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Thermal cycling leads grains to more homogeneous force networks and energy repartition

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ABSTRACT

With the help of molecular dynamics simulations of a realistic granular system, here it is first reported that thermal cycling is able to induce the total system energy to be reallocated to grains, and this makes grains gradually evolve to the energy equilibrium, especially under larger cyclic temperatures. At the same time, the stress in force chains (and on grains) will also get much relieved, and this does not need the decrease in applied pressure. Consequently, the statistical probability distribution of both internal particle forces and energy will become narrower around the most likely value, and their spatial distribution will also become more and more homogeneous. The primary cause behind the above phenomena is that grains within the initial granular system are not in sufficient energy equilibrium, and they were rearranged by thermal excitations to a new steadier packing where grains are closer to energy equilibrium. Besides, it was also observed that for the macroscopic-scale grains, the internal particle energy distribution within the granular system obeys a more general Maxwell-Boltzmann (M-B) distribution which has a more uniform distribution profile than the classical M-B distribution for gases, suggesting that the direct-contact collision may be a more effective channel for the energy interchange between particles than the indirect-contact collision. The results showed here demonstrate that more homogeneous energy reallocations may be a universal phenomenon for granular matter and may have important practical implications for the handling of granular materials.

1. Introduction

Granular materials widely exist in our nature, like sands, rocks and cereal grains. Due to their discrete nature, granular matter often shows the flow behaviors and therefore holds a rich set of unusual behaviors [1]. When a pressure is applied, particles within a granular system are under stress in addition to supporting the weight of the material above them. In the meantime, the filamentary structures, which are also called force networks (or force chains), will then be generated. It has been suggested that force chains are often highly nonhomogeneous in space [2, 3]. In another word, grains within the granular system are in highly different energy states. As the skeleton of granular matter [1, 4], force networks play the dominant role in stability [5], elasticity [6, 7], sound transmission [8, 9] and also thermal and electrical transport phenomena [10–13]. The simplest characterization of force networks is the probability distribution of internal forces within the system $P(F)$. In a typical granular packing, $P(F)$ has an exponential tail at large F, and a plateau at small F [14, 15]. It has been well known that, with the increase in external loads, force chains in granular matter will grow and extend continuously and become increasingly uniform in their appearance. This is not surprising since more and more particles will participate in burdening the load as applied pressure increases.

Just owing to their specific properties, granular materials are also applied in many industrial fields. For example, in fusion reactors the pebble beds, assemblies consisting of pebbles, have been determined as the form of tritium breeders (Li-based ceramics, like Li_4SiO_4 and Li_2O) and neutron multipliers (such as Be and BeO). For a long time, people were attempting to get a deeper insight into granular matter. Many investigations were concentrated on the force networks of static granular matter including their global structure and the probability distribution of internal contact forces [6, 14–21]. These works make people have a good knowledge of the general structure of internal forces inside a granular system. Besides, many researchers investigated the compaction dynamics behaviors of grains under the vibration, tapping, shear deformation and also thermal cycling [22–32], which tell us that the contacts between grains are quite fragile and can be easily destroyed by external mechanical and even thermal excitations.

Although some previous works on the heat transfer in granular systems [10, 33–37] and effect of thermal excitations on grains [29–32, 38,

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39] have been made, very little has yet studied the effect of thermal cycling on the granular system which are under the constant applied pressure. In the previous work [39], it has been observed that temperature changes will degenerate the force networks within a granular system and make their spatial distribution increasingly inhomogeneous. Later, however, we will see that the evolution laws of force networks and stress (energy) state of pebbles for the granular system which is exposed to the thermal cycling under the constant applied pressure are completely different from the situation where grains are not under the applied pressure. About the underlying mechanism, it has still remained elusive to us and needs to be known. As a matter of fact, in many cases granular materials are under pressure and also subjected to thermal excitations. For example, grain heaps on farms often undergo temperature changes from days to nights, so we want to know what would happen to grains, especially the ones at the bottom which are under much stress (in the high energy level). Also, it has been reported that fusion pebble beds are possibly subjected to the periodic mechanical and thermal loads during their practical operation [40], and we desire to predict how the stress (energy) state of pebbles which are under one constant pressure will evolve. These questions concern the evolutions of internal particle forces and energy within a granular system which is exposed to thermal cycling under the constant applied pressure. Moreover, it's known to us that for gases, their microscopic molecules' energy distribution obeys the classical Maxwell-Boltzmann (M-B) distribution. So it's attractive for us to explore the internal particle energy distribution inside a granular system, and we also want to know if there is a difference in the particle energy distributions between gases and the macroscopic-scale grains and the possible behind mechanism.

Recently, in our study it is first founded that thermal cycling is able to induce the fairer reallocations of the total energy of a granular system to grains, which lead grains to gradually evolve to the energy equilibrium. This finding may have important practical implications for the handling of granular materials, like the energy storage in a granular system.

2. Thermal particle dynamics

As we know, some statistical information, like the internal particle forces, and also the pattern of force networks within a granular assembly, are very hard to acquire for experiments [21, 30, 41]. The molecular dynamics simulations, which are also known as the discrete element method (DEM) in engineering, have been proved to be an effective tool to obtain these quantities [30]. In this study, DEM will also be used to solve our problem.

The equations describing particle motions in our DEM procedure are as follows:

Linear motion:

$$m_i \ddot{x}_i = m_i g + F_s \tag{1}$$

Angular motion:

$$I_i \ddot{\boldsymbol{\theta}}_{\boldsymbol{i}} = \sum \boldsymbol{M} \tag{2}$$

where $\ddot{\boldsymbol{x}}_{\boldsymbol{i}}$ and $\ddot{\boldsymbol{\theta}}_{\boldsymbol{i}}$ are respectively the linear and angular accelerations of the particle i. m_i and I_i are respectively the mass and inertia moment. $\mathbf{g}$ is the gravitational acceleration. $\boldsymbol{F}_{\boldsymbol{s}}$ and $\sum \boldsymbol{M}$ are the resultant surface force (contact force) and moment, respectively.

Instead of some complex contact models for elastoplastic and plastic spheres [42, 43], in this study the accurate and efficient nonlinear Hertz-Mindlin contact model [44] was selected to characterize the elastic contact behavior between perfect particles. At the contact surface, the normal and tangential contact forces are as follows:

Normal force:

$$\mathbf{F_n} = -\mathrm{k_n}\boldsymbol{\delta}_{\mathbf{n}}^{3/2} \tag{3}$$

Tangential force:

$$F_t = -k_t \delta_t \tag{4}$$

where $\boldsymbol{\delta}_{\boldsymbol{n}}$ and $\boldsymbol{\delta}_{\boldsymbol{t}}$ are the vectors of normal and tangential deformation, respectively. k_n and k_t are respectively the normal and tangential spring constant.

In DEM simulations, the transition to sliding for a contact is the key incident that determines whether the real behaviors of a granular system could be successfully described. In the current study, the sliding of a contact will occur when the Coulomb friction law is satisfied: $F_t = \mu \mathrm{F_n}$, where μ is the coefficient of static friction, and F_n and F_t are respectively the normal and tangential contact force.

To solve our problem, the heat transfer between grains needs to be taken into account. Through thermal conduction, the heat flux across one contact area can be expressed as the following:

$$Q_{ij} = h_c \Delta T_{ij} \tag{5}$$

where $\Delta T_{ij} = T_j - T_i$ is the temperature difference between the particles i and j. h_c is the contact conductance and is approximated via:

$$h_c = \frac{4k_{s,i}k_{s,j}}{k_{s,i}+k_{s,j}}\left(\frac{3F_n r^*}{4E^*}\right)^{1/3} \tag{6}$$

where E^* and r^* are respectively the effective Young's modulus and radius for the two contacted particles. k_s is the thermal conductivity of solids.

According to the heat flux calculated, we can update the temperature of each particle through the following energy equation:

$$m_i C_{p,i} \frac{dT_i}{dt} = \sum_{j=1}^{N_C} Q_{ij} \tag{7}$$

where N_C is the number of contacts over one grain, C_p is grains' specific heat and t is time. The applied time step dt is in order of 10^{-3} s, which is far smaller than that for the general thermal process of a granular system (~0.1 s, see [10]). However, compared with the time-step restriction in the pure particle dynamics (~10^{-7} s), the applied dt here is orders of magnitude larger, but it is still applicable, as grains under thermal cycling are in the very slowly moving state (one thermal cycle takes about 100 s for this study).

Similar with the previous treatment [30, 39, 45], in simulations the effect of thermal expansion on grains' size is considered as the following:

$$r = r_0(1 + \beta \Delta T) \tag{8}$$

where r_0 is the initial radius of grains, r is the current radius, ΔT is the temperature rise relative to the reference temperature and β is the thermal expansion coefficient.

It's necessary to note that the only one way of energy dissipation through friction was applied in the current study, and the radiant heat transfer is neglected since the temperatures concerned in this study are low enough and the radii of particles are also relatively small [46]. Besides, for simplicity the more complex contact force model including, for example, the damping ratio is not considered here. Moreover, the effect of stagnant interstitial fluids is also out of consideration. This is in line with [30, 36]. These neglects can be expected not to hinder one's observation of the final results.