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Simulations for dynamics of granular mixtures in a rotating drum

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Abstract We present a simple model and carry out simulations to investigate the dynamics of mixtures of granular material within a rotating drum. On the basis of the commonly held belief (supported by considerable experimental evidence) that segregation is due to motion of particles on the active layer, the bulk playing little or no role, we introduce a 2d lattice gas model which takes into account the rotational frequency, frictional forces, and the gravitational field, and represents segregation tendencies via activated effective grain-grain interactions. Our results include the onset of segregation perpendicular to the drum axis, the appearance and subsequent coarsening of bands and peculiarities of the effects of periodic modulation of the drum. Observed effects such as the segregation of rougher (smoother) particles into the bellies (necks) of the modulation are reproduced by our simulation.

Keywords Granular matter, pattern formation, segregation

1 Introduction

Recently, flows of granular material (GM) have received much attention from many disciplines of science and engineering [1–4]. On the one hand, interest to basic science arises from a variety of issues including statistical mechanics and critical phenomena [3–6]. On the other hand, the understanding of the behavior of GM is very important to practical industrial processes such as crushing of particles, transporting, mixing, etc [1, 7–10, 14]. Rotating drums are often used in industries for mixing in the production of several goods such as pharmaceuticals, foods, polymers, semiconductors, etc. However, under certain conditions rotating drums induce segregation [11, 12].

Grains within a rotating drum undergo a sequence of avalanches. When the frequency of the rotation is increased, the time between avalanches becomes shorter than the relaxation time of each avalanche and the motion of grains resembles a continuous flow. The behavior of the granular mixture can be separated into two regions: the active layers and the passive layers [13]. Grains in the active layers flow down the slope like a liquid and grains in the passive layers execute essentially a rigid body motion. The rotating drum removes material from the downstream portion of the active layers and injects material onto the upstream portion. In this way, the average number of grains flowing down the slope is constant. There are two types of segregation observed in rotating drums, radial and axial segregation. Axial segregation involves the formation of single species bands perpendicular to the axis of the cylinder and is always preceded by radial segregation [11, 14]. In this work we restrict our attention to axial segregation. Zik et al. [15] made experiments using a mixture of glass balls and sand subjected to rotation within a drum. They explained segregation as occurring due to an instability nucleated by concentration fluctuations. In addition, they observed that: (i) segregation is due to motion on the surface, the bulk playing no role, (ii) friction is an important factor to be taken into account, and (iii) bands grow due to a coarsening process. They also performed experiments using spatially modulated drums and found that modulation promotes segregation and that rougher particles always develop bands in the bellies of the modulation and smoother particles in the necks. In the following, we will consider these experimental results to be prototypical and will report our theoretical considerations entirely in their context.

2 The model

The study of simple models for granular systems which consider only the essential processes have proved to be very useful for the understanding of the behavior of GM [16]. Our model is a generalization of the so-called KLS model which is a 2d stochastic lattice gas first introduced [17, 18] in order to study the behavior of fast ionic

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conductors and normally simulated on a square lattice where there can be at most one particle per lattice site. The system is in contact with a thermal bath at temperature T. Only nearest-neighbor interactions through a coupling constant J are considered, and a driving field which favors (suppresses) jumps along (opposite to) its direction is introduced. Periodic boundary conditions are imposed and the number of particles in the system is conserved. The time evolution of the probability distribution P is given by the master equation,

$$\frac{dP(\eta)}{dt} = \sum_{\eta'} w_F(\eta' \to \eta) P(\eta') - w_F(\eta \to \eta') P(\eta) \quad (1)$$

where η is a configuration of all the particles, and $w_F(\eta \to \eta)$ are the transition rates. In order to introduce the driving field, local detailed balance is imposed,

$$w_F(\eta' \to \eta) = w_F(\eta \to \eta')\, e^{-\beta[H(\eta')-H(\eta)]}\, e^{\beta\epsilon F} \quad (2)$$

where $\epsilon = \{-1, 0, 1\}$ for jumps opposite, perpendicular, and parallel to the field F, respectively, β is the (dimensionless) inverse temperature and $H(\eta)$ is the Hamiltonian.

$$H(\eta) = \frac{1}{2} J \sum_{ij,i'j'} \sigma_{ij} \sigma_{i'j'} \quad (3)$$

where ij denotes the coordinates of the site and $i'j'$ its nearest-neighbors. Motivated by the observations made in [15], we assume that the passive layers play no role in determining axial segregation. It is therefore sufficient to simulate the motion of grains in 2-dimensional space representing the free surface in the drum. We use a square lattice in rectangular geometry and consider two different types of particles, namely A and B. To represent the experimental situation that different types of particles have different friction forces, since the friction forces depend on the composition of the particle itself and on the neighborhood, we consider two interaction parameters, J_A and J_B (both positive) to signify effective attractive interactions among the particles. For the sake of simplicity we consider that there are no interactions between one species of particle and the other (except for excluded volume). In addition, the total number of particles in the system is conserved and open boundary conditions are imposed. To simulate the rotation of the drum, the system is allowed to evolve during τ time steps. Then, we remove the lowermost row of the lattice, and place it at the uppermost edge, shifting downwards the remaining row of the system. This procedure enables us to define the frequency as $f = 1/\tau$. We introduce new expressions for the effective field and the couplings which have not been used in earlier investigations:

$$F = F_0 \sin(\theta_0(1 - e^{-\alpha f})) \quad (4)$$

$$J_s = J_{0s} e^{-\gamma f} \quad (5)$$

where θ_0 (F_0) is a characteristic maximum angle (field), respectively, α is a characteristic time scale for the field and J_{0s} is the maximum coupling constant for the species s ($s = \{A, B\}$). The dynamic angle of repose is the angle formed by the free surface and the horizontal plane, which we assume to be the same for both species for the sake of simplicity. The expression for the field we have used above assumes that the dynamic angle of repose smoothly increases with frequency. The expression for the couplings is of Arrhenius type which simply means that for frequencies lower than the threshold $1/\gamma$, particles interact negligibly and turn on at frequencies of the order of $1/\gamma$. We introduce this feature to represent the fact that dynamic friction, consequently effective interparticle interaction, is present when the motion of the particles overcomes some typical threshold. It should be noted that our model considers a thermal noise which induces disorder in the system. The temperature parameter $1/\beta$ accounts for the amplitude of such a disorder and must not be confused with a real temperature.

3 Simulation results

We have run a large number of simulations using a lattice of size $L \times M = 36 \times 216$ and keeping the densities of different species fixed $\rho_A = \rho_B = 0.40$. Inspection of snapshot configurations (not shown here) leads us to observe that for high enough frequencies several single species bands develop parallel to the direction of the field. Given that the lattice simulates the free surface, it is obvious that this pattern signifies axial segregation. In order to characterize the degree of order in the system we introduce an order parameter which we call the degree of segregation.

$$\Phi_s = \frac{1}{R} \left[\frac{1}{M} \sum_{i=1}^{M} |P_s(i) - \rho_{0s}| \right] \quad (6)$$

where M is the length of the lattice, $\rho_0 s$ is the global density of particles of type s, $R = 2\rho_{0s}(1-\rho_0 s)$ is a normalization constant, and $P_s(i)$ are the density profiles calculated along the direction of the field, given by

$$P_s(i) = \frac{1}{L} \sum_{j=1}^{L} \delta(\sigma_{ij} - \sigma_s) \quad (7)$$

It is easy to show that for a completely disordered (segregated) system the value of Φ is zero (one). Figure 1(a) shows a plot of Φ_A versus f. We observe that for low frequencies the degree of segregation in the system is low, and that it increases smoothly for higher frequencies. The same behavior is seen in a plot (see Fig. 1(b)) of the average number of bands N_b versus f. We have also studied the time evolution of the model. Figure 2 shows two snapshot configuration obtained at different time t when segregation occurs. At early stages of the evolution we observe that several very thin bands have developed. As the system evolves, the bands become wider and many of them coalesce. Figure 3 shows the evolution of the average bandwidth (a) and the average number of bands (b). We first observe that both quantities evolve very slowly. The average bandwidth always increases with time. However, the average number of bands only increases at early stages of the evolution. In the later stages, it decreases. This means that, while the bands are getting thicker, most of

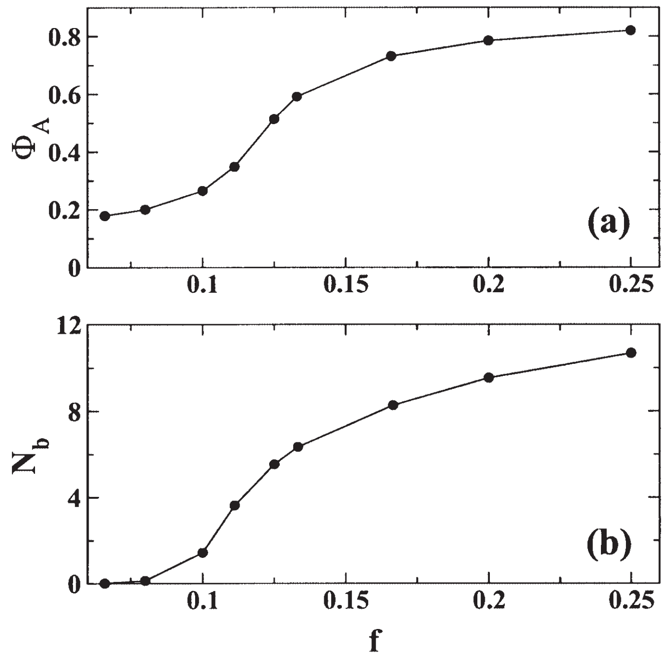

Fig. 1. (**a**) Plot of the degree of segregation Φ_A vs frequency f. (**b**) Plot of the mean number of A-bands vs frequency f

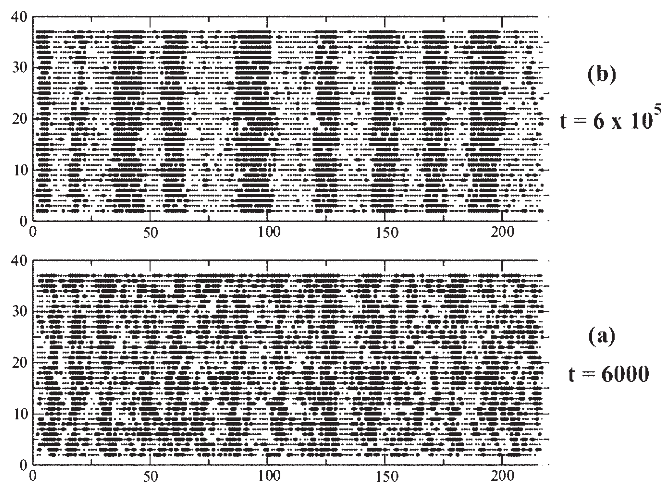

Fig. 2. Typical snapshot configurations obtained at different stages of the evolution of the system for $f = 0.166$

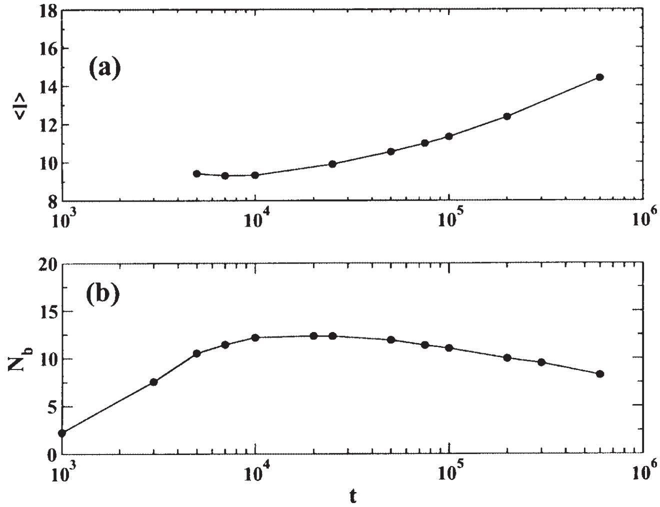

Fig. 3. (**a**) Plot of the mean bandwidth $\langle l \rangle$ versus time t for particles of type A at a frequency $f = 0.166$. (**b**) Plot of the mean number of A-bands N_b versus t for the same frequency

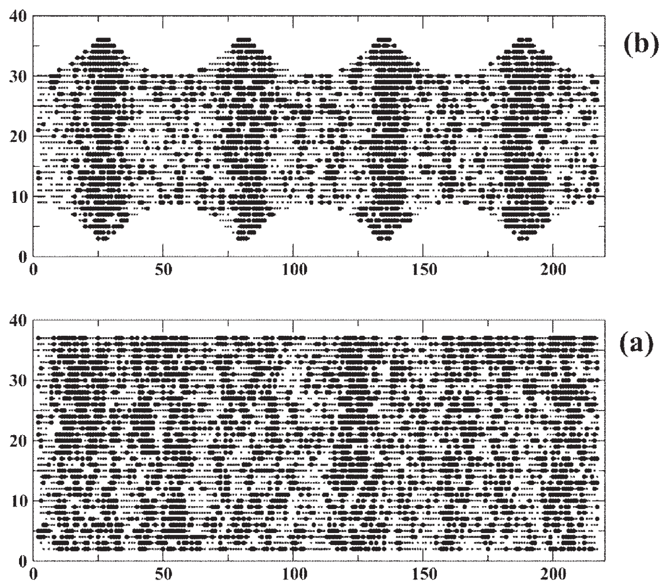

Fig. 4. Typical asymptotic snapshot configurations obtained at a frequency $f = 0.125$. (**a**) Unmodulated lattice. (**b**) Modulated lattice

them disappear because they coalesce. We conclude that we are in the presence of a coarsening process. The segregation mechanism is explained as follows. At very short times local density fluctuations make single species particles to nucleate and form small clusters. When a particle of one species collides with a cluster of another species this particle simply slides since $J_{AB} < J_A, J_B$. In addition, this growing mechanism is influenced by the action of the field which induce single species bands to develop parallel to its direction. This segregation mechanism is in agreement with the one reported by Zik et al [15]. We next report our study of the effect of the introduction of a spatial modulation of the lattice which we associate with a spatial modulation (corrugation) of the drum. Figure 4 shows two snapshot configurations for the modulated and unmodulated cases obtained using the same set of values of the parameters. We first observe that the degree of segregation obtained in the modulated case is distinctly higher. Secondly we observe that black bands always develop at the bellies of the modulations and grey bands in the necks. Figure 5 shows the degree of segregation Φ_A versus time t for the unmodulated and modulated cases. This quantity clearly shows that modulation promotes segregation. In addition, the degree of segregation exhibits two time regimes: a fast time regime at short times and a slow time regime at longer times. The fast time regime occurs at early stages of the evolution since particles can diffuse faster and form several very thin bands through the system. However, after bands have developed it is quite difficult for a particle of one kind to diffuse through a cluster of another kind in order to make a band wider and consequently the process is much slower. In our simulation black particles are the ones provided with the bigger J. Since the coupling constant J is associated with the

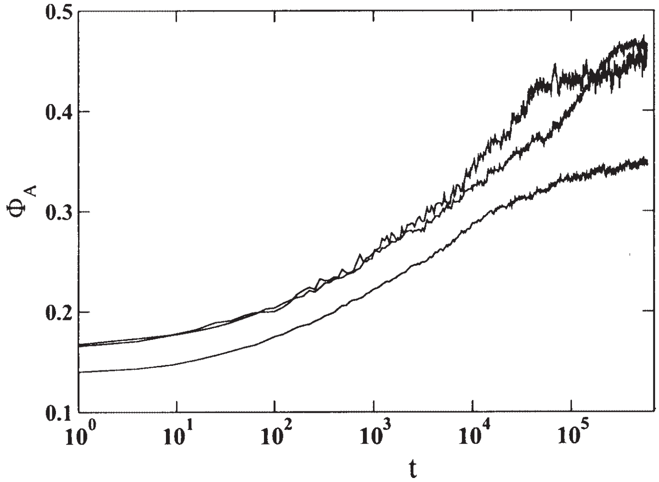

Fig. 5. Plot of the degree of segregation Φ_A versus time t. From bottom to top curves correspond to the unmodulated case, modulation of wavelength $\lambda = 54$, and modulation of wavelength $\lambda = 27$

dynamic friction force, black (grey) particles are the rougher (smoother) particles in the system, respectively. The reason why this selective segregation occurs is as follows. The minimum of every belly is a special position since every particle within this belly will try to flow to the minimum and after arriving to this position it can only escape due to the rotation procedure. In addition, since $J_A > J_B$ in our simulation, particles of type A will cluster sooner. Then, A clusters will develop at the bellies causing B particles to be depleted aside. This finding is again in complete agreement with experimental results [15].

4
Conclusions

We have studied some aspects of the dynamics of a granular mixture within a rotating drum by means of Monte Carlo simulations on a 2d lattice gas model which simulates the motion of grains on the free surface. Our results are in good qualitative agreement with the experimental results we have quoted above. This findings as well as the recent descriptions of the KLS model [18] and the dynamics of granular material [19] both based on a Cahn-Hillard like equation in the presence of a driving force, leads us to conclude that our model has the essential ingredients necessary to explain spatio-temporal features such as the coarsening process of bands observed in axial segregation of GM within rotating drums.

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