Dynamics and stress in gravity-driven granular flow

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We study, using simulations, the steady-state flow of dry sand driven by gravity in two dimensions. An investigation of the microscopic grain dynamics reveals that grains remain separated but with a power-law distribution of distances and times between collisions. While there are large random grain velocities, many of these fluctuations are correlated across the system and local rearrangements are very slow. Stresses in the system are almost entirely transfered by collisions and the structure of the stress tensor comes almost entirely from a bias in the directions in which collisions occur. [S1063-651X(99)14903-1]

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Despite being the *raison d'être* for one of the oldest scientific instruments, an understanding of the dynamics of sand grains in the hourglass remains a mystery that still leaves much to be explored. Recent research into granular material has followed a number of different tracks [1]. The initial state of a diffuse granular gas with velocity fluctuations (about some mean flow velocity $\langle \mathbf{v} \rangle$) drawn from a Maxwell-Boltzmann distribution with characteristic "granular" temperature T, can be described with fluid-mechanical equations using the ideas and machinery of kinetic theory [2–4]. Yet, left to themselves, such systems are unstable to the formation of high-density clusters [5,6]. As the system cools, due to the kinetic energy of the grains being dissipated in the inelastic collisions, correlations in the density and spatial velocity build up and hydrodynamic descriptions based on molecular chaos (mean field assumption) break down [7–9]. If inelastic collapse to a static state is to be avoided, the system must be constantly supplied with energy.

Here, we consider inelastic hard spheres under the influence of gravity in a cylindrical container (chute flow) with a finite probability of reflection p, at the bottom (equivalent to a sieve in an experiment). The dynamics conserve momentum and the energy loss in a collision is proportional to $1-\mu^2$ where μ is the coefficient of normal restitution. (The grain dynamics are the same as those used in [5–7,10] and others). Due to the flow restriction imposed by the sieve at the bottom, the density is very high (around 90% of that of a closed packed configuration). The mean velocity profiles are very similar to those found in quasistatic flows [11,12], a fairly flat region in the middle with exponential boundary layers, or shear zones at the edges. However, as there is no friction in the system and the grains remain separated, a different explanation is required here. We believe the ability of the system to withstand shear in this regime is due to the very long time scales related to the slow glasslike rearrangement of grains. Diffusion is extremely limited, something that is reflected in the finding that both the distribution of distances and times between collisions is a power law. In addition, we find that the stress tensor is not simply related to gradients in the density or velocity fields, as suggested by hydrodynamic-type descriptions of more diffuse granular flows [2,13], but obtains its structure primarily from an anisotropic distribution of collision impact directions. The structure of the stress tensor is thus found to be similar to recently proposed models of stress propagation in static sand in which the direction of the characteristics for stress propagation is fixed [14]. This gives insight into how such models of the static case may be obtained from the dynamics which were involved in the creation of static configurations of grains. Finally, we find large velocity fluctuations in the bulk regions which are free from shear, in agreement with recent experiments [15]. This apparent contradiction with the more accepted view that velocity fluctuations should be zero in the absence of shear [2,13] can be resolved when one takes into account heat flow. It is found that velocity fluctuations are generated in the shear zones and are then conducted to the interior region.

Figure 1(a) shows a snapshot of one of our two-dimensional (2D) simulations. When a grain hits the bottom of the chute, it is reflected with probability p and escapes with probability $1-p$ [16]. Whenever a grain escapes from the bottom a new grain is placed at the top. The grains are polydisperse with the diameter of the ith grain being $d_i=2+\epsilon_d\delta_i$ where the δ_i are independently distributed Gaussian random variables with unit standard deviation, and ϵ_d typically around 0.1–0.2. This polydispersity breaks up the long-range crystalline order which would otherwise be present (crystalline order still persists over a distance of 3–5 grains). When two grains collide, the velocities after collision $\dot{\mathbf{r}}_1'$ and $\dot{\mathbf{r}}_2'$, expressed in terms of the velocities before collision, $\dot{\mathbf{r}}_1$ and $\dot{\mathbf{r}}_2$, are

$$\begin{pmatrix} \dot{\mathbf{r}}_1' \\ \dot{\mathbf{r}}_2' \end{pmatrix} = \begin{pmatrix} \dot{\mathbf{r}}_1 \\ \dot{\mathbf{r}}_2 \end{pmatrix} + \frac{1}{2}(1+\mu) \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \dot{\mathbf{r}}_1 \cdot \mathbf{q} \\ \dot{\mathbf{r}}_2 \cdot \mathbf{q} \end{pmatrix} \mathbf{q}, \qquad (1)$$

where $\mathbf{q}=(\mathbf{r}_2-\mathbf{r}_1)/|\mathbf{r}_2-\mathbf{r}_1|$, and μ is the coefficient of restitution (typically $\mu=0.95$ or $\mu=0.9$ in our simulations). While energy is lost to the internal energy of individual grains, momentum is conserved. For $0<p<1$, a steady-state situation is achieved where a dense column of granular material flows down the chute with a constant (in time) average velocity. Within this column, grains *remain separated*, flying from collision to collision with fairly large velocities. The

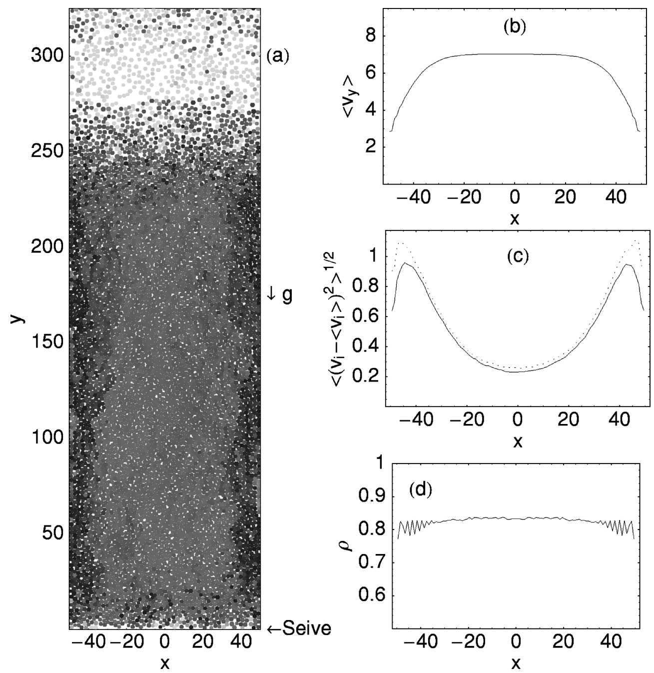

FIG. 1. (a) Sand flow in a two-dimensional cylindrical geometry. Gravity is in the y direction. The color codes the y velocity varying from yellow for fast to blue for slow. Grains are circular with 10% polydispersity, coefficient of restitution $\mu = 0.95$, and the probability of reflection at the bottom is $p = 0.5$. Profiles across the chute at $y = 100$ of (b) average vertical velocity $\langle v_y \rangle$, (c) root mean square velocity fluctuations for the x (solid) and y components (dashed), and (d) average density ρ as a function of x.

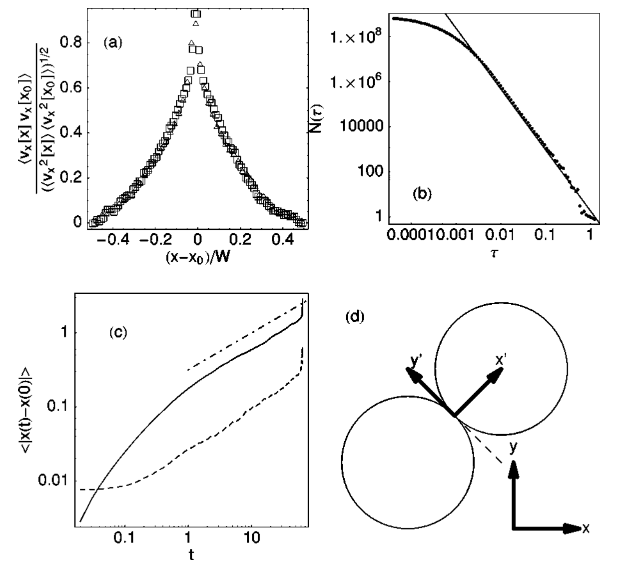

FIG. 2. (a) Correlation function for the x component of velocity shown as a function of the scaled variable $(x - x_0)/W$ where W is the width of the system ($W = 50$ for the triangles and 100 for the squares) and measured from $(x_0, y_0) = (0,133)$, a point at the middle of the column. (b) Unnormalized probability $N(\tau)$ that a ball survives a time τ without suffering a collision, as measured near the center of the column. The straight line indicates the power law $\tau^{-2.75}$. (c) For a grain starting at $r(0) = (0,180)$, the average distance (solid line) a grain moves in the x direction as a function of time; distance between two particles which started out as nearest neighbors (dashed) and power law $t^{1/2}$ expected for normal diffusion (dot-dashed). In (b) and (c) data are from a system of width 50, $p = 0.5$, and $\mu = 0.9$. (d) When two grains collide momentum is transferred in the x' direction across the intervening plane marked by the dashed line.

grains advance between collisions following Newton's equations of motion. Around 10^9 collisions were tracked ($\sim 10^6$ per grain) with an additional 10^8 collisions discarded at the beginning to ensure we had reached steady-state conditions. During this time the grains travel through the system about 20 times. The width of the chute (50 or 100 radii) is comparable or larger than the smallest dimension of situations studied experimentally in three-dimensions in [15].

If, as in the experiments, the pressure is to be independent of the height of the column the side walls must in some way be able to support the weight or absorb momentum in the vertical direction. In order to do this we make collisions with the side walls inelastic in the tangential direction so that after colliding with a side wall, the velocity $\dot{\mathbf{r}}'$ in terms of the velocity before the collision is $\dot{\mathbf{r}}' = (-\dot{\mathbf{r}}_x, \mu \dot{\mathbf{r}}_y)$. (There is nothing special about the choice of μ for the factor by which $\dot{\mathbf{r}}_y$ is decreased.) One can think of this as a very simple model of ''soft'' walls (softer than the grains, e.g., Plexiglas walls and brass balls) or an even simpler model of a rough surface. As we shall see, the boundary layers are exponentially small so that the precise boundary conditions should not affect grain motion in the interior.

Figure 1(b) plots the average vertical velocity in a cross section of the chute. The velocity is flat in the central region, implying an ability to withstand finite shear stresses, with exponential boundary layers, or shear zones. The velocities, and indeed most other quantities, are independent of height in the dense column above a height of approximately half of the chute width, and below a similar distance from the top. These profiles are very similar to those seen in slow and quasistatic flows [13,11,12]. However, the explanation for quasistatic flows involves overcoming the yield stress that arises from static friction [12]. Here there is no friction between the grains and the grains remain separated [and undergo fairly large velocity fluctuations, Fig. 1(c)]. The ability to withstand shear is less surprising when you consider correlations in the velocity fluctuations [17]. Figure 2(a) shows the velocity-velocity correlation function for the x component of velocity. As can be seen, the velocity correlation function scales with system size. As we shall see below, this correlated motion allows for the coherent transfer of momentum across the system from collision to collision, thereby resulting in some of the solidlike properties.

Before examining the process of stress transfer, it is worthwhile to look at the underlying microscopic dynamics, and how these differ from those in a normal fluid or solid material. In diffuse regions, the mean free path can be a very useful quantity to measure [10]. Figure 2(b) shows the (unnormalized) probability $N(\tau)$ that a grain survives a time τ without suffering a collision, measured near the center of the dense column. As can be readily seen, $N(\tau)$ has a power-law dependence on τ:

$$N(\tau) \sim \tau^{-\alpha}, \tag{2}$$

where $\alpha = 2.75 \pm 0.05$. There is a short-time cutoff where $N(\tau) \to \mathrm{const}$ as $\tau \to 0$. In addition, the distance traveled between collisions l is also a power law with the same exponent. This is not that surprising since the moments of the velocity distributions appear to be convergent and thus τ and l are related by some typical velocity. The power law leads to a typical mean free path comparable to the short distance cutoff given by the interparticle spacing. This suggests that particles are tightly confined by their neighbors.

To examine this, it is instructive to look at the observed diffusion of a grain as it travels through the system. Figure 2(c) shows the average distance traveled in the x direction by a single particle (solid line) in a time t and the distance between two particles (dashed line) which started out as nearest neighbors near the top of the column. One sees that diffusion is very limited and that the two particles typically remain nearest neighbors throughout their lifetime in the column. Even the single particle motion is fairly limited moving only of order 1 radius during its lifetime in the column. The single-particle motion is not diffusive [diffusive motion would have $\langle |x(t)-x(0)|\rangle \sim t^{1/2}$] but appears to be approaching this in the long-time limit.

Momentum conservation requires that

$$\partial_t(\rho v_i)+\partial_k(\rho v_i v_k)=\partial_k\sigma_{ik}+\rho g_i, \tag{3}$$

where σ_{ik} is the stress tensor, and all v_k refer to first moments of the velocity distribution. In our steady-state situation the left-hand side is zero. There are two types of contributions to the stress tensor. The first contribution comes from the diffusion of particles [by this we do not mean macroscopic convection, the $\partial_k(\rho v_i v_k)$ term, but the microscopic particle diffusion, present even in the case of no macroscopic flow]. This contribution turns out to be negligible as particles do not diffuse around very much [Fig. 2(c)]. Unlike the often studied granular gas case, in the situation we study here the stress is dominated by momentum transfer during collisions.

Figure 2(d) shows two grains at the moment of collision. The collision results in momentum being transferred in the x' direction across the intervening plane marked by the dashed line in the figure. This gives a contribution to the stress tensor, measured in the (x',y') coordinate system of

$$d\sigma_{x'y'}=\begin{pmatrix} \mathbf{p_c}\cdot\hat{\mathbf{x}}' & \mathbf{p_c}\cdot\hat{\mathbf{y}}' \\ 0 & 0 \end{pmatrix}, \tag{4}$$

where p_c is the momentum transfered from grain 1 to grain 2. Converting to xy coordinates this is

$$d\sigma_{xy}=\begin{pmatrix} (\mathbf{p_c}\cdot\hat{\mathbf{x}})(\hat{\mathbf{x}}\cdot\hat{\mathbf{x}}') & (\mathbf{p_c}\cdot\hat{\mathbf{y}})(\hat{\mathbf{x}}\cdot\hat{\mathbf{x}}') \\ (\mathbf{p_c}\cdot\hat{\mathbf{x}})(\hat{\mathbf{y}}\cdot\hat{\mathbf{x}}') & (\mathbf{p_c}\cdot\hat{\mathbf{y}})(\hat{\mathbf{y}}\cdot\hat{\mathbf{x}}') \end{pmatrix}. \tag{5}$$

The net contribution to the stress tensor is found by averaging over time and dividing by the area over which the average is performed. Figures 3(a) and 3(b) show σ_{yy} and σ_{xy} for one particular case. Figure 3(c) shows how, within statistical errors, $\partial_k\sigma_{ik}+\rho g_i=0$ thus satisfying Eq. (3) (this relationship should be interpreted in the probabilistic sense: it is true "on average"). Interestingly, most of the weight is supported by a shear stress, via $\partial_x\sigma_{xy}$ rather than the pressure gradient $\partial_y\sigma_{yy}\approx 0.014$. Effectively, the column behaves like a solid block sliding down a tube with friction at the walls supporting the force due to gravity. However, the system has

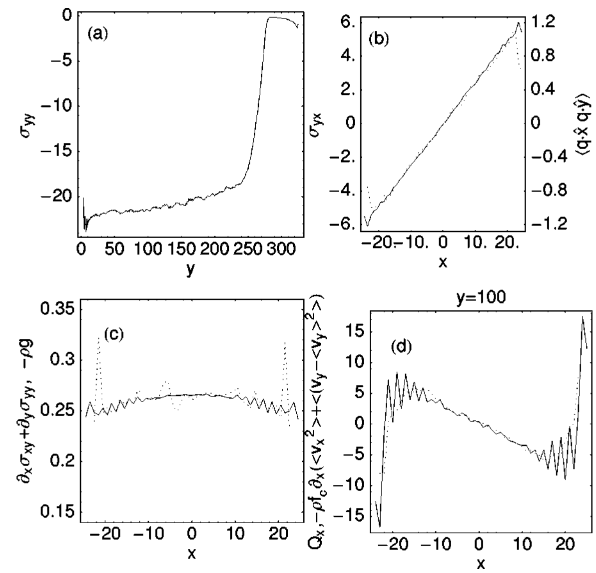

FIG. 3. (a) Diagonal components of the stress tensor σ_{yy} computed from momentum transfer during collisions. (b) Off-diagonal component of the stress tensor, σ_{yx} (solid line and left axes) and correlation between x and y components of a vector $\mathbf{q}$ drawn at every collision from the center of one grain to the center of the other grain (dashed line and right axes). (c) Balancing of body force ρg (solid line) and derivatives of stress tensor $(\partial_x\sigma_{xy}+\partial_y\sigma_{yy})$ (dotted line). The larger fluctuations in ρg near the edge are due to columnar ordering induced by the straight side walls. The statistical error is comparable to the noise level in $(\partial_x\sigma_{xy}+\partial_y\sigma_{yy})$. The data are from the system of width 50, $p=0.5$, and $\mu=0.9$. (d) Heat flow in the x direction Q_x (solid) and $-\rho f_c\frac{1}{2}\partial_x\langle v^2\rangle$ (dotted).

solid properties only in the sense of a glass, as rearrangements do occur, albeit on longer time scales.

Given that things are not isotropic, it is important to see where the structure of the stress tensor comes from. It can arise from both gradients in velocities or from an anisotropic distribution of collision directions. If at every collision one draws a vector from the center of one grain to the center of the other grain and then averages, one finds that there is a definite bias in the collision directions [Fig. 3(b), right axes]. This is consistent with the collision "chains" observed in the simulations and previously by other workers [6,9]. This bias in the collision directions implies a preferred direction to the collision chains. To clarify, we put the momentum transfer from Eq. (1) into the stress tensor from Eq. (5) to get

$$\begin{aligned}\sigma_{ij}&=\frac{1}{t}\sum_{\text{collisions}}-\tfrac{1}{2}(1+\mu)(\dot{\mathbf{r}}_1-\dot{\mathbf{r}}_2)\cdot\hat{\mathbf{q}}\\ &\quad\times\begin{pmatrix} (\hat{\mathbf{q}}\cdot\hat{\mathbf{x}})^2 & (\hat{\mathbf{q}}\cdot\hat{\mathbf{x}})(\hat{\mathbf{q}}\cdot\hat{\mathbf{y}}) \\ (\hat{\mathbf{q}}\cdot\hat{\mathbf{y}})(\hat{\mathbf{q}}\cdot\hat{\mathbf{x}}) & (\hat{\mathbf{q}}\cdot\hat{\mathbf{y}})^2 \end{pmatrix},\\ &\approx-\tfrac{1}{2}(1+\mu)f_c\langle(\dot{\mathbf{r}}_1-\dot{\mathbf{r}}_2)\cdot\hat{\mathbf{q}}\rangle\\ &\quad\times\begin{pmatrix} \langle(\hat{\mathbf{q}}\cdot\hat{\mathbf{x}})^2\rangle & \langle(\hat{\mathbf{q}}\cdot\hat{\mathbf{x}})(\hat{\mathbf{q}}\cdot\hat{\mathbf{y}})\rangle \\ \langle(\hat{\mathbf{q}}\cdot\hat{\mathbf{y}})(\hat{\mathbf{q}}\cdot\hat{\mathbf{x}})\rangle & \langle(\hat{\mathbf{q}}\cdot\hat{\mathbf{y}})^2\rangle \end{pmatrix},\end{aligned} \tag{6}$$

where the sum is over collisions in a (long) time interval t and f_c is the collision frequency. In writing this we have made an assumption, supported by the data, that the factor

$(\dot{\mathbf{r}}_1-\dot{\mathbf{r}}_2)\cdot\hat{\mathbf{q}}$ can be separated from the factors in the matrix when computing averages. In fact, the factors in front of the matrix appear to be nearly a constant, hence the structure of the stress tensor comes almost entirely from the bias in the directions in which the collisions occur [cf. Fig. 3(b)]. Note that there is a striking similarity between the structure of the stress tensor in our model and that of a static model recently proposed in Ref. [14]. In our case, the dynamics of flow automatically drive the system to a ''jamming'' configuration where force chains (as given by the preferred directions of collision) form and the system acquires an ability to withstand shear stress.

Finally, we examine the energy balance. As we saw in Fig. 1(c), there are fairly large velocity fluctuations throughout the flow. This is in agreement with the experiments of Menon and Durian [15], but in apparent contrast to hydrodynamic descriptions of granular flows [2,13], which suggest that velocity fluctuations about the mean flow velocity should be zero in the absence of shear. A resolution to this apparent conflict may be found by examining the energy flow. For our steady-state situations, energy conservation requires

$$0=-\boldsymbol{\nabla}\cdot\mathbf{Q}+\rho g\cdot\mathbf{v}+\boldsymbol{\nabla}\cdot(\boldsymbol{\sigma}\cdot\mathbf{v})+I. \tag{7}$$

From Eq. (1), the (kinetic) energy lost in a single collision is $\delta E=-\frac{1}{4}(1-\mu^2)(\dot{\mathbf{r}}_1\cdot\mathbf{q}-\dot{\mathbf{r}}_2\cdot\mathbf{q})^2$. Averaging over the collisions that occur in a unit area per unit time gives the dissipation I. As the stress balances gravity, the work done by the second and third terms cancel, except for a contribution from $\sigma_{xy}\partial_x\langle v_y\rangle$ in the shear zones at the boundaries. This leaves the ''heat'' flow term $(\boldsymbol{\nabla}\cdot\mathbf{Q})$ to cancel the dissipation in the bulk. One must make a clear distinction here between ''energy flux'' and ''heat flux,'' something that has not been necessary in the diffuse regime [10]. From Eq. (1), the energy flux from one grain to another in a collision is $\delta\mathbf{F}=\frac{1}{2}(1+\mu)[(\dot{\mathbf{r}}_1\cdot\mathbf{q})^2-(\dot{\mathbf{r}}_2\cdot\mathbf{q})^2]\mathbf{q}$. However, part of this energy flux is related to the coherent transfer of momentum (i.e., it is the work done by the stress tensor). As a result, the heat flux is the uncorrelated part of the energy flux, $\mathbf{Q}=\mathbf{F}+(\boldsymbol{\sigma}\cdot\mathbf{v})$. With this done, one can relate the heat flux $\mathbf{Q}$ to the gradient of the granular temperature $T=\frac{1}{2}[\langle v_x^2\rangle+\langle(v_y-\langle v_y\rangle)^2\rangle]$ by $\mathbf{Q}=-\kappa\boldsymbol{\nabla}T$. As demonstrated in Fig. 3(d), the conductivity $\kappa=\rho f_c$, not a terribly surprising result although different from what one finds in the diffuse regime.

In conclusion, we find that the dynamics of gravity driven flow within the regime studied do not fit into previous descriptions of granular flow in the diffuse regime. While the model of instantaneous collisions with only normal forces is not necessarily general to all granular materials, much of the behavior, such as the presence of velocity fluctuations in the absence of shear does agree with experiments [15] on hard grains. While a complete theory requires more work, our results put fairly tight constraints on any such theory as well as providing very helpful information as to what are reasonable (and unreasonable) assumptions in its formulation.

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