

Strain versus Stress in a Model Granular Material: A Devil's Staircase

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The series of equilibrium states reached by disordered packings of rigid, frictionless disks in two dimensions, under gradually varying stress, are studied by numerical simulations. Statistical properties of trajectories in configuration space are found to be independent of specific assumptions ruling granular dynamics, and determined by geometry only. A monotonic increase in some macroscopic loading parameter causes a discrete sequence of rearrangements. For a biaxial compression, we show that, due to the statistical importance of such events of large magnitude, the dependence of the resulting strain on stress direction is a Lévy flight in the thermodynamic limit.

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The mechanical properties of granular media are currently an active field of research, both in the condensed matter physics and in the mechanics and engineering communities [1–3].

Granular packings close to mechanical equilibrium are traditionally modeled, in the framework of continuum mechanics, with elastoplastic constitutive laws [3,4], i.e., incremental stress-strain relations. Such laws, despite their practical success, were never clearly related to grain-level mechanics. Moreover, cohesionless granular systems seem to be quite different from ordinary solids. Many experimental, theoretical, and numerical studies [2,5–8] have recently been devoted to the peculiar features of stress transmission in granular systems at equilibrium, with correlations over length scales significantly larger than the grain size.

Observations of displacement fields and strains, as the system moves from one equilibrium to another, are scarcer. Systems of rigid grains are expected to deform because of rearrangements of the packing, rather than contact elasticity. How such rearrangements average to produce a macroscopic strain, related to stress variations, remains rather mysterious. The rather singular, unilateral form of the local interaction in such systems led some authors [9] to expect quite unusual macroscopic properties, for which the very concept of strain, so familiar in mechanics of solids, would be irrelevant.

Direct grain-level approaches are, in principle, possible by numerical simulations. However, one has then to define a complete mechanical model to enable a calculation of particle trajectories. In practice, dynamical parameters ruling energy dissipation are often chosen according to computational convenience as much as physical accuracy. It would be desirable to assess the influence of such choices on the results.

The present numerical study addresses those problems, as follows.

Disordered, dense assemblies of rigid, circular, frictionless disks are prepared by isotropic compaction. The force law reduces to the condition that contacts transmit repulsive normal forces of unknown magnitude. Then, the di-

rection of the load is gradually altered, thus simulating the biaxial test of Fig. 1. Exploiting the isostaticity property [10–12] of such systems, which is exactly satisfied provided impenetrability is enforced accurately enough, we designed a prescription [12] for the computation of sequences of equilibrium states that we call the geometric quasistatic method (GQSM), in which the only inputs are the geometric data. The strain versus stress evolution in biaxial compression tests is recorded, and a statistical analysis of fluctuations and system size dependence is carried out. Then the GQSM predictions are compared with those of a standard molecular dynamics (MD) method.

First, samples of different sizes are generated (51 samples of $N = 1024$ disks, 23 with $N = 1936$, 10 with $N = 3025$, and 15 with $N = 4900$). Disk diameters are uniformly distributed between 0.5 and 1 (the largest diameter is chosen as unit length), and packed in a loose state within a rigid, square box. After some amount of random mixing (using some dynamical method with energy conservation), we proceed to the isotropic compaction: two of the walls, 1 and 2 in Fig. 1, are now mobile, and

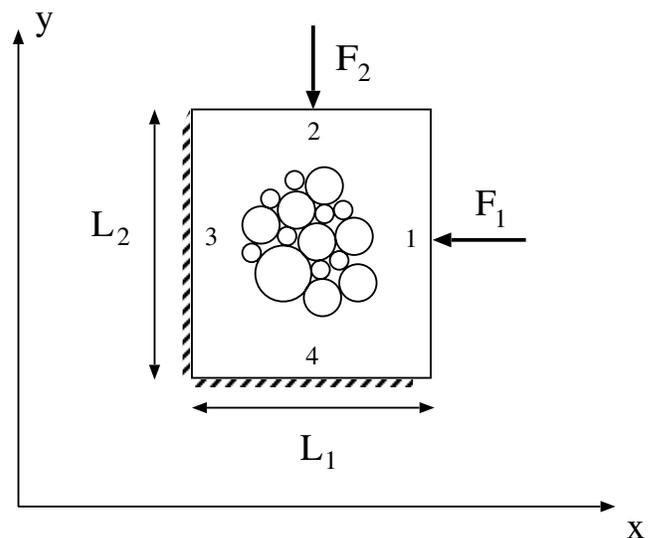


FIG. 1. Sketch of a biaxial compression test.

submitted to compressive external forces F_1 (along the x axis on the figure) and $F_2 = F_1$ (along the y axis). Stress components $\sigma_{11} = F_1/L_2$ and $\sigma_{22} = F_2/L_1$ are kept constant, equal to p , while the system lengths along directions 1 and 2 (L_1 and L_2) decrease. To produce a dense, isostatic equilibrium state, we use the “lubricated granular dynamics” method of Refs. [7,13]. Then, the initial, reference configuration of the biaxial experiment is ready: $F_2 = (p + q)L_1^0$ is gradually increased while $F_1 = pL_2^0$ stays constant; strain components are defined as the relative decrease of lengths $(L_i)_{1 \leq i \leq 2}$, with reference to their initial values $(L_i^0)_{1 \leq i \leq 2}$ as $\epsilon_{ii} = -\Delta L_i/L_i^0$. One also defines the volumetric [14] strain as $\epsilon_v = -\epsilon_{11} - \epsilon_{22}$. We use units such that $p = 1$.

As our main result here, we obtained the $\epsilon(q)$ curves in the thermodynamic limit, as loading parameter q increases monotonically, at constant p . Let us first describe the GQSM procedure. One starts from an equilibrium state in which the force-carrying structure is isostatic. This means that the equilibrium conditions are sufficient to compute all contact force values, on the one hand (the structure is devoid of hyperstaticity, it is not “over-braced” or “overconstrained” [10]), and that the force-carrying structure is rigid (devoid of mechanisms or “floppy modes” [12]), on the other hand. The first of these two properties stems from the condition that two grains need to be exactly in contact to transmit a force to one another [11,12], and cannot interpenetrate. It entails that force values, once equilibrium positions are known, are geometrically determined, all material properties being irrelevant in the limit of rigid grains. The second property is satisfied, for stability reasons, because the grains are circular and contacts do not withstand tension [12]. It entails that an assembly of rigid disks will not deform at all until some initially active contact opens. This cannot occur as long as contact forces are compressive, since this would require the potential energy to increase from equilibrium. As soon as one contact force vanishes, this contact will open [12], because the resulting motion corresponds to an instability. Hence, the following algorithm.

(i) At equilibrium, as q increases from its initial value q_0 , the contact forces depend linearly on q (equilibrium equations are linear). When q reaches some value $q_0 + \delta q$, the force vanishes in one contact, say l_0 .

(ii) Open l_0 , all other contacts being maintained. Because of isostaticity, this entirely determines the initial direction of motion for the whole structure. Keep moving the grains with the same prescription.

(iii) When another contact, say l_1 , closes, the new contact structure (the old one, minus l_0 , plus l_1) is isostatic and may carry the load with geometrically determined contact forces. If there is no traction, a new equilibrium state has been found: go back to step (i). Otherwise, pick up the largest traction, call the corresponding contact l_0 , and go back to step (ii).

This procedure determines a series of equilibrium configurations that are separated by rearrangements occurring

for discrete values of q . The strain versus stress curve is a staircase (see Fig. 2). As long as the same contacts carry the load, the system does not deform; as soon as a rearranging event occurs, strain variables jump to the values corresponding to the next equilibrium configuration. This algorithm clearly involves, in steps (ii) and (iii), an arbitrary ingredient: the prescription that contacts open one by one. The main merit of GQSM, however, is that it does not introduce parameters other than geometric ones.

We now focus on the rise of ϵ_{22} with q , close to the origin, and ask whether the staircase approaches a smooth curve in the thermodynamic limit. (Its initial slope, if finite, would be the effective compliance of the material.) To do so, one studies the statistics of stress (δq) and strain ($\delta \epsilon_{22}$, $\delta \epsilon_{11}$) steps.

Successive δq and $\delta \epsilon$ values are found to be independent, and the width δq of a stability interval is not correlated to the following strain steps. Throughout the investigated q interval, the probability distributions of increments δq , $\delta \epsilon_{22}$, and $\delta W = p \delta \epsilon_v - q \delta \epsilon_{22}$, which is the variation in potential energy corresponding to the current load, do not appreciably change [15]. No significant difference between samples is observed either.

Both q and ϵ_{22} values reached at a given stage can thus be regarded as sums of equidistributed independent random increments. The distribution of stress increments δq is displayed in Fig. 3. It decays exponentially for large δq , and is shifted to smaller and smaller values as N increases, so that the probability distribution of the rescaled increment $\delta q N^\alpha$ is size independent. We denote as δq_0 its average. The exponent can be estimated as $\alpha = 1.16 \pm 0.04$. Stability intervals shrink to zero as N increases: in the thermodynamic limit, any macroscopic load variation entails some motion of the grains. This property of packings of frictionless rigid grains, known as *fragility* [9,12], is unambiguously established by our simulations. The value of α should be related to the shape of the force distribution for small values, and to the varying sensitivity

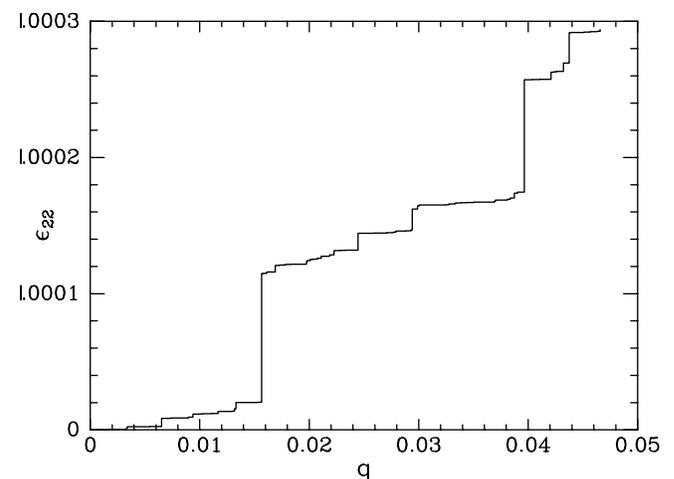


FIG. 2. “Axial” strain ϵ_{22} versus deviator q in one sample with $N = 4900$.

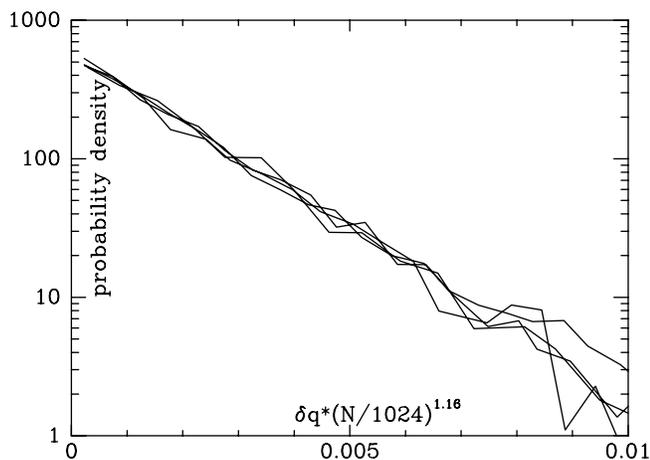


FIG. 3. Probability distribution function for rescaled stress increments $\delta q(N/1024)^{1.16}$ for the four values of system size N .

of the contact forces to macroscopic load increments. The classical central-limit theorem, applied to q increments, will relate for large systems the number of steps M from the beginning of the biaxial compression to the current value of q , as

$$M \sim \frac{q}{\delta q_0} N^\alpha. \quad (1)$$

The distribution of strain increments $\delta \epsilon_{22}$ is shown in Fig. 4. A reduced variable $N^\beta \delta \epsilon_{22} / \delta \epsilon_0$ can also be defined, with an N -independent probability distribution. Remarkably, the (power-law distributed) number c of contact losses (or gains) in one strain step, which tends to grow with $\delta \epsilon_{22}$, does not show any significant size dependence, and contacts that simultaneously open or close are homogeneously scattered throughout the sample, whatever N . We estimated β as $\beta = 2.18 \pm 0.12$. Unlike for stress increments, the distribution now decays as a power law:

$$p(\delta \epsilon_{22}) \sim (\delta \epsilon_{22})^{-(1+\mu)},$$

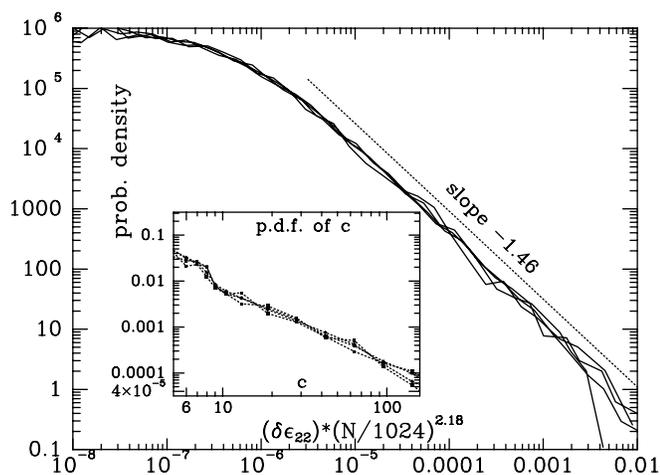


FIG. 4. Probability distribution function for rescaled strain increments $\delta \epsilon_{22}(N/1024)^{2.18}$ for the four values of N . The inset displays the probability distribution function of the number c of lost contacts in one strain step for each system size.

with $\mu = 0.46 \pm 0.03$. As $\mu < 1$, it should be remarked that, although the *typical* strain increment decreases as $N^{-\beta}$ in the limit of large samples, the *average* strain increment does not exist. The standard central limit theorem does not apply, but, due to the power-law decay of the distribution function, one may resort to a generalized central limit theorem [16]. In our case, for a large number M of increments, the asymptotic form of their sum ϵ_{22} is

$$\epsilon_{22} \sim \delta \epsilon_0 N^{-\beta} M^{1/\mu} \xi, \quad (2)$$

with an M -independent random variable ξ abiding by an asymmetric Lévy distribution of index μ .

The stress-strain relationship is obtained on combining Eqs. (1) and (2):

$$\epsilon_{22} = \frac{\delta \epsilon_0}{(\delta q_0)^{1/\mu}} q^{1/\mu} N^{-\beta + \alpha/\mu} \xi. \quad (3)$$

The presence of ξ in Eq. (3) implies that the strain versus stress curve will never express a deterministic dependence. Some size effect—a dependence on N —remains in the thermodynamic limit, unless one has

$$\alpha = \beta \mu. \quad (4)$$

Our estimates of α , β , and μ are compatible with this relation. If it is satisfied, then the distribution of axial strain increments $\Delta \epsilon_{22}$ corresponding to a given, fixed, q increment, Δq , should no longer depend on the system size as soon as N is large enough for Δq to involve, typically, sufficiently many elementary rearranging steps. This was checked, confirming (see Fig. 5), within statistical errors, Eq. (4) and the absence of size effects.

In order to compare the GQSM results to the predictions of more conventional methods, we also simulated biaxial compressions on samples of 1024 and 3025 disks

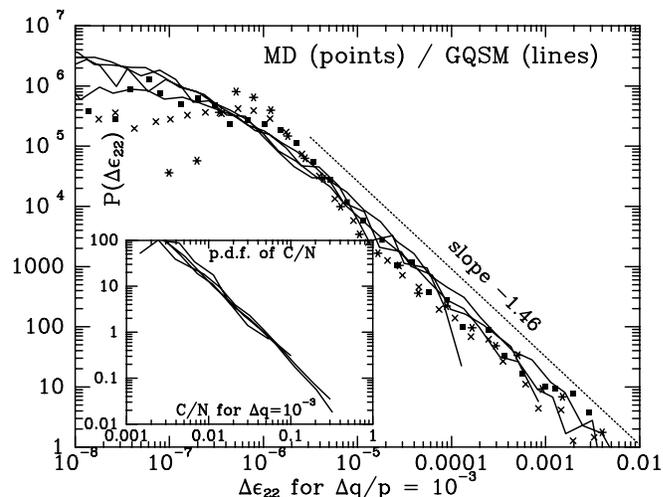


FIG. 5. Probability distribution function for strain increments $\Delta \epsilon_{22}$ corresponding to $\Delta q = 10^{-3}p$ obtained for the four values of N by GQSM (continuous curves) and for $N = 1024$ (crosses) and $N = 3025$ (square dots) by MD. The inset shows the distribution of C/N , where C is the number of lost contacts in one increment Δq , for the different system sizes.

using MD, successively imposing deviator increments $\Delta q = 10^{-3}$. Contacts obey an elastic unilateral law, with a normal stiffness equal to 10^5 . After each stress step, one waits for a new equilibrium state, requesting forces on each grain to balance up to an accuracy of 10^{-3} . Successive strain increments $\Delta\epsilon_{22}^{\text{MD}}$ are uncorrelated and distributed according to the same probability law, which coincides (within statistical uncertainties) as shown on Fig. 5, with that of increments $\Delta\epsilon_{22}$ obtained for the same value of Δq by GQSM. Similarly, the (power-law) distribution of the *fraction* of the total number of contacts that change within one fixed increment Δq does not depend on N (Fig. 5).

We therefore conclude that, in a biaxial test, the axial strain ϵ_{22} dependence on deviator q , as expressed by Eqs. (3) and (4), is a Lévy stochastic process. It does not become deterministic in the thermodynamic limit, but it is devoid of size effect: the strain versus stress curve approaches a devil's staircase with a dense set, on the q axis, of discontinuities of random magnitudes. Moreover, it appears not to depend on dynamical parameters (at least within the accuracy of the present study) and to be determined by the sole system geometry. These results apply, without appreciable change in the statistics, throughout the interval $0 \leq q/p \leq 0.2$.

The evolution of ϵ_v (which can be of either sign, typically 1 order of magnitude smaller than ϵ_{22}) is somewhat more complicated, since successive increments $\delta\epsilon_v$ are not equidistributed (unlike δW). Leaving a discussion of volumetric strains to a future publication, let us further comment here on the behavior of axial [14] strains.

Our results preclude the existence of a constitutive law in the usual sense. As q is increased, ϵ_{22} is typically of order $q^{1/\mu}$, but its actual value is essentially unpredictable, with the remarkable consequence that macroscopic models for granular mechanics should be of a stochastic, rather than deterministic, nature. Of course, such a behavior might be limited to frictionless grains, and is thus perhaps more relevant for some colloidal glasses than for sand, although important fluctuations and high noise levels were sometimes reported for soil materials or glass beads. One does obtain an extremely noisy curve on numerically compressing our system at constant strain rate instead of controlling the stress: understandably, between two equilibrium states that can be relatively far apart, the contact structure does not consistently oppose any given level of stress, and the observed response depends on dynamical parameters. Laboratory tests, at constant strain rate, on such systems would be sensitively influenced by the apparatus itself. It will be interesting to study the dependence of parameter μ on grain shape and polydispersity. Preliminary MD results on dense random packings of monodisperse spheres in 3D yielded Lévy-distributed large strain steps with a value of μ in the 0.4–0.6 range.

Physically, large strain increments are due to rearrangements involving many contact changes [GQSM steps (ii) and (iii) have to be repeated]. Had we resorted to the

approximation of small displacements (ASD), in which all relevant quantities are dealt with to leading order in the displacements, then, as shown in Ref. [12], no iteration of steps (ii) and (iii) would have been necessary. Within the ASD, contacts are replaced one by one, and we have checked that the resulting strain increment distribution does possess an average value. This geometric approximation would ensure [12] uniqueness of the equilibrium state and a one-to-one correspondence between stress and strain. The ASD was used for slightly polydisperse disks on a triangular lattice, in which case it can be justified and constitutive laws are obtained [12,13] (the second listing of Ref. [11] proposes an independent implementation of the GQSM, with the ASD). The distinctive mechanical features of model granular assemblies that are reported here are thus due to the motion of the system in configuration space along a tortuous path between local minima in a complex potential energy landscape. Cooperative rearranging events are also observed in glassy relaxation [17], which might open interesting perspectives.

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