Recent advances in jamming: Packing probabilities, geometrical families, and anharmonicity

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Jamming Phase Diagram

Simulations of Jamming

\[ T > T_g \]

Temperature (T), packing fraction (\( \phi \))

\[ \sigma > \sigma_y \]

Shear stress (\( \sigma \)), packing fraction (\( \phi \))

\[ \phi = \frac{A_{circles}}{A_{box}} \]
Jamming along the $\phi$-axis

$V(\vec{r})$

Mechanically stable packing

Degenerate minima

overlapped

Mechanically stable packing

non-overlapped
Focus Questions

• Are jammed packings points or continuous geometrical families in configuration space?

• Are jammed packings equally probable? If not, what determines their probabilities? How do the probabilities depend on packing-generation protocol?

• Can the vibrational response be determined from static jammed packings?
http://jamming.research.yale.edu/

The O'Hern group in the Summer 2010: (back row from left to right) Carl Schreck, Thibault Bertrand, Robert Hoy, and Mark Shattuck; (front row from left to right) Tianqi Shen, Alice Zhou, Corey O'Hern, Sarah Penrose, Amy Werner-Allen, S. S. Ashwin, and Guo-Jie Gao.

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The O’Hern Group

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2. Dr. Robert Hoy, Ph.D. in Physics, The Johns Hopkins University (protein nanogels, polymer collapse)
3. Dr. Vijay Kumar, Ph.D. in Physics, Centre for Condensed Matter Theory, Indian Institute of Science, Bangalore, India (energy flow in granular media)
4. Dr. Maria Sammalkorpi, Ph.D. in Electrical Engineering, Helsinki University of Technology (intrinsically disordered proteins)
5. Thibault Bertrand, 1st year Ph.D. student in Mechanical Engineering & Materials Science (granular packings)
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8. Jared Harwayne-Gidansky, 2nd year Ph.D. student in Electrical Engineering (polymer collapse)
9. Alice Zhou, 2nd year Ph.D. student in Molecular Biophysics & Biochemistry (protein-protein interactions)
10. Tianqi Shen, 3rd year Ph.D. student in Physics (protein nanogels)
11. Carl Schreck, 5th year Ph.D. student in Physics (granular packings)
What are jammed granular packings?

Distinguishing features of granular media: athermal, dissipative, driven
Jammed = mechanically stable (MS) configuration with extremely small particle overlaps; net forces (and torques) are zero on each particle; stable to small perturbations
Disorder versus Order

\[ Q_6 = \frac{1}{N} \sum_{k=1}^{N} \left( \frac{1}{n_k} \sum_{j=1}^{n_k} e^{i6\theta_{jk}} \right) \]

- ellipses
- dimers
- polydispersity

\( Q_6 \)
Are jammed packings points in configuration space?
Deposition Algorithm in Simulations

• All geometric parameters identical to those for experiments
• Terminate algorithm when $F_{\text{tot}} < F_{\text{max}} = 10^{-14}$
• Vary random initial positions and conduct $N_{\text{trials}} = 10^8$ to find ‘all’ mechanically stable packings for small systems $N=3$ to 10.

$$\bar{g} = \frac{m_s g}{k \sigma_s}$$
Mechanically Stable Frictionless Packings

• Distinct MS packings distinguished by particle positions \( \{ \vec{r}_i \} \)
• # of constraints ≥ # of degrees of freedom
Configuration Space of Mechanically Stable Packings

\[ R = \left\{ \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N \right\} \]

- \( \Delta R_D \) = distance in configuration space between distinct MS packings
- \( \Delta R_C \) = error in measuring distinct MS packings
Separation in Configuration Space

- MS frictionless packings are discrete points in configuration space
Discrete MS Packings

\[ \bar{r}_c = \frac{1}{N} \sum_{i=1}^{N} \bar{r}_i \]

- simulations
- experiments
How is the quantitative agreement between sims and exps?

- 95% of distinct MS packing match; others are unstable in sims
Are jammed packings equally probable?
Sorted Probabilities

- $7 \times 4$ orders of magnitude variation in probabilities in simulations (experiments)
MS Packing Probabilities Are Robust

- Rare MS packings in exps are rare in sims; frequent MS packings in exps are frequent in sims
What determines the packing probabilities?
Protocol Dependence of Granular Packings

slow quench rates: basin-depth dominated

fast quench rates: basin-volume dominated
Rate dependence and basin volume

- Fast rate; $\phi_f=0.622$
- Slow rate; $\phi_f=0.730$
- Fast rate; different IC; $\phi_f=0.730$
Density landscape for hard spheres

\[ \phi_d^{-1} \left( \{ \vec{r} \} \right) = \frac{6V}{\pi N \min_{mn} |\vec{r}_m - \vec{r}_n|^3} \]

N. Xu, D. Frenkel, and A. J. Liu, xxx.lanl.gov/cond-mat1101.5879
Method 1 (small l): Probability to return to a given MS packing

\[ \phi_i^{MS}, \{ \vec{r} \}_i^{MS} \]

\[ \{ \vec{r} \} = \{ \vec{r} \}_i^{MS} + l \bar{e}_r \]

\[ f_i(l) = \frac{M_i}{M} \]

Distance in config. space

Distance in config. space
Distinct N=4 Packings

Polarizations

floater
Particle-label permutations
Method 2 (large $l$): Random initial conditions

$\phi_1, \{\vec{r}\}_1$

$\phi_2, \{\vec{r}\}_2$

$\phi_3, \{\vec{r}\}_3$

$\phi^{-1}_d$

Distance in config. space

$$l = \sqrt{(x_1 - x_{10})^2 + (x_2 - x_{20})^2 + \cdots + (x_N - x_{N0})^2 + (y_1 - y_{10})^2 + (y_2 - y_{20})^2 + \cdots + (y_N - y_{N0})^2}$$

$$f_i(l) = \frac{M_i}{M}$$
Basin Volumes

\[ P_i = \frac{V_i}{L^{dN}} \]

\[ V_i = \int_0^{\sqrt{dN}} S_i(l) dl \]

\[ S_i(l) = A_{dN} f_i(l) l^{dN-1} P_i N_s ! N_l ! \]
Weighted/Unweighted basin profile functions

- Probability of MS packing determined by large $l$, not core region $l_c$
- Large probability near peak in MS packing separation distribution
Floaters

Particles with fewer than 3 contacts
Future Directions

• Probability for MS packings determined by large $l$, not nearby regions of configuration space
• Study $\phi_i$ and quench rate dependence of probabilities
Vibrational Response in Granular Media

Figure 1: [left] Sound (force) propagation at 4 times and [right] frequency response to a sinusoidal vertical compression of a packed composite material under constant pressure.
Harmonic Solids

- Atomic and molecular systems
- Pair potentials have 'double-sided' minimum and are long-ranged
- Equilibrium positions are well-defined
- Vibrations at low T captured using harmonic approximation

\[
\overline{r}_0^i = \langle \overline{r}^i(t) \rangle_t
\]
Causes of nonharmonicity in granular solids

- Nonlinear Hertzian interaction potential ✗
- Dissipation from normal contacts ✗
- Sliding and rolling friction ✗
- Inhomogeneous force propagation

- Breaking existing contacts and forming new contacts
Model Particulate Media

\[
V_{RS}(r_{ij})/\varepsilon = \begin{cases} 
\alpha^{-1} \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^\alpha & r_{ij} \leq \sigma_{ij} \\
0 & r_{ij} > \sigma_{ij}
\end{cases}
\]

\[
\alpha = 2 \text{ linear} \\
\alpha = 5/2 \text{ Hertzian}
\]

Total potential energy \[ V = \sum_{\langle i,j \rangle} V(r_{ij}) \]
Harmonic approximation: Normal Modes from Dynamical Matrix

\[ M_{\alpha, \beta} = \frac{\partial^2 V(\vec{r})}{\partial r_\alpha \partial r_\beta} \bigg|_{\vec{r}=\vec{r}_0} \]

\( \alpha, \beta = x, y, z, \text{ particle index} \)
\( \vec{r}_0 = \text{ positions of MS packing} \)

Calculate d N- d eigenvalues; \( m_i = \omega_i^2 > 0 \).
Density of Vibrational Modes via Dynamical Matrix

\[ D(\omega)\,d\omega = N(\omega + d\omega) - N(\omega) \]

- Why \( D(\omega) \)?
- Formation of plateau in \( D(\omega) \)
  (excess of low-frequency modes)
  as \( \Delta \phi = \phi - \phi_j \to 0 \)

Are jammed particulate systems harmonic?

\[ \vec{r}_i' = \vec{r}_i + \delta \hat{e}_6 \]

- Deform system along each ‘eigenmode’ \( \omega_i \)
- Run at constant NVE, measure power spectrum of grain displacements
- Does system oscillate at frequency \( \omega_i \) from dynamical matrix?
Power-spectrum of particle displacements

- System becomes strongly nonharmonic at extremely small $\delta$
- First spreads to `harmonic’ set of $\omega$ (NH1); then continuum of $\omega$ (NH2)
$N=12$
$\Delta \phi = 10^{-5}$
$\text{Mode}=6$
$\delta/\sigma = 10^{-5}$
N=12
\[ \Delta \phi = 10^{-5} \]
Mode = 6
\[ \delta/\sigma = 10^{-3} \]
Strongly Anharmonic Behavior
Are large jammed packings composed of highly probable sub-systems?
Delaunay triangle packings
Distribution of tile numbers

\[ P_M(\Delta N^*_2) \]

\[ P_N(\Delta N^*_7) \]
• Average values converge quickly with $N$
• ‘Compatibility’ rules determine large $N$ values
Future Directions

- Form triangles, quadrilaterals, pentagons,… out of all links (from Delanauy triangulation) that surround particles.
When do jammed packings form continuous geometrical families?
Continuous Range of Boundary Conditions, $L$

- Electromagnetic Shaker
- $r_j$
- $\sigma$
- $L_{\text{min}}$ to $L_{\text{max}}$
Continuous Range of Boundary Conditions, $L_{\text{min}}$ to $L_{\text{max}}$

1. Enumeration: large number of unrelated $L$ (sim)

2. Dynamics: Quasistatic compression/decompression (sim, exp)
(a) 

(b) compression

(c) decompression
How do slow, dense shear flows sample MS packings... with equal probability?

Quasi-static Couette Shear Flow $\dot{\gamma} \rightarrow 0$

Quasi-static shear flow at zero pressure

1. Initialize MS packing at zero shear strain
2. Take small step shear strain $x_i' = x_i + \Delta \gamma y_i$
3. Minimize energy
4. Find nearest MS packing at P=0 using growth/shrink procedure
5. Repeat steps 2, 3, 4
Quasistatic Shear Flow at Zero Pressure
Rearrangement events cause system to switch geometric families.
Complete Family Tree

Small systems sample only negligible fraction of available geometric families!
Sensitivity to Initial Conditions: $N \geq 12$
Noise-generation Mechanism: Collinear Particles

\[ \gamma = \gamma_0 - \Delta \gamma \]  

\[ \gamma = \gamma_0 \]
Frictional Geometric Families

(a)

(b)
Sticky Disks

- Study $C/\varepsilon \rightarrow 0$ limit
- 50 - 50 binary mixtures of disks with $R_2/R_1=1.4$
Bond Percolation
Rigidity Percolation
Rigidity Percolation Exponents

\[ \Delta^2 \]

\[ n_s(\phi_p) \]

\[ N_{\text{perc}} \]

\[ \nu = 1.92 \]

\[ D = 1.88 \]

\[ \tau = 2.04 \]
Contact Percolation in Repulsive Disks
## Percolation Critical Exponents

<table>
<thead>
<tr>
<th></th>
<th>Nature</th>
<th>sticky</th>
<th>repulsive disks</th>
<th>Rod (a=3)</th>
<th>Rod (a=6)</th>
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<tbody>
<tr>
<td>η</td>
<td></td>
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<td>1.127</td>
<td>0.734</td>
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<td>φc</td>
<td>0.558</td>
<td></td>
<td>0.676</td>
<td>0.520</td>
<td>0.381</td>
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<td>D</td>
<td>1.89</td>
<td>1.88±0.04</td>
<td>1.907±0.013</td>
<td>1.900±0.004</td>
<td>1.908±0.018</td>
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<tr>
<td>τ</td>
<td>2.06±0.02</td>
<td>2.04±0.04</td>
<td>2.01±0.03</td>
<td>1.99±0.03</td>
<td>1.97±0.03</td>
</tr>
<tr>
<td>v</td>
<td>1.6±0.1</td>
<td>1.92±0.03</td>
<td>1.376±0.065</td>
<td>1.404±0.055</td>
<td>1.420±0.044</td>
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</table>
Cyclic Compression and Decompression
Packings of ellipse-shaped particles

bidisperse

\[
\begin{array}{c|c}
 a_1 & b_1 \\
\hline
 a_2 & b_2 \\
\end{array}
\]

\[
\frac{a_1}{b_1} = \frac{a_2}{b_2} = \alpha
\]

\[
\frac{a_1}{a_2} = 1.4
\]

compression method-fixed aspect ratio \(\alpha\)
Pairwise Repulsive Interactions: True Contact Distance

\[ V(r_{ij}) = 0 \]

\[ V(r_{ij}) = \begin{cases} 
\frac{\varepsilon}{\alpha} \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^\alpha & \text{if } r < \sigma_{ij} \\
0 & \text{if } r \geq \sigma_{ij}
\end{cases} \]

\( \alpha = 2; \) linear springs
Average Contact Number

\[
N(2d - 1) = N\frac{\langle z \rangle_{iso}}{2}
\]

\[
\langle z \rangle_{iso} = 2(2d - 1)
\]

- Not a discontinuous jump from \(<z> = 4\) to 6.
- Quartic modes to the rescue!
Two gaps in spectrum over range of aspect ratios
Onset of first gap depends on aspect ratio
Second gap closes at large aspect ratios
Rotational/Translational Character of Eigenmodes

\[ T_i = \sum_{j=1}^{N} \left[ (e_{xi}^j)^2 + (e_{yi}^j)^2 \right] \quad T_i = 1 - R_i \]
What is the difference between between a dimer and an ellipse?

\[ \alpha = \frac{a}{b} \]
Structural Properties

\[ \langle z \rangle \]
\[ \Phi \]

- **dimers**
- **ellipses**