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Dynamic equilibrium in granular flow obtained by a nonlinear dynamic equation

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We derive a nonlinear diffusion equation for a void density in the diffusing-void model of granular assembly [Phys. Rev. Lett. **67**, 828 (1991)] and present numerical solutions when the assembly is in dynamic equilibrium. We find that the solutions exhibit unique features of the real granular flow patterns in a confined geometry with and without obstacles; notable examples are the V-shaped kink at the free surface, stagnant solids near the wall, and the shock front below the obstacle accompanied by the empty region.

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In a recent paper [1], a discrete-random-walk model termed the diffusing-void model [2] was proposed to study the unusual properties of granular flows. The model is based on the assumption that the flow of granular particles in a confined geometry is caused by the upward motion of voids that result from the escape of granular particles through an orifice. The model is *linear* because the walker performs biased random walk. It is, however, *nonlinear* at or near the boundaries because the walker proceeds only when there are available sites. For example, the cascading process at the free surface, where the walker simply rolls up, is *not* a diffusion process but a distinctively nonlinear process. In addition, when the walker hits an obstacle, it stops there, which is again a nonlinear process. In the discrete random-walk model [1], these nonlinear processes can be easily incorporated by imposing a simple rule derived from observing the motion of grains: the walker performs a biased random walk only through available nearest-neighbor sites.

In order to study the dynamics of granular flows, however, we recognize that it is essential to find a dynamic equation that can deal with the nonlinear processes mentioned above and correctly describe at least the most simple flow patterns of the granular particles. The purpose of this paper is to present such a dynamic equation and study its behavior. This is an extension of our recent efforts along this direction [3], where an attempt has been made to derive a dynamic equation of motion for the grains by considering the continuity equation and the microscopic force balance equation of the coarse-grained granular materials. A similar attempt has been made to derive a dynamic equation of motion for the sandpiles in the hydrodynamic limit based on pure symmetry arguments [4], and the equation derived in Refs. [3] and [4] happens to be identical except for the derivative term along the vertical axis. The equation to be derived in this paper contains a step function. When this step function is approximated by a *linear* function, the equation is similar to those in [3] and [4], *except for* a higher-order diffusion term along the x axis, which is irrelevant in RG calculation, but appears to be important in real simulation: it extends the region of kink at the free surface substantially. Thus the most simple form of our dynamic equation reduces to those discussed in [3] and [4]. It appears that the underlying physics of granular flows should be simple, at least in the simple granular flow problems considered in this paper, and it is our belief that the simple rule proposed in [1] and summarized above would be sufficient in describing the flow patterns. Mathematically identical formulation of this rule might be to replace the drift velocity by a step function. Complexity and nonlinearity seem to enter in when we try to approximate this step function by a smooth function.

In this paper, our attention is focused on the most simple granular flow patterns, namely the flow of granular particles in a rectangular box through a hole at the bottom (orifice) [Fig. 1(a)]. Experiment indicates that the free surface soon develops a V-shaped kink with a tip angle given by the angle of repose, after which the free surface retains its shape. The diffusing void that enters at the bottom then cascades upward upon reaching the free surface and stays permanently where it has stopped, either at the corners or at the free surface [Fig. 1(b)]. The equation of motion for the diffusing void *inside* the box, when it is free from boundary effects, is simply the biased diffusion equation [1,2]

$$\partial_t \Psi = -\nabla \cdot \mathbf{J} = D_x \partial_x^2 \Psi - v \partial_y \Psi \ , \quad (1)$$

where $\Psi(x,y,t)$ is the density of the hole, D_x is the diffusion constant along the x axis, and v is the drift velocity along the y axis due to the gravity. The current density $\mathbf{J}$, corresponding to Eq. (1) is

$$\mathbf{J} = -D \partial_x \Psi \hat{\mathbf{x}} + v \Psi \hat{\mathbf{y}} \ . \quad (2)$$

Note that this equation is good only when the walker is away from boundaries such as the free surface and the obstacle. We now have to add nonlinear terms to adequately take into account the motion of the particle at the boundaries, notably at the free surface and at or near an obstacle (at the vertical wall, we impose the reflecting boundary conditions). To this end we now make the following three observations.

First, the void must stop moving vertically when the void reaches the free surface where the void density is 1 (complete void). We model this by assuming that the void velocity goes to zero when the void density is 1. The ideal case would be to take v as a step function, which requires infinitely many terms to represent. For simplicity, however, we take a linear function $v(\Psi)=v_0(1-\Psi)$, for which case the current density due to *drift*, J_d, becomes

$$\mathbf{J}_d=v_0(1-\Psi)\Psi\hat{\mathbf{y}}\ , \tag{3}$$

with v_0 constant.

Second, by the same argument, the diffusion along the x axis must vanish when $\Psi=1$. Thus we take

$$\mathbf{J}_x=-D_x(1-\Psi)\partial_x\Psi\hat{\mathbf{x}}\ . \tag{4}$$

Finally, in the diffusing-void model the void executes a *biased* random walk. But when we take into account the microscopic force balance equation along with the continuity equation and then go to *the hydrodynamic limit*, the gradient term along the vertical axis must appear [3], adding a new *diffusion* term to the vertical current density. Thus, we find that the total current

$$\mathbf{J}_y=-D_y\partial_y\Psi\hat{\mathbf{y}}+\mathbf{J}_d\ . \tag{5}$$

By imposing the continuity equation $\partial_t\Psi+\nabla\cdot\mathbf{J}=0$, we then arrive at the nonlinear dynamic equaton for the void density Ψ:

$$\partial_t\Psi=D_x[\partial_x^2\Psi-\partial_x^2(\Psi^2/2)]+D_y\partial_y^2\Psi-v_0(\partial_y\Psi-\partial_y\Psi^2), \tag{6}$$

which is a special form of the generalized diffusion equation [3,4]

$$\partial_t\Psi=D_\perp\nabla_\perp^2(\Psi+a_1\Psi^2+\cdots)+D_\parallel\partial_\parallel^2\Psi$$
$$+\lambda_0\partial_y\Psi+\lambda_1\partial_y\Psi^2+\cdots\ . \tag{7}$$

The most significant term in (6) is the last term, which is responsible for the most unique features of granular flows, such as the development of a kink at the free surface, the formation of dead zones, the appearance of a shock front, and the occurrence of an empty region below the obstacle. Note that this nonlinear term results from approximating the step function by a linear function [5]. Now, without the diffusion term along the y axis, the density quickly builds up at the top, eventually winning over the diffusion along the x axis, no matter how big it is. Thus, the diffusion along the y axis is necessary to counterbalance the drift term. The second nonlinear term in Eq. (6) is irrelevant in RG calculation [3,4] and thus it might not be really necessary. Its presence, how-

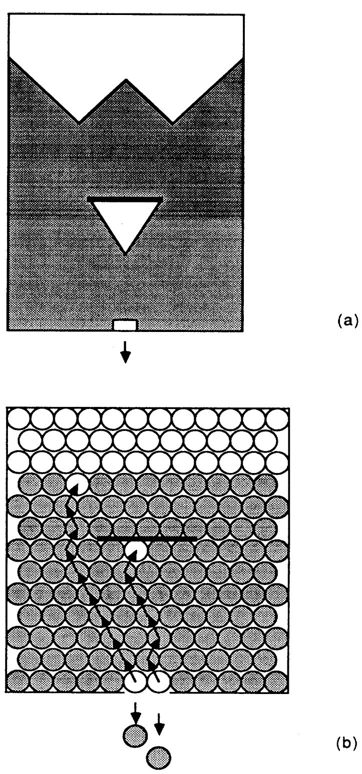


FIG. 1. (a) The most simple granular flow patterns. Granular particles are confined in a two-dimensional box that has a hole at the bottom. The free surface soon reaches the V shape with a tip angle given by the angle of repose. (b) Upon discharging a particle through a hole (or an orifice), a void is created that performs a biased walk upward. The void moves only when there are available nearest sites; otherwise it stops and stays there permanently.

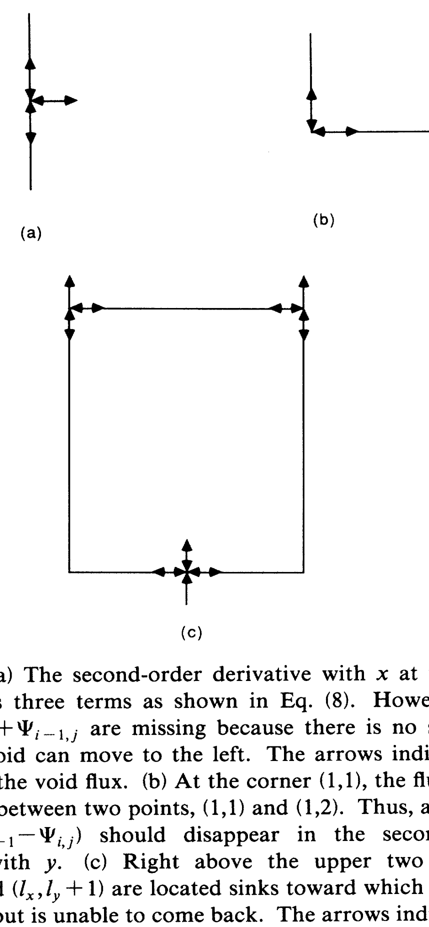
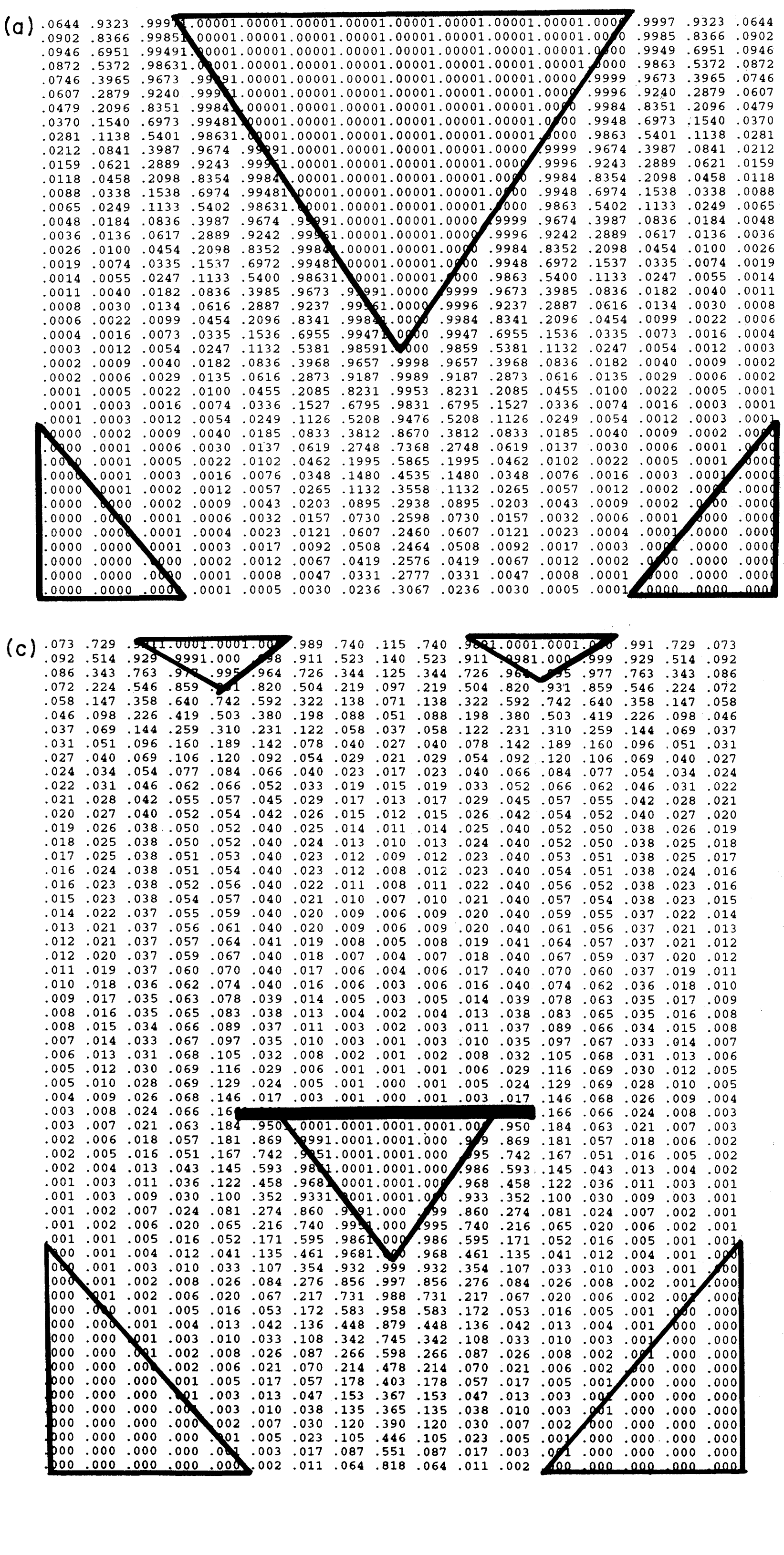


FIG. 2. (a) The second-order derivative with x at the wall (i,j) contains three terms as shown in Eq. (8). However, the terms $-\Psi_{ij}+\Psi_{i-1,j}$ are missing because there is no site into which the void can move to the left. The arrows indicate the direction of the void flux. (b) At the corner (1,1), the flux along the y axis is between two points, (1,1) and (1,2). Thus, again the terms $(\Psi_{i,j-1}-\Psi_{i,j})$ should disappear in the second-order derivative with y. (c) Right above the upper two corners $(1,l_y+1)$ and (l_x,l_y+1) are located sinks toward which the void diffuses out but is unable to come back. The arrows indicate the direction of the void flux by which we find Eq. (11). Right below the orifice, we place a source term that constantly generates voids. When the rate of void generation equals the rate of death at the upper two corners, we reach the dynamic equilibrium.

ever, is certainly important at least in our numerical solutions. Without it, the kink region in Fig. 3(a) shrinks substantially. We have not yet carried out large-scale simulations to sort out its relevance numerically.

We now solve Eq. (6) numerically and obtain the steady-state density profile as well as the current density profile that is equivalent to the stream function.

We show a form similar to the *master equation* on a discrete lattice. The discrete equivalent master equation for (6) in a two-dimensional grid point (i,j) is



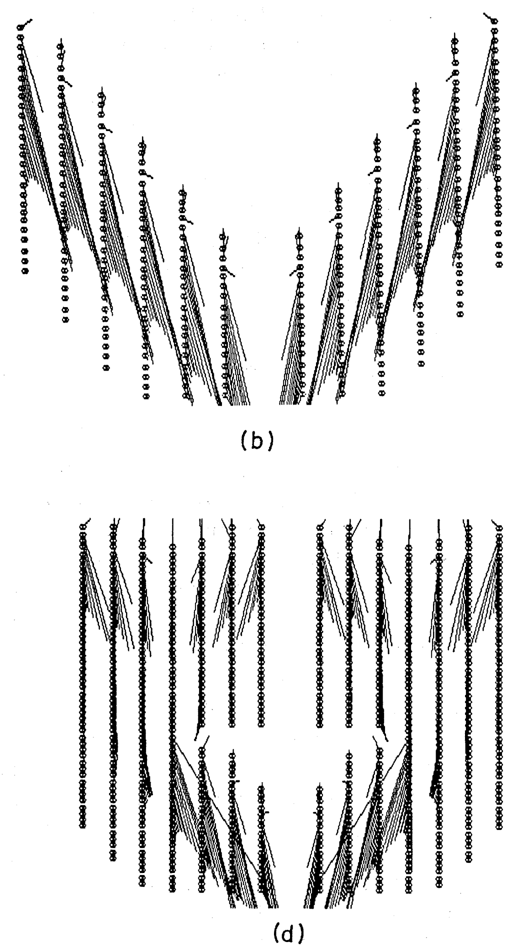


FIG. 3. (a) Steady-state current density profile Ψ after the system has reached the dynamic equilibrium. The profile is generated by numerically solving the nonlinear equation (7) iteratively. In this run, $D_1=0.1$, $D_2=1.0$, $v_0=1.0$, $l_x=13$, and $l_y=41$. Note the V-shaped region with $\Psi=1$ near the top and the triangular region with $\Psi=0$ near the wall. The regions with $\Psi=0$ are termed "stagnant solids." In real granular flows the angle of the triangular region is given by the "angle of repose." (b) Stream lines obtained by (4) and (5). The length of the tail at a given point is proportional to the magnitude of (c). Steady-state current density profile in the presence of an obstacle and stream lines (d). A one-dimensional obstacle is placed symmetrically in the middle of the box. In this run, $v_0=1.0$, $D_1=0.1$, $D_2=1.0$, $v_0=1.0$, $l_x=19$, and $l_y=61$. Note the appearance of stagnant solids near the wall, the shock front, and the empty region below the obstacle.

$$\partial_t \Psi_{ij}(t) = D_1(\Psi_{i+1,j} - 2\Psi_{ij} + \Psi_{i-1,j}) - D_1'(\Psi_{i+1,j}^2 - 2\Psi_{ij}^2 + \Psi_{i-1,j}^2)/2 + D_2(\Psi_{i,j+1} - 2\Psi_{ij} + \Psi_{i,j-1}) - \lambda(\Psi_{ij} - \Psi_{i,j-1} - \Psi_{i,j}^2 + \Psi_{i,j-1}^2) , \quad (8)$$

with $D_1 = D_x/\Delta x^2$, $D_1' = D_1/2$, $D_2 = D_y/\Delta y^2$, $\lambda = v_0/\Delta y$. The two-dimensional box has a width l_x and height l_y. One of the reasons in using the master equation is to deal with the boundaries. For example, each term in the master equation has a physical meaning. Consider the second term in the right-hand side of Eq. (8), where flux comes in to (i,j) from $(i+1,j)$ and $(i-1,j)$ and goes out from (i,j) into $(i+1,j)$ and $(i-1,j)$. Consider now points at the left wall for $2 \le j \le l_y - 1$, in which case particles can come and go only between (i,j) and $(i+1,j)$. Thus, the first term on the right-hand side of the above equation becomes [Fig. 2(a)]

$$D_1(\Psi_{i+1,j}(t) - \Psi_{ij}(t)) , \quad (9)$$

while at (1,1) the third term also should be modified [Fig. 2(b)] as

$$D_2(\Psi_{i,j+1}(t) - \Psi_{ij}(t)) . \quad (10)$$

At other boundary points, one can easily modify Eq. (7).

We now simulate the *dynamical steady state* by introducing a source term with a constant source density, say, α just below the orifice and two sinks at $(1, l_y+1)$ and (l_x, l_y+1) [Fig. 2(c)]. At the corner $(1, l_y)$, the first term of Eq. (8) has the same form as in Eq. (9), but the third term now modifies to [Fig. 3(d)]

$$D_2(\Psi_{i,j-1}(t) - 2\Psi_{ij}(t)) . \quad (11)$$

We now present numerical solutions of Eq. (8). In Fig. 3(a) is shown the steady-state density profile Ψ with $D_1 = 0.1$, $D_2 = 1.2$, and $v = 1$. The numbers represent hole densities Ψ at each point. Note the appearance of a V-shaped region with $\Psi = 1$, which is precisely the kink region shown in Fig. 1. When we increase D_1, the V-shaped region shrinks and eventually disappears because voids diffuse out too fast along the x axis. Also, near the wall, there are regions where the hole densities $\Psi = 0$, indicating that holes are unable to penetrate. This is a region termed "stagnant solids." The boundary lines that divide this region from the bulk define the so-called "angle of response." In Fig. 3(b) is shown the streamlines obtained by (4) and (5). Most flow occurs near the center and near the free surface.

With an obstacle in the middle of the box, the steady-state density profile is shown in Fig. 3(c) and its current density in Fig. 3(d). Flow patterns near the top and near the walls are similar to those seen in Fig. 3(a). There are, however, some differences. First, the vertical current density J_y right below the empty region near the top is negative: the hole is pushed from above. This is probably due to the influence of the boundary. Second, while the hole densities increase as one goes up toward the free surface, there are columns below the free surface where the density oscillates [fourth and fifth columns in Fig. 3(c)]. It is not clear whether this is a genuine feature of the real system or an artifact of the model equation. Note that the flow patterns near the obstacle exhibit noble phenomena unique in granular flows: the appearance of stagnant solids above the obstacle with $\Psi \approx 0$ and the empty region below the obstacle with $\Psi = 1$. The two lines under the obstacle beyond which the voids cannot penetrate (because $\Psi = 1$) have been termed a *shock front* in [1] because of their similarity with the supersonic flow: streamlines change abruptly after crossing the shock front. Note that the shock must be distinctively nonlinear. As demonstrated in Fig. 3, Eq. (6) indeed yields the remarkably similar flow patterns seen in the real experiment (see Fig. 1 of Ref. [1]).

In summary, we have derived a nonlinear dynamic equation and showed how its solutions produce unique features seen in the most simple granular flow patterns. The equation is relatively simpler to solve than the usual kinetic equations [6]. It is a continuum equation and so offers a way to handle the dynamics analytically, often a hindrance in the cellular-automata approach [7]. It also does not require the large-scale computation typical in molecular-dynamics simulations [8]. It appears that the dynamic equation derived in this paper might enable us to describe the somewhat more complex dynamics displayed by granular materials under various circumstances [9]; notable examples would be the convective flow patterns [10] that appear when the granular materials are subjected to vibrations and the segregation of Brazilian nuts [11]. However, it might be possible that Eq. (6) needs to be modified along the direction briefly mentioned in [5] in order to study more complex flow patterns of the granular particles, which are currently underway.

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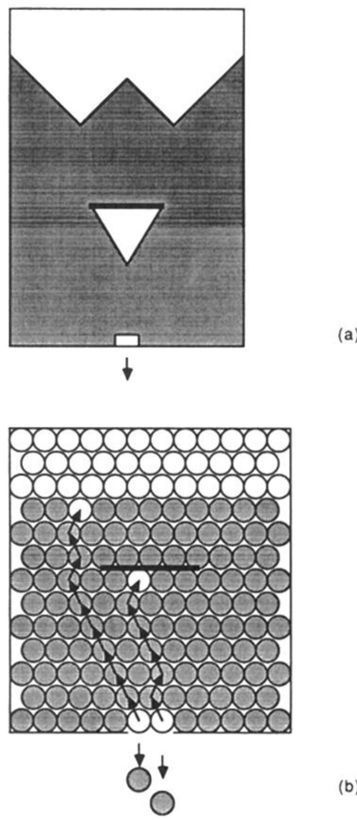

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