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RELAXATION TIME IN WET GRANULAR 2D SYSTEMS OF NONSPHERICAL PARTICLES

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Abstract. We apply the genetic algorithms - search procedures, to study the relaxation process in two-dimensional wet granular medium of non-spherical grains. We examine the equilibration of granulates under so-called tap dynamics and examine the dependence of relaxation times on system topology and on boundary conditions. Numerical computation are performed in the framework of genetic algorithm for sizes up to $N = 200^2$ sites.

1. Introduction

The behaviour of granular materials is of great technological interest. Especially, the granular materials are widely encountered in pharmaceuticals and agricultural products. Unfortunately, the basic physical understanding of granular media is not yet complete. Due to such complex phenomena as: disorder, pattern formation, threshold dynamics or segregation there is no strong theoretical approaches to the granular systems. Therefore, simplified models and computer modelling has come to play an important role in attempting to understand the nature of granular matter.

The mechanical behaviour of granular materials has been largely studied in the framework of continuous models treating granular flows as hydrodynamic field of particles. On the other hand, the investigation of the materials at the grain scale using discrete element modelling provides a valuable description of many micro--mechanical aspects of granular state of matter.

If one adds a wetting liquid to a granulate, there occur capillary bridges which exert forces on the particles. These forces are the main reason for the strongly changed mechanical properties of wet granular matter compared to the dry case. Since the formation of he liquid bridges strongly depends on the microscopic geometry of granulate an appropriate description of the packing is essential. According to experimental and theoretical investigations [1] an average bridge number varies from $n \approx 3.3$ to $n \approx 4.7$ par site, in order to maintain respectively, the loose or dense packing of an ensemble of horizontally shaken glass beads at water contents of ≈0.2%. Thus, we examine triangular, square and hexagonal 2D lattices with the site - coordination numbers equal to 6, 4 and 3, respectively to cover the range of possible number of interactions between neighbouring grains.

The local, on-site physical properties randomly change from site to site in order to represent different beads arrangements and we employ the spin - glass concept to describe such local random properties. So, the system is characterized by the following energy functional:

$$E\{\varepsilon_{ij}\} = -\sum_{i \neq j} (\varepsilon_{ij} S_i S_j - 1) \tag{1}$$

The sum runs over all pairs nearest neighbours and $\varepsilon_{ij} = \pm 1$ are quenched random numbers, characterized the local random interactions, established via capillary bridges, between grains at sites i and j. $i,j = 1,2,...,L$. Here, we restrict our analysis to ellipsoidal grains. They can have two possible onsite orientations: in plane or vertical, so their states can be characterized by an internal degree of freedom $S_i = \pm 1$. The grains are placed on vertices of a square, triangular or honeycomb lattice. The model consists of $N = L^2$ grains. We report results for L = 40, 60, 80, 100, 200, 300 and for open and periodic boundary conditions [4].

The behaviour of the disordered granulate is determined by the occurrence of geometrical frustration. Two nearest - neighbours grains can be freely oriented if they satisfy the interaction $\varepsilon_{ij} S_i S_j = 1$, otherwise they feel strong repulsion and they stay in an energetically costly configuration. The frustrated loops of grains are the same as frustrated loops in spin-glass magnets or in frustrated liquids of molecules with geometrical hindrance.

The aim of the present work is to analyze how the frustration slow down equilibration processes in wet dense granular ensembles.

2. Computational method and results

Our simulation are based on genetic programming. Genetic algorithms were pioneered by Holland [3], and have been used in diverse areas of science and technology, mainly in optimisation. The basic idea is to break up mathematical objects into their building blocks, and to use these blocks in the same way that nature uses genetic material and chromosomes to evolve ever fitter individuals. The processes of natural selection and survival of the fittest tend to make suitable blocks of objects combine with other useful blocks, while useless parts eventually disappear.

We combine genetic algorithm evolution with Monte Carlo philosophy of acceptance of new generation with respect to the minimal energy of new and old generations. Each step is accepted with the usual Metropolis probability depending on the energy change according to functional (1). Specifically, we apply the modified genetic algorithm (modGA) with tournament selection. The structure of modGA is given in [5].

Formation of liquid bridges between a given pair of grains is a random phenomena and so, the strength and the nature of resulting effective forces between

particles are also random. If a granulate consists of non-spherical particles, their local arrangement will be disordered as is the case of generic spin glass systems, i.e. systems with quenched disorder and randomness. Quenched disorder is common to many condensed matter systems. Due to its presence in the systems the translational invariance is broken and common approaches relay on the introduction of replicas in order to re-establish this invariance. Slow, glassy - like equilibration due to the presence of many metastable states on large length scales is the main obstacle to the numerical and experimental study of disordered systems. Granular systems represent an important paradigm for the study on non-equilibrium stationary states. Due to the dissipative nature of the interactions, these systems have to be considered as open systems and therefore concepts from equilibrium thermodynamics cannot be applied in a straightforward way. Nevertheless, a 'granular temperature' can be defined in terms of the kinetic energy per particle and so-called tap dynamics replaces the scenario of conventional thermo-dynamical equilibration [2].

Relaxation process in granular systems resembles a process called 'aging', presents in glassy-like systems. Aging means a very slow evolution with time, called 'age', of the physical properties of the system.

To study this 'aging'-relaxation process, we record two types of one-time quantities: the energy density of the granulate and the Hamming distance between an instantaneous configuration and a configuration related to the energy minimum, presumably the global one.

In our picture an 'age' of a sample is identified with the sequence of populations produced by modGA. For each population, the number of 'flipped' grains is $r \times p_{mut} \times n_{pop} \times N$, where r - number of configurations selected to reproduction, p_{mut} - probability of mutation, n_{pop} - size of population, and $N = L \times L$ - size of the system. We used the numbers: $n_{pop} = 480$, $r = n_{pop}/3$, $p_{mut} = 0.0075$. Thus, from population to population at least $1.2N$ grains change its orientation (in contrary to few changes performed during a typical Monte Carlo or Simulated Annealing time step).

In Figure 1 we present an example of time evolution of minimal energy of modGA population of 480 samples. Typically, we take 500 generation for each realizations of frozen disorder given by effective interactions ε_{ij}, see Equation (1), and we average over 10 disorder realizations. As a result we obtain an approximation to the averaged minimal energy in the form

$$\ln\left\langle E_{\min}\left\{\varepsilon\right\}\right\rangle_{av} = \text{const} - t/\tau_R \tag{2}$$

where: τ_R is the relaxation time of averaged minimal energy configuration. We report calculated τ_R in Table 1.

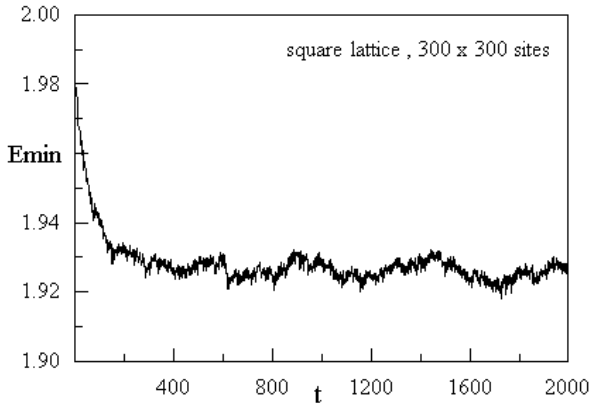

Fig. 1. Evolution of minimal energy of modGA-populations for some random realization of ε_{ij} (Equation (1)), for a square lattice with open boundary condition

Table 1. The relaxation times τ_R of systems with different geometries. L is the linear size of the systems and we used open and periodic boundary conditions

L	square open b.c.	square periodic b.c.	triangular open b.c.	triangular periodic b.c.	hexagonal open b.c.	hexagonal periodic b.c.
40	$2.5 \cdot 10^3$	$2.56 \cdot 10^3$	$3.3 \cdot 10^3$	$3.3 \cdot 10^3$	$2.1 \cdot 10^3$	$2{,}1 \cdot 10^3$
60	$5 \cdot 10^3$	$4.5 \cdot 10^3$	$5.7 \cdot 10^3$	$5.5 \cdot 10^3$	$3.6 \cdot 10^3$	$4 \cdot 10^3$
80	$6.2 \cdot 10^3$	$6.6 \cdot 10^3$	$8.3 \cdot 10^3$	$8.3 \cdot 10^3$	$5.5 \cdot 10^3$	$5.2 \cdot 10^3$
100	$7.8 \cdot 10^3$					
200	$19 \cdot 10^3$					

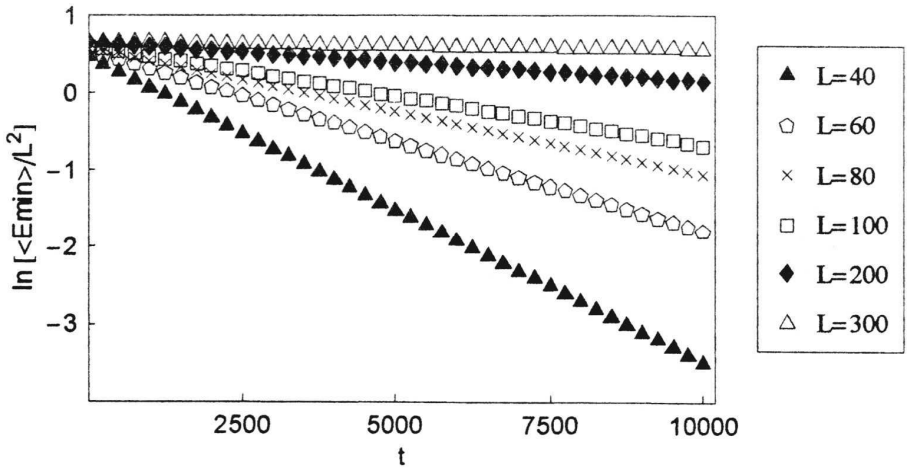

Fig. 2. Plot of $\ln\left\langle E_{\min}\left\{\varepsilon\right\}\right\rangle_{av} = \text{const} - t/\tau_R$, from Equation (2), for quadratic lattice with open boundary conditions and for different system's size

In Figures 2 and 3 we plot $\ln\left\langle E_{\min}\{\varepsilon\}/L^2\right\rangle_{av}$ resulting from Equation (2). We averaged the results over 10 realization of disorder $\{\varepsilon\}_{ij}$ for each considered geometry and size of system.

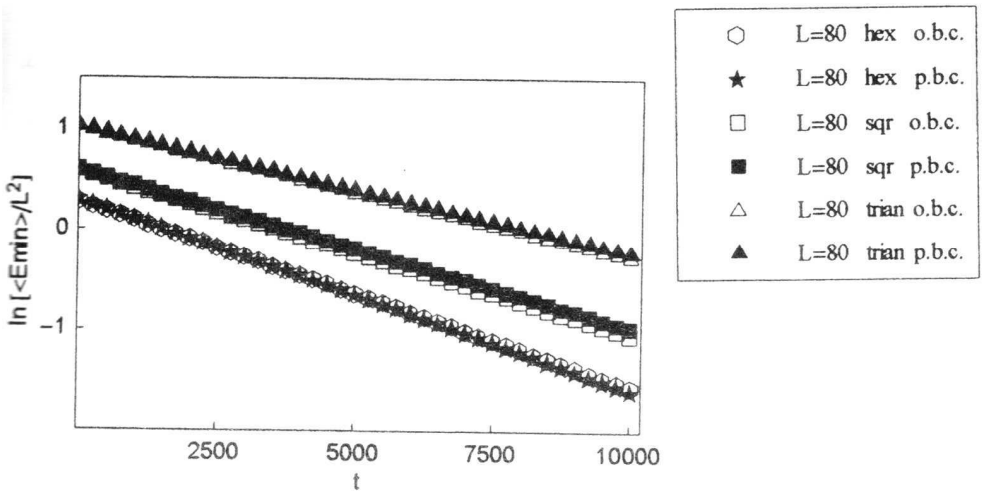

Fig. 3. Plot of $\ln\left\langle E_{\min}\{\varepsilon\}\right\rangle_{av}$, from Equation (2), for different geometry and boundary conditions, o.b.c. - means open boundary conditions, p.b.c. is for periodic boundary conditions, hex - honeycomb, train - triangular, sqr - square lattices

We also measured the Hamming distance (Δ_{Hamm}) between configurations with the lowest energy of a given population and the configuration which corresponds to the lowest energy within whole mod-GA evolution. Δ_{Hamm} between two configurations is the number of grains which differ in their orientation. This quantity serves as an auxiliary parameter to control the convergence of evolution.

3. Conclusions

In conclusion, we studied the evolution of two-dimensional granular system within tap dynamic, a model for horizontally shaken dense grains ensemble. By the calculation of relaxation time using genetic-algorithm-evolution scheme we find much quicker convergence of granulate to stationary metastable states than equilibration observed within picture generated by typical Monte Carlo dynamics. The main difference is due to massive, large scale of changes in grains configurations performed by selection, crossover and mutation operations during the genetic algorithm evolution compared to restricted scale of grain's rearrangements allowed by Monte Carlo dynamics.

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