Compression of Particles in a 3-Dimensional Granular System

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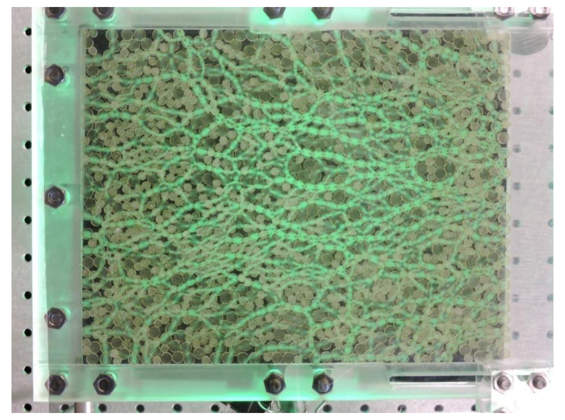
Introduction

We consider the systems of particles exposed to compression, with the main goal of developing better understanding of the properties of force networks, the mesoscopic structures characterized by a size which is large compared to the particle size, but small compared to the domain size.

Computationally, we consider 3-Dimensional systems of bidisperse particles. To compress the system, the walls move inward at a small constant speed. The system is then relaxed by decreasing the velocity of the walls. The system is defined as being relaxed if the particle contacts are at a force less than 0.1, or the average velocity of the particles is less than 0.1 times the velocity of the compression of the walls. The simulation runs until the system reaches a packing fraction of 0.75. Using various techniques discussed in what follows, we analyze the properties of force networks that form in the system as it is being compressed.

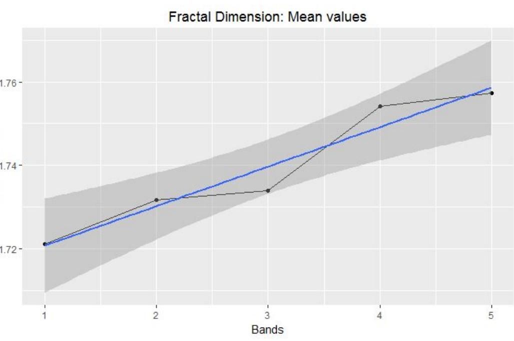
Experiment



Experimental Setup:

- photoelastic particles sitting on a plane
- pressure applied by rubber bands from right hand side
- polarization filter for detecting forces on particles

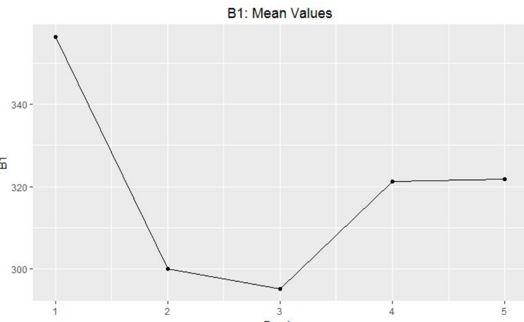
Objective: computing fractal dimension and Betti numbers (introduced in Topology and Percolation section) and influence of increasing pressure.

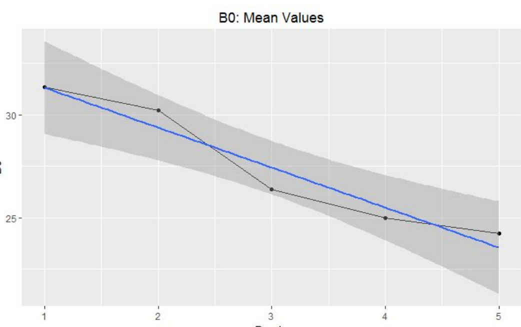


Fractal dimension, D_f:

- values of $D_f \sim 1.75$, consistently with [6]
- D_f slightly increases as applied pressure is increased, as shown in [6]

Betti numbers:
We observe a decreasing trend for B_0 (number of clusters) values with increasing force applied on the right boundary. The values of B_1 do not show a specific trend.

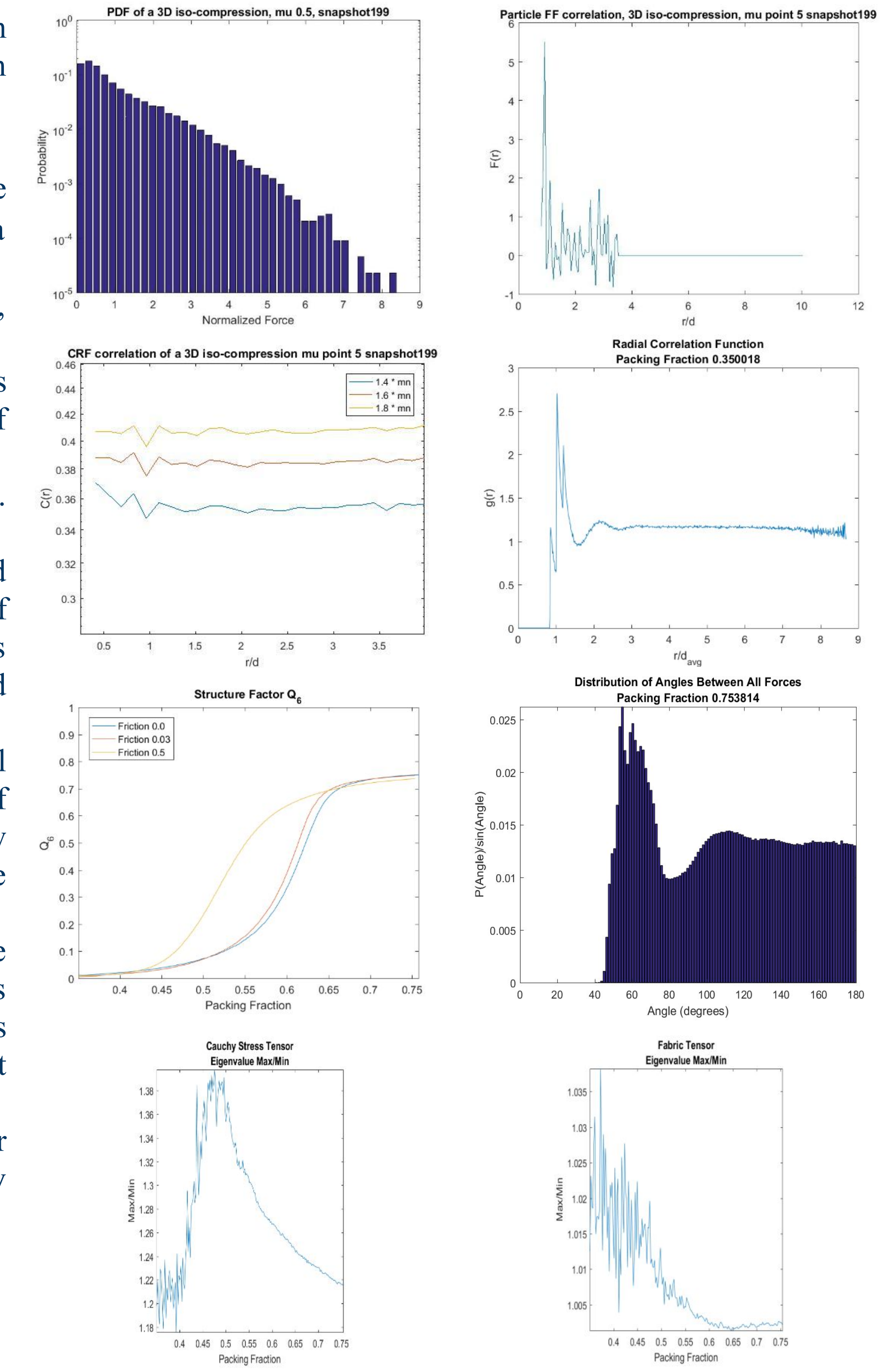




Classical Measures

Probability Distribution Function: This measure gives the probability of finding a force of a certain magnitude. The main finding (see figure) is that the probability of finding a force decays exponentially with the force magnitude.

Correlation: Force Force Correlation: calculated with $F(t) = \left(\sum_i\sum_{j>i}\delta(|r_{ij}-r|)(f_i-f)(f_j-f)\right)/\left(\sum_i\sum_{j>i}\delta(|r_{ij}-r|)\right)$ where r_{ij} is the distance between particles i and j, f_i is the total force acting on particle i, $\delta(c)$ is the Dirac delta function, and $<f>$ is the mean force of the system.
CRF Correlation: calculated with $C(r, f_{cut})=<(f_i-<y>)(f_j-<y>)>/\sigma_y^2$ where f_i is the force acting on contact i, $<y>$ is the mean of all the force contacts, and y^2 is the variance of y.
Radial Correlation: calculated with $g(r)=1/(4\pi r^2\, drN_r\,\rho_0)\sum_{i=1}^{N}\sum_{i\neq j}^{N}\delta(r-r_{i,j})$ where N is the number of particles in the system, N_r is the number of particles that were included for the distance r, ρ_0 is the number density of the system, and $r_{i,j}$ is the distance between particles i and j.
Results: peak in correlation at approximately one particle diameter in radial and force-force correlation. Larger friction resulting in higher correlation.
Structure Factor: Describes the sixfold symmetry of contact points between particles in a system, calculated by $Q6=1/N\sum_{i=1}^{N} 1/(C_i-1)\sum_{k=1}^{Ci-1}cos(6\theta_k)$ where N is the number of particles in the system, C_i is the number of contacts on particle i, and θ_k is the angle between two consecutive contacts at the particle. Our conclusion is that the systems approach the crystalline structure over time, but never perfectly reach it (Q_6 is never 1), and although friction affects structure over time, it does not strongly impact structure after complete compression.
Cauchy Stress Tensor and Fabric Tensor: The Cauchy stress tensor is a matrix that describes the overall direction of forces within a system. The fabric tensor is a similar matrix that considers only the positions of particles, not the forces between them. We use these matrices to analyze the anisotropy of the system, or how uniform the system is in terms of either particle forces or particle positions. Both plots exhibit the same behavior of being very noisy before a certain packing fraction, then "calming down" after that point.
Angle Distributions: We also looked at the distribution of angles between contacts in the system. The motivation behind this is similar to the structure factor Q_6, where we are expecting to find 60 degree angles representative of tetrahedrons formed by hexagonal sphere packing. For strongly compressed systems, there is a clear peak around 60 degrees, and a mostly flat distribution after about 110 degrees. This lines up with what we saw in Q_6: there are many 60 degree angles, but they are not an overwhelming majority.
Results: Our results provide significant information about the properties of force fields in compressed granular systems. These results, that are in general consistent with the ones found in the literature [1, 5-8], are currently further being analyzed to extract in more detail the influence of the friction coefficient and system size.



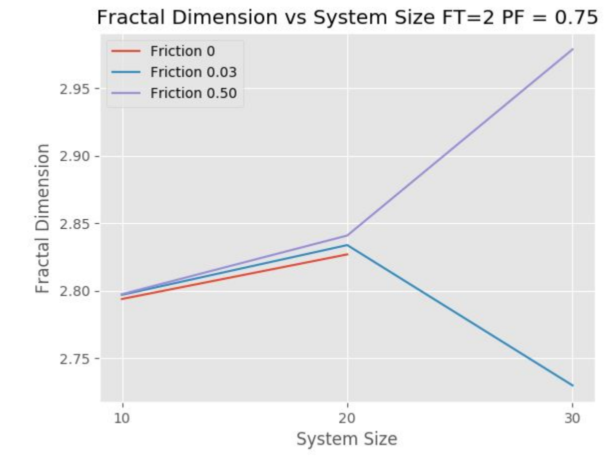
Percolation and Fractal Dimension

- Fractal Dimension is a measure of the space-filling capacity of a pattern relative to the dimension it is embedded in.
- We compute this as the Minkowski "Box-Counting" Dimension, D_f, for the Percolating Cluster:

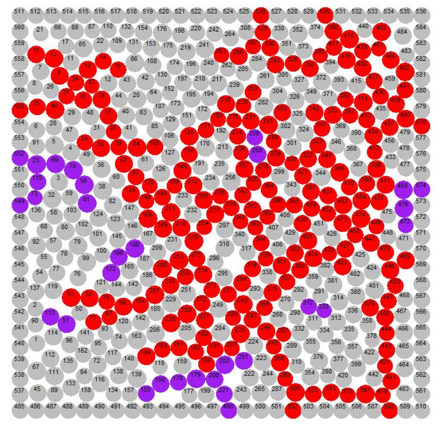
$$D_f \log(1/L) \propto \log(N)$$

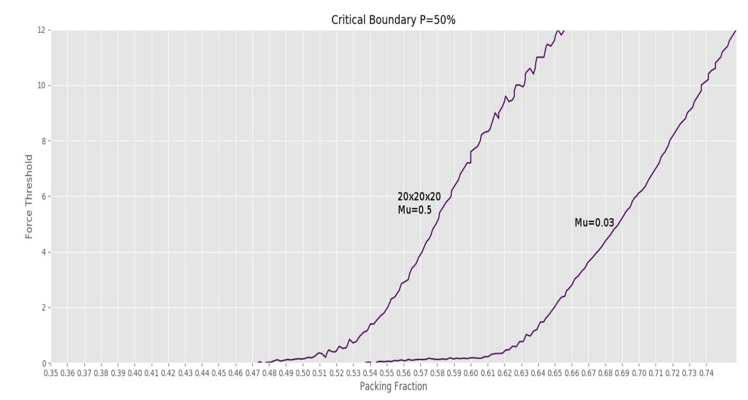
with L the box length and N the number of boxes.

- D_f of the percolating cluster on the critical boundary is related to one of the critical scaling exponents [6], [9].



Percolation in particulate systems is a collection (cluster) of particles that connect opposite boundaries of the enclosing box. We can focus on particles that experience total forces above specified threshold, F_{th}, and study percolation properties as F_{th} changes.

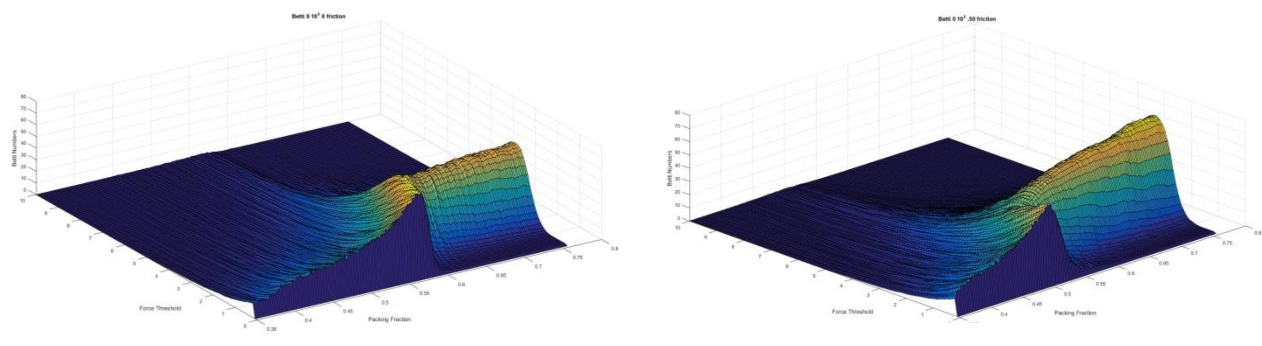


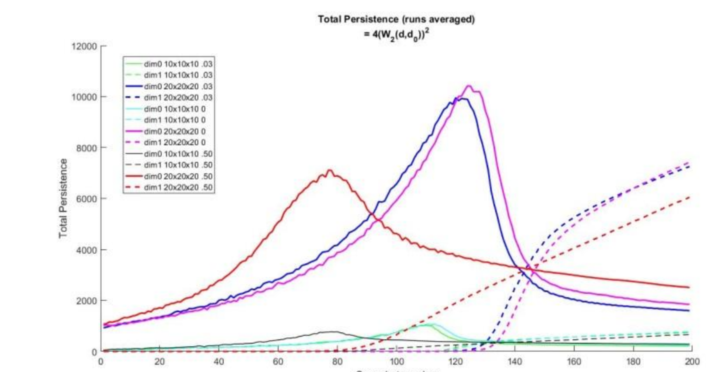


We find the force threshold, F_{th}, for which the probability of percolation is P=0.5. The rise in the force threshold curve corresponds to the jamming transition, similarly as in [7] for 2D systems.

Topology

Simplicial complex: The topological space under consideration in this section is the simplicial complex formed by considering particles under forces (of a certain varying force threshold). These particles are the 0-cells and their force chains the 1-cells.
Total Persistence: We used total persistence, a measure of how far a persistence diagram is from the empty diagram, to get a first approximation of how the persistence diagrams change as system size and friction changes. Although we cannot directly compare two systems because we have approximated an n-dimensional distance by 1-dimensional distance, it provides a range of how far the persistence diagrams of each system might be from each other. This is calculated by $Pers_p(d)=\sum_{x\in d}(2inf_{y\in\Delta}(||x-y||_\infty))^p$, where we use $p = 2$.
Betti Numbers: We also computed the Betti numbers of each system. These count the number of connected components (Betti 0), loops (Betti 1), and 2 dimensional bubbles (Betti 2).
Results: Total persistence graphs corroborated the results of percolation techniques – system size increases the total persistence (more particles lead to more Betti generators in each dimension, except 2) but does not qualitatively affect the behavior. Friction causes the maximum total persistence in dimension 0 to occur at lower packing fractions, due to the system jamming sooner because of the higher friction locking particles together. This jamming decreases the number of connected components, lowering the total persistence of dimension 0. Higher friction causes the dimension 1 total persistence to grow at lower packing fractions but makes the growth linear.
The Betti numbers offer a more interesting result: as expected, there is a steady local maximum at or near normalized force threshold 1 (the average force), and there is a local maximum along packing fractions for low force thresholds which shrinks for high force thresholds. However, there is also a ridge connecting these two local maxima, a result previously unseen in 2D systems. As before, system size only scales the Betti numbers, but friction causes the local max along packing fractions to shift to lower packing fractions and lowers the maximum, emphasizing and elongating the local maximum at force threshold 1.





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