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Cellular automata models of granular flow

G. William Baxter and R. P. Behringer
Department of Physics and Center for Nonlinear Studies, Duke University, Durham, North Carolina 27706
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Simple experiments demonstrate the importance of particle irregularity on the flow of granular materials. We introduce cellular automata to model these flows with rules that are derived from experiments. Automata that model nonspherical particles can reproduce a number of important features of the physical flows, including alignment of the particles, the formation of a complex channel region, the formation of defects in the body of the material, and the overall shape of the upper free surface of the material.

The dynamics of sand is a challenging problem that has attracted recent as well as past interest.[1-12] While this has been an historically and technically important problem, relatively little progress has been made in comparison to that achieved in the dynamics of Newtonian fluids. Traditional theoretical descriptions of granular flow have taken a continuum mechanics approach.[1-4] More recently, molecular dynamics, i.e., integration of Newton's equations for a collection of particles (with assumed collisional properties), has been used to try to understand the "microscopic" behavior of granular flows.[5-7]

Both approaches have limitations. Often, the continuum equations are difficult to solve for all but the simplest geometries, or they are subject to strong instabilities when linearized.[8] Still at issue are the correct constitutive laws for these theories. These models are most appropriate for smooth particles; yet many interesting and technologically important flows involve rough or otherwise nonspherical particles which contain additional degrees of freedom. Molecular dynamics simulations are limited by the number of grains which they can follow, and by the fact that the computational complexity increases significantly for nonspherical grains.

Cellular automaton models avoid each of these problems. These models use well-defined rules, uncomplicated by instabilities, with a simplicity that allows a simulation to follow a large number of particles (10^5-10^6) even if "particle irregularity" is included and a fairly small computer is used. Automata are particularly valuable in modeling granular flows because they can test the importance of each microscopic feature. In addition, they provide testable predictions for length and time scales and structures of a particular symmetry, which may be expected in physical experiments. Automata models for sand flows (in this case sand avalanches) have been used[9,10] as a probe of self-organized criticality. There, the concern was less with understanding the mechanisms of granular flows and more with obtaining model systems which showed structure over a large range of temporal and spatial scales. As such these models fall short of describing real sand avalanches.[11] In this work, we take a different point of view. Specifically, we use automata models as a probe of a necessary piece of physics which must be included if an accurate description of real granular materials is to be achieved. However, we do not claim that the model is rigorous or that better models could not be constructed.

In this work, we will focus on one particularly simple type of flow, flow from a hopper, which is poorly understood at the basic level, but also has obvious technological applications. Simpler flows, such as steady flow through a uniform channel are possible. However, flow in a hopper shape is one of the simplest geometries in which particle irregularity plays a demonstrably important role.[12]

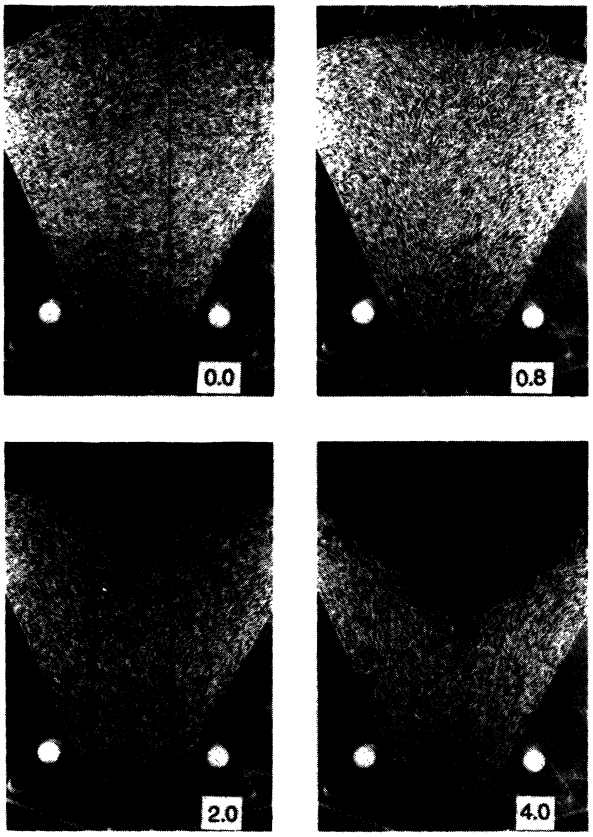

FIG. 1. Photographs of seed flowing from hopper. The hopper angle is set to 60° which corresponds to the angle used in the automata studies. The first photograph shows the full hopper. The numbers under subsequent pictures show the elapsed time in seconds. The physical dimensions of each image are 14×21 cm^2.

The effect of particle irregularity in the flows is probably best understood by considering a material in which the particles have a well-defined uniform nonspherical shape. A useful example of such a material is grass seed, and we will use it as a convenient paradigm. In particular, Fig. 1 shows part of a series of photographs of the flow of seed out of a thin Plexiglas wedge. The thickness of the hopper, 1.2 cm, is about twice the length of a seed. We call particular attention to several features seen in these flows: (1) nearly all the particles are aligned with the face of the hopper, and very few are normal to the vertical faces, making the flows nearly two-dimensional; (2) within the plane, there is a long-range orientational order of the grains; (3) the flow takes place in a central region with stagnant material on either side, and within the flowing region, the grains tend to orient vertically; (4) the upper free surface exhibits a number of complex shapes; (5) there are a number of interesting smaller structures within the bulk, including small star-shaped defects and somewhat larger circular structures; (6) the flow rate, as measured on a time-scale of a few seconds, is steady independent of the height of the layer in spite of the obvious time dependence in these flows.

We turn now to the modeling of these flows with cellular automata. Our automata use a regular 2D triangular lattice with hexagonal symmetry. Lattice sites can be occupied by walls or grains or may be vacant, i.e., a hole. Walls are placed initially and never move or change. A grain at a site i has a *state* consisting of an orientation O and a direction of motion $\hat{v}$. There are three directions for O, each parallel to a basis vector of the lattice: 0° (vertical) or $\pm 60°$. The direction of motion $\hat{v}$ of a grain can be toward any of its six nearest neighbors or the grain can be at rest. The automata use a two step rule consisting of an *interaction step* and a *propagation step*. Iteration n begins with the *interaction step* in which a new O and $\hat{v}$ are chosen *simultaneously* for each site i by minimizing an "energy function" defined by

$$E_i = E_{\text{gravity}} + \sum_{\text{NN}} E_{\text{inter}} , \tag{1}$$

where NN represents nearest neighbors. E_i depends on the state of the grain at site i and the states of its six nearest neighbors at the previous iteration $n-1$. Specifically, E_i is computed for all 21 possible states of the grain at site i. The new state of the grain at site i at iteration n becomes the one that minimizes E_i (subject to the constraint that $\hat{v}$ may only be toward holes). If several allowed states share the same lowest energy (a rare occurrence), one is chosen at random. Also, as in the physical system, grains are not allowed to change their state unless they are adjacent to a moving grain or have a hole in one of the three sites beneath them. At the conclusion of the interaction step, each site is set to its new state.

Following the interaction step, the propagation step occurs. Every grain is moved one lattice spacing along its new direction of motion $\hat{v}$ (i.e., $\hat{v}$ of the chosen minimum of E_i in the last interaction step). Due to the nature of the interaction step, it may happen that multiple grains have $\hat{v}$ directed toward the same hole. In this case, the candidate with the lowest E_i (from the interaction step) is moved and all other competing candidates have their $\hat{v}$'s set to rest. The propagation step completes the nth iteration.

We now consider the various terms in E_i. The first term reflects the fact that grains prefer to move downward in a gravitational field. E_{gravity} has the form

$$E_{\text{gravity}} = \begin{cases} \Delta \text{ if 1 or more adjacent sites below are holes and } \hat{v} \text{ not toward one of these,} \\ 0.0 \text{ otherwise.} \end{cases} \tag{2}$$

The second term takes into account the interaction of a grain with its nearest-neighbor grains

$$E_{\text{inter}} = F^{\alpha}_{\text{shear}} F^{\beta}_{\text{orient}} F^{\chi}_{\text{dilation}} . \tag{3}$$

The factors on the right-hand side model the effects of relative motion, relative orientation, and dilation, respectively. Specifically,

$$F_{\text{shear}} = |\hat{v}_N - \hat{v}_i| + 0.1 . \tag{4}$$

Here $\hat{v}_N$ is the direction of motion of a neighbor at the $(n-1)$th iteration and $\hat{v}_i$ is a possible direction of motion of the particle at the nth iteration.

$$F_{\text{orient}} = \begin{cases} S \text{ if both grains are aligned along one of their velocity vectors,} \\ 1.0 \text{ otherwise,} \end{cases} \tag{5}$$

where $S \leq 1$. The case $S = 1$ or $\beta = 0$ correspond to spherical particles.

$$F_{\text{dilation}} = \begin{cases} \dfrac{1}{d} \text{ if } d \leq \dfrac{1}{1-C}, \\ 0.2 \text{ otherwise,} \end{cases} \tag{6}$$

where d is the mean spacing (i.e., time-average spacing) of the grains, and C is a parameter which can be set to a positive value (less than one) if the particles are cohesive. For any two neighboring grains, the term F_{shear} is near zero if they are both at rest or have the same direction of motion and increases in proportion to the difference in their directions of motion. The term F_{orient} is smaller if the grains are aligned and larger otherwise. Note that an orientational interaction must be distinct from a frictional interaction, since an irregular particle can cause a torque about the center of mass of a neighbor even in the absence of friction. Finally, the term F_{dilation} approaches zero as

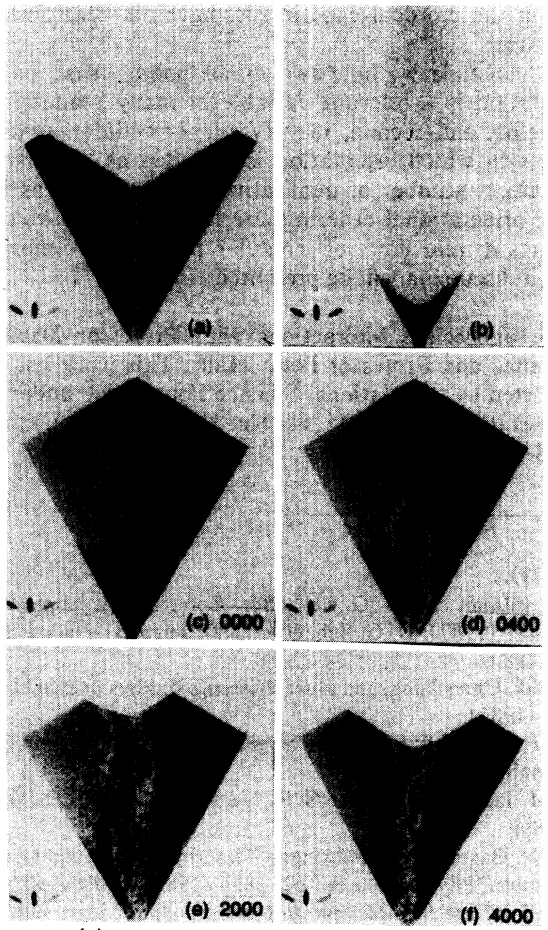

FIG. 2. (a) Results for a structureless model in which the power β of the orientation term F_{orient} has been set to 0. (b) The filling process. (c)–(f) Flow states of a structured automaton with the time given by the iteration number. (Parameters: wedge angle 60°, $\Delta=3.0$, $C=0.2$, $S=0.01$, $\alpha=3.0$, $\beta=1.0$, $\gamma=2.0$.) The shading gives the orientation. Holes are indicated by white.

the grains move farther apart. The exponents α, β, and γ provide a convenient way to vary the relative strengths of the different components in the interaction term.

An important issue is the initial state of the system, before the material is allowed to flow. The initial state of a physical experiment is typically prepared by raining the material into the hopper [see also Fig. 2(b)]. Because the grains interact during this process, the initial state is not characterized by random orientation, but typically has orientational order. The model "hopper" is filled by placing rest grains with random orientations in a Gaussian density distribution along the top row of the lattice at each iteration. These are allowed to fall into the hopper as shown in Fig. 2(b). The same set of flow rules is used during the filling and emptying process. The emptying process is initiated by replacing wall points blocking the outlet with holes. Grains moving into holes at the bottom row of the outlet channel are effectively removed from the grid by replacing them with holes.

We turn now to results obtained from this model. The simplest automaton results when the orientation effect is turned off by setting $\beta=0$. In this case [Fig. 2(a)], grain motion occurs within a central core which approaches a constant width in the horizontal direction as time progresses. Within this core, the density is uniformly lowered, and the flow is relatively structureless. As the flow progresses, the upper surface develops a shape characteristic of physical flows in this geometry. Automata with these characteristics resemble the flow of smooth spheres.[12]

We now consider the effect of orientational interactions. We first show the number of particles falling out per iteration in Fig. 3 for 6000 iterations, enough to substantially empty the hopper. In Fig. 3, we have averaged the number of particles per iteration over (a) five and (b) eleven successive iterations. Interestingly, there is no monotonic variation in the flow rate, a fact that is consistent with experiments.[12] However, a power spectrum computed from

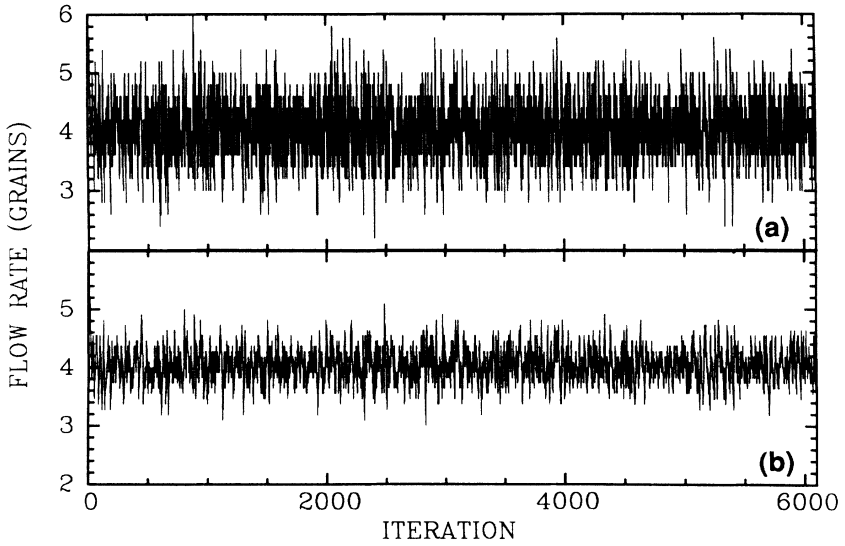

FIG. 3. (a) The number of automata particles falling out per iteration averaged over five iterations for 6144 iterations. (b) is averaged over eleven iterations. These data are from the automaton of Fig. 2. Qualitatively similar results are obtained if the orientation is turned off.

the flow rate is flat, corresponding to white noise. At present, there are no data for the flow rate for the physical particles on short-time scales, so the automaton provides a testable prediction in this regard.

Figures 2(c)–2(f) show several iterations out of a long sequence, for parameters which are specified in the caption. The shading indicates the orientations. [In this example, the shaded region of Fig. 2(c) has 0% holes.] Note that there is significant correlation of the particle orientations over a range comparable to the macroscopic dimensions of the container. The qualitative large-scale features seen in real flows, as typified in Fig. 1, are correctly captured by the automaton. The automaton also contains structure in the flowing center region which is qualitatively similar to the physical flow. However, some of the smaller features, such as star-shaped defects, which are seen in the physical experiments have not been found in the model.

To conclude we note two major points: first, particle orientation is a relevant variable in many granular flow problems, and second, in very simply cellular automata models in which orientation is included as a dynamical variable, a number of qualitative features, such as long-range orientational ordering, are found which have counterparts in real flows of irregular particles. A more extended discussion will be presented elsewhere.[13]

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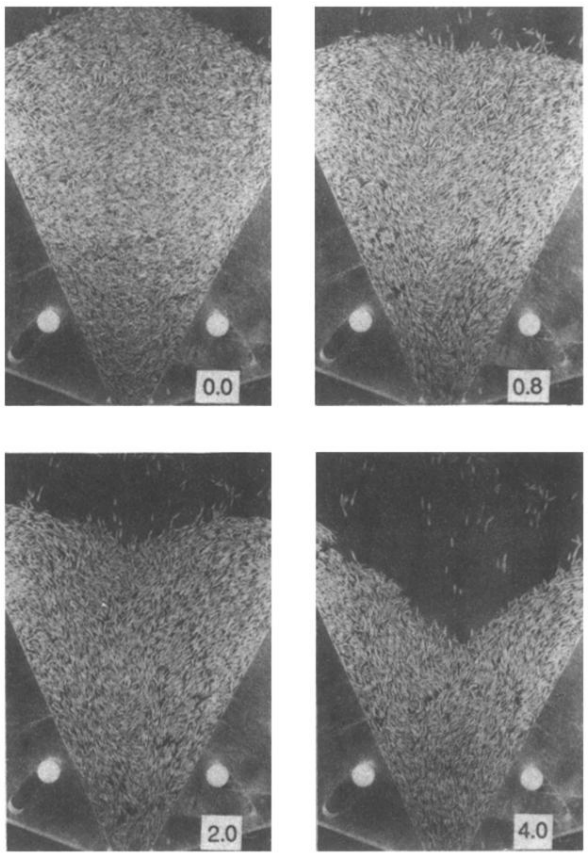

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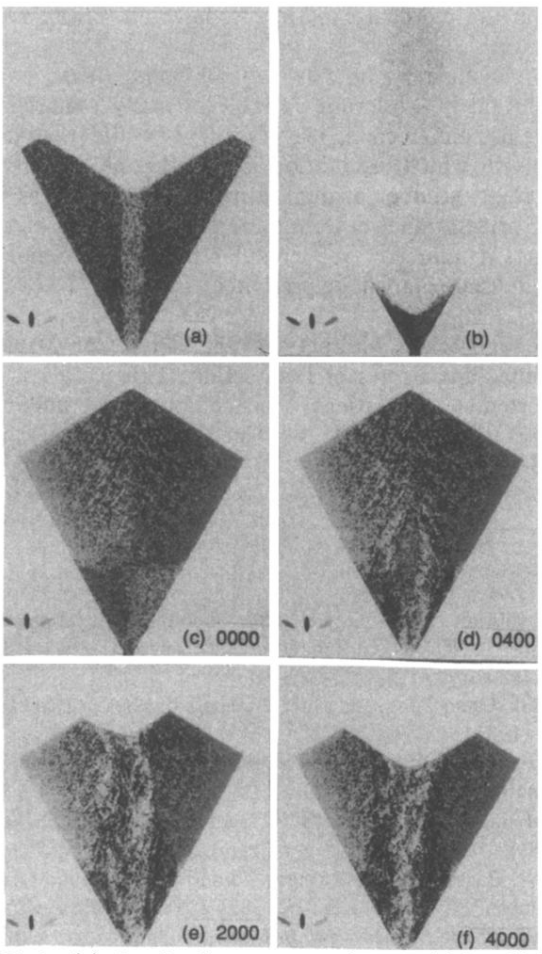

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