## Swirling granular matter: From rotation to reptation

Michael A. Scherer,<sup>1</sup> Volkhard Buchholtz,<sup>2</sup> Thorsten Pöschel,<sup>2</sup> and Ingo Rehberg<sup>1</sup>

<sup>1</sup>Institut für Experimentelle Physik, Otto-von-Guericke-Universität, Postfach 4120, D-39016 Magdeburg, Germany

<sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, Invalidenstraβe 110, D-10115 Berlin, Germany

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Experiments and numerical simulations of granular material under swirling motion of the container are presented. At low packing densities the material rotates in the same direction as the swirling motion of the container (rotation). At higher densities the cluster of granular material rotates in the opposite direction (reptation). The change of the direction of the motion of the cluster takes place at a critical packing density while the diffusion coefficient changes significantly. The measured critical density of the packing is in good agreement with results obtained by molecular-dynamics simulation. [S1063-651X(96)50611-2]

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The fascination of the flow behavior of granular material such as sand is due to the fact that under certain circumstances it behaves like a fluid: An hourglass is the most popular example. Its solid-like behavior is obvious as well: A pile of sand is stable and it can undergo plastic deformation; however, unlike a fluid, it does not flow freely under gravity. Instead there is a finite angle of repose of sandpiles. The exotic behavior of granular matter and the sometimes unexpected observations have stimulated many scientists to focus their scientific interest on sandlike materials (see, e.g., [1-4]). We describe a fairly surprising effect that demonstrates to a certain extent both the similarity and the dissimilarity between granular material and fluid. The experiment is extremely robust, easily visualizable, and can be performed even as a kitchen table experiment using a bunch of marbles and a pot. The basic idea is to move the pot in a swirling motion, the motion one frequently uses to stir up the bouquet of a glass of wine. If the pot contains only one or a few spheres, they will follow the rotation of the swirl in a fashion similar to the wine in the glass. When one successively increases the number of spheres the angular velocity of the cluster decreases with increasing packing density. At a certain critical packing density an intriguing effect appears: The angular velocity becomes negative, i.e., the cluster rotates in the opposite direction. Now the collective behavior is more reminiscent of a pancake rotated by the swirling motion of a frying pan. The first regime of motion we call "rotation," the second one "reptation." These two different regimes are also observed in vibrational mills that are used to grind feed material [5]. There the reptation mode is important to transport feed material from the bottom of the mill to the grinding zone. In this paper we present a quantitative description of this crossover effect, which is accompanied by a moleculardynamics simulation. The numerical results are qualitatively and quantitatively in good agreement with the experimental findings. This is surprising because the effect, although qualitatively robust, turns out to be quantitatively very sensitive to small changes of the parameters of the granulate. In particular, we found a strong sensitivity of the effect with respect to the condition of the surfaces of the spheres. The fairly small granular system presently seems to be the only one where each single particle of the experiment can be simulated using molecular-dynamics (MD) technique. Hence the phenomenon can serve as a benchmark for the validity of different types of numerical simulations such as MD or event driven techniques. The experiment presented here seems to be very suitable for enlightening the transition from solidlike to fluidlike behavior in granular matter.

The experimental setup is shown in Fig. 1. A Petri dish of inner diameter 9.0 cm is mounted on a table performing a circular vibration, i.e., each point of the table moves along a circular line during one oscillation period. For the experiments presented here, its frequency is chosen to be 2.5  $sec^{-1}$  and the amplitude of the swirling motion is 1.27 cm. A camera is fixed on the oscillating table; thus the analysis can be done in a comoving frame by visual inspection of the image displayed on a monitor. In between the Petri dish and the camera there is a glass plate with a marker that is fixed in the laboratory frame. Thus the position of the marker relative to the dish indicates the direction of the momentary acceleration. The Petri dish is partially filled with a monolayer of ceramic spheres (density 1.74 g/cm<sup>3</sup>) of diameter 1.223  $\pm 0.035$  cm. The number of particles ranges between 1 and 42, where 42 corresponds to the closest possible packing of spheres. We want to focus here only on the packing density dependence of the effect. The dependence on the amplitude, the frequency, the material properties, etc., is planned to be discussed in more detail in a forthcoming paper.

The system described above was simulated using molecular dynamics of spheres of mass m and radii R moving on an ideally smooth plane. We applied the soft-particle ansatz by Cundall and Strack [6] including the interaction between colliding particles in normal and tangential directions. Instead of linear damping we applied the force derived in [7]. Two



FIG. 1. Experimental setup.

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colliding particles *i* and *j* at positions  $r_i$  and  $r_j$  with angular velocities  $\Omega_i$  and  $\Omega_j$  "feel" the force

$$\vec{F}_{ij} = F_{ij}^N \vec{n} + F_{ij}^T \vec{t}, \qquad (1)$$

with

$$F_{ij}^{N} = -Y\xi_{ij}^{3/2} - \gamma_{N}\sqrt{\xi_{ij}}\dot{\xi}_{ij},$$
 (2)

$$\xi_{ij} = 2R - |\vec{r}_i - \vec{r}_j|,$$
 (3)

$$F_{ij}^{T} = \operatorname{sgn}(v_{ij}^{\operatorname{rel}}) \min\left(\frac{m}{2} \gamma_{T} |v_{ij}^{\operatorname{rel}}|, \mu| F_{ij}^{N}|\right)$$
(4)

$$v_{ij}^{\text{rel}} = (\vec{r}_i - \vec{r}_j)\vec{t} + R(\Omega_i + \Omega_j).$$
(5)

 $Y=8 \times 10^6$  g cm<sup>-0.5</sup> sec<sup>-2</sup> is the measure for the restoring force as given by the Hertzian contact model [8],  $\gamma_N = 600$ g sec<sup>-1</sup> cm<sup>-0.5</sup> and  $\gamma_T = 3000$  sec<sup>-1</sup> are the damping coefficients in normal and tangential direction, and  $\mu = 0.5$  is the Coulomb friction coefficient. The parameter Y has a usual order of magnitude for MD simulations in the spirit of the soft-particle ansatz.  $\gamma_N$  and Y have been chosen to give a reasonable coefficient of restitution, which we have experimentally determined to be of the order of 0.5 for a velocity of about 5 m/sec. The value of  $\gamma_T$  is inspired by previous work on this subject [9]. The unit vectors in normal and tangential direction are given by

$$\vec{n} = \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|},$$
 (6)

$$\vec{t} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|}.$$
(7)

Equation (5) describes the relative velocity of the surfaces of the particles at the point of contact. Equation (4) takes the Coulomb friction law into account, saying that two particles slide on top of each other if the shear force overcomes  $\mu$ times the normal force. For the integration of Newton's equations we applied a Gear predictor-corrector method of fifth order [10].

The time series of images in Fig. 2 visualize the motion of 26 spheres [11] in a counterclockwise rotating Petri dish at low packing density. They have been taken at time intervals T/5, with T being the period of the driving motion of the Petri dish. The evolution of the positions of the white spheres in Figs. 2(a)-2(f) indicates that the cluster of spheres also rotates in counterclockwise direction. Figures 2(g)-2(l) show, corresponding to Figs. 2(a)-2(f) snapshots from the molecular-dynamics simulation using the same parameters as the experiment.

When the number of spheres is increased the rotation becomes slower. At a fairly well-defined packing density it stops rotating. Increasing the packing density leads to a different kind of motion, which is displayed in Fig. 3 for the case of 37 spheres. Now the cluster rotates in the opposite direction. This motion is better described by the term reptation. Animated sequences of the motion are available [12].



FIG. 2. Temporal behavior of a system of 26 spheres during one counterclockwise cycle of the swirl. The arrow shows the direction of the momentary acceleration. The lower six figures show the corresponding molecular dynamics simulation.

The experimental snapshots show a white arrow that indicates the direction of the momentary inertial force. It is obtained by drawing a vector from the small white cross through the center of the Petri dish. The small white cross is



FIG. 3. Temporal behavior of a system of 37 spheres. Top, the experiment; bottom, molecular-dynamics simulation.



FIG. 4. Angular velocity of the cluster of particles (top). The solid circles show the experimental data, while the crosses show the results of a molecular-dynamics simulation. For  $N_c = 32$  we observe the reversal of the direction of the rotation. The particle numbers according to Figs. 2 and 3 have been marked by *L* and *H*, respectively. The lower part of the figure shows the diffusion coefficient *D* derived from the simulation due to Eq. (11). For *N* approaching  $N_c$  the diffusion coefficient changes significantly.

the marker on the glass plate that is fixed in the laboratory frame as mentioned above; hence it rotates in the comoving frame. This procedure shows that the phase shift between the crescent-shaped area and the inertial force is different in the rotation and the reptation mode.

The most striking feature of the motion of the cluster is the dependence of the direction and the absolute value of its angular velocity on the particle number, i.e., the packing density as presented in the upper part of Fig. 4. To obtain the experimental data indicated by the solid circles, the time for a single particle located near the wall for one complete path around the container is measured. The inverse of this time is shown for different numbers of spheres. The effect of the change of the sign of the rotation is thus clearly demonstrated. This method of measurement is not sufficiently well defined for a small number of particles. A particle located at the edge of the cluster does not remain there, but has a tendency to migrate inward, which makes the characterization of the cluster movement by tracing an individual particle meaningless. Therefore, in the case of low particle numbers N < 23 the experimental method breaks down.

In order to avoid those difficulties in the simulation we used a slightly different measurement method for the rotation velocity drawn in Fig. 4 (crosses). The motion of the center of mass is extracted from the numerical data

$$f = \left(\frac{1}{N}\sum_{i=1}^{N} \frac{\vec{r}_{i}^{*} \times \vec{v}_{i}^{*}}{|\vec{r}_{i}^{*}|^{2}}\right)_{t},$$
(8)

where  $\langle \rangle_t$  denotes the time average.  $\vec{r_i^*}$  and  $\vec{v_i^*}$  are the relative position and velocity of the *i*th particle with respect to the position and velocity of the center of mass:

$$\vec{r}_i^* = \vec{r}_i - \frac{1}{N} \sum_{j=1}^N \vec{r}_j,$$
 (9)

$$\vec{v}_i^* = \vec{v}_i - \frac{1}{N} \sum_{j=1}^N \vec{v}_j.$$
 (10)

The experiment and the simulation agree quantitatively, showing that the rotation velocity decreases with particle number. For a critical number of particles  $N_c = 32$  we observe the reversal of the direction of the rotation. To obtain the experimental equivalent of Eq. (8) requires computer aided image analysis, which is currently under development. While in the experiment the rotation velocity is measured from the velocity of particles close to the wall of the Petri dish only, in the simulation the velocity is calculated due to Eq. (8) taking into account data of *all* particles. Hence the particles close to the center of mass having lower rotation velocity lead to lower values of *f* for the results of the simulation (see Fig. 4). One can get a visual impression of the described behavior in [12].

The change of the sense of rotation might be caused by the change of the dynamical structure of the cluster, which depends on the packing density. For high densities one finds that the cluster rolls like a rigid body along the inner wall of the Petri dish, i.e., the neighborhood relations of the particles do not change significantly in time. At lower packing density the bulk of particles behaves more fluidlike, i.e., the relative positions of the particles change quickly in time. A quantitative measure of this effect is given by the diffusion coefficient D shown in the lower part of Fig. 4:

$$D = \frac{1}{\pi} \left\langle \frac{d}{dt} \left( \sum_{i=1}^{N} \sum_{j \in U(i) \neq i} (\vec{r}_i - \vec{r}_j)^2 \right) \right\rangle_t.$$
(11)

Here U denotes the surrounding of the *i*th particle defined by

$$j \in U(i)$$
 if  $|\vec{r_i} - \vec{r_j}| \leq R_U$ . (12)

In our simulation we used  $R_U = 3$  cm. As indicated by Fig. 4, the diffusion coefficient changes significantly for N approaching  $N_c$ .

The agreement between the experimental results and numerical calculation is remarkable when considering the fact that the theory applies idealized boundary conditions and particle interactions. From a technical point of view, it is an important advantage that this experiment can obviously serve as a test for the quality of theoretical models describing the behavior of granular matter, which is a field where robust and reproducible experimental effects are not easily obtained.

While our idealized numerical simulation has at least demonstrated that the observed reversal phenomenon is a robust one, we cannot claim at this point to have understood its physical mechanism. We believe that both theoretical models and experimental variations of the geometry might help to catch the physical essence of the effect. Moreover, we believe that the crossover of the diffusion coefficient is connected with the Reynolds dilatancy, an observation that deserves further investigation. Thus an experimental attempt to check the predictions for the diffusion coefficient is currently under development. In some of the currently ongoing variations of the experiment, it occurred to us that the relationship between the packing density and the frequency has a fine structure, which might be caused by an interplay between the Reynolds dilatancy and finite-size effects. Another interesting feature is the dependence of the rotation on the frequency and amplitude of the swirling motion. Preliminary measurements show sharp crossovers between different particle trajectories when varying the frequency. Finally, it seems that rings of different rotation of the granulate are possible in large containers, an observation that might be

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interesting in connection with the grinding efficiency of vibrational mills.

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- [11] The black and white spheres have been checked to have identical mechanical properties. In test series we did not find effects such as segregation that might originate from different bulk or surface properties.
- [12] The animated sequences mentioned in this paper can be found via World Wide Web under URL http://summa.physik.huberlin.de/~volkhard/swirl.html. The following six "movies" from the simulation can be accessed: (a) 26 particles recorded by a resting camera, (b) a camera moving with the dish, (c) a camera moving with the center of mass of the particles, and (e)–(g) the same for 37 particles.