.

Table 1: State parameters and elastic moduli of different groups of packings. The values of elastic moduli are calculated with the error $\pm 2\%$.

	\bar{Z}	\bar{G} [MPa]	\bar{K} [MPa]	μ_i
S1	5.36	131.7	167.5	10^{-4}
$p_0 = 100$ kPa	5.10	115.8	160.1	0.05
	4.99	105.1	155.5	0.1
	4.88	95.5	151.0	0.3
S2	5.48	183.8	218.8	10^{-4}
$p_0 = 200$ kPa	5.21	158.6	207.2	0.05
	5.07	144.3	199.8	0.1
	4.88	120.2	188.1	0.3
S3	5.72	289.8	316.0	10^{-4}
$p_0 = 500$ kPa	5.48	254.3	299.6	0.05
	5.29	225.5	287.1	0.1
	4.90	163.1	257.5	0.3
S4	5.85	394.3	409.8	10^{-4}
$p_0 = 1$ MPa	5.72	361.2	395.8	0.05
	5.50	324.0	375.9	0.1
	5.02	229.3	331.1	0.3
S5	6.65	1083.5	1005.2	10^{-4}
$p_0 = 10$ MPa	6.31	974.3	952.5	0.05
	6.15	922.4	928.1	0.1
	5.92	842.7	897.0	0.3

Results. – We analyze the various packings to determine which parameters affect the incremental response of the aggregate. Because of the loading path, there are particles in the packing, that are not touching or have only one contact; these are the so-called “rattlers” that do not carry any force during the incremental loading applied to evaluate the elastic moduli. In order to reproduce the situation in physical experiments, we use all the particles to calculate the solid volume fraction, but use only the particles with more than two contacts to define the coordination number and χ (*e.g.*, [23]). We also note that the number of rattlers in the packing depends on the coordination number itself, decreasing when \bar{Z} increases.

As a first result of our simulation, we see that for the same confining pressure aggregates may exhibit different coordination numbers (fig. 1). Therefore pressure and coordination number are independent variables.

By collecting packings obtained by similar protocols (identical μ_i , fig. 3) and packings with similar \bar{Z} (fig. 4), we are able to study the dependence of the elastic moduli on the confining pressure only. We see that for ϕ and \bar{Z} fixed, shown in fig. 4, \bar{G} and \bar{K} both vary as $p_0^{1/3}$, while for ϕ and μ_i fixed (fig. 3), the moduli scale in a different way with pressure. The departure from the Hertz average strain theory is more pronounced for \bar{G} than for \bar{K} . That is, in packings with fixed \bar{Z} , particles experience an increase of the overlapping with the pressure and the behavior of the aggregate naturally follows Hertz’s law [5,6]. For the other set of packings created by the same protocol, there is a variation of the structure of the aggregate as \bar{Z} varies with

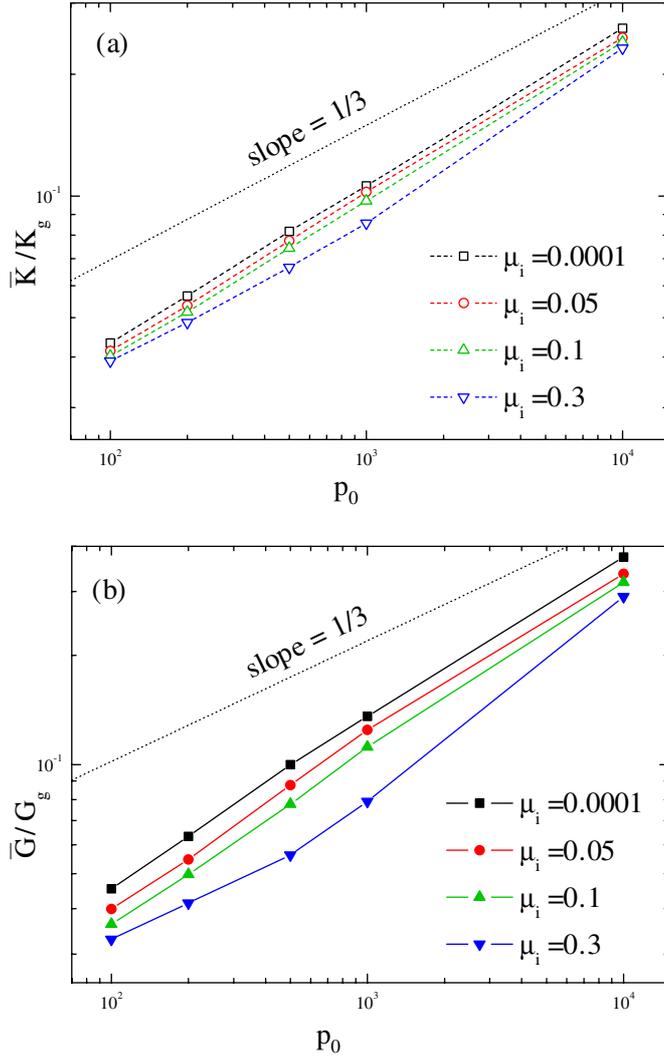


Fig. 3: Elastic moduli \bar{K} and \bar{G} , normalized by the material moduli G_g and K_g , vs. the confining pressure p_0 , for four groups of packings realized by the same protocol determined by μ_i .

the pressure. Consequently, there is more than a simple overlapping among particles with the increase of the pressure, evidenced by the departure of the $p_0^{1/3}$ -dependence in fig. 3 [7,22]. We find that there is a non-trivial dependence of the moduli on the coordination number which goes beyond the usual pressure-induced increments of \bar{Z} found previously [7]. This is associated to fluctuations in the coordination number, in particle translation and rotation [10]. These fluctuations can all be related to \bar{Z} . We will next try to elucidate this dependence.

We focus on the micro-structure of the aggregate and, in particular, we consider the number of particles in contact through the coordination number \bar{Z} and the parameter χ . For packings having similar \bar{Z} , we find that the contact distribution function collapses irrespective of the confining pressure, see fig. 5. Consequently, we may relate the coordination number to the fluctuation in the number of contact per particle. This is corroborated by plotting

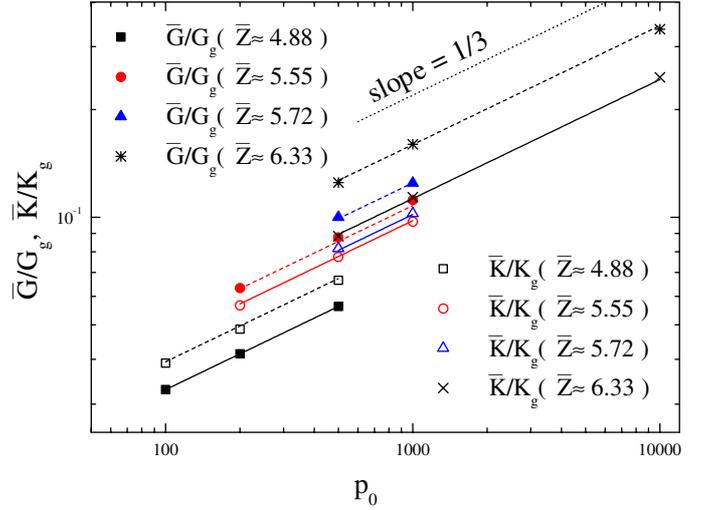


Fig. 4: Normalized elastic moduli, vs. the confining pressure p_0 , for four groups of packings with similar coordination numbers: $\bar{Z} \approx 4.8$, $\bar{Z} \approx 5.5$, $\bar{Z} \approx 5.7$ and $\bar{Z} \approx 6.3$.

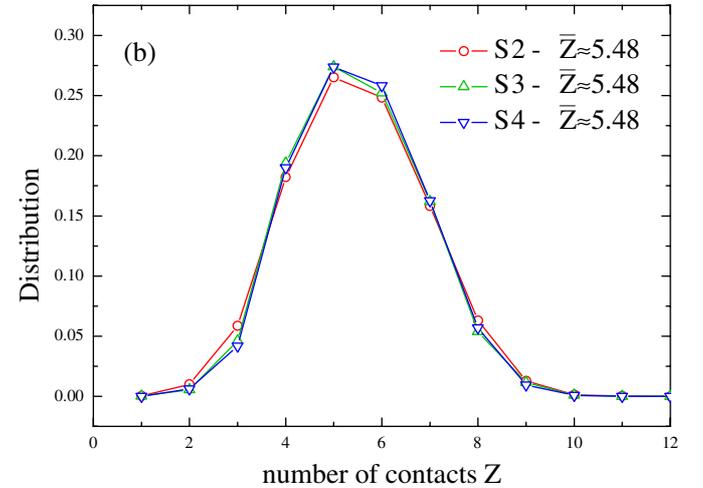
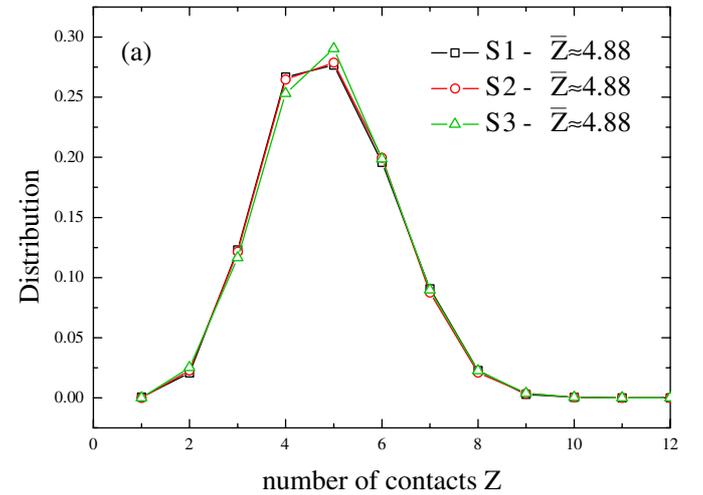
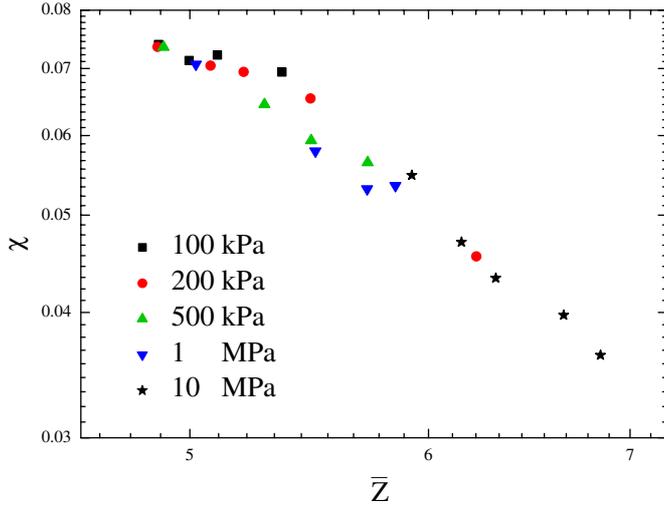
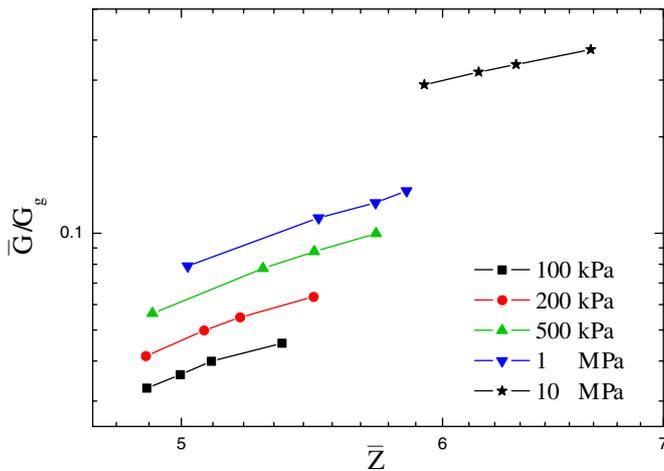
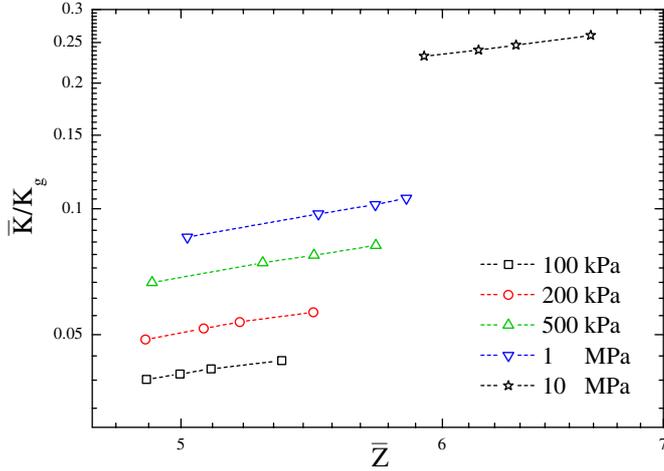
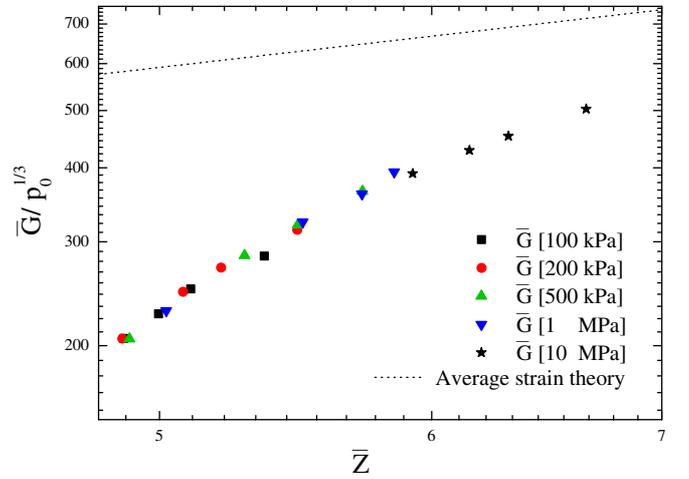
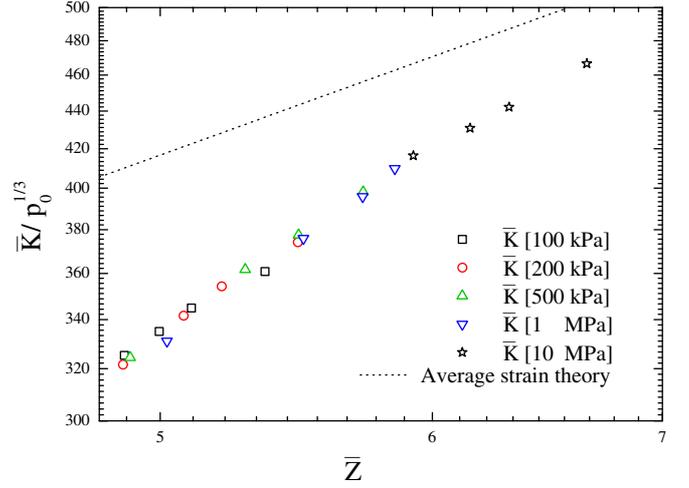


Fig. 5: Distribution function for two groups of packing having similar number of contacts per particle, (a) $\bar{Z} = 4.88$ and (b) $\bar{Z} = 5.48$.


 Fig. 6: Relation between χ and coordination number \bar{Z} .

 Fig. 7: Elastic moduli \bar{K} and \bar{G} , normalized by the material moduli G_g and K_g , vs. the coordination number \bar{Z} , for four groups of packings with the same confining pressure p_0 .

 Fig. 8: Elastic moduli \bar{K} and \bar{G} , normalized by $p_0^{1/3}$, vs. the coordination number \bar{Z} : all the data collapse into unique curves.

χ vs. \bar{Z} in fig. 6. Then, we show the dependence of the measured elastic moduli on \bar{Z} , using groups of packings with the same confining pressure p_0 (fig. 7). While in fig. 8 we plot the bulk and shear moduli normalized by the confining pressure ($p_0^{1/3}$), obtaining unique curves. Predictions from the average strain theory are also proposed.

Finally, it is interesting to focus on the ratio of the elastic moduli, $\eta = \bar{G}/\bar{K}$ [24]. In this ratio the $p_0^{1/3}$ pressure dependence cancels out and, for packings with the same ϕ , all that remains is a pure dependence on \bar{Z} . The plot of η vs. \bar{Z} (fig. 9) results in a universal curve independent of the confining pressure. That is, once the initial state has been achieved, a measurement of the overall shear and bulk modulus can be associated with a unique coordination number. Such a universal curve reveals a dependence on \bar{Z} that strongly deviates from the prediction of the average strain theory based on the Hertz contact that predicts that η is constant. Our results clearly demonstrate the influence of the microstructure characterized by \bar{Z} .

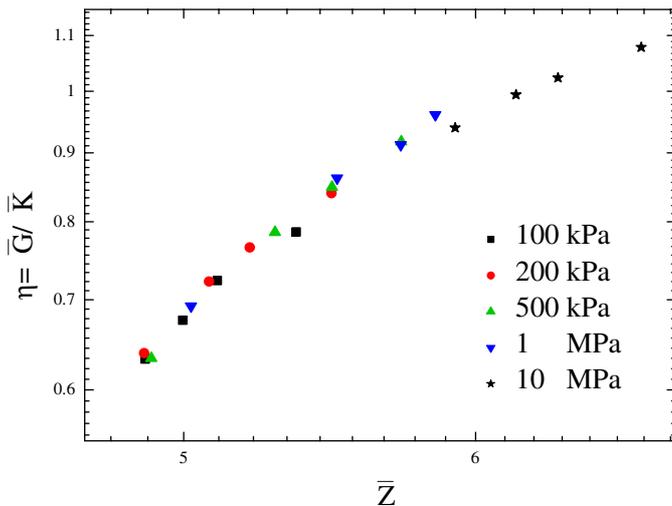


Fig. 9: Variation of η vs. the coordination number.

We note that the relation between η and \bar{Z} reveals a tendency of the ratio of the elastic moduli to decrease with the coordination number. Numerical simulations are in progress to study in more detail packings with lower coordination number and to provide information about the behavior of the assembly near the isostatic point [25–27].

Conclusions. – We have investigated the relevant statistical parameters to describe the elastic response of a dense granular material. In particular, in addition to usual variables such as (p_0, ϕ, \bar{Z}) , we also considered the fluctuation in the number of contacts per particle. We employed a numerical protocol to simulate initial states for an aggregate of particles that is typically characterized by the confining pressure and solid volume fraction. However, using loading history we obtained packings with the same pressure and solid volume fraction, but different elastic responses. We associated this difference to the coordination number. We find a non-trivial dependence for \bar{K} and \bar{G} on \bar{Z} which cannot be captured by the average strain theory. Thus, we conclude that more sophisticated theories, taking in account relaxation of grains, due the disordered micro-structure of the packing, are needed to fully understand the elastic response of granular material.

HAM acknowledges support from DOE, Geosciences Research Program and NSF. LLR acknowledges support from M.I.U.R. - Cofin 2005.

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