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Bistability in simulated granular flow along corrugated walls

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We investigate binary impacts of solid grains obeying a force scheme often used in the molecular dynamics simulation of rapidly flowing granular media. A thorough analysis of the force equations shows that the deceleration of a free grain upon grazing impact on an array of "wall grains" depends dramatically on the initial velocity relative to the wall so that in certain situations a bistability in the granular flow appears. We explain why this is an artifact of the modelization inherent in the force scheme and we illustrate our findings with some sample simulations.

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The flow of granular materials presents a scientific problem of considerable technological importance. Due to complicated interactions and strong fluctuations, no generally accepted theory of granular flow exists so far. Precision experiments are difficult because granular media are not a very well-defined material and the influence of the interstitial medium and of triboelectrification is not easy to control. Therefore, in recent years the simulation of granular flows has become a widely used research tool. Molecular dynamics methods [1] with dissipative two-particle forces ("granular dynamics") [2] have especially been used extensively [3].

Granular dynamics studies rely on suitable assumptions for the forces. It is crucial to understand the limits of their validity in order to avoid misinterpretation of simulation results. In the following we show that a popular implementation scheme using soft particles and corrugated walls gives rise to a phenomenon not recognized so far: Depending on the initial conditions two stationary states with different flow velocities may appear (bistability). This effect is unlikely to occur in reality. However, due to modelization, it is quite naturally encountered in granular dynamics simulations.

For the sake of simplicity and clearness we refer to one specific two-particle force law in two dimensions which serves as a prototype for other similar ones and contains the basic granular interaction properties (inelasticity and friction). The particles are "soft," meaning that they can penetrate into each other. Their overlap is interpreted as a measure of the elastic deformation of the colliding grains. Real deformations are much more complicated [4]: For instance, a head-on collision and a grazing one both with the same overlap in simulation would produce completely different elastic restoring forces in reality. The corrugated walls are made of grains with the same properties as the free grains, but with infinite mass. Particle rotation is not taken into account.

Consider a collision of two grains (Fig. 1). We separate the relative velocity and the interparticle force into normal and shear components using the unit vectors $\vec{n}$ and $\vec{s}$ as defined in Fig. 1: $\vec{v}_{\rm rel} = v_N\vec{n} + v_S\vec{s}$ and $\vec{F}_{12} = F_N\vec{n} + F_S\vec{s}$. If the two particles overlap ($\xi \equiv r_1 + r_2 - |\vec{x}_2 - \vec{x}_1| > 0$), there is a repulsive normal force which we assume to be proportional to ξ. In order to make head-on collisions dissipative, a damping term linear to the normal velocity $v_N \equiv \dot{\xi}$ is added, such that for grain 1

$$F_N = -k_N\xi - \gamma_N m_{\rm red}\dot{\xi} \ . \tag{1}$$

The presence of the reduced mass $m_{\rm red} = m_1m_2/(m_1 + m_2)$ in the damping term has the effect that collisions with wall grains (infinite mass) are more dissipative than those with another free grain. The shear force F_S is related to the normal force by the Coulomb law of friction

$$F_S = -|\mu F_N|{\rm sgn}(v_S) \ , \tag{2}$$

where μ is the Coulomb coefficient of dynamic friction.

Other approaches to the normal force are of the general form

$$F_N = k_N\xi^\alpha - \gamma_N\xi^\beta\dot{\xi}^\gamma, \tag{3}$$

where the exponents α, β, and γ depend on the physical model motivating the force. For instance, integrating Hooke's law plus a viscous damping term over the contact area of two inelastic spheres leads to the Hertz-

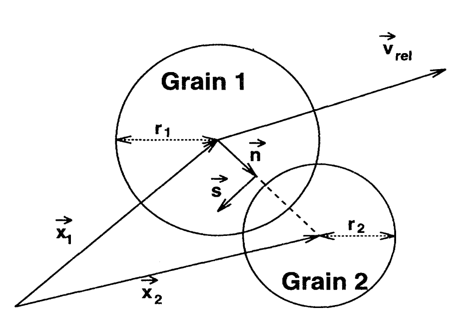

FIG. 1. Definition of quantities describing binary impact.

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Kuwabara-Kono force $\alpha = 3/2, \beta = 1/2, \gamma = 1$ [5]. We used this force to check the generality of our results obtained with (1).

The advantage of the simple damped harmonic oscillator force (1) is that its analytic solution with initial overlap $\xi(0) = 0$ and initial relative normal velocity $v_N^i = \dot{\xi}(0)$ allows the calculation of useful quantities like the collision time

$$t_{\rm col} = \pi \left(\frac{k_N}{m_{\rm red}} - \frac{\gamma_N^2}{4} \right)^{-1/2} , \tag{4}$$

the coefficient of normal restitution (ratio between final and initial normal velocity) $e_N \equiv v_N^f / v_N^i = \exp(-\gamma_N t_{\rm col}/2)$, and the maximum overlap during collision $\xi_{\max} \le v_N^i t_{\rm col}/\pi$, where the equality holds for elastic grains ($\gamma_N = 0$).

An accurate simulation reproducing the analytic results of a collision with relative errors of the order 10^{-4} requires a time step

$$\Delta t \approx t_{\rm col}/50. \tag{5}$$

According to (4) the time step Δt scales essentially with $1/\sqrt{k_N}$. Therefore in most simulations k_N is chosen as small as possible, but sufficiently large to satisfy the condition that $\xi_{\max}$ remains much smaller than the grain diameter for the impact velocities to be expected during the simulation. However, it should always be checked that the simulation results do not depend sensitively on k_N. Luding *et al.* [6] pointed out that for dense granular packings small values of k_N lead to qualitatively different behavior than realistically large ones: $t_{\rm col}$ becomes so large that a column of N beads falling onto a rigid plate behaves like an array of $N-1$ coupled damped oscillators rather than N distinct grains undergoing successive collisions.

Here we consider less dense, flowing granular materials. The phenomenon is also an effect of high collision times due to low force constants, but related to high shear velocities v_S at the corrugated boundary of a granular flow. For illustration, we take a vertical pipe. Gravitation accelerates all particles downwards in the y direction. Braking only occurs at the walls and is essential for reaching a steady state. The braking efficiency can be quantified by the change of the y component of the velocity, Δv_y, upon a particle-wall collision. This is the key quantity for understanding the effect we want to describe.

First consider the impact of a grain on one single wall grain as sketched in Fig. 2. If we suppose the impact to be grazing and v_y^i much larger than v_x^i, then F_S is mainly responsible for braking in y direction and we may write

$$\Delta v_y \propto \int_{t_{\rm cont}} F_S(t)\, dt \ , \tag{6}$$

where $t_{\rm cont}$ is the total time of shearing contact. When the initial velocity v_y^i is low, $t_{\rm cont}$ is determined by the normal contact time $t_{\rm col}$ as defined by (4). Inserting (2) then yields

$$\Delta v_y \propto \int_{t_{\rm col}} \ddot{\xi}\, dt. \tag{7}$$

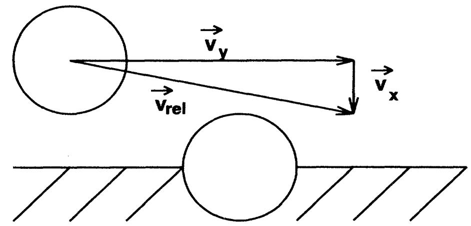

FIG. 2. Impact of a free grain with a grain imbedded in a wall.

In the limit $\gamma_N = 0$, the integral is equal to $-2v_N^i$ and v_N^i is proportional to v_y^i, so that we have $\Delta v_y \propto v_y^i$ for low v_y^i. However, for higher v_y^i, the time needed for the two grains to traverse each other in absence of the normal force, $t_{\rm trav} \propto 1/v_y^i$, becomes shorter and shorter, so that eventually the contact time $t_{\rm cont}$ is determined by $t_{\rm trav}$ instead of $t_{\rm col}$. Thus rewriting (6) as $\Delta v_y \propto t_{\rm trav}\bar{F}_S$, where $\bar{F}_S$ is some mean over F_S during the contact, we obtain $\Delta v_y \propto 1/v_y^i$ in the regime of high v_y^i. The transition between the two regimes is determined by the condition $t_{\rm trav} = t_{\rm col}$, so that we have a critical velocity

$$v_{\rm crit} \propto t_{\rm col}^{-1} \propto k_N^{1/2}. \tag{8}$$

In summary, we find that Δv_y is proportional to v_y^i up to some critical v_y^i which is proportional to $\sqrt{k_N}$ and then decreases like $1/v_y^i$, i.e., the braking efficiency goes down. By analogous reasoning, the same holds true for the velocity change in the x direction, Δv_x. We address the linear increase as the normal regime, and the $1/v_y^i$ decrease as the regime of *soft-sphere brake failure.*

To illustrate, we simulated the impact situation sketched in Fig. 2. Here, we used a free grain of diameter 1 mm and mass 1 mg and a wall grain of diameter 0.66 mm. The parameter values were $k_N = 2000$ N/m, $\gamma_N = 10000\ {\rm s}^{-1}$ ($\Rightarrow e_N = 0.70$), $\mu = 0.5$, and the collision time was $t_{\rm col} = 7.07 \times 10^{-5}$ s. The initial position of the free grain's center was 0.82 mm above the wall line, and v_x^i was set to zero, so that the free grain flew on a line parallel to the wall and the maximum linear overlap ξ of the two grains was 0.01 mm by initial condition. We measured Δv_y and Δv_x as a function of v_y^i. Figure 3 shows the results. Both Δv_y and Δv_x start off linearly, then the slope decreases, the curves go through a maxi-

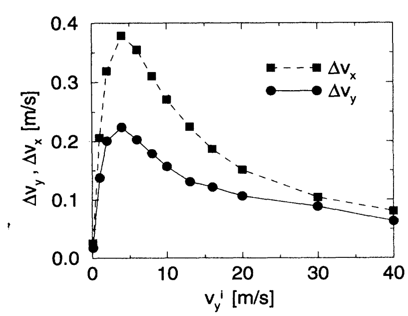

FIG. 3. Δv_y and Δv_x as a function of v_y^i with parameters as given in the text.

mum and bend back to the abscissa in a $1/v_y^i$ fashion. In Fig. 3, we only show the curves for one specific k_N value, but due to the scaling properties of $\Delta v_y(v_y^i)$ discussed above, they also represent the results for $k_N' = \beta k_N$ by scaling both axes with $\sqrt{\beta}$. Note that what is shown in Fig. 3 is not a time step dependent property. One can do the same simulation with identical parameters, but with a time step smaller by a factor 100, and get the same results. Nor is it peculiar to the normal force (1) used here; the general argument (7) only refers to the friction force (2). Moreover, test simulations with other normal forces (Hertz-Kuwabara-Kono) lead to results similar to those of Fig. 3.

So far we have only discussed the interaction of a free grain with one wall grain. Now we replace the single wall grain of Fig. 2 with an array of wall beads along the y axis. As could be seen in Fig. 3, v_x^f tends to zero in the brake failure regime. Figure 3 was obtained with $v_x^i = 0$; if we let $v_x^i > 0$, and have a v_y^i far in the brake failure regime, it may happen that the free grain is not reflected by the wall grain but just wanders through it. If there is an array of wall grains, the free grain enters the next wall grain, and possibly further wall grains until in the end it *is* reflected. But then again, on its way through the wall it was in shearing contact with several grains instead of just one; and the deeper it penetrates into the wall, the less grazing, the more head on, and therefore the more dissipative the contacts become. Thus we expect that with wall arrays $\Delta v_y(v_y^i)$ must ultimately increase again, constituting what might be called an *emergency brake.*

This was checked in a simulation where free grains were shot on an array of wall grains (setup similar to Fig. 2). We varied v_y^i and v_x^i. If we imagine the array to be the wall of a tube, we can associate v_y^i with the mean axial particle velocity and v_x^i roughly with the standard deviation of the mean particle velocity in x direction, σ_{v_x}, which in turn is the square root of the granular temperature in that direction. Experience shows that the axial velocity is much higher than the mean "radial" velocity's standard deviation, so that the range of v_x^i is chosen from 0.1 to 0.5 m/s and the range of v_y^i is from 0.1 to 40 m/s. Because the result of a test impact with fixed v_x^i and v_y^i depends strongly on the initial position (which determines the contact point), we varied the initial position of the free grain over 10 points distributed equidistantly over a length equal to the "wavelength" of the wall, along a line parallel to the wall array. Then Δv_y is given by the mean over the 10 different initial positions.

Figure 4 shows Δv_y as a function of v_y^i with the same parameters as before, and Fig. 5 shows the mean number of contacts as a function of v_y^i. The onset of the multiple contact regime (number of contacts ≥ 2) is observed at a velocity of about 10 m/s, which coincides well with the velocity at which Δv_y begins to increase again. As in the case of only one wall grain, increasing k_N shifts v_{crit} towards higher v_y^i, so that the maximum in the $\Delta v_y(v_y^i)$ diagram gets higher and shifts right.

Characteristics of $\Delta v_y(v_y^i)$ like the one shown in Fig. 4 can lead to bistable behavior in a granular dynamics simulation. Consider again a vertical pipe. The velocity loss Δv_y at the walls constitutes essentially the only mechanism for braking the center-of-mass motion. In a steady state, the overall deceleration due to braking balances the acceleration g to gravitation. This condition may be written as

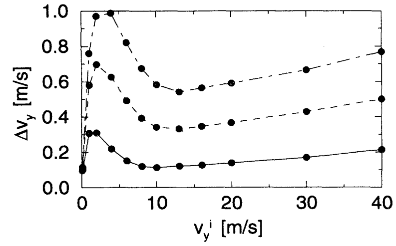

FIG. 4. Δv_y as a function of v_y^i with v_x^i as parameter; $v_x^i = 0.1$ m/s (solid line), 0.3 m/s (dashed line), 0.5 m/s (dot-dashed line).

$$g = \dot{n}\Delta v_y \ , \tag{9}$$

where $\dot{n}$ is the fraction of all particles colliding with the wall per unit time. Now we argue that the right hand side of (9) is a monotoneously increasing function of Δv_y: $\dot{n}$ is roughly proportional to σ_{v_x} and the volume fraction of grains, both taken near the wall. The latter is essentially a constant for fixed global volume fraction. Velocity fluctuations are roughly proportional to Δv_y. This is obvious for σ_{v_y}, but should also be true for σ_{v_x} because of "thermalization" inside the granular system. These crude estimates suggest that $\dot{n}\Delta v_y$ increases quadratically with Δv_y. Hence (9) implies that a unique value of Δv_y is required for a steady state.

The steady-state condition (9) can thus be visualized by drawing a horizontal line in the $\Delta v_y(v_y^i)$ diagram. Its intersections with the v_x^i curves give potential steady states. Positive slope of $\Delta v_y(v_y^i)$ at the intersection means that the steady state is stable; if by some fluctuation the mean velocity gets higher, the velocity loss Δv_y also increases so that the system decelerates again. Negative slope of $\Delta v_y(v_y^i)$ characterizes an unstable steady state. If a system has two stable steady states (bistability), it depends on the initial conditions which of them is reached.

However, stability alone does not determine which of the steady states is selected. In Fig. 4 there is a continuum of curves $\Delta v_y(v_y^i)$ distinguished by different v_x^i. As mentioned before, v_x^i can be associated with the velocity

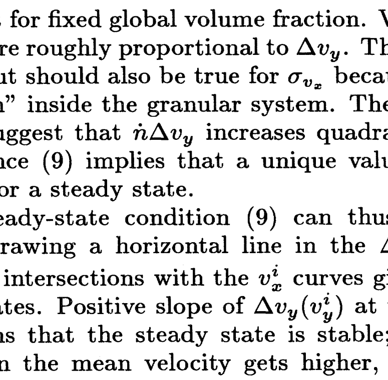

FIG. 5. Number of contacts during impact as a function of v_y^i with v_x^i as parameter; $v_x^i = 0.1$ m/s (solid line), 0.3 m/s (dashed line), 0.5 m/s (dot-dashed line).

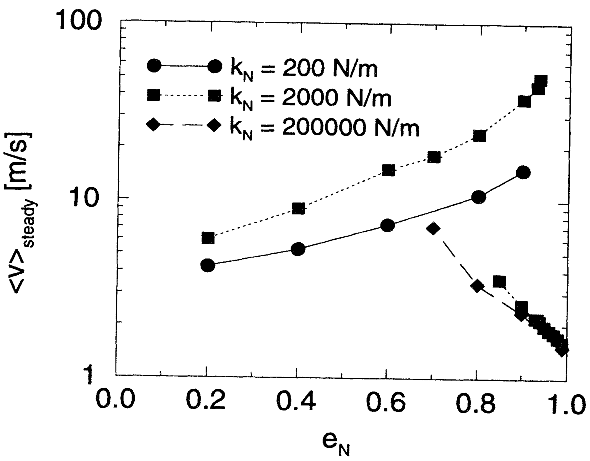

FIG. 6. Steady-state mean velocity in a vertical tube as a function of the coefficient of restitution e_N.

fluctuation σ_{v_x} or with the square root of the granular temperature. In the steady state it should be related to Δv_y, however the precise relationship is not known. Our simulations indicate that it is nearly the same in both steady states, if there is a bistable situation.

As an example, we present simulation data obtained in a two-dimensional (2D) vertical pipe of width 2 cm, filled with slightly polydisperse grains of mean diameter 1 mm which fall down due to gravitation ($g = 10$ m/s^2). The walls were made up of grains of diameter 0.66 mm, the 2D volume fraction of the beads was 0.55, and the Coulomb coefficient was $\mu = 0.5$. We recorded the steady-state mean velocity of the grains as a function of their coefficient of restitution e_N for different values of k_N (Fig. 6).

We first discuss the case $k_N = 2000$ N/m. Starting the simulation with low initial mean velocities, we get a branch of slow steady states on the elastic side of the diagram (e_N near 1); this branch gets unstable at $e_N \approx 0.85$. On the other hand, starting the simulation with high initial mean velocities $\approx$ 5–10 m/s yields a branch of fast steady states which extends over the whole width of the diagram. For $e_N > 0.85$, both branches coexist, and we have bistability. A detailed analysis which we do not give here shows that the slow branch follows the normal steady states, whereas the fast branch belongs to steady states produced by the soft-sphere emergency brake.

If k_N is given a lower value ($k_N = 200$ N/m), the normal branch still exists for nearly elastic grains, but it is so short that we do not plot it here. The soft-sphere branch shifts to lower velocities because the emergency brake begins to function at lower v_y^i for softer grains.

For a larger $k_N = 200\,000$ N/m, the normal branch extends farther into the region of inelastic grains, but still becomes unstable at $e_N \approx 0.7$. The emergency-brake branch lies at much higher velocities and is not plotted. Note that with $k_N = 200\,000$ N/m, the collision time $t_{\text{col}} = 7.07 \times 10^{-6}$ s is of the same order of magnitude as realistic contact times [4], so that it does not make sense to increase k_N very much above this value; furthermore, the simulations become very time consuming.

In summary, we have discussed the "brake failure" effect due to the usage of soft spheres and the Coulomb law of friction in combination with a corrugated wall. In addition to the normal steady state, it introduces an "emergency-brake" steady state into the granular dynamics simulation of rapid granular flow bounded by arrays of wall grains. If the flow velocity in a granular flow along corrugated walls becomes higher than $v_{\text{crit}} \propto \sqrt{k_N}$, the system will accelerate to the (unphysical) emergency-brake steady state. The microscopic reason for this is that the force equations allow two grains to traverse each other almost without losing relative velocity, if the collision is grazing and the initial relative velocity is large compared to v_{crit}. With real grains, this is not possible due to unsymmetric deformation during contact.

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