RESEARCH OUTPUTS / RÉSULTATS DE RECHERCHE

From particle segregation to the granular clock

Lambiotte, R.; Brenig, L.; Salazar, J.M.

ELSEVIER

From particle segregation to the granular clock

R. Lambiotte [a], J.M. Salazar [b,*], L. Brenig [a]

[a] *Physique Statistique, Plasmas et Optique Non-linéaire, Université Libre de Bruxelles,*
Campus Plaine, Boulevard du Triomphe, Code Postal 231, 1050 Bruxelles, Belgium
[b] *Université De Bougogne-LRRS UMR-5613 CNRS, Faculté des Sciences Mirande, 9 Av. Alain Savary, 21078 Dijon Cedex, France*

Abstract

Recently several authors studied the segregation of particles for a system composed of mono-dispersed inelastic spheres contained in a box divided by a wall in the middle. The system exhibited a symmetry breaking leading to an overpopulation of particles in one side of the box. Here we study the segregation of a mixture of particles composed of inelastic hard spheres and fluidized by a vibrating wall. Our numerical simulations show a rich phenomenology: horizontal segregation and periodic behavior. We also propose an empirical system of ODEs representing the proportion of each type of particles and the segregation flux of particles. These equations reproduce the major features observed by the simulations.
© 2005 Elsevier B.V. All rights reserved.

1. Introduction

Granular fluids are assemblies of moving macroscopic solid grains, including common materials such as sand, powders, cereals, etc. Their ubiquity in various industrial processes (e.g., pharmaceutical, food) as well as in geophysics and astrophysics motivates a better understanding of their properties [1]. Due to the inelastic interaction between the grains, these systems have a natural tendency to cool down by successive dissipative collisions leading to a macroscopic state of rest. Nevertheless, when these systems are supplied with an external energy source (e.g., a vibrating wall), they reach a dynamic stationary state whose macroscopic behavior presents some similarities with a classical liquid or a gas. Moreover, granular fluids exhibit a rich and peculiar phenomenology, for instance, non-Gaussian velocity distributions, non-equipartition of energy, anomalous transport coefficients, a natural

* Corresponding author.
E-mail addresses: rlambiot@ulb.ac.be (R. Lambiotte),
jmarcos@u-bourgogne.fr (J.M. Salazar), lbrenig@ulb.ac.be
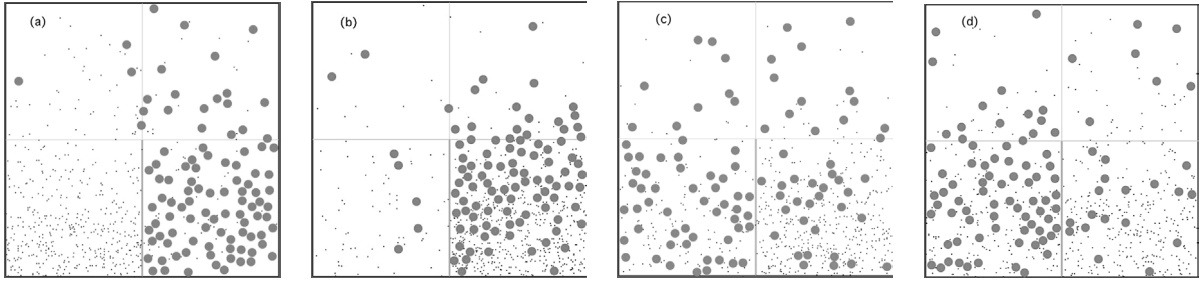(L. Brenig).

Fig. 1. (a), (b), (c), (d) Snapshots of the oscillation at different times. In (a), one plots the initial condition, with the small discs in box L and the large discs in box R. In (b), one may observe the transfer of small discs into box 2 and the vertical segregation. In (c), the transfer of large discs into box L has started. In (d), most of large discs are in box L.

tendency to form dense and dilute regions [2], shearing instability, etc. Recently, a significant progress has been achieved in the understanding of these phenomena by applying the kinetic theory and the resulting hydrodynamical equations. Some years ago a generalized Maxwell Demon experiment [3] has been devised that shed light on one of the most amazing properties of granular media. This experience consists of a box divided into two equal compartments by a vertical wall at the bottom and going up to the middle of the box, leaving the upper half of the box undivided. The box is filled with identical inelastic particles submitted to gravitation and the energy is supplied by a vibrating wall (Fig. 1). For a high energy input, the system presents a homogeneous steady state, while when the energy input is decreased, a phase transition occurs and an asymmetric steady state prevails. This asymmetric steady state has been first studied theoretically by Eggers [4] in a slightly modified configuration with a separation wall extending throughout the entire height of the box. This wall contains a small hole at a given height through which particles can be exchanged. In this formulation was assumed that the exchange of particles between the compartments corresponds to an effusive process and it was considered that the mean energy of the granular system decreases when the density increases. This last feature of granular systems is a consequence of the inelasticity of collisions between particles and is responsible for the symmetry breaking in the Maxwell Demon experiment. Indeed, an asymmetric fluctuation in the system induces a decrease of the mean energy in the denser compartment. Consequently, the escaping rate of grains from this compartment is reduced and the grains have higher tendency to flow from the dilute compartment towards

the dense compartment. This argument has been successfully verified by both molecular dynamics simulations [5] and hydrodynamic approaches [6].

In this Letter, we focus on a Maxwell Demon simulation with the same experimental setting as described in the first paragraph (Fig. 1) and characterized by two equal components. The binary system is composed by two kinds of smooth hard discs, whose dynamics depends on a large number of parameters. Here we have assumed that particles are characterized by the diameters σ_1, σ_2 and by the same mass ($m = 1$). Concerning the restitution parameter α it was set equal to 0.95. The particles evolve under gravity $\mathbf{g}$ (which acts along the y-direction), in a rectangular two-dimensional box (Fig. 1) of height H and width W, and moving ballistically between successive collisions. The collision rule between grains i and j reads:

$$\mathbf{v}'_i = \mathbf{v}_i - \frac{1}{2}(1+\alpha)\boldsymbol{\epsilon}(\boldsymbol{\epsilon} \cdot \mathbf{v}_{ij})\mathbf{v}'_j$$
$$= \mathbf{v}_j + \frac{1}{2}(1+\alpha)\boldsymbol{\epsilon}(\boldsymbol{\epsilon} \cdot \mathbf{v}_{ij}) \qquad (1)$$

with $\mathbf{v}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$ and $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$. The primed velocities are the post-collisional velocities and the unprimed ones the velocities before the collision. $\boldsymbol{\epsilon} \equiv \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|}$ is the unitary vector along the axis joining the centers of the two colliding spheres. These rules have been often used to study fluidized granular materials and have been proven to reproduce the specific phenomenology of granular fluids. The equations of motion of the N particles are solved numerically using the event-driven algorithm [7]. In our simulations, the box is divided in two equal compartments, box L (left) and box R (right) of width $W/2$, by a wall parallel to the y-direction of height $H/2$. The walls

are elastic except the ground which is a thermalizing wall at a given temperature T_G injecting the energy to the system. For this we used the dimensionless parameter $\gamma \equiv \frac{T_G}{mgH}$ relating the gravity and the energy input. The system studied is composed by 500 *small* particles and 100 *big* particles. The diameter ratios analyzed were 8.0 and 4.0 and in both cases we obtained the same dynamical scenario as we will show below. It is important to point out that this way of injecting the energy into the system has no intrinsic frequency and does not introduce any essential differences when compared to an injection of energy by a vibrating wall.

2. Dynamical regimes

In the one component case the dynamical system is described by the proportion of particles on the left

$$n^{\mathrm{L}}(t) \equiv \frac{N^{\mathrm{LEFT}}(t)}{N}.$$

It is known that when γ is decreased a transition occurs [5]. That is, for $\gamma > \gamma^*$ on average the particles distribute themselves uniformly over the two compartments: $n^{\mathrm{L}}(t) = 1/2$ and for $\gamma < \gamma^*$, one of the compartments gets denser, leading to an asymmetric stationary solution $n^{\mathrm{L}}(t) \neq 1/2$. This symmetry breaking is entirely due to the inelastic coupling between density and temperature explained in the introduction. For a binary granular fluid other key features come into play. Indeed, when granular media are shaken, particles of different sizes tend to separate vertically [8,9]. Moreover, the system exhibits non equipartition of energy (i.e., the mean energy of the different species is different [10]) and as we will see below this is reflected by a difference in the granular temperature for each kind of particles. The coupling of these phenomena with the horizontal spatial instability described above leads to a surprising new phenomenon, namely the emergence of an oscillatory regime. In the following, the state of the system is characterized by two dynamical variables: the proportions of small ($n_1^{\mathrm{L}}(t) = N_1^{\mathrm{LEFT}}(t)/N_1$) and big ($n_2^{\mathrm{L}}(t) = N_2^{\mathrm{LEFT}}(t)/N_2$) particles on the left, respectively. In our simulations we identified three well-defined regimes, separated by the critical values γ^* and γ^{**}, with $\gamma^* > \gamma^{**}$ (Fig. 2):
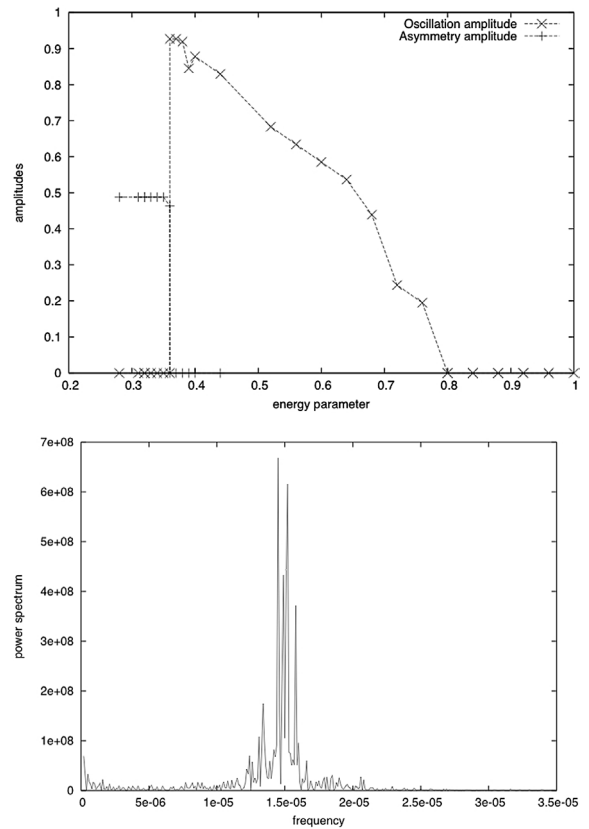

Fig. 2. In the upper figure, bifurcation diagram obtained from event-driven simulations, as a function of the energy parameter γ. The amplitudes are the oscillation amplitude, characterizing the oscillation regime and an asymmetry amplitude, defined by $A_{\mathrm{Asym}} \equiv \langle |n(t) - \frac{1}{2}| \rangle$, which characterizes the asymmetric regime. In the lower figure, discrete Fourier transform of the autocorrelation of the signal in the periodic regime ($\gamma = 0.48$) calculated for long runs (5×10^8 collisions).

- *Stationary homogeneous regime* ($\gamma > \gamma^*$). If the shaking of particles is vigorous enough, the particles are uniformly distributed over the two compartments. In this regime, which has been also observed for a case of a monodispersed distribution of particles, the system homogenizes like a classical elastic fluid: $n_1^{\mathrm{L}}(t) \approx 1/2$ and $n_2^{\mathrm{L}}(t) \approx 1/2$. The stability of this solution has been corroborated by simulations with different initial conditions.
- *Periodic regime* ($\gamma \leqslant \gamma^*$). When γ is decreased below the critical value γ^*, i.e., when the energy input is lowered, a new behavior appears: the two

densities of particles evolve periodically in time with the same frequency but separated by a phase delay (Fig. 3). This is what we call a granular clock. The mechanism behind these oscillations is the following: suppose one starts the experiment with the small discs in box L and all the large discs in box R (Fig. 1(a)). Initially, the net flux of the small discs is directed towards the compartment of the large discs (Fig. 1(b)) since the latter suffer more collisions (the collision frequency is proportional to the diameter) and dissipate more energy, favouring the clustering instability. Progressively, the small discs accumulate in the box R and consequently a vertical segregation takes place. Our simulations show that the large discs are pushed upwards in the box (Fig. 1(c)). This vertical asymmetry, in the box R, increases the probability of escaping of the large discs and diminishes the probability of escaping of the small discs. This will induce a flow of large discs towards the box L, while small discs continuing to flow from L towards R. Hence, most of the large discs finish in box L and box R becomes richer on small discs (Fig. 1(d)). This situation is the opposite of the initial condition. Then, the whole process reverses and the initial state is recovered by the same mechanism. Hence, one oscillation has been taken place. Obviously, the motion of large discs drives the oscillation and this may explain the observed phase delay between the two signals. The power spectrum for long time runs of this regime consists of a well-defined peak (Fig. 2) surrounded by smaller peaks. When γ is decreased below the threshold γ^*, the size of the small peaks increases with respect to the main peak. The fact that this effect increases with the distance to the bifurcation point seems to indicate that some non-resonant intrinsic nonlinearities start to play a relevant role. This property has been also observed in the solutions of the model proposed in the next section. It is important to point out, that in our simulations the mean energy of the large discs is lower than the small ones, as reported by Wildman and Parker for a binary system of grains [10].

- *Stationary asymmetric segregated regime* ($\gamma < \gamma^{**}$). Finally, when the input energy is lowered further a stationary asymmetric state appears characterized by a horizontal symmetry breaking. Initially, the system behaves as in the periodic regime but in this case the input energy is reduced and the number of large discs which escape from the box R is not large enough to launch the oscillation. As long as the vertical segregation takes place, small discs get trapped below the large discs in box R, in such a way that only large discs can flow from box R to box L. Hence, an asymptotic steady state is reached in which box L is mainly composed of large discs. It is interesting to mention that Barrat and Trizac [11] have already observed such stationary asymmetric state for a binary Maxwell Demon simulation without gravity.

The succession of the above regimes is summarized in the bifurcation diagram of Fig. 2. In addition to the regimes described above we also observed a transition regime characterized by intermittent oscillations between the two opposite steady asymmetric steady states. This regime, which appears near the transition between the periodic and the asymmetric states, may be associated to the action of the internal noise on the dynamics of the macroscopic variables near the phase transition. One should note that the intermittent regime complicates the study of the second transition and does not allow a clear determination of the system frequency at that point. Nonetheless, results obtained from the theoretical model proposed in the next section seem to indicate that the frequency at the transition point goes abruptly to zero.

3. Model

In this section we introduce a simple empirical system of dynamical equations reproducing qualitatively well the regimes observed in the above described simulations. The formulation has been inspired by a model proposed by Eggers [4] for the Maxwell Demon experiment with only one of disc diameter composition. By using a hydrodynamic approach Eggers was able to find, under certain approximations, an expression for the escaping rate from one compartment in terms of the proportion of particles in the considered compartment only. If n denotes the proportion of particles, in say the left compartment, then its time evolu-

tion can be written as:

$$\frac{\partial n}{\partial t} = -nF(n) + (1-n)F(1-n),$$

where the escape rate per particle, $F(n)$, is a decreasing function for large values of n. This feature represents the typical granular effect that in high density regions the average kinetic energy is reduced by the number of inelastic collisions, leading to a reduction of the escaping rate. In the right-hand side appears a loss term, the escaping flux, and a gain term which has the same functional structure as the gain term but in this case it depends on $(1-n)$, the proportion of particles in the right compartment. This last point guarantees the existence of a steady homogeneous solution; $n = 1/2$. In fact, the steady state condition leads to three stationary solutions: the homogeneous one and two asymmetric configurations that are in good quantitative agreement with numerical simulations. These results are robust for a large class of functions $F(n)$.

Concerning the two-component problem described in the last section, we are looking for a model, as simple as possible, that can be able to reproduce the sequence of regimes obtained when decreasing the energy input, namely the homogeneous steady state, the oscillating regime and the asymmetric steady state. Given the inherent complexity of the system, we will only require in this work a qualitative agreement with simulations. For this, we define two variables in the left compartment; the proportions of small, n, and large, m particles. The corresponding proportions in the right half-box are $(1-n)$ and $(1-m)$, respectively. Here we assumed that the escape rate of the grains from the left half-box is of the form

$$F(n, m) = e^{-(n^2 + Rm^2)/A},$$

where A is a positive parameter representing the balance between energy input and inelasticity of collisions. This parameter decreases with the inelasticity ($A = \infty$, for elastic collisions). The positive parameter R describes the fact that the cross section of big particles is larger than for small particles (the cooling effect of the big particles is larger).

The vertical segregation phenomena is taken into account, qualitatively, by introducing two more dependent variables s_L and s_R describing the influence of segregation on the escaping rate in the left and right compartments, respectively. We assume that these

variables change the escape rate per particle. For example, in box L they reduce the escaping rate for small particles while they increase it for large particles. This last point is in agreement with the discussion of the previous section. By construction, the *segregation variables* vanish when there is no vertical segregation. The next step consists in assuming that these variables reach, respectively, the values nm and $(1-n)(1-m)$ asymptotically. This expression qualitatively reproduces the fact that there should be no segregation if a box is composed by only one component, while segregation effects should be maximum if there are as many small and large particles in the box. It is important to point out that the supplementary variables s_L and s_R have no direct physical interpretation, they are formal variables used to mimic the segregation effects observed on the dynamics of the system. In our formulation these variables are necessary to reproduce the observed phenomenology. By considering all the points described in this section the modeling equations can be written as:

$$\frac{\partial n}{\partial t} = -nF(n, m)(1 - s_L)$$
$$\qquad + (1-n)F(1-n, 1-m)(1 - s_R),$$
$$\frac{\partial m}{\partial t} = -mF(n, m)(1 + s_L)$$
$$\qquad + (1-m)F(1-n, 1-m)(1 + s_R),$$
$$\frac{\partial s_L}{\partial t} = -\lambda(nm - s_L),$$
$$\frac{\partial s_R}{\partial t} = -\lambda\big((1-n)(1-m) - s_R\big). \qquad (2)$$

The parameter λ in the two last equations introduces the relaxation time of the segregation mechanism. By construction, the symmetric regime ($n = \frac{1}{2}$, $m = \frac{1}{2}$) is always a solution of the dynamics of the system. The dynamical equations (2) have been solved numerically and they exhibit the three regimes observed by our event-driven simulation. In Fig. 4 is depicted the bifurcation diagram obtained for the model which as can be seen is very similar to the one obtained by event-driven simulations (Fig. 3). It is important to point out that other functional dependences for the escaping rate of the discs have been tested and indeed they did not show qualitative differences. For complementarity, in our analysis we introduced an additive noise into Eq. (2) and some features of the simulations that were not observed in the deterministic model
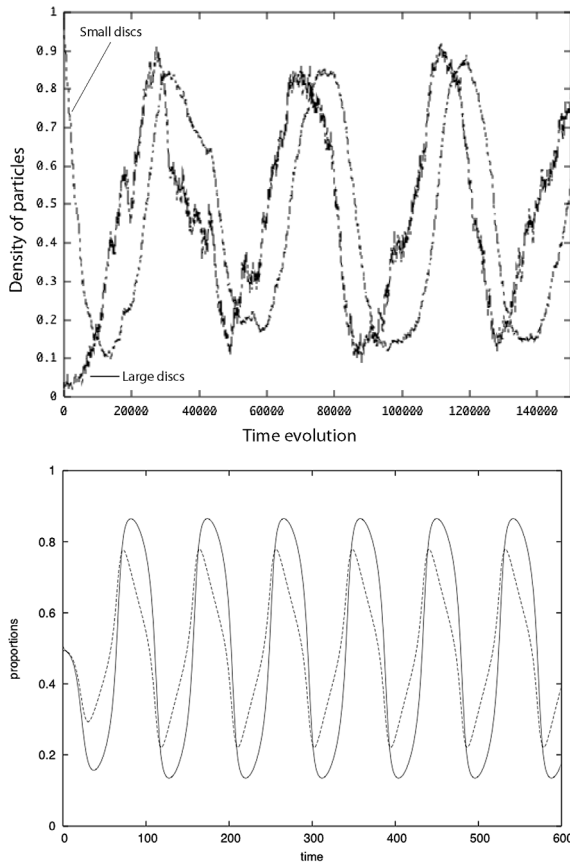
Fig. 3. Typical time evolution of the densities in the periodic regime, respectively, for the simulations ($\gamma = 0.58$) and for the proposed model ($\lambda = 0.1$, $R = 3.0$, $A = 1.67$).

Fig. 4. (a) Bifurcation diagram for the modeling equations [4], for $\lambda = 0.1$, $R = 3.0$. (b) Phase diagram, $\lambda = 0.1$.

are accessed. Namely, the intermittent regime and the presence of satellite peaks around the frequency of the deterministic oscillations. One must keep in mind that, although the proposed model is relatively simple, it has been formulated by adapting the escaping rate proposed by Eggers for a binary mixture of disc.

4. Conclusions

A Maxwell Demon experiment composed by a binary mixture of grains with two different diameters has been studied by means of event-driven simulations. It has been found that the phenomenology of this system is richer than the case of single diameter grain case. In the former case we found a symmetric steady state,
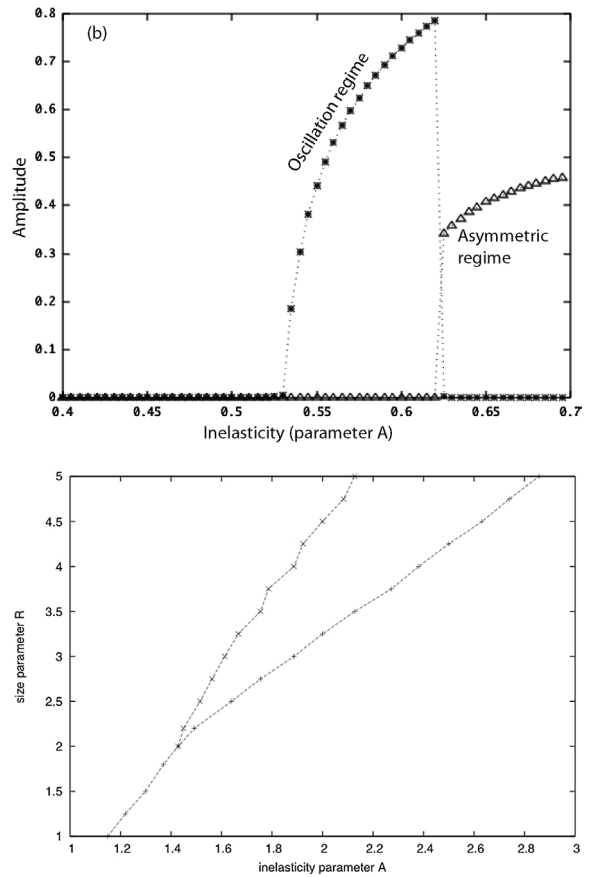
an oscillatory regime, an intermittent behavior and a stationary asymmetric regime featuring grain segregation. We have performed simulations over a wide range of parameters values for constructing the bifurcation diagram and for deducing accurately the power spectrum of the system. The observed oscillation phenomenon is mainly due to the combination of two typical granular effects; a vertical segregation with large particles above the smaller ones and the horizontal instability related to the clustering effect. Moreover, we have proposed a qualitative model for studying binary mixtures of grain inspired on the model proposed in [4] for the experiment with only one species of discs. In order to recover the phenomenology obtained by the simulations, we have introduced into our proposition a segregation mechanism through two new variables. The numerical integration and the linear stabil-

ity analysis of our dynamical model (Eq. (2)) showed its excellent ability to reproduce the major dynamical features obtained by simulations, namely, (a) transition from a symmetric regime to an oscillation regime (Hopf bifurcation) characterized by a delay between the signal of the small and the large discs, (b) passage from the oscillation regime to an asymmetric steady regime.

It worthwhile to remain that binary demon experiments have been already performed by Van der Weele et al. [5]. Even when these authors do not observed an oscillatory segregation regime (granular clock) they suggested, based on their experimental results, that the key factor leading to an horizontal segregation instability may be the difference on the disk radii. In our simulations the radius ratio used was relatively large (8.0 and 4.0). This last may lead to think that the observed dynamics may be restricted to a particular set of parameters. Nonetheless, both our simulations and our modeling equations reproduce undoubtedly the major dynamical features observed by experiments [12] and the results reported by Barrat and Trizac for a binary mixture of grains (without gravity). Recent numerical simulations developed by Marconi [13] seem to corroborate the existence of the granular clock. Presently, we are working on a reformulation of our system of equations (Eq. (2)) which will allow to represent both the horizontal and vertical segregation in such a way that it permits to measure experimentally the parameters associated to the segregation mechanisms. The results of the last approach will be presented in a forthcoming paper.

References

[1] H.M. Jaeger, S.R. Nagel, R.P. Behringer, Rev. Mod. Phys. 32 (1996) 1259.
[2] I. Goldhirsch, G. Zanetti, Phys. Rev. Lett. 70 (1993) 1619.
[3] H.J. Schlichting, V. Nordmeier, Math. Naturwiss. Unterr. 49 (1996) 323.
[4] J. Eggers, Phys. Rev. Lett. 83 (1999) 5322.
[5] K. Van der Weele, D. Van der Meer, M. Versluis, D. Lohse, Europhys. Lett. 53 (2001) 328.
[6] J. Brey, F. Moreno, R. Garca-Rojo, M.J. Ruiz-Montero, Phys. Rev. E 65 (2001) 011305.
[7] S. Luding, E. Clément, A. Blumen, J. Rajchenbach, J. Duran, Phys. Rev. E 49 (1994) 1634.
[8] A. Rosato, K.J. Strandburg, F. Prinz, R.H. Swendsen, Phys. Rev. Lett. 58 (1987) 1038.
[9] D.C. Hong, P.V. Quinn, S. Luding, Phys. Rev. Lett. 86 (2001) 3423.
[10] R.D. Wildman, D.J. Parker, Phys. Rev. Lett. 88 (2002) 064301.
[11] A. Barrat, E. Trizac, Mol. Phys. 101 (2003) 1713.
[12] R. Mikkelsen, D. Van der Meer, K. Van der Weele, Phys. Rev. Lett. 89 (2002) 214301.
[13] U.M.B. Marconi, private communication. We were aware of the studies from Marconi after we have written the present Letter.