Generating ensembles and measuring mixing in a model granular system

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Abstract. A major open question in the field of granular materials is the identification of relevant state variables which can predict macroscopic behavior. We experimentally investigate the mixing properties of an idealized granular liquid in the vicinity of its jamming transition, through the generation of ensembles of configurations under various boundary conditions. Our apparatus consists of a two-dimensional aggregate of particles which rearrange under agitation from the outer boundaries. As expected, the system acts like a slow liquid at low pressure or low packing fraction, and jams at higher pressure or high packing fraction. We characterize mixing in the system by computing the topological entropy of the braids formed by the trajectories of the grains. This entropy is shown to be well-defined and very sensitive to the approach to jamming, reflecting the dynamical arrest of the assembly.

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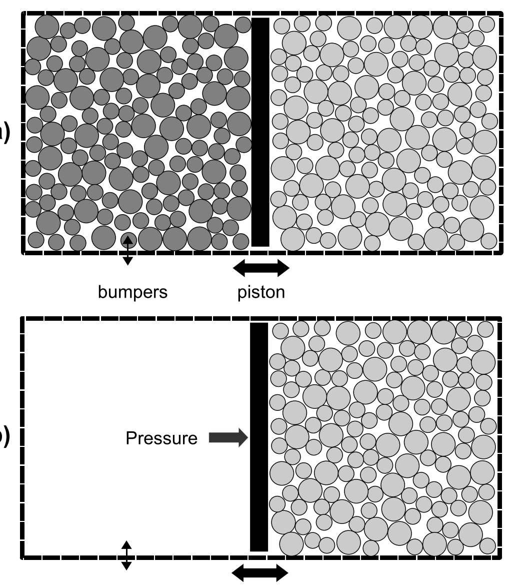
Our current knowledge of granular materials does not allow us to make accurate descriptions about the state of the system based on a complete set of state variables. One promising approach has been the use of techniques drawn by analogy to equilibrium statistical mechanics, allowing us to connect the microscale (grain-level) behavior to the macroscale behavior. We are particularly interested in the extent to which state variables such as the pressure, volume, and temperature-like variables such as Edwards compactivity [1] describe the state of the system and make predictions about its dynamics.

In particular, realistic models suitable for predictive purposes in natural and industrial systems will need to accurately account for a specified choice of boundary constraint. However, experiments have largely been conducted with only a single type of boundary constraint, making it difficult to compare behaviors in a controlled fashion. For instance, dense granular materials respond differently to constant-pressure or constant-volume constraints [2, 3] and even a small change in packing fraction significantly affects the stresses within the sample [4]. In this paper, we describe experimental methods used to examine a system under three interchangeable boundary constraints: $P = const.$, $V = const.$, and equilibration between two subsystems at constant total volume. Using these techniques, we have begun to determine what role the pressure and volume constraints play in the equation of state and dynamics.

The granular material studied is a monolayer of disks resting upon on a horizontal air table, which provides ultra-low friction with the bottom of the particles. The grains are free to move horizontally, but are contained within a 1 m $\times$ 2 m area cell. Two key advantages are obtained through the study of a two-dimensional material: grains are at a uniform gravitational potential and all grains within the system can be simultaneously visualized. To generate new configurations, we inject energy

(a)



(b)

FIGURE 1. Schematic of the apparatus used to measure the dynamics under (a) volume equilibration (b) and constant pressure conditions. In the volume-equilibration case, an equal number of particles with different properties are placed in "thermal" contact and allowed to equilibrate under agitation from the sidewalls. In the constant-pressure (or constant-volume, not shown) case, the properties of a single set of particles are examined.

FIGURE 2. Photograph of large and small particles, showing unique identifier patterns.

into the system by means of an array of 60 randomly activated coil bumpers located around the outer boundary of the system (see Figure 1). Three operating conditions of the system are possible: (1) a single, constant-volume system, (2) a single, constant-pressure system for which one wall (a piston) is attached to an adjustable weight via a pulley, and (3) two subsystems placed in contact via a piston constrained to move along the long axis of the system. During a typical experimental run, $\approx 10^4$ different configurations are obtained through the agitation of bumpers. These bumpers are randomly-triggered solenoids paired so as to exert zero net torque on the system, providing an efficient and random evolution between nearby configurations in the ensemble.

We primarily use three experimental tools for investigating the phase-space of the mixture: changing the number of grains (for constant-volume experiments), changing the piston pressure (for constant-pressure experiments), and altering the material properties of the grains. We probe the importance of grain-material properties by using one of two types of particles: one family possesses a coefficient of friction and coefficient of restitution of $\mu = 0.5$ and $\varepsilon = 0.33$, while the other family has $\mu = 0.85$ and $\varepsilon = 0.51$. In all cases, we use a binary mixture composed of grains differing only in diameter, chosen to suppress crystallization. The ratio of these species is fixed at one-third large grains and two-thirds small grains with diameter of $d_L = 8.6$ cm and $d_S = 5.8$ cm, respectively.

Each configuration is recorded by a high-resolution color CCD camera mounted above the air table. Because we are interested in the long-term diffusive and mixing properties of the system, it is important not to exchange the identity of "identical" particles even when images are separated at times slow compared to the rearrangement timescale of the aggregate. Therefore, we have developed an image analysis technique which identifies each grain by a unique identifier. Each particle is marked with a 3×3 array of colored dots, as shown in Figure 2. The unique identifier consists of a vector composed of four 4-bit elements represented by the colors magenta, cyan, yellow, and green. This allows for accurate tracking of 256 disks in the mixture (or 512 disks within the equilibration study, where the separation of the two subsystems allows for the re-use of the unique patterns on each side). The full 3×3 pattern provides two methods for error-correction during the tracking process: two copies (one color-inverted from the other) of the four-element identifier, plus an error-correcting bit formed from the sum of the numeric value of these colors. The nine dots are arranged in an unevenly-space array so that there is a unique orientation which can be identified. The particles are initially located using high-contrast white rims located at the edge, after which their identities are established and adjacent image frames are connected into trajectories.

For each equilibration run, we prepare the apparatus with an identical number N of particles on each side, with each side populated by particles of only one of the two types. To probe the volume-equilibration of the system as it approaches a jammed state, we perform experiments at a series of increasing values of N (corresponding to a packing fraction range from $\phi \approx 0.76$ to 0.83). All other variables are held constant. The particle trajectories allow for many different types of measurements of the properties of the granular aggregate: local or global packing fractions (and fluctuations), mean squared displacements, and the braiding of trajectories. In addition, the position of the piston provides a macroscopic measure of the state of the system. We will describe results from several of these types of measurements below.

The packing fraction, ϕ, is known to have a significant effect on the macroscopic and microscopic behavior of granular materials. At a low packing fraction, granular materials can exhibit Brownian motion similar to that of a liquid [5, 6, e.g]. At low ϕ in our system, we observe that grains are in frequent, sustained contact with their neighbors, but the force chains are not yet system-spanning. We observe highly diffusive trajectories such as those shown in Figure 3(a). In contrast, the individual grains of an instance with a higher packing fraction (larger N) start to resemble a solid, and exhibit caged dynamics. In Figure 3(b), individual trajectories tracked and plotted over the span of 300 seconds have a mean displacement less than the grain diameter. The narrow range $0.77 < \phi < 0.79$ corresponds to the jamming transition and is of particular interest.

An alternative way to visualize this change in dynamics is to map the location of select grains within a hori-

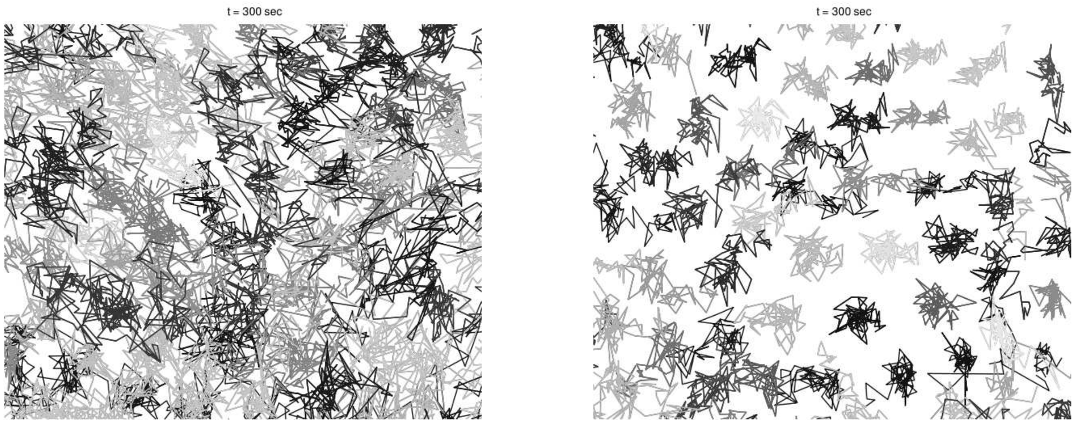


FIGURE 3. Trajectories of individual particles over during 300 seconds, plotted for one side of a volume-equilibrated sample with (a, left) $\phi = 0.77$ and (b, right) $\phi = 0.79$. Each line segment in the trajectory respresents the displacement of the grain during 2 seconds. Different grayscale values represent different particles.

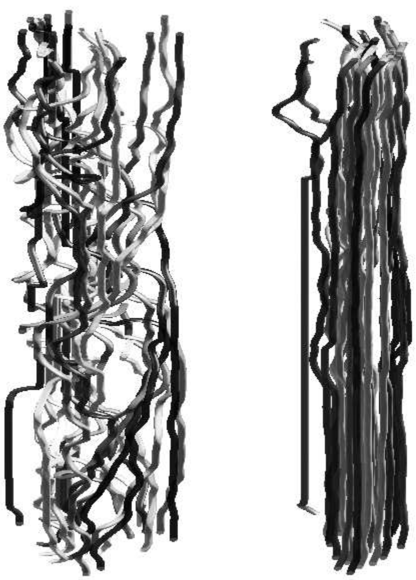


FIGURE 4. Space-time trajectories of twenty individual particles (not necessarily neighbors) at (a, left) $\phi = 0.77$ and (b, right) $\phi = 0.79$, each sampled from one side of an equilibrated sample.

zontal plane and evolve time along the vertical axis. By making such a space-time plot, we can observe the braiding of the trajectories, as shown in Figure 4. We can characterize the mixing of the system by computing the degree of braiding created by all such trajectories of the grains, as has previously been done for fluids [7, 8] to quantify the degree of mixing in a chaotic flow. As shown in Figure 5(a), the degree of braiding (calculated via the methods described by Thiffeault [7]) grows linearly in time, corresponding to exponential growth in the separation of trajectories. This corresponds to a Lyapunov exponent, and the technique provides a lower bound on the topological entropy S:

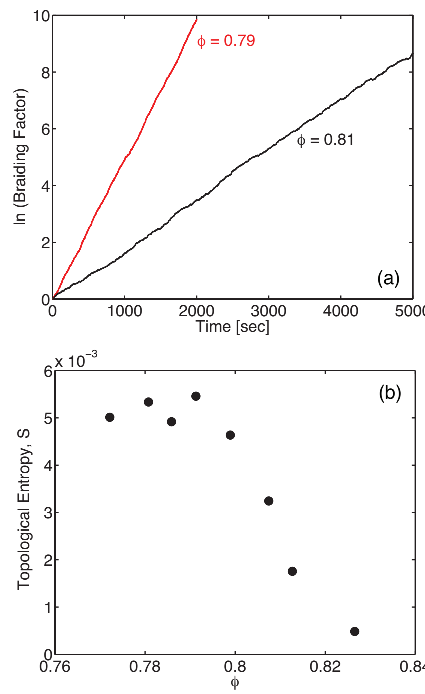


FIGURE 5. (a) Linear growth in braiding factor as a function of time at $\phi = 0.79$ and $\phi = 0.81$. (b) Braiding entropy S as a function of ϕ.

$$S = \lim_{t\to\infty} \frac{1}{t} \log\left(\text{braiding factor}\right), \qquad (1)$$

which we plot as a function of ϕ in Figure 5(b). We observe a dramatic change in the topological entropy of the system at the crossover near $\phi = 0.79$, as described above. Therefore, the reduction in topological entropy approximately corresponds to caging dynamics and the dynamical arrest of the assembly.

The experiments described in this paper are ongoing, and having a single apparatus capable of examining a granular system under constant volume, constant pressure, or equilibration, will yield a better understanding of the mechanics driving the material behavior.

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