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Density patterns in two-dimensional hoppers

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Recent experiments by Baxter *et al.* [Phys. Rev. Lett. **62**, 2825 (1989)] showed the existence of density waves in granular material flowing out of a hopper. We show, using molecular dynamics simulations, that this effect is a consequence of static friction and find that these density fluctuations follow a $1/f^{\alpha}$ spectrum. The effect is enhanced when the opening angle of the hopper decreases.

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Moving dry granular media, like sand, show a rich variety of rather astonishing and scarcely understood phenomena [1,2]. Famous are the so-called "Brazil nut" segregation [3–5] and the heap formations that occur under vibrations [6–8]. More recently a series of experiments have given evidence that under certain circumstances density patterns are generated inside the flowing medium. Baxter *et al.* [9], for instance, visualized wavelike patterns emanating from the outlet of a two-dimensional wedge-shaped hopper using x rays. Also previous authors [10–12] had noted the formation of similar structures. Brown and Richards [13] explained the density fluctuations during the outflow with nonrandom dilatant waves but their experiments with a single layer had limitations due to irregular sticking to the plate. Similarly rather erratic shocklike density waves have been observed in flow through pipes [14] and down inclined planes [15]. Another experimentally observed ubiquitous phenomenon in granular media seems to be $1/f^{\alpha}$ noise. Liu and Nagel [16] recently measured the acceleration of a particle inside a bulk of glass beads that were excited by a small amplitude vibration. Its Fourier spectrum in time showed power law decay over many orders of magnitude. Baxter *et al.* [17] also observed power law decay in the frequency dependent forces that act on the wall of a hopper. For avalanches going down the slope of a sandpile theoretical considerations of self-organized criticality [18] led to the proposal that their size and lifetime distributions were power laws which was in fact only verified experimentally on very small piles [19].

The existence of these erratic density and force inhomogeneities is intimately related to the ability of granular materials to form a hybrid state between a fluid and a solid: When the density exceeds a critical value which some authors call the critical dilatancy [20,21], granular materials are resistant to shearlike solids. In regions where the density is below this value they will behave almost like fluids which, e.g., can be seen under vibrations and flow through a pipe. In the presence of density fluctuations the rheology therefore can become rather complex. Two microscopic facts seem to be responsible for the strong density fluctuations: On the one hand, one has in granular media solid friction between the grains. This means that when particles are pushed against each other a finite force is needed to start or maintain a relative tangential motion between them. On the other hand, a granular material is internally disordered giving a natural source of noise. We conclude from our molecular dynamics studies that the strong nonlinearity coming from friction produces instabilities in the density which enhance the fluctuations coming from the noise.

Various attempts have been made to formalize and quantify the complicated rheology of granular media. Continuum equations of motion [22], a cellular automaton [23], and a random walk approach [24] have been proposed. But none of them has yet been able to explain these heterogeneous waves. This is why we chose to study these phenomena using molecular dynamics (MD) simulations of inelastic particles with static and dynamic friction in two-dimensional systems. In fact, MD simulations [25] have already been applied to granular media to model segregation [5], outflow from a hopper [26,27], shear flow [28], convection cells on vibrating plates [29,30], avalanches on a sandpile [31], flow through a pipe [14], and others.

We consider a system of N spherical particles of equal density and with diameters d either all equal or chosen randomly from a Gaussian distribution of width w around $d_0 = 1$ mm. These particles are placed into a hopper having an opening angle θ and at the bottom an opening of diameter D. When two particles i and j overlap (i.e., when their distance is smaller than the sum of their radii) three forces act on particle i.

(1) An elastic restoration force using a Hertzian contact law

$$\mathbf{f}_{\rm el}^{(i)} = -Y[|\mathbf{r}_{ij}| - \tfrac{1}{2}(d_i+d_j)]^{1.5}(\mathbf{r}_{ij}/|\mathbf{r}_{ij}|) \, , \tag{1a}$$

where Y is the Young modulus and $\mathbf{r}_{ij}$ points from particle i to j.

(2) A dissipation due to the inelasticity of the collision

$$\mathbf{f}_{\rm diss}^{(i)} = -\gamma m_{\rm eff}(\mathbf{v}_{ij}\cdot\mathbf{r}_{ij})(\mathbf{r}_{ij}/|\mathbf{r}_{ij}|^2), \tag{1b}$$

where γ is a phenomenological dissipation coefficient and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ the relative velocity between the particles.

(3) A shear friction force which in its simplest form can be chosen as

$$\mathbf{f}_{\rm dyn}^{(i)} = -\gamma_s m_{\rm eff}(\mathbf{v}_{ij}\cdot\mathbf{t}_{ij})(\mathbf{t}_{ij}/|\mathbf{r}_{ij}|^2) \, , \tag{2a}$$

where γ_s is the shear friction coefficient and $\mathbf{t}_{ij} = (-r_{ij}^{y}, r_{ij}^{x})$ is the vector $\mathbf{r}_{ij}$ rotated by 90°. Equation (2a) is a rather simplistic description of shear friction which is proportional to the relative velocity of the particles. In order

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to allow for static situations of blocking in a hopper due to arching it is important to include real static friction, i.e., which does not depend on the velocities but rather the relative angle of the surfaces [32]. When two particles start to touch each other, one puts a "virtual" spring between the contact points of the two particles. Let δs be the *total* shear displacement of this spring during the contact and $k_s \delta s$ the restoring frictional force (static friction), then this reads

$$\mathbf{f}^{(i)}_{\text{friction}} = -k_s \delta s \ , \tag{2b}$$

where δs is the shear displacement integrated over the entire collision time. The maximum possible value of the restoring force in the shear direction is then, according to Coulomb's criterion, proportional to the normal force $F_n := f^{(i)}_{\text{el}} + f^{(i)}_{\text{diss}}$ multiplied by the friction coefficient μ [5,31]. Cast into a formula this gives a friction force

$$\mathbf{f}^{(i)}_{\text{shear}} = -s \min(f^{(i)}_{\text{dyn}} + f^{(i)}_{\text{friction}}, \ \mu |F_n|) \ , \tag{2c}$$

where the sign s is taken from the sum of the forces in the shear direction. When particles are no longer in contact with each other the spring is removed. Since we found that omission of the rotational degree of freedom for our model does only slightly change the results quantitatively [26,29] we do not consider it here in order to save some computer time. In fact, when particles have strong deviations from the spherical shape, rotations are strongly suppressed.

When a particle collides with a wall the same forces act as if it would have encountered another particle of diameter d_0 with infinite mass at the collision point. The walls are in fact made out of small particles themselves and in order to introduce roughness on the wall these particles are chosen randomly from a distribution of two radii. The only external force acting on the system is gravity $g \approx -10$ m/s^2.

As initial positions of the particles we considered that they are placed at random positions inside a space several times as high as the dense packing. The initial velocities are set to zero. After that the particles are allowed to fall freely under gravity. Using a Hertzian type elastic force in Eq. (1a) does not give a well defined collision time and we took a Young modulus of $Y = 10^6$ g/s^2 and a time step of $\Delta t = 2 \times 10^{-4}$ s and ran our program on 8 or 16 processors of an Intel iPSC/860 and an IBM RS/6000-550.

In Fig. 1 we see a snapshot of the outflowing particles at four different time steps for material parameters consistent with the experiment of Baxter *et al.* [9]. We clearly see that close to the outlet large holes appear which then propagate in an attenuated form upwards. These patterns quickly vary in time. When the opening angle θ of the hopper is reduced the contrast in the patterns becomes more pronounced. The holes are in general stretched in the horizontal direction but their shape seems rather random. Particularly striking are these structures when watched in a movie. When the static friction μ between balls is switched off and we use a low shear force ($\gamma_s \ll \gamma$) the structures disappear and the density of the outflowing particles becomes homogeneous. This agrees with Baxter *et al.*'s experimental observation that density patterns only occur for rough and not for smooth sand. When the friction with the walls is switched off the density waves also disappear since there is nothing left to support them.

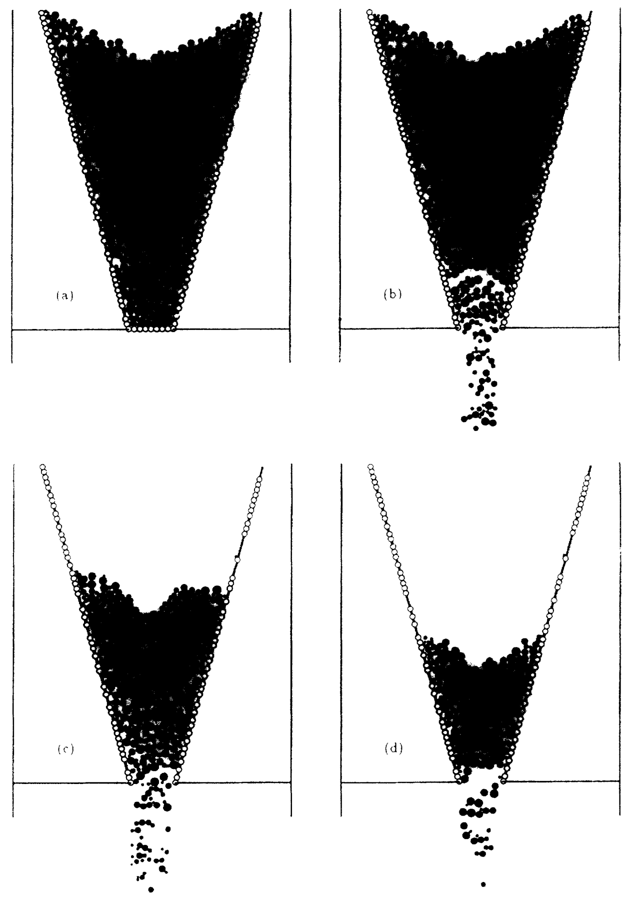

FIG. 1. In this sequence, we show the outflow behavior with static friction for an initial configuration of roughly 1500 particles. The parameters were chosen as the following: γ=500 Hz, γ_s=100 Hz, k_s=1000 g/s^2, θ=30°, D=8d_0, μ=0.5. (a) Initial configuration, (b) after 10 000 iterations, (c) after 100 000 iterations, (d) after 140 000 iterations

A more quantitive approach can be made by measuring the local densities ρ. We binned space in units of 1.56d_0 and counted the number of particles that have their center of mass inside the box averaged over 100 consecutive iteration steps. This density is plotted in Fig. 2 as a function of time and space. We see that the low density regions form curved stripes pointing downwards and indicating rather short living waves. This agrees well with Baxter *et al.*'s observation that for small opening angles the density waves flow downwards. We see no regular structure in the distance and magnitude of the waves in our simulations. They rather look like independent shock waves with random amplitudes coming in a random sequence. Larger waves usually have small densely packed precursors. Strong similarities can in fact be seen with space-time plots of the density of granular media in pipes [14] and of cars on highways having traffic jams [33].

In Fig. 3(a) we see the density profile as a function of time for a point six particle diameters above the outlet. In the beginning, the rather flat region indicates a near blocking but generally no regularity can be seen. The Fourier transformed data averaged over four components are shown in a log-log plot in Fig. 3(b). Clearly they fall on a straight line over nearly two decades. The slope is about -2.7 ± 0.2 obtained

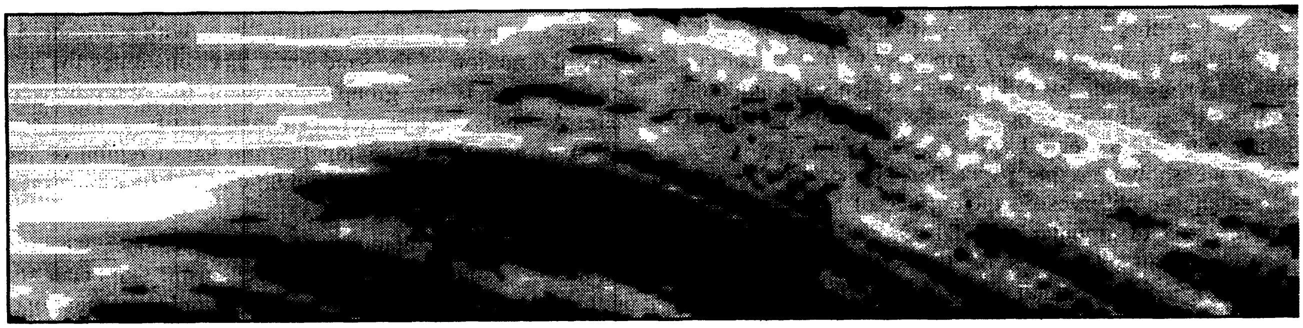

FIG. 2. This figure shows the spatial density fluctuations (vertical axis) for a typical outflow simulation as a function of time (horizontal axis) for $\gamma=100$ Hz, $\gamma_s=500$ Hz, $k_s=1000$ g/s^2, $\theta=10°$, $D=10d_0$, and $\mu=0.5$. Dark areas mark regions with lower densities.

by a least square fit. This means that we have found $1/f^\alpha$ noise which might give rise to alternative experimental verifications since such $1/f^\alpha$ fluctuations in hopper outflows are not yet, to our knowledge, clearly experimentally established [9,13,17]. We checked the stability of our algorithm and the reliability of our data by using different time steps Δt and found that the power spectrum did not change for time steps smaller than 5×10^{-4} s.

When particles of equal size are taken we observed equally well developed density patterns and find roughly the same power law decay of the spectrum. The effect is reduced when the diameter D of the outlet becomes too large. If it is too small the flow of sand can entirely stop due to arching. The critical diameter D_0 when this arching sets in has been studied before with similar techniques [26] where it was found that D_0 is larger when the particles have the same size. When we consider smooth walls, i.e., all wall particles having the same radii, we do not find density waves and the power spectrum looks significantly different. It shows an upwards curved slope with increasing frequency which one also finds when configurations block during the outflow. A similar effect was also found in simulations of flow on an inclined plane [34].

Baxter *et al.* also observed that there exists a critical angle θ_0 above which stagnation regions exist next to the walls of the container. We also found these regions; one example is shown in Fig. 4.

We have observed in a very simple modelization that density waves are generated and distributed with frequency like $1/f^\alpha$. Two ingredients were found essential to generate them: static friction and a large enough surface roughness of the walls. The static friction tends to align the particles, i.e., to form fronts of particles moving exactly with the same vertical velocity. These fronts are nucleated randomly at the walls. Their size distribution (density contrast) comes by it-

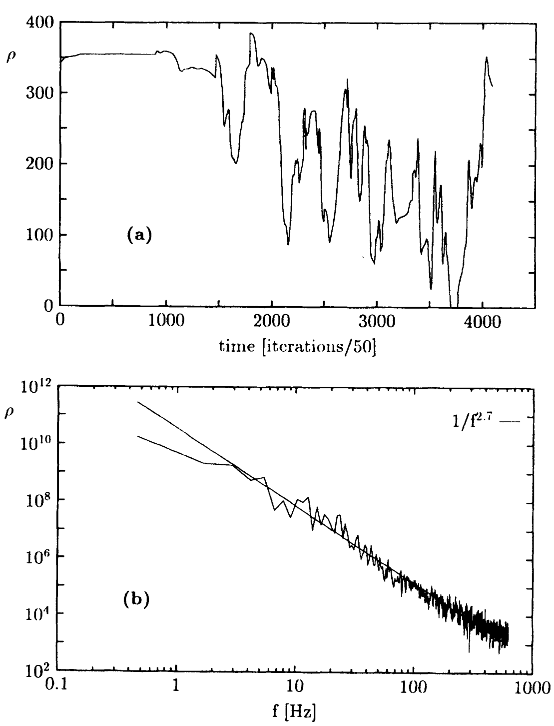

FIG. 3. We consider an outflow sequence for the same parameter values as in Fig. 1 but we constantly fill in particles from above. (a) Shows the density fluctuations $6d_0$ above the hole. One clearly sees a quite random behavior after an initial near blocking. (b) Shows the log-log plot of the fast Fourier transform (FFT) analysis of the density fluctuations. A straight line with slope -2.7 is drawn obtained from a least square fit.

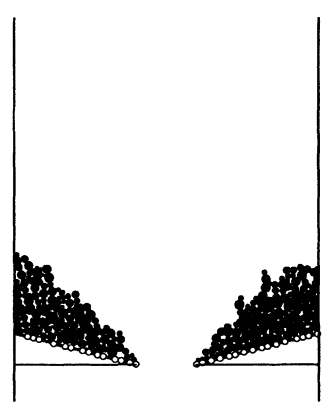

FIG. 4. Due to static friction, 314 particles remain in the hopper for an opening angle of $\theta=150°$ ($\gamma=100$ Hz, $\gamma_s=0$ Hz, $k_s=1000$ g/s^2, $D=10d_0$, and $\mu=0.5$).

self into a critical state, namely, a power law distribution. It therefore has the properties of self-organized criticality (SOC) [18]. It is, however, very important to notice that our simulations were made for rather small systems as compared to real systems. It could therefore be that for systems of millions of particles a cutoff exists in this power law.

We have shown in this paper that similar to the avalanches that one observes on the surface of a sandpile also inside the bulk of granular material one has avalanche behavior which, like the ones on the surface, shows self-organized criticality on small scales [19]. Surface avalanches for large piles, however, seemed to have a characteristic size due to inertia [35]. In fact, avalanches in the holes rather than in the mattered substance could be relevant here and one might speculate that the bulk avalanches might be a better example for asymptotic SOC than the ones on the surface. The mechanisms that generate the patterns are similar but not identical to the original sandpile models. While the static friction similarly generates waiting times with a threshold it is not the motion of the sand itself that constitutes the avalanches but it is the group velocity of the holes between them: An individual particle can easily go from one dense region to the other by flying fast through a region of low density. There is therefore a backflow of information similar to the jamming on highways [33].

Although our simulations are two dimensional, we think that they do capture the essential mechanisms that occur also in three-dimensional experiments. It should be mentioned that in fluidized beds (low Bagnolds number) where the granular medium is surrounded by a fluid and the hydrodynamic interactions become important a similar phenomenon to the one described here, called slugging, is observed [36]. The mechanisms involved seem, however, quite different.

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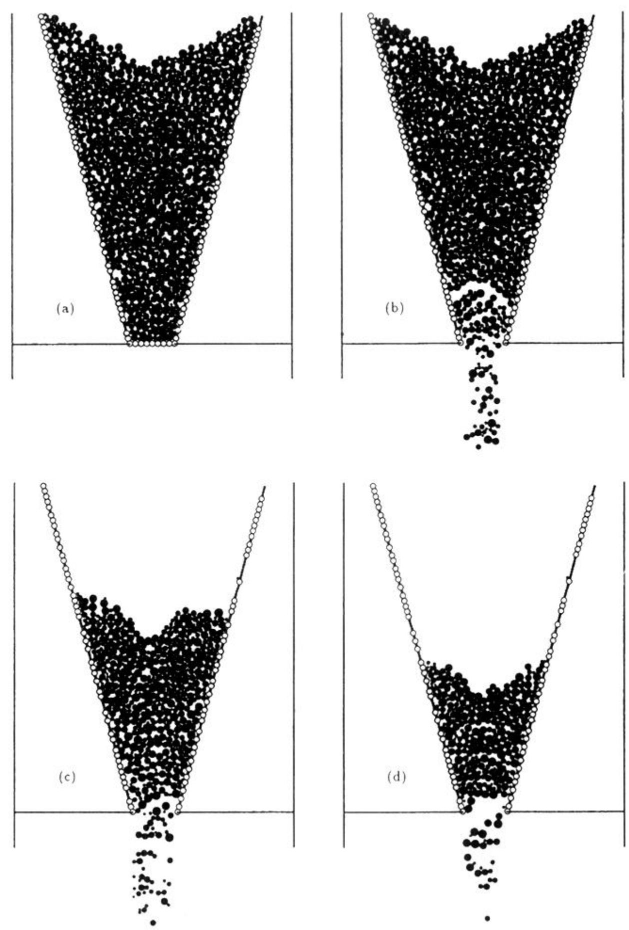
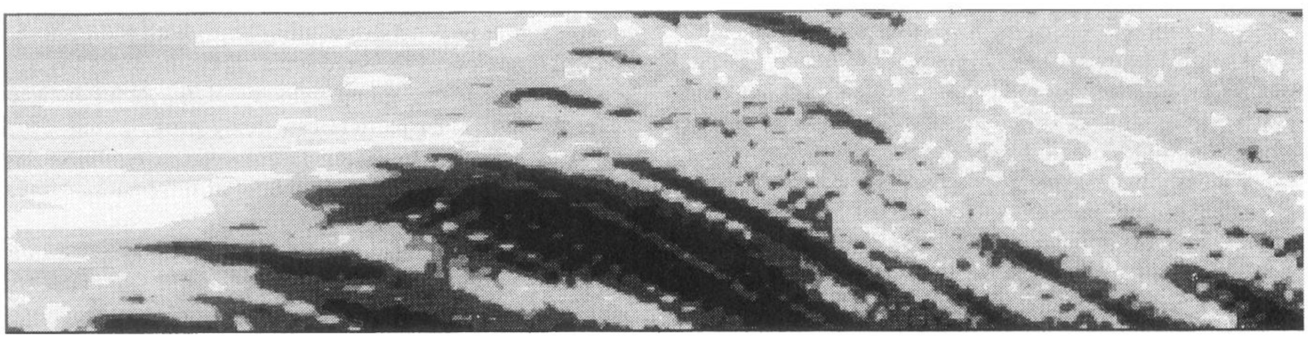


FIG. 1. In this sequence, we show the outflow behavior with static friction for an initial configuration of roughly 1500 particles. The parameters were chosen as the following: $\gamma=500$ Hz, $\gamma_s=100$ Hz, $k_s=1000$ g/s^2, $\theta=30°$, $D=8d_0$, $\mu=0.5$. (a) Initial configuration, (b) after 10 000 iterations, (c) after 100 000 iterations, (d) after 140 000 iterations



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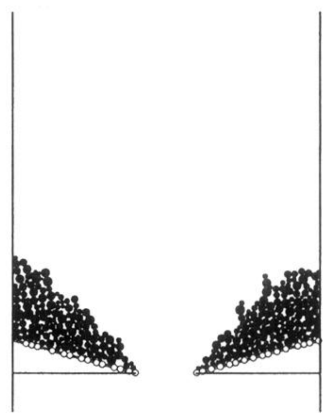

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