Granular Matter (2011) 13:211–214
DOI 10.1007/s10035-010-0247-y

ORIGINAL PAPER

A cellular automaton for segregation during granular avalanches

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Received: 5 August 2010 / Published online: 30 January 2011

Abstract Segregation is a complex and poorly understood phenomenon that is prevalent in many industrial and natural granular flows. When grains flow down a slope [1–5], are spun in a rotating drum [6–8] or shaken in a box [9], we observe those grains organising into intriguing patterns. Kinetic sieving is the dominant mode of segregation in granular avalanches, where separation of particles occurs according to size. Using a cellular automaton we have modelled kinetic sieving as the swapping of particles in a one-dimensional system. From the cellular automaton we have deduced a continuum model to describe the segregation.

Keywords Granular flow · Cellular automata · Kinetic sieving · segregation

1 Motivation

The authors would like to begin by mentioning that this work was the result of inspiring discussions with Prof. Vardoulakis, with whom we were initially aiming at establishing a new mathematical theory of segregation. Before too long, we found in the literature two distinctively comprehensive and successful theories essentially predicting similar patterns [1,2]. Our interest was then to step back and search for the simplest explanation to this problem. This is the aim of this paper.

Many theories have been developed to explain segregation in granular avalanches, in particular those involving kinetic sieving mechanisms [1,2]. Cellular automata have been used to model a variety of granular systems [10,11], including segregative systems [12–14].

Kinetic sieving is a result of local fluctuations in the porosity of a granular avalanche [2]. These cause internal voids to be produced, which are in turn filled with particles under the influence of gravity. Since it is more likely that a small particle will fit in any given void, there is a net movement of small particles downwards through the bulk, and a corresponding net movement of large particles upwards (Fig. 1a). We ignore the mechanism by which very small particles spontaneously fall through the pore throats, with almost no help from external perturbations.

In the field of kinetic sieving, two main theories are those described by Gray and Thornton [1] and Savage and Lun [2]. They both describe thin, rapidly flowing avalanches of bi-disperse mixtures down an inclined chute. Gray and Thornton use a binary mixture theory to find concentration shocks which define their solutions. Savage and Lun use a maximum entropy argument and a statistical approach to describe their steady state concentration profiles.

2 Approach

We define a cellular automaton that works in a regular one-dimensional lattice, where the diameter of each particle, d_i, is a Boolean variable attached to each discrete position i of the lattice. We then define a rule which specifies the time evolution of the diameter at each site.

In Fig. 1b, either of the two particles indicated could fall into the available space. It has been observed [2] that the smaller particle is more likely to fall into the pore, and so this has a greater probability of occurring. This is expressed in simplest terms as two particles swapping places. With some frequency f:

IE acknowledges grant DP0986876 from the ARC.

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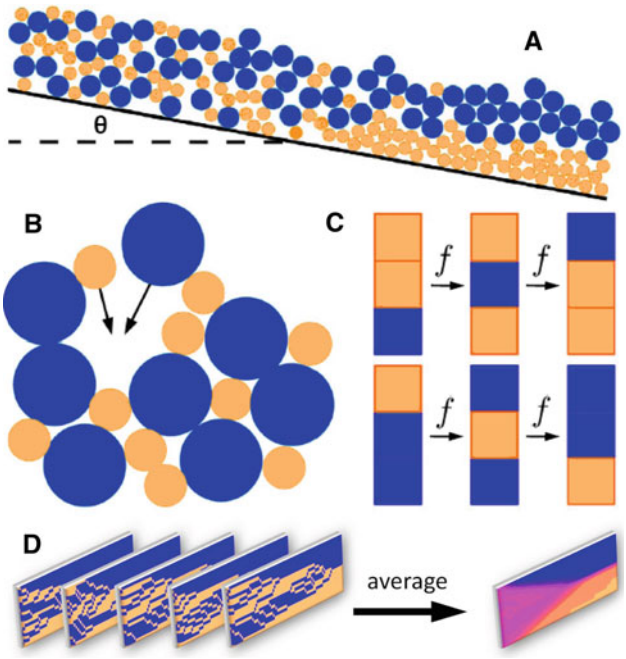

Fig. 1 Schematics of segregation and corresponding cellular automaton rule. *Orange* are small particles, *Blue* are large particles. **a** Effect of kinetic sieving on particles flowing down an inclined slope. **b** Two particles attempting to fall into an available space. **c** The automaton mechanism, where large and small particles swap places with frequency f. **d** Individual simulations are averaged to produce mean model behaviour

$$d_i \Leftrightarrow d_{i-1} \quad \text{if } d_i < d_{i-1}.$$

Here the double arrow indicates that the variables representing the diameters have swapped positions at cells i and $i-1$. Figure 1c illustrates two iterations of the rule on a three particle system. In both cases, the small particles swap with the large particles, creating segregation. We consider a purely non-diffusive system, in which large particles cannot move down and small particles cannot move up. We run our simulation simultaneously in many instances, and average the particle diameter at each point across these simulations (Fig. 1d).

We generalise our model with the inclusion of a swapping frequency, f, which defines the rate of segregation as a function of the shear strain rate [15] that drives the kinetic sieving process, $\dot{\gamma}$. We can then describe the tendency for our mechanism to occur as a function of the height z such that $f \propto \dot{\gamma}$.

The simplest case of flow is that of plug flow, where the down slope velocity is constant along the depth. For this case, $\dot{\gamma} = 0$ and we expect no segregation. A more complicated case is that of simple shear. Here we use a linear velocity profile, giving us a constant shear rate, and $f_1 = k$ where k is a non-dimensional frequency of swapping.

For a more accurate representation of shallow particle flow down an inclined plane, we assume that the shear rate

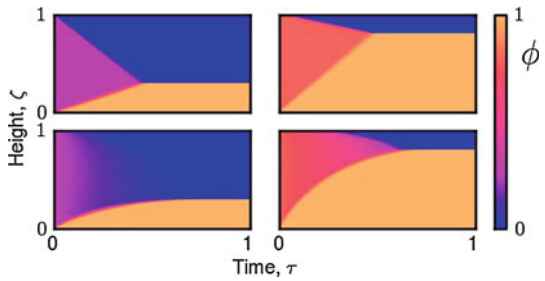

Fig. 2 Time evolution for two different shear flows. The *top* row assumes simple shear, i.e. $f_1 = k$, while the *bottom* row assumes Bagnold shear, i.e. $f_2 = k\sqrt{1-\zeta}$. The system is initially filled with a mixture of 30 and 80% (*left* to *right*) small concentration. *Colour bar* represents small particle concentration ϕ

is approximated by Bagnold shear [16–18], where $f_2 = k\sqrt{1-\zeta}$, $\zeta = \frac{z}{H}$ and H is the avalanche depth.

In our model, $\zeta = \frac{i}{N}$, where N is the total number of cells in the vertical direction. We define a non-dimensional time $\tau = j\frac{k}{N} = t\frac{kU}{H}$. The first equality refers to the cellular automaton, where j is the time step. The second equality refers to the physical time t, where U is the average bulk velocity across the depth.

The cellular automaton outputs the time evolution of the flow for any applied shear regime and initial mixture. The flow is described by ϕ, the small particle concentration. We find ϕ by summing the number of small particles at a given height across all of the simulations, and dividing by the total number of simulations.

For a homogeneous initial condition, we start the system as a randomly generated sample with given concentration of small particles, ϕ_0. As in [12] we begin at the bottom of the system, working our way up, checking if each particle has on average smaller particles above it. If it does, it swaps at frequency f with the above particle. For stability, we work in half time steps, checking only for particles in odd or even rows. This stops particle from moving many times in a single time step. The top row is never explicitly checked, but has small particles taken out of it by the row below.

3 Results

The top of Fig. 2 shows the behaviour of a system undergoing simple shear flow. This is described by $f_1 = k$, i.e. the frequency is constant over the height. Three sharp concentration shocks develop during the time evolution, marking the boundaries between the two fully segregated states and the mixed state. The shocks are linear, and move towards a discrete triple point. The height of this point depends on the initial concentration of the particles ϕ.

The bottom of Fig. 2 outlines the case of Bagnold shear, i.e. $f_2 = k\sqrt{1-\zeta}$. Because of the large swapping frequen-

cies at the base of the flow, a concentration shock develops. At the top of the flow, however, the swapping frequency is uniquely zero, and a second concentration shock does not develop. In this case, there is no robust definition of complete segregation. In a flow of infinite width relative to the grain size, segregation would never fully occur.

We do not expect a concentration shock at the top of the flow. This is in contrast to suggestion by both Gray and Thornton and Savage and Lun. Experimental tests [2,19] generally involve a small number of particles (flows typically 10–20 particles deep and with minimal width) and full segregation may occur because the problem becomes stochastic in nature with insufficient realisations of the segregation statistics.

When looking at the Bagnold shear case it is evident that the small particles saturate the bottom before the large particles saturate the top. Is one faster than the other?

To answer this, we look at a case of heterogeneous initial conditions. We define two regions of mono-disperse particles such that the large particles are below the small particles. The insets of Fig. 3 picture large particles moving upwards through the bulk (3D), and small particles moving downwards (3B). These two cases correspond to distinctly different aspect ratios between the upper and lower regions, 9:1 and 1:9.

We place a 'gate' at some height δ, and time until 90% of the contaminating particles have passed beyond this gate. The curves at the right of Fig. 3 plot this time, τ_{90}, for a range of values of δ for both simulations. The idea is to present a competition between the two particles—a race to pass a gate at a similar distance from their initial point.

We see that for any distance moved by the particles, the small particles (yellow line) take longer to reach the gate. It should be noted at this stage that we only consider small size differences between the two species, and do not account for filtration of very small particles through the bulk. Also, the time for one particle to go from the top to the bottom, or the bottom to the top will be the same. The reason the times vary in intermediate lengths is due to the asymmetry of the shear strain rate. For example, if the asymmetry was inverted, it would be the smaller particles that trickle faster than the large particles float. Using this understanding, it my be possible to tailor industrial processes to obtain faster separation times.

4 Continuum model

By averaging over a sufficiently large number of simulations, cellular automaton can be used to represent continuum flow equations [20] by looking at the flux of volume fraction ϕ between adjacent cells over time. Over one time step, the flux that moves downwards out of a point (ζ, τ) is the product of the swapping frequency at that height $f(\zeta)$, the amount of that size present at that height $\phi(\zeta, \tau)$ and the available space to move into. A small particle will only move if it is larger than the average particle below it and so the available space can be expressed as $1 - \phi(\zeta - \Delta\zeta, \tau)$. Taking conservation of mass over a single time step we get:

$$\phi(\zeta,\tau)\Delta\zeta + f(\zeta+\Delta\zeta)\phi(\zeta+\Delta\zeta,\tau)(1-\phi(\zeta,\tau))\Delta\tau = \phi(\zeta,\tau+\Delta\tau)\Delta\zeta + f(\zeta)\phi(\zeta,\tau)(1-\phi(\zeta-\Delta\zeta,\tau))\Delta\tau$$

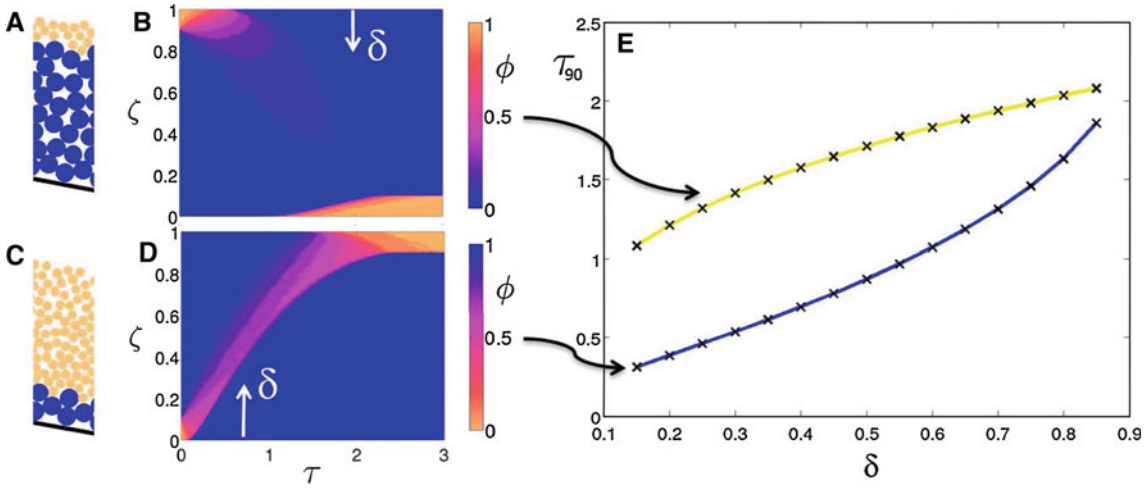

Fig. 3 **a** An initial configuration of small particles sitting above large particles. **b** These small particles sinking to the *bottom* of the flow, under Bagnold shear. **c** An initial configuration of large particles sitting below small particles. **d** These large particles rising to the *top* of the flow, under Bagnold shear. **e** The time for 90% segregation, τ_{90} at a particular height δ. The *blue line* is large particles moving upwards, and the *yellow line* is small particles moving downwards

Taking $f(\zeta) = k\dot{\gamma}$, we represent the segregation mechanism in terms of the variation of shear strain with height. In continuum terms this can be expressed as:

$$\frac{\partial \phi}{\partial \tau} = k \frac{\partial (\dot{\gamma} \phi (1 - \phi))}{\partial \zeta}$$

This continuum formula differs from that described by Gray and Thornton [1], as it replaces a constant segregation co-efficient S_r with a contribution due to shear strain rate $\dot{\gamma}$. Gray and Thornton's continuum formulation in one spatial dimension is:

$$\frac{\partial \phi}{\partial \tau} = S_r \frac{\partial (\phi (1 - \phi))}{\partial \zeta}$$

Our model predicts that in a physical flow, such as that approximated by Bagnold shear, a concentration shock develops at the bottom of the flow only. The appearance of a shock at the top of the flow is a result of the small number of particles being observed. Flow near the free surface in Bagnold shear can be approximated by plug flow, corresponding to a situation with extremely slow segregation.

This paper could be viewed in a different light by seeing the cellular automaton as an effective numerical tool to solve partial differential equations. These problems are known to be extremely challenging to solve [21] and such a simple approximate solution, which handles shocks and rarefactions without qualms, is of great help.

Acknowledgments We would like to thank the members of the Particles, Grains and Complex Fluids Group at the University of Sydney, in particular Dr. Pierre Rognon and Dr. Bjornar Sandnes for useful discussions.

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