Testing the Equal-Probability Assumption for Jammed Particle Packings[1]

Guo-Jie GAO[2], Jerzy BŁAWZDZIEWICZ[3] and Corey S. O'HERN[3]

Summary

The Edwards' and similar statistical descriptions for athermal particulate systems assume that all jammed configurations at a given volume fraction ϕ are equally likely. Although recent numerical simulations and experiments have provided indirect evidence that the Edwards' equal probability assumption is valid, there have been no direct tests. In our work, we focus on small systems in two dimensions and are thus able to generate nearly all mechanically stable disk packings and obtain the probabilities with which these packings occur. We have studied two experimentally relevant packing generation protocols, a compression/decompression scheme and quasi-static shear flow at zero pressure, to assess how the packing probabilities depend on protocol. We find that the mechanically stable packings are not equally likely for either protocol. Our results suggest that the equal probability assumption for granular and particulate systems is suspect and should be investigated in more detail.

1. Introduction

There have been several attempts to construct statistical mechanical descriptions of athermal particulate systems, for example, the Edwards' entropy description for granular materials[1]. An essential assumption of the Edwards' framework is that all jammed configurations at a given packing fraction ϕ are equally likely. However, this assumption has not been directly tested.

Most previous numerical and experimental work on statistical descriptions of granular media has only provided indirect tests of the Edwards' hypothesis. For example, Nowak, et al.[2] have performed experiments in which they vertically shake a granular material and obtain a well-defined effective temperature from density fluctuations. Makse, et al.[7] have performed numerical simulations of quasi-static granular shear flow and find that an effective temperature defined using the ratio of the diffusion constant and viscosity is consistent with an effective temperature defined from the Edwards' entropy. Consistency of different definitions of effective temperature provides only indirect evidence of the validity of Edwards' hypothesis for slow, dense granular flows.

In this work, we investigate the Edwards' assumption directly by creating mechanically stable disk packings in small systems—the number of particles N ranges from 6 to 20. We focus on small systems because we can generate nearly all mechanically stable packings and accurately measure the probability with which they occur. We employ two experimentally relevant packing-generation protocols: 1) a procedure in which we successively compress or decompress a square cell followed by energy minimization until the disks are just in contact and 2) quasi-static shear flow at zero pressure. Fig. 1 shows the probability density $P_k(\phi)$ to obtain a mechanically stable packing versus the packing fraction ϕ_k at which they occur using the first protocol for $N = 10$. In second method, we initialize the system with an unsheared mechanically stable packing and monitor the system as it evolves from one mechanically stable packing to another as a

1. Manuscript received on April, 3, 2007.
2. Graduate Student, Department of Mechanical Engineering,Yale University, New Haven, CT.
3. Associate Professor, Department of Mechanical Engineering, Yale University, New Haven, CT.

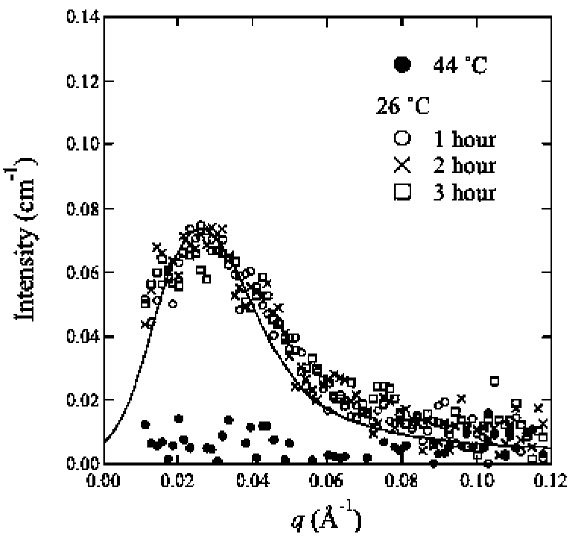

Fig.1 The probability density $P_k(\phi)$ to obtain a jammed packing at a particular packing fraction ϕ_k using the compression/decompression scheme for $N = 10$. The inset is a close-up of the packing fraction range $\phi = [0.7420, 0.7455]$. Notice that there are strongly varying probabilities within a small range of ϕ.

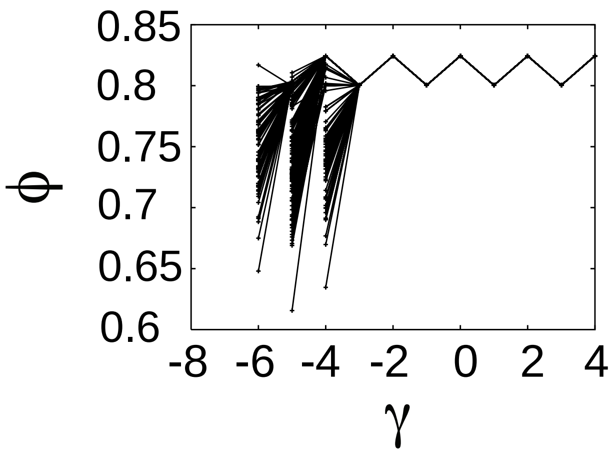

Fig.2 Packing fraction ϕ as a function of shear strain γ during quasi-static shear flow at zero pressure for $N = 10$. Each curve represents a different initial mechanically stable packing. Only integer shear strains are shown and all of the final trajectories are periodic at large shear strain with period 2. The trajectories have been shifted so that they overlap at large shear strain.

function of increasing shear strain γ. The mechanically stable packings obtained during the shear flow at integer values of shear strain are identical to those found using the compression/decompression protocol. We find that regardless of the initial mechanically stable packing, for small systems the shear flow settles on a periodic trajectory—alternating among only a few mechanically packings that were the most frequent packings found using the compression/decompression protocol. Fig. 2 shows the evolution of the mechanically stable packings during shear flow for integer shear strains with $N = 10$ particles.

For both packing-generation methods, we find that the mechanically stable packings do not occur with equal probability. For the compression/decompression protocol the mechanically stable packings have strongly varying probabilities even within a small range of ϕ. For the quasi-static shear flow at zero pressure, the systems settle into periodic trajectories and thus do not sample all mechanically stable packings during shear flow. These results show that the Edwards' equal probability assumption for athermal particulate systems should be reconsidered.

2. Quasi-static shear flow at zero pressure

The first protocol for creating mechanically stable packings (compression/decompression coupled with energy relaxation) has been described in our previous paper[9] and thus we will not provide further details here. In this work, we focus instead on the second protocol—quasi-static shear flow at zero pressure. We implement the following steps to perform quasi-static shear flow at zero pressure: we select an unsheared mechanically stable packing as our initial condition, shift all particles by a small shear strain increment $x_i' = x_i + y_i\Delta\gamma$, where $\Delta\gamma = 10^{-4}$, and implement Lees-Edwards shear periodic boundary conditions, relax the sheared configuration using energy minimization at fixed shear strain, use the compression/ decompression scheme to find the nearest mechanically stable packing with no particle overlaps, and then repeat these steps for a sufficiently large total shear strain. This protocol allows the system to evolve from one mechanically stable packing to another as a function of shear strain. Since we are using Lees-Edwards boundary conditions, configurations that have been sheared for integer strains are subject to the same boundary conditions as those that are unsheared. Thus, we can directly compare the mechanically stable packings that occur at integer shear strains in shear flow at zero pressure to those found using the compression/decompression packing-generation protocol. Typical sequences of mechanically stable packings explored at integer strains during shear flow at zero pressure are shown in Fig. 2 for $N = 10$. Note that for these small systems there is an initial transient, but then the system behaves periodically and only samples a few mechanically stable packings (two in Fig. 2) at large shear strain.

3. Results and discussion

In our previous study [9], we identified correlations between the frequency with which mechanically stable packings occur and features of the potential energy landscape near the energy minimum corresponding to a given packing. The basins near the frequent minima tended to be larger and possess larger barriers than less frequent minima. This raises an interesting question concerning the evolution of the mechanically stable packings during quasi-static shear flow. Do the periodically occurring mechanically stable packings at large shear strain correspond to the most frequent mechanically stable packings in the compression/decompression protocol? Our preliminary data in Fig. 3 shows that there is a significant overlap between the periodically occurring packings during shear flow and the most frequent packings from the compression/decompression protocol. Thus, the shear flow appears to target the mechanically stable packings with the largest basins of attraction and steepest barriers.

Another interesting feature of the quasi-static shear flow at zero pressure is for small systems the evolution from one mechanically stable packing to another is deterministic, i.e. the sequence of mechanically stable packings that the system visits is not random. However, when the system size increases above roughly $N = 18$ particles, the evolution becomes non-deterministic as shown in Fig. 4. The blue-highlighted portion of ϕ versus γ that extends from $\gamma = 0$ to 25 repeats from $\gamma \approx 115$ to 140. However, the trajectory diverges from the periodic pattern for $\gamma > 140$. To study the non-deterministic behavior in more detail, we will add thermal noise during the shear flow and determine the noise strength above which the evolution becomes non-deterministic. In future work, we will also employ a transfer matrix method to describe how the system evolves from one mechanically stable packing to another during shear flow. We will initialize the system with an unsheared mechanically stable

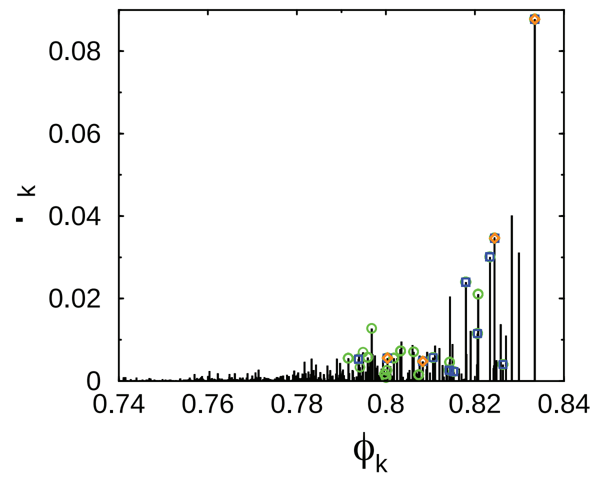

Fig.3 The probability density $P_k(\phi)$ to obtain a mechanically stable packing as a function of ϕ_k for the compression and decompression packing-generation protocol for $N = 10$. We also show the mechanically stable packings that occur during shear flow at zero pressure after shear strain $\gamma = 1$ (green circles), 2 (blue squares), and $\gamma > 6$ (orange diamonds).

packing and then determine to which mechanically stable packing the system evolved after unit shear strain. By doing this for all initial mechanically stable packings, we can form a map that tells us how each initial mechanically stable packing evolves under shear.

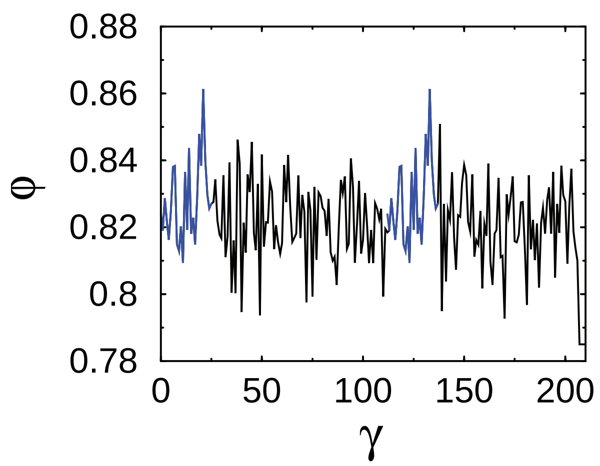

Fig.4 ϕ versus shear strain γ sampled at integer strains during quasi-static shear flow for a 20-particle system. The blue portions correspond to a possible periodic trajectory, however, the trajectory for $\gamma > 140$ becomes non-periodic.

References

[1] A. Mehta and S. F. Edwards: Statistical Me-

chanics of Powder Mixtures, *Physica A*, Vol.157 (1989), pp.1091–1100.

[2] E. R. Nowak, J. B. Knight, E. Ben-Naim, H. M. Jaeger and S. R. Nagel: Density Fluctuations in Vibrated Granular Materials, *Phys. Rev. E*, Vol.57 (1998), pp.1971–1982.

[3] J. B. Knight, C. G. Fandrich, C. N. Lau, H. M. Jaeger and S. Nagel: Density Relaxation in a Vibrated Granular Material, *Phys. Rev. E*, Vol.51 (1995) , pp.3957–3963.

[4] C. Josserand, A. Tkachenko, D. Mueth and H. Jaeger: Memory Effects in Granular Materials, *Phys. Rev. Lett.*, Vol.85 (2000), pp.3632–3635.

[5] P. Philippe and D. Bideau: Compaction Dynamics of a Granular Medium under Vertical Tapping, *Europhys. Lett.*, Vol.60 (2002) , pp.677–683.

[6] O. Pouliquen, M. Belzons and M. Nicolas: Fluctuating Particle Motion during Shear Induced Granular Compaction, *Phys. Rev. Lett.*, Vol.91 (2003), pp.014301-1–014301-4.

[7] H. A. Makse and J. Kurchan: Testing the Thermodynamic Approach to Granular Matter with a Numerical Model of a Decisive Experiment, *Nature*, Vol.415 (2002), pp.614–617.

[8] J. M. Luck and A. Mehta: A Column of Grains in the Jamming Limit: Glassy Dynamics in the Compaction Process, *Eur. Phys. J. B*, Vol.35 (2003), pp.399–411.

[9] G. Gao, J. Blawzdziewicz and C. O'Hern: Frequency Distribution of Mechanically Stable Disk Packings, *Phys. Rev. E*, Vol.74 (2006), pp.061304-1–061304-20.