Convection Cells in Vibrating Granular Media

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We present molecular dynamics simulations of granular material submitted to vibrations in a two-dimensional system. We find various types of convection cells, due either to the existence of walls or to spatial modulations in the amplitude of the vibration. The direction of the motion relative to the walls depends on shear friction. We measure the strength of the convection velocity and find a characteristic resonance frequency as in experiments. We propose an explanation for the mechanisms that are at the origin of the different motions.

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Many astonishing, scarcely understood phenomena are encountered when granular materials like sand or powder move. Examples are the so-called "Brazil nut" segregation [1-3], heap formation under vibration [4-6], and density waves emitted from outlets [7]. All these effects seem to eventually originate in the ability of granular materials to form a hybrid state between a fluid and a solid: When the density exceeds a certain value, the critical dilatancy [8], it is resistant to shear like solids, while below this density it will "fluidify." This fluidified state can be rather complex, especially in the presence of density fluctuations and density gradients, giving rise to the mentioned phenomena.

Various attempts have been made to formalize and quantify the complicated rheology of granular media. Continuum equations of motion [9], a thermodynamic dynamic formalism [10], a cellular automaton [11], and a random walk approach [12] have been proposed. But so far only in rare cases has it been possible to make quantitative predictions satisfying experiments. This is because much basic understanding of the relevant mechanisms is still lacking—even for the concept of fluidization various definitions are possible [13].

An experimental setup particularly suited to study this fluidization is putting sand on a loudspeaker or on a vibrating table [4-6,14-17]. Under gravity the sand jumps up and down and although kinetic energy is strongly dissipated, collisions among its grains reduce its density, thereby allowing it to flow. Under certain circumstances flow between top and bottom can occur in the form of convection cells. Such cell flow has been observed experimentally in the case of inhomogeneities in the amplitude of the vibration, for instance when the plate is driven at the center and fixed at the boundary [16]. Convection occurs also within the heaps [4-6] and might even be the "motor" for the heap formation.

In this Letter we present the first numerical evidence for the occurrence of convection cells due to inhomogeneities in the vibration amplitude. We also report convection-cell generation due to the existence of walls, an effect that has also been observed recently [18,19]. We study two-dimensional systems and perform molecular dynamics (MD) simulations of inelastic particles with an additional shear friction. In fact, MD simulations [20,21] have already been applied to granular media to model segregation [3], outflow from a hopper [22,23], shear flow [24], and vibrating conveyor belts [25].

Let us consider a system of N spherical particles of equal density and with diameters d chosen randomly from a homogeneous distribution of width w around $d_0=1$ mm. These particles are placed into a container of width L that is open on the top and has either periodic boundary conditions or fixed walls in the horizontal direction. When two particles i and j overlap (i.e., when their distance is smaller than the sum of their radia) three forces act on particle i: (1) an elastic restoration force

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

where Y is the Young modulus (normalized by the mass), $m_i \propto d_i^2$ the mass of particle i, and $\vec{r}_{ij}$ points from particle i to j; (2) a dissipation due to the inelasticity of the collision

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

where γ is a phenomenological dissipation coefficient and $\vec{v}_{ij}=\vec{v}_i-\vec{v}_j$ the relative velocity; (3) a shear friction force that mimics to some degree the effect of static friction

$$\vec{f}_{\rm shear}^{(i)}=-\gamma_s m_i(\vec{v}_{ij}\cdot\vec{t}_{ij})\vec{t}_{ij}/|\vec{r}_{ij}|^2\,, \tag{1c}$$

where γ_s is the shear friction coefficient and $\vec{t}_{ij}=(-r_{ij}^y,r_{ij}^x)$ is the vector $\vec{r}_{ij}$ rotated by 90°. As compared to other modelizations of the forces acting between grains [3,22,24] our Eqs. (1) are simpler since we neglect Coulomb friction and the rotation of particles. In fact, static friction should be proportional to the normal force but the term of Eq. (1c) is always needed to halt the tangential relative motion [3]. We did these simplifications on purpose in order to have fewer, in our opinion unimportant, fit parameters. Under realistic deviations from a spherical shape of the particles, rotations are strongly suppressed and in recent flow simulations the effect of normal forces on friction was found to be negligible [22]. When a particle collides with a wall the same forces act as if it had encountered another particle of diameter d_0 at the collision point. Two forces act on the system: On one hand gravitation $g \approx -10$ m/s^2 pulls each particle down; on the other hand the bottom of the container is subjected to a vibrating motion described by

$$z_0(t) = A(x)\sin(2\pi f t), \tag{2}$$

where f is the frequency and the amplitude A can have an explicit spatial modulation of the form

$$A(x) = A_0[1 - B\cos(2\pi x/L)]. \tag{3}$$

Two initial positions of the particles are considered: They are either placed regularly on the bottom of the container or put on random positions inside a space 7 times as high as the dense packing. The initial velocities are either zero or randomly chosen. After that the particles are allowed to fall freely under gravity and relax for a time that corresponds to ten or twenty cycles of the vibration. The displacements, velocities, and energies are then measured by averaging over up to 200 cycles. We use a fifth-order predictor-corrector MD simulation with $(2\text{-}6)\times 10^3$ iteration steps per cycle which can be vectorized on the Cray-YMP, running at about 10 μs per particle update for $N=200$.

Let us first consider the case of a spatial modulation in the amplitude of the vibration, i.e., $B \neq 0$, using periodic boundary conditions. In Fig. 1(a) we see the displacements of the particles after fifteen cycles for $B=0.5$. Clearly the particles flow upwards in the center where the amplitude of the vibration is larger and form two convection cells. If the dissipation coefficient γ is increased by a factor of 10 the convection is completely suppressed while it is quite insensitive to γ_s, including for $\gamma_s=0$. The elastic modulus also has only a very weak influence as long as it remains larger than 10^3 (in units of d_0) and so we chose a very small value compared to that of experimental materials in order to save computer time. The initial condition plays no noticeable effect, showing that convection is no transient effect. The polydispersity of the particles only slightly distorts the shape of the convection cells as compared to the case $w=0$. We also considered a model in which particles lose energy each time they collide with each other in order to mimic the effects of a real two-dimensional experimental setup [14] and found the same effects when γ is decreased correspondingly.

The strongest convection for the aforementioned parameters is obtained around 60 Hz and it increases dramatically with the amplitude A_0. This resonance seems to be the driving force of the convective motion. In Fig. 1(b) one sees a snapshot of the positions of the particles close to this resonance. In the upper part of the packing, especially in the center where the amplitude is strongest, the particles are not in contact anymore. Therefore static friction cannot be effective on the top and a heap would not be stable. For this reason we think that it is rather unlikely that the heap formation can be traced back to resonances due to spatial inhomogeneities of the vibrating plate.

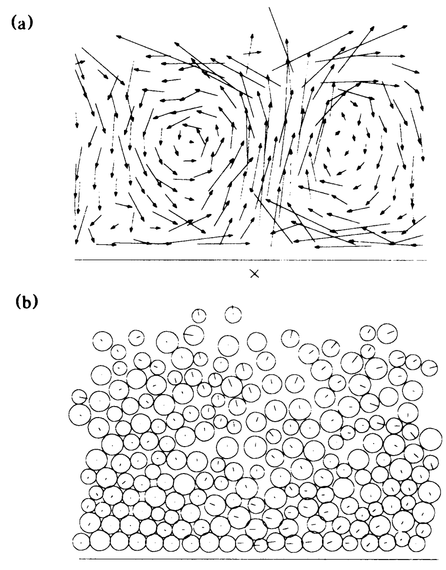

FIG. 1. Convection cells obtained with periodic boundary conditions using 200 particles in a box of size $L/d_0=20$ with $A_0=0.5d_0$, $B=0.5$, $w=0.5$, $Y=5000/d_0$, $\gamma=50g$, $\gamma_s=200g/f$. (a) Displacement of the particles after fifteen cycles for $f=100$ Hz; (b) snapshot of the particles and their velocities (lines) averaged over all time steps of the last fifteen cycles closer to the resonance, $f=50$ Hz.

The strength of the convection can be measured quantitatively by recording the average vertical components of the velocities of the particles in the center, v_1, and at the edges, v_2, of the cells of Fig. 1. These quantities have also been measured experimentally by Rátkai [16]. In Fig. 2 we see these velocities plotted as functions of frequency and amplitude of the vibration. As already mentioned above and also seen in the experiment [16], the convection is strongest around a characteristic resonance frequency given by the position of the maximum in Fig. 2 which increases for decreasing dissipation coefficient γ. In this resonance region the statistical error bars are quite large. The strength of the resonance strongly depends on the amplitude and at $A_0=0.3$ it virtually disappears.

A completely different type of convection can be caused by the existence of fixed vertical walls without any modulation of the amplitude, i.e., for $B=0$. In Fig. 3 we see various cases. As long as $\gamma_s \neq 0$ there is at each wall a very strong downward motion [Fig. 3(a)] giving rise to a circulating current. The particle positions at the end of one cycle are shown in Fig. 3(b) and one sees that there are long horizontal holes in the packing. The particles falling downward tend to separate vertically but horizontal neighbors stay together due to the shear friction γ_s which synchronizes their velocities. In Fig. 3(c) we see

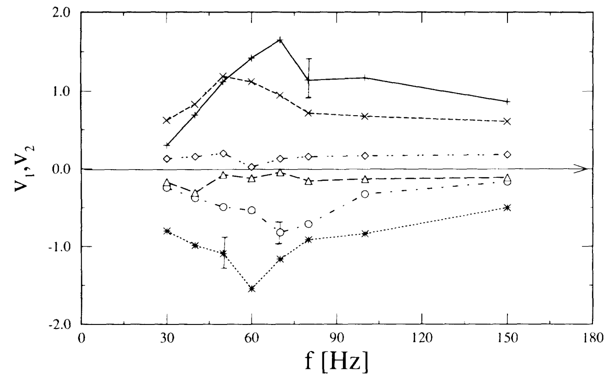

FIG. 2. Average vertical components of the velocity in the center (v_1) and the sides (v_2) of the cell as function of the frequency f for amplitudes $A_0=0.7d_0$ (+ for v_1 and $*$ for v_2), $A_0=0.5d_0$ (× for v_1 and ○ for v_2), and $A_0=0.3d_0$ (◇ for v_1 and △ for v_2). All other parameters are as in Fig. 1.

what happens when the aspect ratio is changed by halving the height of the packing. The two convection cells remain attached to the walls, showing that the walls are at the origin of these cells. One also recognizes a slight heap formation at the wall which might be a first sign of the famous sand heaps discovered by Faraday [4-6]. In Fig. 3(d) we see that when $\gamma_s=0$ there is still a convection cell but the motion of the particles at the wall can now be either upward or downward. This effect prevails when the shear friction is only suppressed during collisions with the walls and not at particle-particle collisions.

The average total kinetic energy $\langle E\rangle$ of the packing is another measure for the strength of the flow. In Fig. 4 we see how it decreases with the dissipation coefficient γ in the presence of walls and with $B=0$. The effect is rather weak and the statistical error bars are quite large so that both a linear or an exponential decay of the form $\langle E\rangle \propto \exp(-c\gamma)$ seem possible.

Let us analyze the origin of the convection due to fixed vertical walls. In the case of no shear friction the vertical walls do not transfer any vibrating motion of the container but represent only a steric hindrance to the flow. In this case, the following scenario applies: When, after levitating from the plate, the packing falls back on the bottom of the container only the horizontal component of the velocities of the particles arriving first will survive collisions with the downwards vertical motion of the rest of the packing that follows behind. So flow parallel to the bottom plate will spontaneously appear and is reinforced at each cycle. This parallel flow will only survive in regions where it is coherent and the size of these regions will grow due to the reinforcement. When one of these regions collides with a vertical wall the flow must go upwards since it cannot go anywhere else. This explains not only the orientation of the convection but also why the convection cells are attached to the walls as seen in Fig. 3(c). The driving force for these cells is therefore the horizontal flows along the bottom plate.

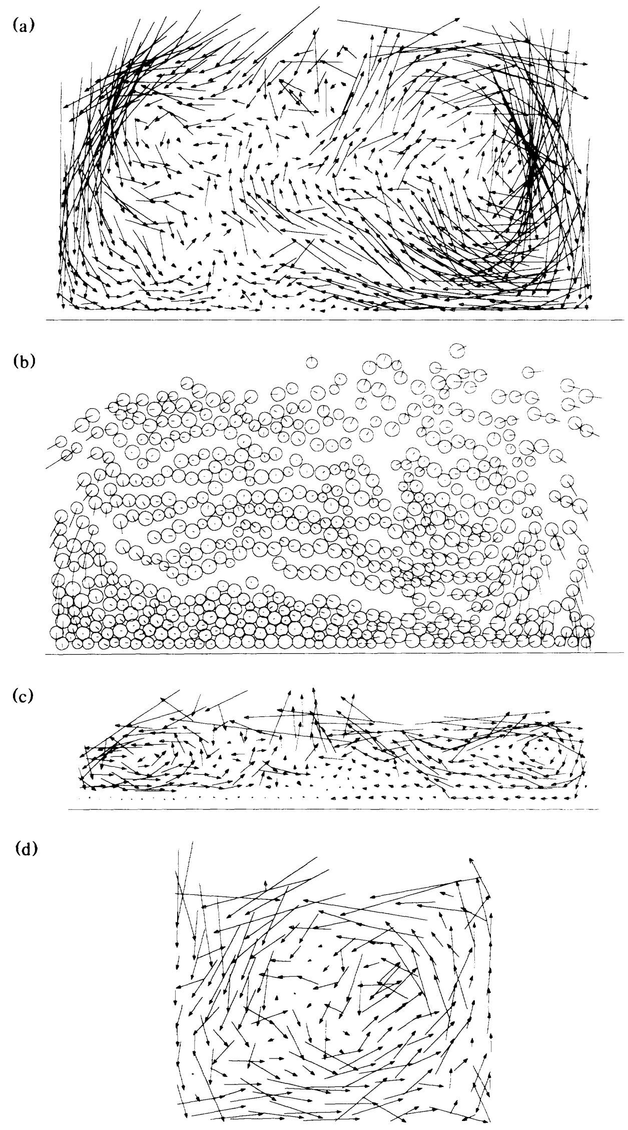

FIG. 3. Convection cells due to fixed vertical walls for $B=0$, $w=0.5$, $Y=5000/d_0$. (a) Displacements after eight cycles and (b) snapshot of the positions of the particles for $f=20$ Hz, $N=600$, $L=46d_0$, $A_0=1.25d_0$, $\gamma=80g$, $\gamma_s=100g$; (c) $f=20$ Hz, $N=300$, $L=44d_0$, $A_0=1.1d_0$, $\gamma=80g$, $\gamma_s=100g$, averaged over ten cycles; (d) $f=100$ Hz, $N=200$, $L=20d_0$, $A_0=0.5d_0$, $\gamma=50g$, $\gamma_s=0$, averaged over fifteen cycles.

When shear friction with the wall is present a different mechanism sets in: While the particles are pushed up and start to levitate, the packing is still quite compressed and so a strong pressure is exerted on the walls giving rise to a strong shear friction while the relative motion of the particles with respect to the walls is upward. When afterwards the particles fall back and have downward relative motion with respect to the wall the packing is much looser and the shear friction much less efficient. Therefore the upward motion of the particles with respect to

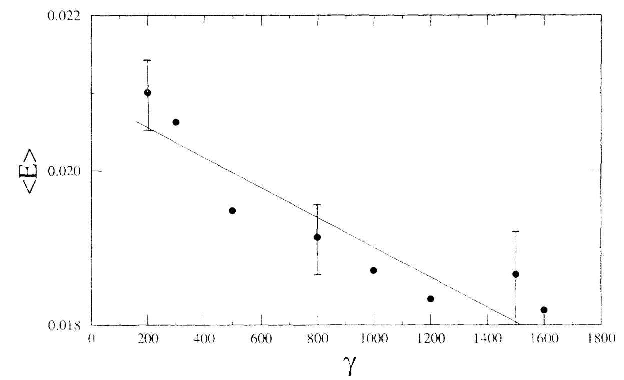

FIG. 4. Average kinetic energy $\langle E \rangle$ as function of the dissipation coefficient γ for $N=150$, $f=20$ Hz, $A_0=1.25d_0$, $B=0$, $w=0.5$, $Y=5000/d_0$, $\gamma_s=100g$, averaging over twenty cycles and using 6000 iteration steps per cycle. The full line is a linear fit to the data; the error bars are statistical.

the wall is slowed down stronger resulting in a net drag down along the wall. If γ_s is strong enough this effect can overcome the effect described in the above paragraph and the convection can reverse its orientation.

We have shown via a rather simple two-dimensional description of a granular medium as an ensemble of inelastic spherical particles with shear friction that various types of convection can occur when such an ensemble is placed on a vibrating plate. First, one can have resonances coming from spatial variations in the amplitude of the vibration. Second, horizontal flows that are generated close to the bottom can collide with a fixed vertical wall acting just as an obstacle to the flow and give rise to a circular motion. Third, in the presence of shear friction with a vertical wall a downward drag force along the wall is exerted on the particles acting opposite to the circular flow. We have investigated how the strength of the convection depends on the initial conditions, the frequency and the amplitude of the vibration, the dissipation, the elastic moduli, the number and size distribution of the particles, etc., and presented quantitative predictions. Since it is not straightforward to determine the material constants corresponding to γ and γ_s, a comparison with experiments still involves two fit parameters. A more realistic model including real static and dynamic friction, rotations of particles, and eventually varying particle shapes is needed to establish a closer contact between model parameters and material constants.

It is not clear whether any of the discussed convection mechanisms are at the origin of the well-known heap instabilities with surface avalanches [4-6]. Although we have observed the appearance of weak finite slopes close to walls a larger number of particles must be simulated over longer times to be conclusive. Work in this direction is in progress. In addition, three-dimensional simulations should also be performed.

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