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Departure from elasticity in granular layers: Investigation of a crossover overload force

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ABSTRACT

Aiming at characterizing the departure from elasticity in granular materials, we study, by means of numerical molecular dynamics simulations, the stress response of a layer submitted to increasing overload forces. Comparing normalized stress profiles to a reference small overload case, $\sim 0.1\langle m\rangle g$, we compute root mean square (RMS) differences, averaged over several independent realizations, as a function of the overload force. The results indicate two different regimes for these RMS data: an elastic plateau at small overload values and an increase of the RMS at large forces. This increase is due to small (and frequent) as well as large (and rare) rearranging events. We show that one can extract from both of these contributions a crossover value for the overload force, which separates the two regimes.

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1. Introduction

During the last years the description of dense granular materials has been matter of debate and progress (see, e.g., [1,2]) both in the physics and engineering communities. Experiments and simulations of these systems have shown a rich variety of behaviors, where elastic, plastic, jamming or glassy features are observed [3–7]. Some of them concern the characterizations of the elastic-like response of a granular slab to externally imposed forces [8–10] and the transition to a hyperbolic-like response when the system size is sufficiently small [11].

Very recently, some macroscopic descriptions were applied to relatively small systems (slabs of depth of ten to a hundred grain diameters) showing that there is a minimal scale on which macroscopic concepts can be applied to granular systems [12], and that a regime of linear response exists [11]. In this work we are interested in characterizing the limit of the elastic behavior exploring stress response functions when this linear regime starts to fail – the departure of elasticity. To this end we specialize on a relatively simple and quite well studied system, i.e. that of a two-dimensional rectangular slab comprising polydisperse disks. Gravity is accounted for and an additional external force (or overload) is applied to a single particle at the top of the system. We focus in particular on the calculation of the stress on the floor (which has been measured in several experiments [8,9]).

In this paper we investigate the departure from elasticity by testing the linearity of the response at different values of the overload magnitude. More precisely, comparing the normalized stress profiles to the reference situation where the applied force is $F_0 = 0.1\langle m\rangle g$, we compute the Root Mean Square (RMS) difference as a function of the overload force F. The rest of the paper is organized as follows. In the next section, we present the numerical procedure used for preparing the granular packings and computing the stresses. Our results are discussed in Section 3. Conclusions and perspectives for further investigations are presented in the last section.

2. Numerical procedure

Our aim is to perform extensive simulations of assemblies of grains, in order to provide precise two-dimensional numerical data of stress response functions. The control of all the parameters of the simulations, as well as the ability of measuring both micro (grain size) and macro (system size) quantities, ensure a useful and interesting feed back to the experiments and the models. The sim-

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Table 1
The units used in the simulation. $\langle m\rangle$ denotes the mean particle mass, and g is the gravitational acceleration.

Quantity	Normalization	Comments
Length	$L_0 = 1$	system width
Mass	$m_0 = 1$	largest grain mass
Force	$W_0 = \langle m\rangle Ng = 1$	total system weight
Energy	$E_0 = L_0\langle m\rangle Ng = 1$	
Time	$\tau_0 = \sqrt{L_0\langle m\rangle Ng/m_0} = 1$	

ulations are performed using a classical molecular dynamics (MD) algorithm in three successive stages: preparation, deposition and overloading that are briefly described in the following.

We consider a grain-by-grain (GG) preparation (for further information, see [10]) in which a polydisperse set of N grains is considered, with radii homogeneously distributed between $R_{\min} < r_i < R_{\max} = 2R_{\min}$, where $i = 1, \ldots, N$ is the label of the particles. We start by putting $2\sqrt{N}$ similar fixed particles on a horizontal line which will be used as the support for deposition – the bottom layer – and apply horizontal periodic boundary conditions. These bottom grains are chosen in such way that the distances between them are small enough to avoid grain evasion.

Each grain is deposited individually, by choosing a random initial position and a vanishing initial velocity. The next particle is deposited after the system reach an equilibrium configuration. The equilibrium criteria consists in verifying the following tests, which are applied after each period of 100 MD time steps:

(1) the total kinetic energy is very close to zero, smaller than some very low threshold ($\sim 10^{-15}$);
(2) the residual layer weight, i.e. the sum of all forces on the bottom, subtracted to the sum of the weight of all the grains, is lower than a minimal tolerance ($\sim 10^{-10}$);
(3) the force balance on each particle is lower than some small number ($\sim 10^{-7}$).

As consequence, all particles possess at least two contacts with their neighbors, ensuring stable mechanical equilibrium. Besides, the number of gained or lost contacts between particles is zero; also there are no sliding contacts during these time steps. Once these criteria are all satisfied (this typically takes several millions MD time steps and few days of CPU processing in a Xeon 2.4 GHz station) the deposition is stopped, and the overloading phase can begin.

The grains interact through elastic and friction forces. They obey classical Newton motion equations and under molecular dynamics rules – velocity Verlet with 3rd predictor–corrector scheme [13]. The rheology of the contacts is modeled by means of two springs, with k_n and k_t for the normal and tangential contact stiffness, respectively, and a damping coefficient g_n chosen in order to get a critical damping in the normal direction. We choose $\mu = 0.5$ for the contact friction (the dynamic and static friction coefficients are considered identical). This model is similar to the commonly used model of Cundall and Strack [14]. The time step dt used in the MD is fixed as $dt = t_s/50$, where $t_s = \sqrt{m_0/k_n}$ is the characteristic period of oscillation of the normal contact for the grain with smallest mass in the layer (m_0). In order to simplify the simulations, the values for these parameters are defined considering normalized quantities – see Table 1. Expressed in these units, we used $k_n = 1000$, $k_t = 0.75k_n$ and $g_n = 30$. The typical contact deformation close to the bottom is on the order of 0.1% of $R_{\max}$, i.e., the particles are much softer than real glass beads, but still rather rigid.

The overload phase consists in the application of a force F to a single grain of the surface. The applied force is increased linearly from 0 to F with a force increment of $10^{-4}\langle m\rangle g$ in each MD step, and is subsequently kept fixed. The equilibrium criteria are those described above, except that the sum of the forces at the floor has to be equal to the weight of all the grains *plus* the applied force F. Let us use the label 'b' for the static packing *before* the overload is applied, and 'a' for the packing for which static equilibrium is reached again *after* the external force F has been added. The response of the system is computed as the difference between the stress profiles obtained at the 'a' and 'b' states independently.

The stresses are computed in terms of microscopic quantities. Under very general considerations, it was shown [15,16] that an exact expression of the stress tensor $\sigma_{\alpha\beta}$ at position $\vec{r}$ for a static assembly of grains (i.e., the kinetic part of the stress is zero; we consider only the contact stress in the present paper) is given by

$$\sigma_{\alpha\beta}(\vec{r}) = \frac{1}{2}\sum_{i,j;i\neq j} f_{ij\alpha} r_{ij\beta} \int_0^1 ds\, \phi[\vec{r} - \vec{r}_i + s\vec{r}_{ij}]. \tag{1}$$

In this expression, Roman indices are particles labels, whereas Greek ones denote the Cartesian coordinates. $\vec{r}_{ij} \equiv \vec{r}_i - \vec{r}_j$, where $\vec{r}_i$ is the center of mass of particle i, are the 'branch vectors', and $\vec{f}_{ij}$ is the force particle j applies on particle i. $\phi(\vec{R})$ is an arbitrary coarse graining (CG) function which is normalized, positive semi-definite with a single peak at $\vec{R} = \vec{0}$, and has a typical width w, the CG length scale. Note that $\sigma_{\alpha\beta}$ depends, in general, on the choice of ϕ and in particular on the CG scale, However, it has been checked that, for a range of values $d < w < 10d$ (d is the mean grain diameter), this dependence is weak, especially after ensemble averaging [12]. Here we have chosen a Gaussian CG function [17] with a CG width $w = 6d$, a value which is also small enough not to be sensitive to the finite thickness of the layer. We show in Fig. 1 some typical stress response profiles obtained for a single realization (i.e. no ensemble average over several loads), ranging over 4 orders of magnitude in the applied force.

The codes were developed in Fortran language. A typical run for a single layer with 3720 particles, ~30 overload points and 25 different force magnitudes tested for each point, takes about 20 days of CPU processor in a Xeon 2.4 GHz server and generates about 400 Mbytes of data to be analyzed.

3. Results and discussion

The linearity test is illustrated in Fig. 1, in which we compare individual bottom stress rescaled profiles measured of the same layer in response to loadings with different values of F. For small values of the extra force, the contact forces are linear in F, so that the rescaled profiles are indistinguishable. For larger values of F however, one can clearly observe deviations from linearity.

In order to quantify these deviations from linearity, we calculate the root mean square (RMS) differences of the rescaled profiles compared to a small force reference profile, $F_0 = 0.1\langle m\rangle g$. In each realization, a grain is chosen at the top surface and we plot the RMS as a function of function of the overload force magnitude, F. This RMS curve starts with a plateau for the smaller force values. This plateau means that, within fluctuations, the response profiles are linear, which corresponds to the elastic regime. Increasing further the overload force, the RMS value depart from this plateau. This departure in generally smooth, with, besides, few rather abrupt changes. Examining such an abrupt change with smaller force steps, we could check that they really correspond to sudden jumps, in general associated to the loss or the gain of a contact involved in a major force chain close to the overloaded grain.

As we expect the behavior of the RMS curve to be the result of respectively small and larger contact or grain rearrangements, it is interesting to consider these two aspects separately. For this pur-

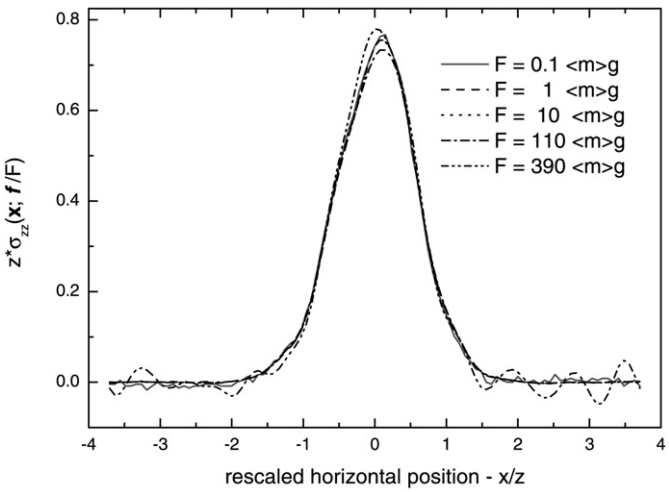

Fig. 1. Stress response profiles normalized by the vertical distance from overload point to the layer bottom. Five different values of F are shown, ranging 4 orders of magnitude for a single realization. Note the remarkable linearity comparing the stress response profiles.

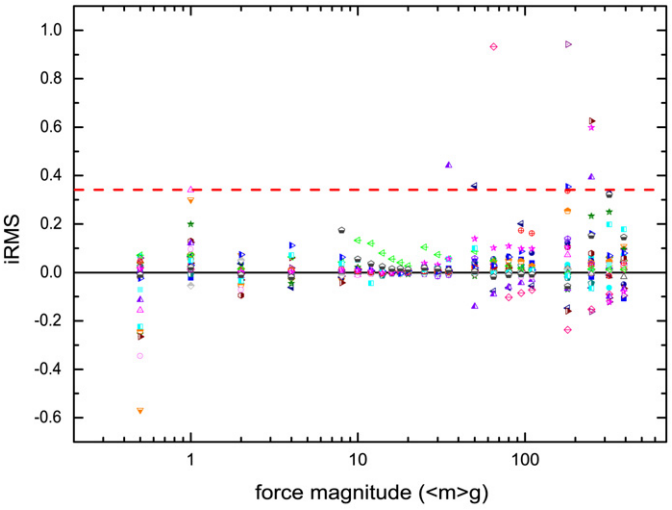

Fig. 2. Incremental values of the RMS difference to the reference profile $F_0 = 0.1\langle m\rangle g$ as a function of the overload force F. All 28 individual realizations computed in this layer are shown – different symbols correspond to independent realizations. The dashed line indicates the threshold considered here (0.33, see text).

pose, we compute, for each overload force step, the corresponding relative increment of the RMS differences defined as

$$iRMS(F_j) = \frac{RMS(F_j) - RMS(F_{j-1})}{RMS(F_j) + RMS(F_{j-1})}, \tag{2}$$

where $RMS(F_j)$ is the RMS value associated to the overload F_j. This incremental RMS is displayed as a function of F_j in Fig. 2 for each single realization in the studied layer. We can see that, most of the data lie close to the zero–y-axis, which means that the relative change in the RMS from a value of the overload force to the next is small. Few points, however, have an iRMS value which can be large. They correspond to these abrupt changes. Taking a threshold value (here we chose 0.33, which corresponds to a doubling of the RMS), we can discriminate between these two types. Once this threshold was reached, the stress response of the respective sample is no longer considered in the ensemble averaging. In Fig. 3, we display an example of such RMS curves, averaged over the 28 different realizations. The elastic plateau is clearly visible for overload forces up to a crossover overload force $F_c \simeq 30\langle m\rangle g$. Beyond this value, the linearity of the response begins to fail. At

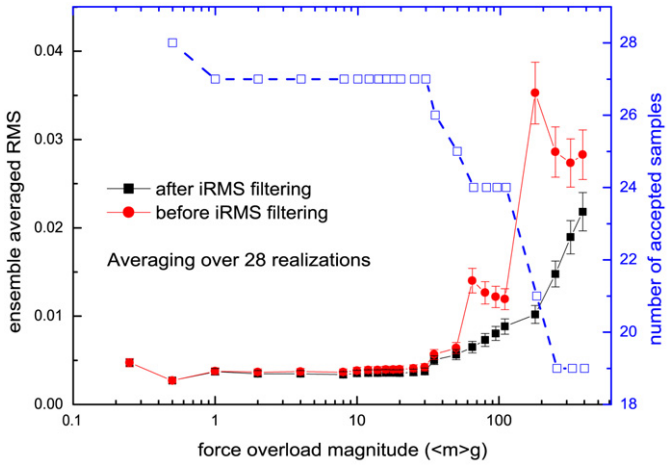

Fig. 3. Ensemble average RMS difference to the reference profile $F_0 = 0.1\langle m\rangle g$ as a function of the overload force F. In this layer, 28 overloads have been computed. Note the difference in the RMS plot after the iRMS threshold has been considered, removing the sudden variations in the RMS values. The dashed line corresponds to the number of accepted realizations – note the different scale in the right axis – i.e. those which pass this iRMS criterion.

the same time, the number of data points above the iRMS threshold increases, meaning that both small and large rearrangements start to be important for the same overload amplitude. Importantly, the value of the threshold is quantitatively relevant for the large-F regime, but not for the determination of F_c. As already mentioned, large iRMS values seem to be associated to crucial contact rearrangements in the force network. However, the precise study of these rearrangements is beyond the scope of the present paper.

4. Conclusions and perspectives

We have studied the departure from the elastic response of a granular layer submitted to a localized force. This departure has been investigated through a test on the linearity of the response. We have shown that it can be attributed to both large and small rearrangements of the packing when the overload increases. We have identified a crossover overload which separates the elastic and non-elastic regimes. Interestingly in this example, this crossover value $F_c \simeq 30\langle m\rangle g$ is on the order of the pressure force felt by a grain at the bottom without overload – the layer depth is approximately 25 grain diameters. Further investigation is needed to explore the effect of the system size on this crossover force. Attention will also be devoted to the role of the inclination of the layer with respect to the gravity – we expect F_c to vanish at the avalanche angle.

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