

Scale Separation in Granular Packings: Stress Plateaus and Fluctuations

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(Received 24 November 2005; revised manuscript received 16 March 2006; published 28 April 2006;
publisher error corrected 2 May 2006)

It is demonstrated, by numerical simulations of a 2D assembly of polydisperse disks, that there exists a range (plateau) of coarse-graining scales for which the stress tensor field in a granular solid is nearly resolution independent, thereby enabling an “objective” definition of this field. Expectedly, it is not the mere size of the system but the (related) magnitudes of the gradients that determine the widths of the plateaus. Ensemble averaging (even over “small” ensembles) extends the widths of the plateaus to subparticle scales. The fluctuations within the ensemble are studied as well. Both the response to homogeneous forcing and to an external compressive localized load (and gravity) are studied. Implications to small solid systems and constitutive relations are briefly discussed.

DOI: [10.1103/PhysRevLett.96.168001](https://doi.org/10.1103/PhysRevLett.96.168001)

PACS numbers: 45.70.Cc, 46.65.+g, 61.46.-w

Continuum descriptions of matter comprise equations of motion for appropriate sets of macroscopic fields [1]. It is helpful (though not required) when these fields or the constitutive relations do not depend on the averaging scale within a certain range of scales (larger than microscopic and smaller than the scales characterizing field gradients); see, e.g., [2]. These “plateaus” of scales define the macroscopic fields and their fluxes in a “scale independent” way. The corresponding constitutive relations are local (expressed in terms of gradients of the fields) when scale separation exists. The Navier-Stokes equations and solid elasticity are typical examples.

Recent studies render support to the notion of scale separation in nanoscale solids and granular matter, as their mechanics lends itself to description by elasticity for a range of loads [3–10]. The short correlation length of the contact forces in static granular matter [11] suggests that such plateaus should indeed exist. In this Letter, we study the scale dependence of the stress response in polydisperse granular packings. We show that even in small systems where stress gradients may be large, stress plateaus can be identified (though they may be quite narrow in some cases); expectedly, the widths of the plateaus are related to the gradients of the stress field. Ensemble averaging increases these widths. The scale dependence of the fluctuations within the ensemble is studied as well.

The considered model is a two-dimensional (2D) rectangular slab in the x - z plane, periodic in the x direction. It comprises 3600 polydisperse frictional disks, whose radii are uniformly distributed in the range (R_{\min} , $R_{\max} = 2R_{\min}$). The aspect ratio is about 7. Gravity acts in the $-\hat{z}$ direction. It is prepared by sequentially dropping the grains from rest at random horizontal positions above the

top of the system. The floor comprises about 160 non-touching grains, whose centers are constrained to reside at $z = 0$, and whose radii are randomly chosen from the range ($1.2R_{\min}$, R_{\max}), which ensures that bulk particles cannot percolate through the floor. Similar systems have been studied experimentally both in two and three dimensions [3,4,12,13].

The force model used in the simulations is essentially that of Cundall and Strack [14]: overlapping disks are coupled by both normal and tangential springs, of respective stiffnesses, $k_n = 1.5 \times 10^4 \frac{\langle m \rangle g}{R_{\max}}$ and $k_t = 0.5k_n$, where $\langle m \rangle$ is the mean particle mass and g the gravitational acceleration. A linear viscous damping force (dashpot) acts in the normal direction (parallel to the line connecting the centers of the disks), the damping coefficient chosen to correspond to critical damping. The tangential forces are limited by the Coulomb condition, with a coefficient of (both static and dynamic) friction, $\mu = 0.5$. The simulation is run until it reaches a numerically static state [15]. To this system we apply either a uniform external load (at its top) or a vertical compressive force acting on one particle at the top of the system. In the latter case the displacement gradients are large near the point of application of the force and decay with distance from this point; the effects of the local gradients on the widths of the plateaus can thus be studied in the same system. The external load is linearly increased from zero to its final value, F_0 , in a time comparable to the typical relaxation time to static equilibrium. The load is subsequently kept fixed, and the system is relaxed to a new numerically static state. The system’s response is linear in the magnitude of the force for loads not exceeding a few times $\langle m \rangle g$, as in Ref. [8]. The response obeys superposition when two external forces

are applied, and is reversible to the slow removal of the force [15]. Below we specialize to the range of loads for which the response is linear. Findings for single realizations as well as “ensemble averages” over different realizations of the disorder are presented. The results reported here pertain to the normal stress *response* of the system (at the floor), i.e., the difference between the floor stress for the loaded system and the (near-uniform) floor stress of the unloaded system.

The stress field, $\sigma_{\alpha\beta}(\mathbf{r})$, at point \mathbf{r} , is given (without the kinetic stress term, which vanishes in the static limit) by the following exact expression, which is fully compatible with the general equations of continuum mechanics (for both static and time dependent states) [6,16–18]:

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

where i, j are particle labels, α, β represent Cartesian components, $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$, where \mathbf{r}_i is the center of mass of particle i , and \mathbf{f}_{ij} is the force exerted by particle j on particle i . The coarse-graining (CG) function, $\phi(\mathbf{R})$, is a positive semidefinite normalized function, with a single maximum at $\mathbf{R} = 0$, and width w (the CG scale). The sign convention here is that compressive stress is positive.

The validity of the equations of continuum mechanics (unlike the constitutive relations) is not resolution limited [with Eq. (1) defining the stress field]; see, e.g., [6,16]. The actual values of the stress depend on the choice of ϕ and w . For “large” CG scales the dependence of the stress on the choice of ϕ is weak for “reasonable” CG functions, such as [16,19]: $\phi(\mathbf{R}) = 1/(\pi w^2)H(w - |\mathbf{R}|)$, where H is the Heaviside function, and the Gaussian, $\phi(\mathbf{r}) = \frac{1}{\pi w^2} e^{-(|\mathbf{r}|/w)^2}$ (in 2D). Gaussian CG functions yield smoother stress fields than the Heaviside function, for obvious reasons [15]. The stress field of Eq. (1) corresponds to the Born-Huang [20] (or Irving-Kirkwood [21]) formula in the limit of large CG scales.

Experimentally [3,4], the normal stress at the floor, σ_{zz} , is given by $\sigma_{zz}(x) = -\frac{1}{L} \sum_i f_{iz} H(\frac{L}{2} - |x - x_i|)$, where L is the CG length (gauge area in experiments), f_{iz} is the force acting on the floor particle i and x_i is its position. An identical expression can be obtained from Eq. (1) by substituting the anisotropic CG function $\phi(\vec{r}) = \frac{1}{L} H(\frac{L}{2} - |x - x_i|) \delta(z)$ [15].

As a theoretical basis for defining ensembles for granular solids is lacking, one usually averages (with equal weights) the desired entities over randomly generated realizations, subject to some constraints, such as the construction protocol of the system. It is not *a priori* clear [22] whether these averages indeed yield typical values. In order to study the effect of ensemble averaging, we prepared 10 different samples; this rather small ensemble was extended as follows. To each of the realizations we applied an external load $F_0 = 7\langle m \rangle g$ to different particles at the

top of the slab. We verified that the corresponding fluctuations were nearly statistically independent when these positions were separated by distances exceeding about half the height of the system. The CG response profiles were therefore ensemble averaged over ensembles of effective sizes, N_e , up to $N_e = 110$. The x coordinate of the load defines $x = 0$.

The inset of Fig. 1 presents the response of the system to uniform forcing at its top both for the case of vertical forces (uniaxial vertical stress) and oblique ones (a combination of vertical stress and horizontal shear). Forces of magnitude $7\langle m \rangle g/n_t$ were applied to each of the $n_t \sim 150$ particles whose centers resided at $z \geq 20.5\langle d \rangle$, where $\langle d \rangle$ denotes the average diameter of a particle. The response is quite flat for $w \geq \langle d \rangle$ even for a single realization, and flatter for an average over five realizations. In contrast, in the inhomogeneous case (with a localized force at $x = 0$), we obtain narrower plateaus. Figure 1 depicts the response at $x = 0$ in this case. Even for a single realization, one observes a (narrow) plateau. The deviations from the plateau at large values of w are due to the large-scale (macroscopic) spatial dependence of the average stress. For the case studied here, the mean response function (for w of a few particle diameters and $N_e = 110$; see Fig. 4) can be well fitted by a Gaussian of half-width, $W \simeq 17.5\langle d \rangle$ (except at the tail), hence (ignoring small scale fluctuations) the convolution involved in the coarse-graining process yields, for $w \gg d$, a (approximate) Gaussian of half-width $\sqrt{W^2 + w^2}$, in agreement with the results obtained by direct coarse graining.

The presence of a plateau suggests that the stress is “locally homogeneous;” however, since the forcing is macroscopically inhomogeneous, the width of the plateau depends on position, as shown in Fig. 2. In order to study this dependence in more detail, we define the plateau

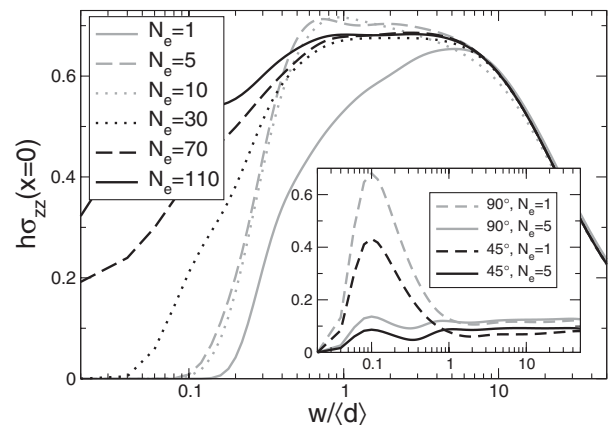


FIG. 1. Mean response to a force at $x = 0$, vs CG width, w , for different ensemble sizes, N_e . The CG function is Gaussian, and the unit of σ_{zz} is F_0/l , where $l \approx 160\langle d \rangle$ is the width of the system; h is the height of the system. Inset: the response to homogeneous forcing at 45° and 90° to the horizontal.

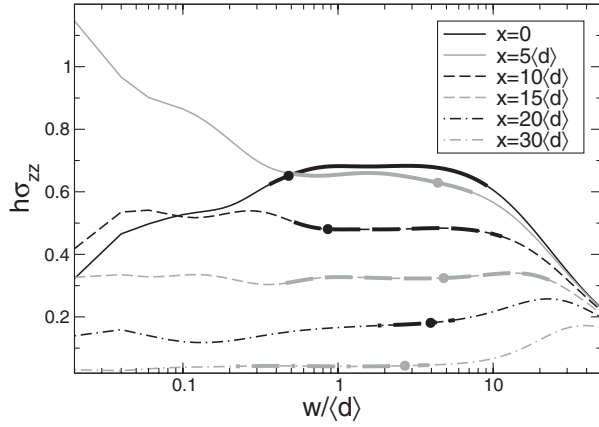


FIG. 2. Mean response at different x coordinates at the floor vs CG width, w , for an ensemble size $N_e = 110$. The thickened parts correspond to the plateaus; \bullet marks w_0 .

width Δw as the largest connected range of w for which $|\left[\sigma_{zz}(w)/\sigma_{zz}(w_0)\right] - 1| < \epsilon$, for a given tolerance ϵ (maximizing Δw over $0 < w_0 < 5\langle d \rangle$). Figure 3 presents the dependence of Δw on x for $\epsilon = 5\%$ and $N_e = 110$. The plateau widths can be rather small (a few particle diameters) in parts of the system, as may be expected considering the inhomogeneity of the response in this relatively small system. The dependence of Δw on x is related to the shape of the macroscopic response. One expects Δw to be smaller where the response is less homogeneous. In Fig. 3 we plot the first and second derivatives of the response (calculated for $w = 4\langle d \rangle$). In general, Δw appears to be anticorrelated with the second derivative of the response, rather than the first derivative. The reason seems to be that the average over a symmetric segment around x , of a profile which is locally linear (on average) and whose fluctuations are essentially uncorrelated, yields basically the same (coarse-grained) value at x almost irrespective of the width of the segment, w . It is easy to verify that the size of the plateau should be given by $(\Delta w)^2 \left| \frac{\partial^2 \sigma_{zz}}{\partial x^2} \right| \approx \epsilon |\sigma_{zz}|$; the peak in Fig. 3 corresponds to a region where $\frac{\partial^2 \sigma_{zz}}{\partial x^2}$ vanishes and there the plateau size depends on the next even (fourth) derivative of σ_{zz} .

The dependence of Δw on N_e for several values of x is shown in the inset of Fig. 3. As expected, ensemble averaging smoothes small scale fluctuations: while for $N_e = 1$ the plateaus start at $w \geq \langle d \rangle$ (see also Fig. 1), they probably extend down to $w = 0$ as $N_e \rightarrow \infty$. Note that not only the forces fluctuate among the realizations, but also the particle positions. The plateau widths seem to practically saturate already for $N_e \approx 50$, suggesting that the fluctuations in the ensemble are not strong.

The wide distribution of contact forces in granular materials [11,23] may suggest the existence of strong stress fluctuations. However, since the force correlations are rather short ranged [11], their fluctuations are well smoothed by spatial averaging. Denote the standard deviation

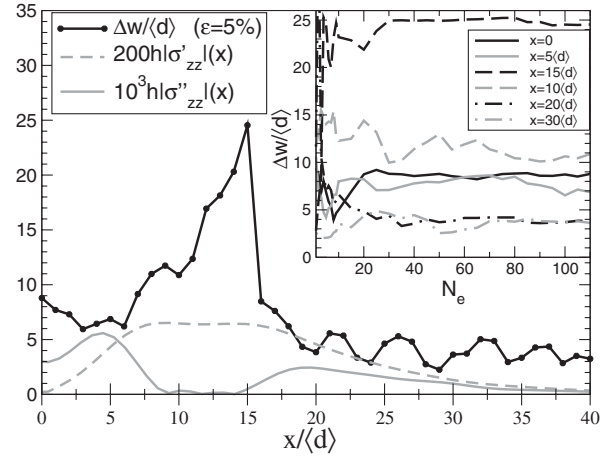


FIG. 3. The width of the plateau, Δw , vs the x coordinate, for an ensemble size $N_e = 110$ and tolerance $\epsilon = 5\%$, as well as the first and second derivatives of the response (for $w = 4\langle d \rangle$). Inset: Δw vs N_e at different x coordinates.

tion (in the ensemble) of the response by $\Delta \sigma$. The relative standard deviation, $\Delta \sigma_{zz}/\sigma_{zz}$, as a function of the CG scale w , for different ensemble sizes, is presented in the inset of Fig. 4. With increasing N_e , $\Delta \sigma_{zz}/\sigma_{zz}$ seems to saturate to a well-defined limit (for a given w). The relative stress fluctuations at fixed x seem to approximately satisfy $\Delta \sigma_{zz}/\sigma_{zz} \propto w^{-2/3}$. While an explanation of this possible “scaling” is still lacking, we believe it is quite surprising that the fluctuations at small values of w (clearly related to the force and particle position fluctuations) share the same (approximate) scaling with those at large values of w , which sample large-scale fluctuations and the spatial variation of the stress.

The dependence of the stress field (for w within the plateau) and its fluctuations on the absolute horizontal

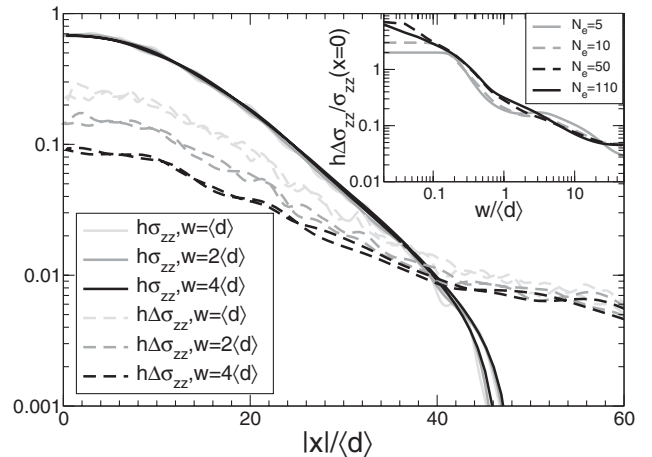


FIG. 4. Mean response and its standard deviation vs $|x|$ at the floor, for several values of the CG width w , for an ensemble size $N_e = 110$. Inset: relative standard deviation of the response at $x = 0$, vs w , for different N_e .

distance from the load, $|x|$, is presented in Fig. 4. The fluctuations ($\Delta\sigma$) seem to decay nearly exponentially with x , at least not too far from $x = 0$. The decay length depends on w . However, the mean stress decays faster than exponentially at large x (basically as a Gaussian), in conformity with the linear elastic solution for this case; the sharp drop near $|x| = 50\langle d \rangle$ is due to the fact that the response becomes negative over a small interval, as expected from linear elasticity [4,19]. A similar study of a Lennard-Jones glass in the linear response regime, with a localized force applied in the interior (rather than the boundary) is presented in Fig. 7 of [7] for 2D and Fig. 8 of [10] for 3D systems (the dependence on w is not discussed in [7,10]). In our case the mean stress (calculated at the boundary) decays faster than exponentially, while in [7,10] the stress is calculated in the bulk, and decays algebraically (both results are consistent with linear elasticity). This renders the relative fluctuations, in our case, non-negligible at large distances, as opposed to the decay with distance found in [7,10]. Our findings suggest that this decay only characterizes intermediate distances (or possibly a wall effect), whereas asymptotically the relative standard deviation is finite (see Fig. 4).

In summary, our findings indicate that the magnitudes of the local gradients of the macroscopic fields (stress in the above case) determine the widths of the plateaus. Although large gradients are expected in nonuniformly forced small systems, the size of the system is not the main factor that limits these widths. The mere existence of the plateaus (which can be as small as 3–5 particle diameters) suggests that continuum theories may be valid for granular and mesoscopic solid systems, but one may need to go beyond simple linear descriptions. The saturation of the results for small ensembles (e.g., 40–50 realizations) due to the short range of force correlations suggests that appropriate constitutive relations can be derived for such systems. Although this Letter is restricted to the linear response regime, we believe that the plateaus will continue to exist even near fluidization (they do exist in the fluid regime), hence, the above approach should be relevant to a rather large range of loads.

We thank E. Clément, F. Léonforte, A. Tanguy, and J.-L. Barrat for useful discussions. C.G. acknowledges support from a Chateaubriand grant. A.P.F.A. is grateful for the support of the CNPq and CAPES (Brazil). A.P.F.A., C.G., I.G., and P.C. express their gratitude to Arc-en-Ciel-Keshet exchange program. I.G. gratefully acknowledges partial support from the ISF, Grant No. 689/04, GIF, Grant No. 795/2003, and BSF, grant No. 2004391.

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