Basins of attraction of mechanically stable packings on the density landscape

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Stress Fluctuations

Glass Formation
• What is probability with which granular packings occur?
• Edwards’ hypothesis

• Athermal
• Driven
• Dissipative
• Finite system size
Protocol Dependence of Granular Packings

slow quench rates: basin-depth dominated

fast quench rates: basin-volume dominated

<\phi_j>
Mechanically Stable Frictionless Packings

- Distinct MS packings distinguished by particle positions $\{\vec{r}_i\}$
- # of constraints $\geq$ # of degrees of freedom
Sorted Probabilities

- 7 (4) orders of magnitude variation in probabilities in simulations (experiments)
Rate dependence and basin volume

- Fast rate; $\phi_f = 0.622$
- Slow rate; $\phi_f = 0.730$
- Fast rate; different IC; $\phi_f = 0.730$
<table>
<thead>
<tr>
<th>$N^*$</th>
<th>$N_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>6</td>
<td>46</td>
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<tr>
<td>8</td>
<td>500</td>
</tr>
<tr>
<td>10</td>
<td>3983</td>
</tr>
<tr>
<td>12</td>
<td>16935</td>
</tr>
</tbody>
</table>
What determines MS packing probabilities: Density landscape for hard spheres

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

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

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

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

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

- red dot: return to i
- blue dot: change to j

\[ l = \sqrt{(x_{i_f} - x_{i_0})^2 + (x_{2_f} - x_{2_0})^2 + \cdots + (x_{N_f} - x_{N_0})^2 + (y_{i_f} - y_{i_0})^2 + (y_{2_f} - y_{2_0})^2 + \cdots + (y_{N_f} - y_{N_0})^2} \]
Method 2 (large l): Random initial conditions

\[ \phi_1, \{\vec{r}\}_1 \]

\[ \phi_2, \{\vec{r}\}_2 \]

\[ \phi_3, \{\vec{r}\}_3 \]

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

\[ l = \sqrt{(x_{i_f} - x_{i_0})^2 + (x_{2_f} - x_{2_0})^2 + \cdots + (x_{N_f} - x_{N_0})^2 + (y_{i_f} - y_{i_0})^2 + (y_{2_f} - y_{2_0})^2 + \cdots + (y_{N_f} - y_{N_0})^2} \]
Basin Volumes

\[ P_i = \frac{V_i}{L^{dN}} \quad V_i = \sqrt[1]{dN} \int_0^\infty S_i(l) dl \]

\[ S_i(l) = A_{dN} f_i(l) l^{dN-1} P_i N_s ! N_l ! \]

polarizations and permutations
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
Collapse for $l > l^*$

• Complete enumeration not necessary to determine $P_i$
Floaters

Particles with fewer than 3 contacts
Conclusions and 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