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LETTER TO THE EDITOR

Why shape matters in granular compaction

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Abstract

We present a stochastic model of dynamically interacting grains in one dimension, in the presence of a low vibrational intensity, to investigate the effect of shape on the statics and dynamics of the compaction process. Regularity and irregularity in grain shapes are shown to be centrally important in determining the statics of close-packing states, as well as the nature of zero- and low-temperature dynamics in this columnar model.

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The fact that shape matters crucially in the efficient packing of objects is an everyday experience. Coffee grains can be shaken into a closely packed state far more readily than marbles, where necks and pores remain even in the most ordered state. This letter is devoted to a simple stochastic dynamical model in one dimension, demonstrating the effect of shape in closely packed systems, such as glasses or densely packed granular media; see [1] for a review, and [2] for recent investigations of lattice models of granular systems. A more general version of the model, where lattice sites can be empty, has been described elsewhere [3, 4]. The present model, and some of its generalizations, will be investigated in more detail in [5].

1. The model

Our model consists of a column of N sites, each of which is occupied by a grain. Grains are indexed by their depth $n = 1, \dots, N$, measured from the top of the column. Grains are assumed to be anisotropic in shape. They take, for simplicity, two possible orientations, referred to as ordered and disordered. We define orientation variables by setting $\sigma_n = +1$ if grain number n is ordered, and $\sigma_n = -1$ if grain number n is disordered. A configuration of

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the system is uniquely defined by the N orientation variables $\{\sigma_n\}$. While ordered grains are perfectly packed, disordered grains are imperfectly packed. Each disordered grain leaves a void space ε on the site it inhabits.

Non-trivial dynamical interactions between the grains are such as to minimize the void space locally. These lead to frustration between competing grain orientations which seek to minimize interstitial voids. Under the influence of a dimensionless vibration intensity Γ , this system undergoes cooperative reorganizations reminiscent of glassy dynamics [6]. From a phenomenological point of view, we model the above by a stochastic dynamics, defined by the following transition rates per unit time:

$$\begin{cases} w_n(\sigma_n = + \rightarrow \sigma_n = -) = \exp(-n/\xi_{\text{dyn}} - h_n/\Gamma) \\ w_n(\sigma_n = - \rightarrow \sigma_n = +) = \exp(-n/\xi_{\text{dyn}} + h_n/\Gamma). \end{cases} \quad (1)$$

The dynamical rules (1) fully define the model. In these formulae, Γ is a dimensionless measure of the vibration intensity, which will also be referred to as temperature. The dynamical length ξ_{dyn} is a phenomenological parameter which controls the spatial dependence of dynamical behaviour [5]. (In earlier work [3] ξ_{dyn} was shown to determine the extent to which order propagates down the column in the glassy regime, a perspective that is maintained here.) Finally, and most importantly, the ordering field h_n acting on the orientation σ_n of grain number n is *compacting* (see later); it reads

$$h_n = \varepsilon m_n^- - m_n^+ \quad (2)$$

where m_n^+ and m_n^- are the numbers of ordered and disordered grains, respectively, above the grain number n

$$m_n^+ = \frac{1}{2} \sum_{k=1}^{n-1} (1 + \sigma_k) \quad m_n^- = \frac{1}{2} \sum_{k=1}^{n-1} (1 - \sigma_k) \quad (3)$$

so that $m_n^+ + m_n^- = n$. Hence h_n represents the excess void space [7] of the system. Equation (2) shows that a transition from an ordered to a disordered state for grain number n is *hindered* by the number of voids that are already above it, i.e., it represents a compacting dynamics. Our model is thus fully directed in time and space; the orientation of a given grain only influences the grains below it and at later times. The free surface of such a system under vibration could be expected to have maximal mobility; the free volume generated by vibration [8] would decrease with increasing depth in the column.

In the limit of a vanishing vibration intensity ($\Gamma \rightarrow 0$), the probabilistic rules (1) become the following deterministic updating formula

$$\sigma_n \rightarrow \text{sign } h_n = \text{sign } (\varepsilon m_n^- - m_n^+) \quad (4)$$

provided $h_n \neq 0$ (see below).

2. Statics

Ground states are defined as being the configurations such that the static counterpart of (4)

$$\sigma_n = \text{sign } h_n = \text{sign } (\varepsilon m_n^- - m_n^+) \quad (5)$$

holds for all grains $n = 1, \dots, N$. In other words, in a ground state each orientation σ_n is aligned along its local field h_n .

We mention for completeness that the case $\varepsilon < 0$ is a generalization of earlier work [3], with a complete absence of frustration and a single ground state of ordered grains. In the

present situation ($\varepsilon > 0$), a rich ground-state structure is achieved, because of frustration [9], whose nature depends on whether ε is rational or irrational. The rotation number

$$\Omega = \varepsilon/(\varepsilon + 1) \quad (6)$$

fixes the proportions of ordered and disordered grains in the ground states, $f_+ = \Omega$, $f_- = 1 - \Omega$, and their difference $\langle \sigma_n \rangle = f_+ - f_- = 2\Omega - 1$ can be seen as a spatially averaged ‘magnetization’.

- For irrational ε , equation (2) implies that all the local fields h_n are non-zero. A unique quasi-periodic ground state is thus generated [5], which can be constructed by the cut-and-project method, along the lines of a geometrical approach developed for quasi-crystals [10]. The local fields h_n lie in a bounded interval $-1 \leq h_n \leq \varepsilon$.
- For rational $\varepsilon = p/q$, with p and q mutual primes, $\Omega = p/(p + q)$, and some of the h_n can vanish. The equation $h_n = 0$ means that grain number n has a perfectly packed column above it, so that it is free to choose its orientation. For $\varepsilon = 1/2$, for example, we can visualize that each disordered grain carries a void half its size, so that units of perfect packing must be permutations of the triad $+ - -$, where the two half voids from each of the $-$ grains are filled by the $+$ grain. The dynamics selects two of these patterns, $+ - -$ and $- + -$. More generally, orientational indeterminacy occurs at points of perfect packing such that n is a multiple of the period $p + q$. Each ground state is a random sequence of two patterns of length $p + q$, each containing p ordered and q disordered grains. The model therefore has a zero-temperature configurational entropy (or ground-state entropy) per grain:

$$\Sigma = \ln 2/(p + q). \quad (7)$$

Associating (ir)regular grains with (ir)rational void spaces, this has the appealing physical interpretation that irregularities in grain shapes lead to a unique state of close packing (such that all jagged edges are well meshed together), while regular grains have a huge degeneracy of such states (as in the fabled greengrocer problem [11]).

3. Zero-temperature dynamics

We now turn to the zero-temperature dynamics (4), starting with a disordered initial configuration.

- For irrational ε , the application of this dynamics causes the quasi-periodic ground state to be recovered downwards from the top of the column. The depth of the ordered boundary layer grows ballistically with time:

$$L(t) \approx V(\varepsilon)t. \quad (8)$$

The velocity $V(\varepsilon) = V(1/\varepsilon)$ varies smoothly with ε , and diverges as $V(\varepsilon) \sim \varepsilon$ for $\varepsilon \gg 1$ [5]. The rest of the system remains in its disordered initial state. When $L(t)$ becomes comparable with ξ_{dyn} , the effects of the free surface begin to be damped. In particular, for $t \gg \xi_{\text{dyn}}/V(\varepsilon)$ we recover the logarithmic coarsening law $L(t) \approx \xi_{\text{dyn}} \ln t$, observed in related work [3, 12] to model the slow dynamical relaxation of vibrated sand [13].

- For rational ε , as mentioned above, the local field h_n may vanish. The corresponding orientation is updated according to $\sigma_n \rightarrow \pm 1$ with probability $1/2$, leading to a dynamics which is stochastic even at zero temperature. Here, even the behaviour well within the boundary layer ξ_{dyn} contains many intriguing features, while the dynamics for $n \gg \xi_{\text{dyn}}$ again takes place on a logarithmic scale [5]. We therefore focus on the limit $\xi_{\text{dyn}} = \infty$.

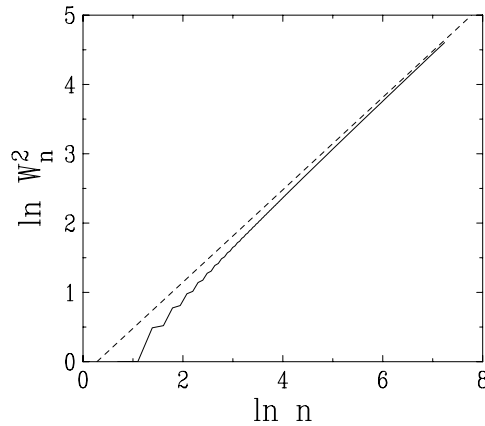


Figure 1. Log–log plot of $W_n^2 = \langle h_n^2 \rangle$ versus depth n , for zero-temperature dynamics with $\varepsilon = 1$: full line, numerical data; dashed line, fit of asymptotic behaviour, leading to equation (9).

The main result is that zero-temperature dynamics does not drive the system to any of its degenerate ground states. The system instead shows a fast relaxation to a non-trivial steady state, independent of its initial condition. The local fields h_n have unbounded fluctuations in this steady state, which are reminiscent of the density fluctuations about the mean packing fraction observed in granular systems [13, 14], especially around the so-called random close packing density [7, 15], which is the highest density achievable in practice by extensive dynamical processes.

Figure 1 demonstrates the anomalous roughening law

$$W_n^2 = \langle h_n^2 \rangle \approx An^{2/3} (A \approx 0.83). \quad (9)$$

The local fields h_n are approximately Gaussian distributed. The following scaling argument explains the observed roughening exponent $2/3$. Let h_n be the position of a fictitious random walker at time n . The noise in this random walk originates in the sites $m < n$ where the local field h_m vanishes. It is therefore proportional to $\sum_{m=1}^{n-1} \text{Prob}\{h_m = 0\}$, hence the consistency condition $W_n^2 \sim \sum_{m=1}^{n-1} 1/W_m$, yielding the power law (9). A more detailed derivation will be given in [5]. Roughly speaking, the walker obeys a diffusion equation, with a diffusion constant scaling as the inverse distance to its starting point. This is reminiscent of the domain-growth mechanism in the low-temperature coarsening regime of the Ising chain with Kawasaki dynamics [16]; the power law $L(t) \sim t^{1/3}$ for the mean domain size (analogous to $W_n \sim n^{1/3}$) can be understood from the picture of diffusing domains, whose diffusion constant scales as the inverse of their length. The anomalous roughening law (9) is the most central feature of the zero-temperature steady state observed for rational ε .

If the grain orientations were statistically independent, i.e., uncorrelated, we would have the simple result $\langle h_n^2 \rangle = n\varepsilon$, while equation (9) implies that $\langle h_n^2 \rangle$ grows much more slowly than n . Orientational displacements are thus fully anticorrelated. More precisely, figure 2 shows that the orientation correlations $c_{m,n} = \langle \sigma_m \sigma_n \rangle$ scale as [5]

$$c_{m,n} \approx \delta_{m,n} - \frac{1}{W_m W_n} F\left(\frac{n-m}{W_m W_n}\right). \quad (10)$$

The scaling function F is even, positive, and it obeys $\int_{-\infty}^{+\infty} F(x) dx = 1$, expressing that spin fluctuations are asymptotically totally screened (i.e., fully anticorrelated). This is similar to the bridge collapse seen in displacement–displacement correlations of strongly compacting

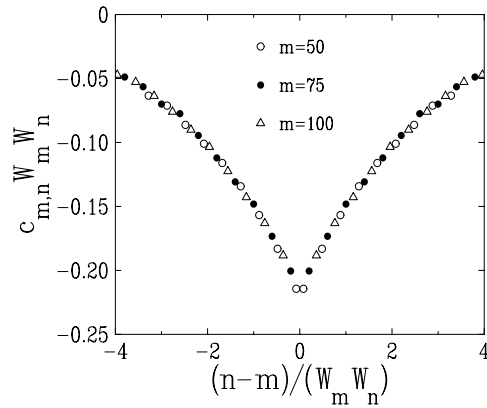


Figure 2. Scaling plot of the orientation correlation function $c_{m,n}$ for $n \neq m$ in the zero-temperature steady state with $\varepsilon = 1$, demonstrating the validity of equation (10), and showing a plot of (minus) the scaling function F .

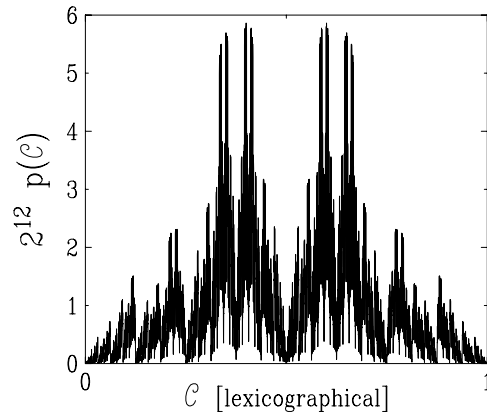


Figure 3. Plot of the normalized probabilities $2^N p(C)$ of all the configurations in the zero-temperature steady state for $N = 12$ and $\varepsilon = 1$, against the configurations C sorted lexicographically.

grains [14]; grain orientational displacements in the direction of vibration were there seen to be strongly anticorrelated in jammed regions, as each grain tried to collapse into the void space trapped by its neighbours. We remark that temporal anticorrelations have also been observed in recent experiments investigating the properties of cages near the colloidal glass transition [17]. Interestingly, correlations transverse to the shaking direction were found to be rather small [14], thus, in self-consistency terms justifying the choice of a column model in the present case.

Figure 3 shows a plot of the normalized probabilities $2^N p(C)$ of all the configurations C in the zero-temperature steady state of a system with $N = 12$ grains and $\varepsilon = 1$, directly measured in a very long simulation. The probabilities are plotted against the $2^{12} = 4096$ configurations, sorted lexicographically (read down the column). This plot exhibits a rugged structure on this microscopic scale; some configurations are clearly visited far more often than others. We suggest that this behaviour is generic, i.e., the dynamics of compaction in the jammed state

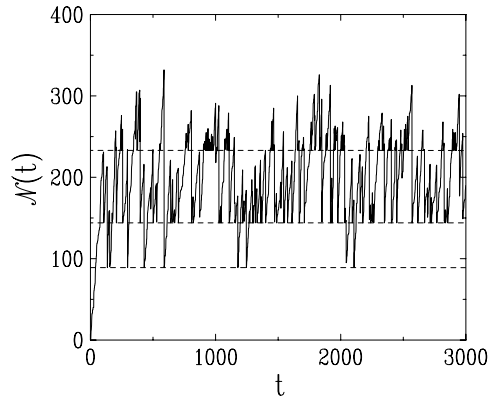


Figure 4. Plot of the instantaneous depth $\mathcal{N}(t)$ of the ordered layer, for $\varepsilon = \Phi$ (the golden mean) and $\Gamma = 0.003$. The dashed lines denote leading nucleation sites given by Fibonacci numbers, from bottom to top, $F_{11} = 89$, $F_{12} = 144$, and $F_{13} = 233$.

leads to a microscopic sampling of configuration space which is highly non-uniform. In spite of this fine structure, the steady-state entropy

$$S = - \sum_{\mathcal{C}} p(\mathcal{C}) \ln p(\mathcal{C}) \quad (11)$$

is not far from the estimate $S_{\text{flat}} = N \ln 2$ along the lines of Edwards' flatness hypothesis [18]. Indeed, for $N = 12$ (data of figure 3), we have $S = 7.839$ against $S_{\text{flat}} = 8.318$. In other words, the entropy reduction [19] $\Delta S = S_{\text{flat}} - S = 0.479$ is small, compared to the absolute value of the entropy per grain.

4. Low-temperature dynamics

Low-temperature dynamics induces drastic changes in the case of ε irrational. (Since zero-temperature dynamics remains stochastic in the rational case, we do not expect low-temperature dynamics to introduce qualitative differences there.) For a low but non-zero Γ , there will be a few mistakes, i.e., orientations which are not aligned with their local field according to equation (5). The *a priori* probability of observing a mistake at site n scales as

$$\Pi(n) \sim \exp(-2|h_n|/\Gamma). \quad (12)$$

Hence the sites n so that $|h_n| \sim \Gamma \ll 1$ will be preferred nucleation sites for mistakes, and thus dominate the low-temperature dynamics. It turns out that those sites are such that $n\Omega$ is close to an integer. The magnitude of the excess void space is least here, leading to the least cost for a misalignment.

Choosing the golden mean $\varepsilon = \Phi = (\sqrt{5} + 1)/2$ for concreteness, the preferred nucleation sites are given by the Fibonacci numbers: $n = F_k \approx \Phi^k/\sqrt{5}$. Then $\Pi(F_k) \sim \exp(-2\Phi^2/(\sqrt{5}\Gamma F_k))$. Let us denote the instantaneous position of the uppermost mistake by $\mathcal{N}(t)$. This depth divides an upper boundary layer, ordered in the quasi-periodic ground state, from a disordered lower zone, characterized by the anomalous roughening law (9). The mistake is itself advected ballistically with velocity $V(\Phi) \approx 2.57$, just as with zero-temperature dynamics, until another mistake is nucleated above it.

Figure 4 shows a typical sawtooth plot of the instantaneous depth $\mathcal{N}(t)$, for a temperature $\Gamma = 0.003$. The ordering length $\langle \mathcal{N} \rangle$ is expected to diverge at low temperature, as mistakes

become more and more rare. From a more quantitative point of view, the most active Fibonacci site F_k is such that the nucleation time $1/\Pi(F_k)$ is comparable to the advection time to the next nucleation site F_{k+1} . This yields

$$\langle \mathcal{N} \rangle \sim 1/(\Gamma |\ln \Gamma|). \quad (13)$$

The ordering length therefore diverges linearly at low temperature, up to a logarithmic correction. A similar law is predicted for all the irrational values of ε with typical Diophantine properties [5]. This mechanism, where mistakes appear at preferred nucleation sites, is reminiscent of the phenomenon of hierarchical melting observed in incommensurate modulated solids [20].

Both $\langle \mathcal{N} \rangle$ and ξ_{dyn} retain the flavour of a boundary layer separating order from disorder. Within each of these boundary layers, the relaxation is fast, and based on single-particle relaxation, i.e., individual particles attaining their positions of optimal local packing [12, 14]. The slow dynamics of cooperative relaxation only sets in for lengths beyond these, when the lengths over which packing needs to be optimized become non-local. This in turn leads, as in reality [7], to hysteresis, i.e., a dependence on the initial state of the packing.

Remarkably, all of these features were obtained at a qualitative level in the glassy regime of a much simpler model [3]. On the one hand, this allows us to speculate that the shape-dependent ageing phenomena seen there could be retrieved here, i.e., that conventional ageing phenomena would only be seen for irregular grains (irrational ε). On the other hand, it is tempting to ask if the directional causality of the dynamical interactions present in this model and the earlier one [3] could be responsible for their qualitative similarity, and thus be a necessary ingredient for modelling glassiness.

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