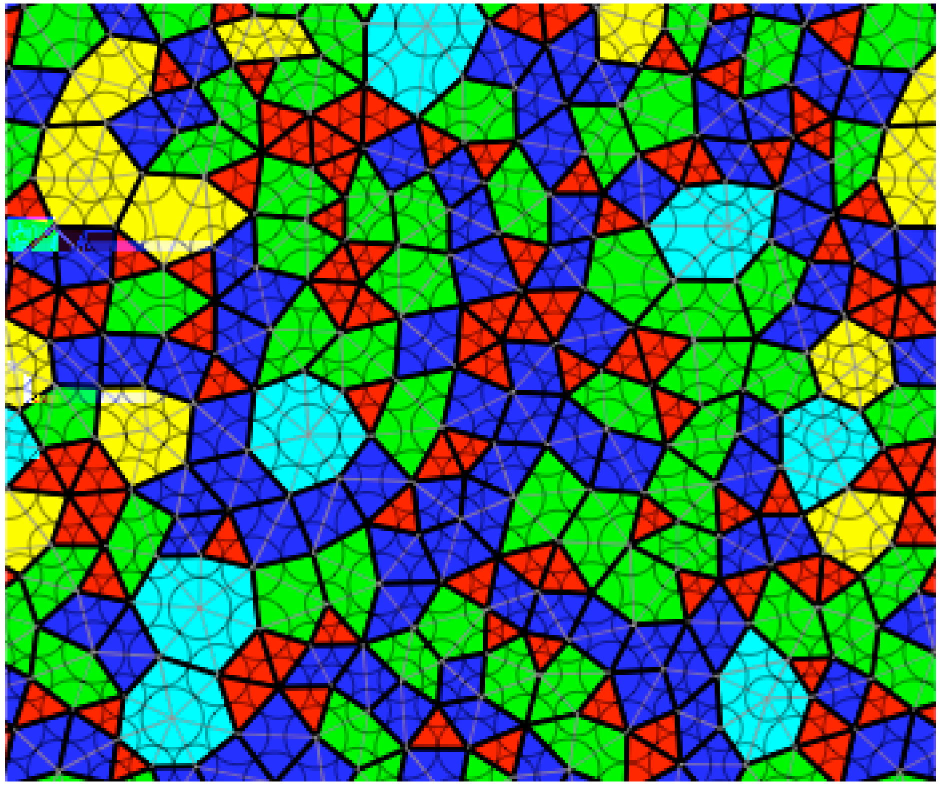
Recent advances in jamming: Packing probabilities, geometrical families, and anharmonicity



Prof. Corey S. O'Hern
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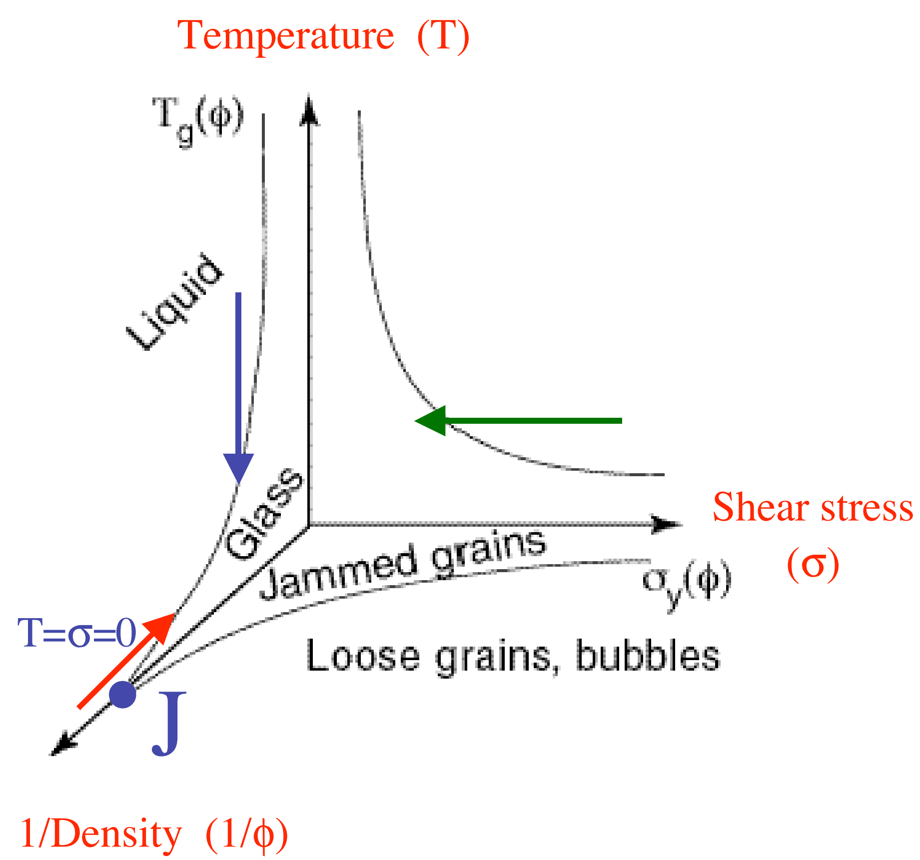
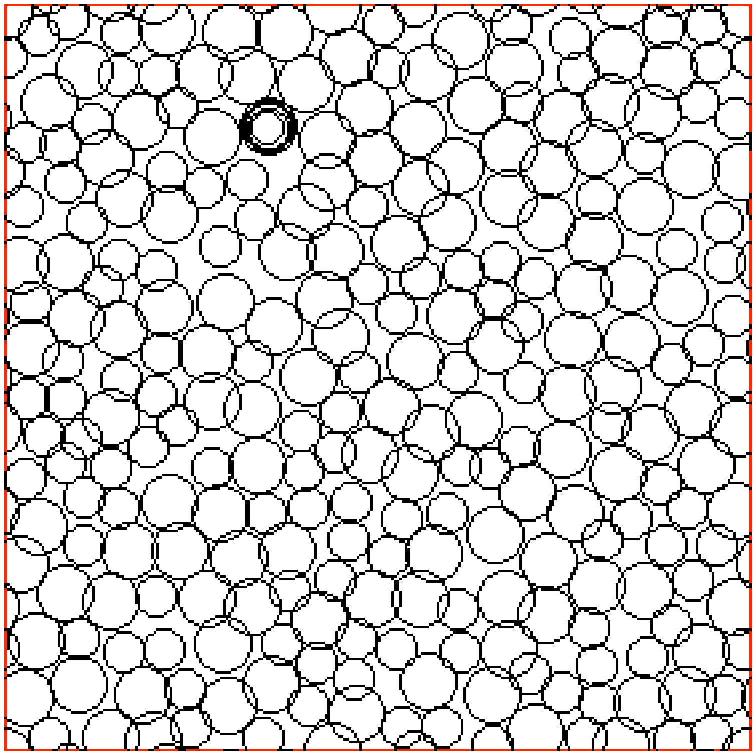
Jamming Phase Diagram



Liu and Nagel, Nature 396 (1998) 21
O'Hern, Silbert, Liu, Nagel, PRE 68 (2003) 011306.

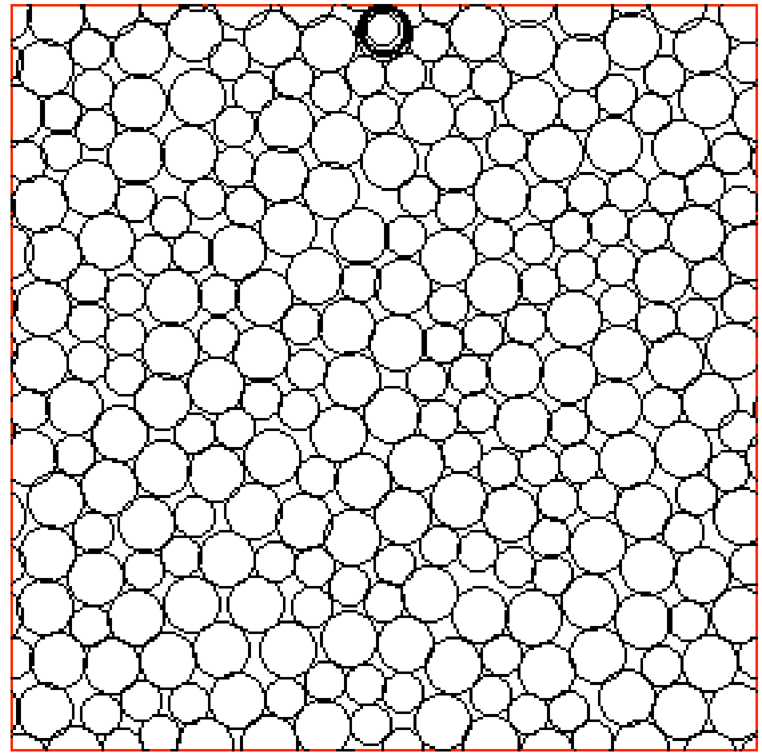
Simulations of Jamming

$T > T_g$



Temperature (T), packing fraction (ϕ)

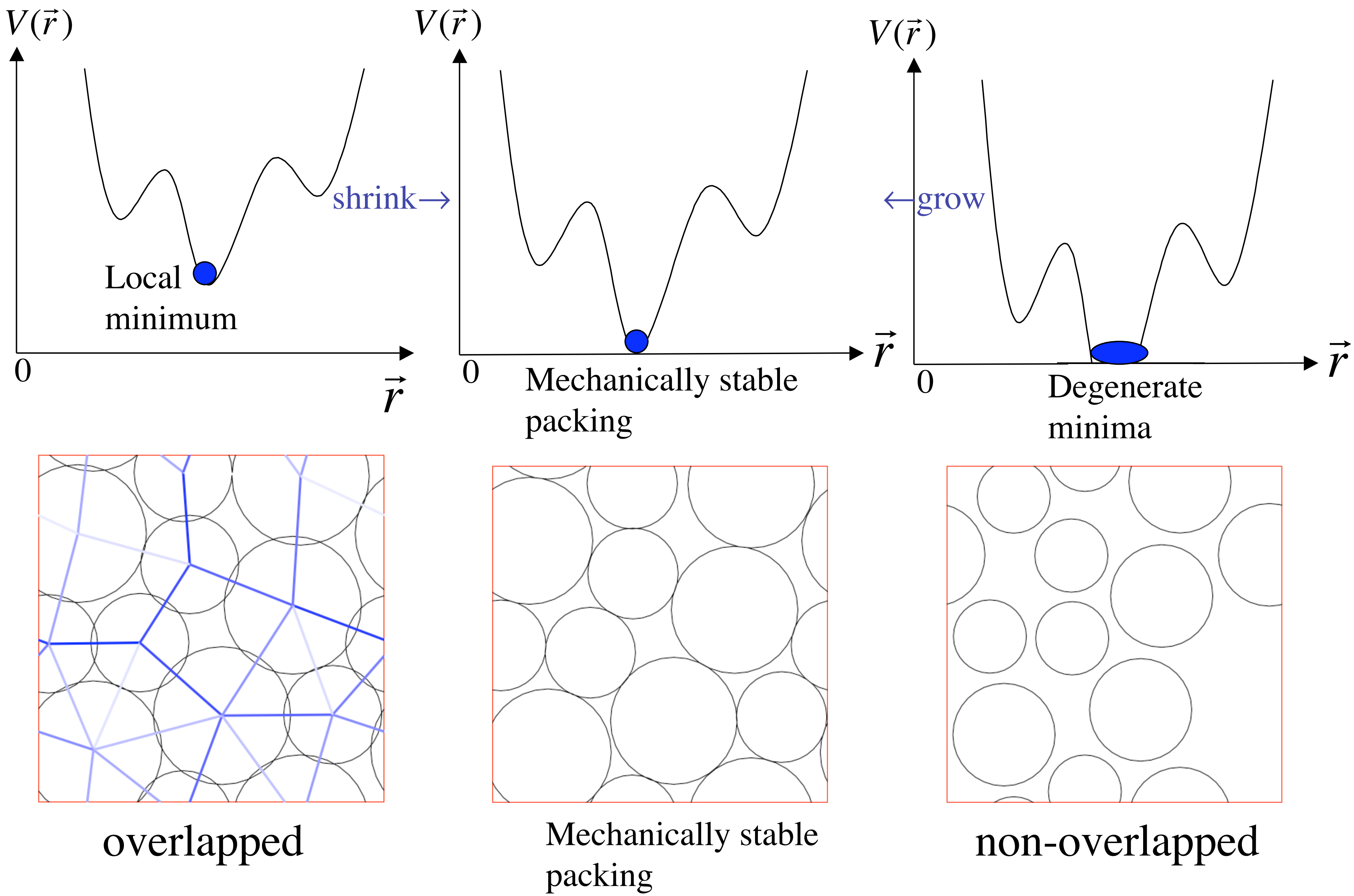
$\sigma > \sigma_y$



Shear stress (σ), packing fraction (ϕ)

$$\phi = \frac{A_{circles}}{A_{box}}$$

Jamming along the ϕ-axis



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?

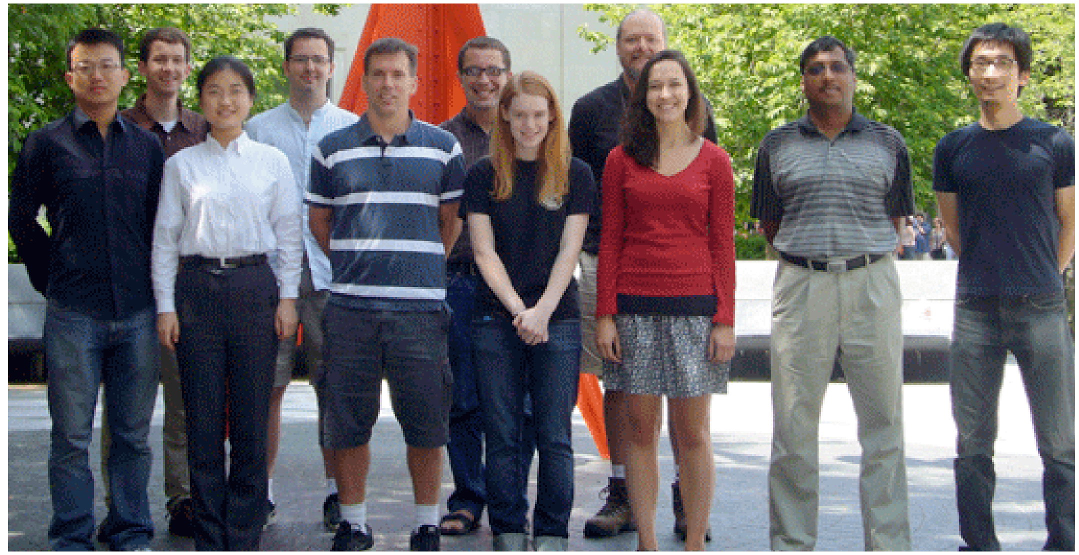
- Can the vibrational response be determined from *static* jammed packings?

The O'Hern Group

Yale SCHOOL OF ENGINEERING & APPLIED SCIENCE

Theoretical & Computational Studies of Soft and Biological Materials

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.

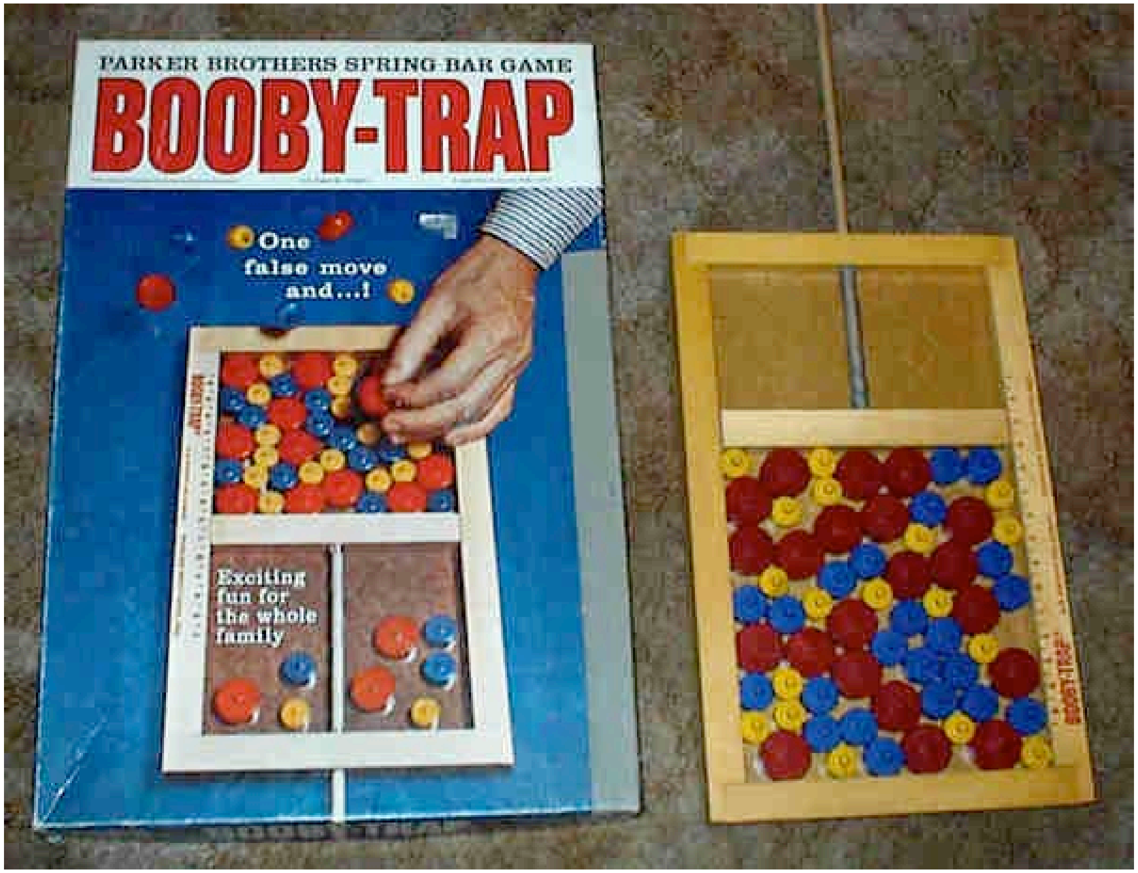
NSF DMS-0835742, Duration: 9-1-08 to 8-31-12
NSF CBET-0967262, Duration: 2-15-10 to 2-14-13
DTRA BRBAA08-H-2-0108, Duration: 4-1-10 to 3-31-15
NSF-PHY-1019147, Duration: 7-1-10 to 6-30-15
NSF-DMR-1006537, Duration: 9-1-10 to 8-31-13
NIH-R21-NS-070251-01A1, Duration: 7-1-11 to 6-30-14

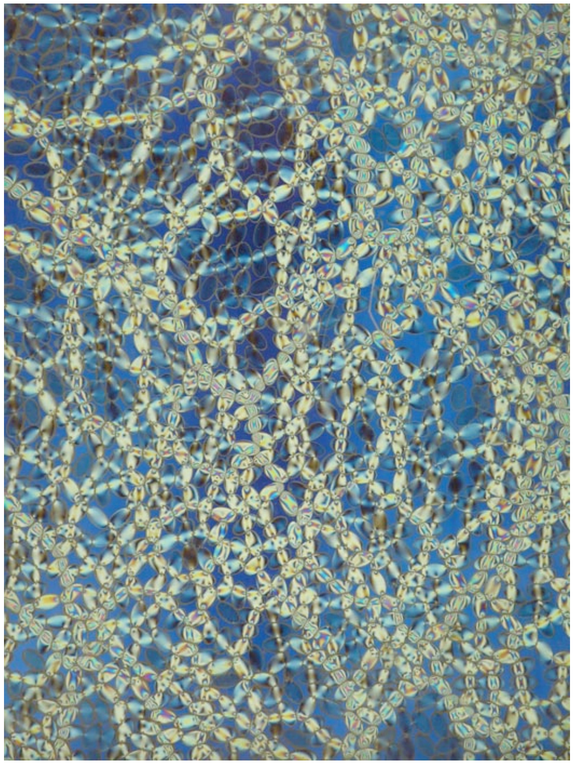
The Raymond and Beverly Sackler Institute for Biological, Physical and Engineering Sciences | Yale

The O'Hern Group

1. Dr. S. S. Ashwin, Ph.D. in Physics, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India (protocol dependence in granular media)
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)
6. Wendell Smith, 1st year Ph.D. student in Physics (asphaltines)
7. Minglei Wang, 1st year Ph.D. student in Mechanical Engineering & Materials Science (optics of amorphous materials)
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?

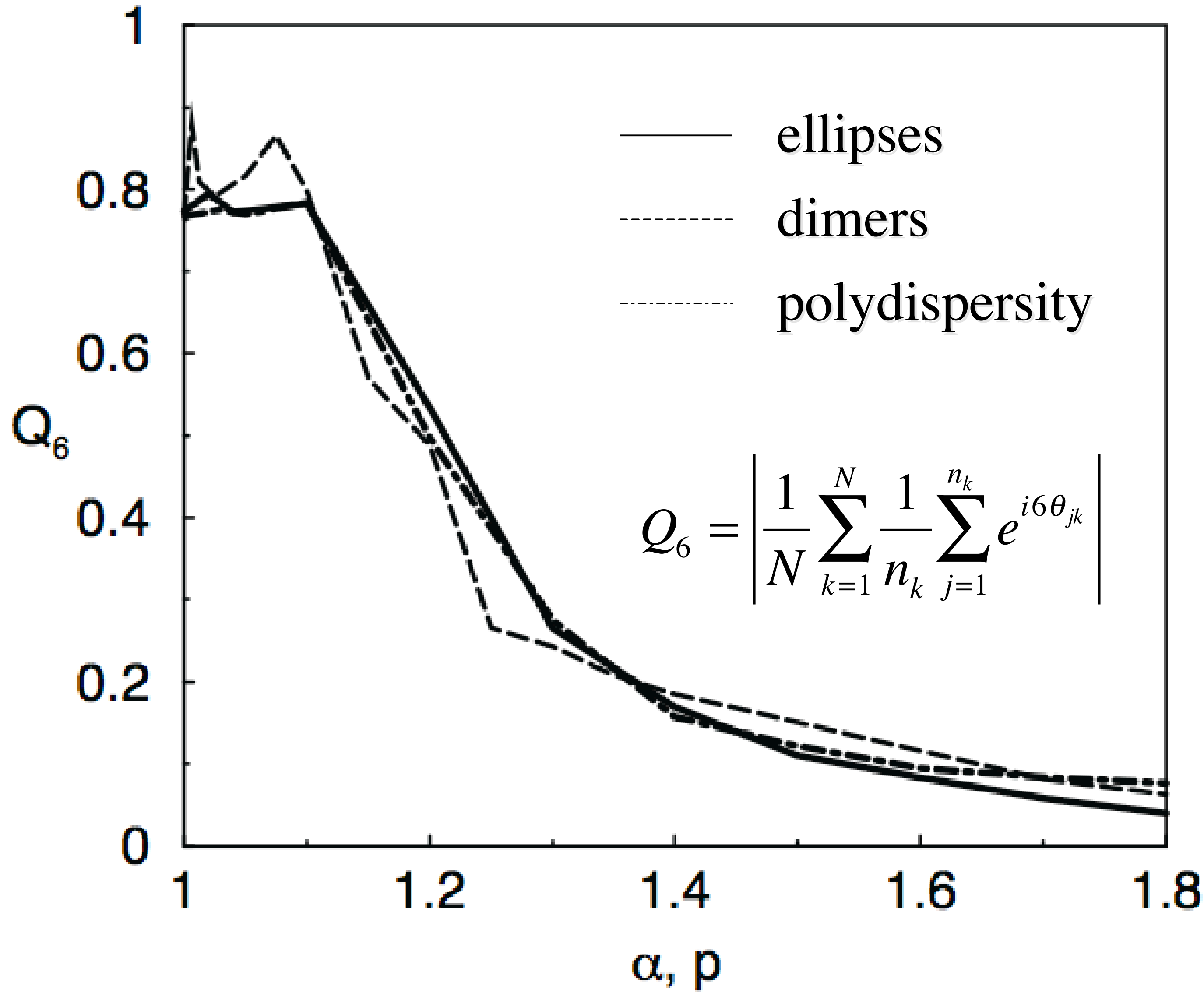




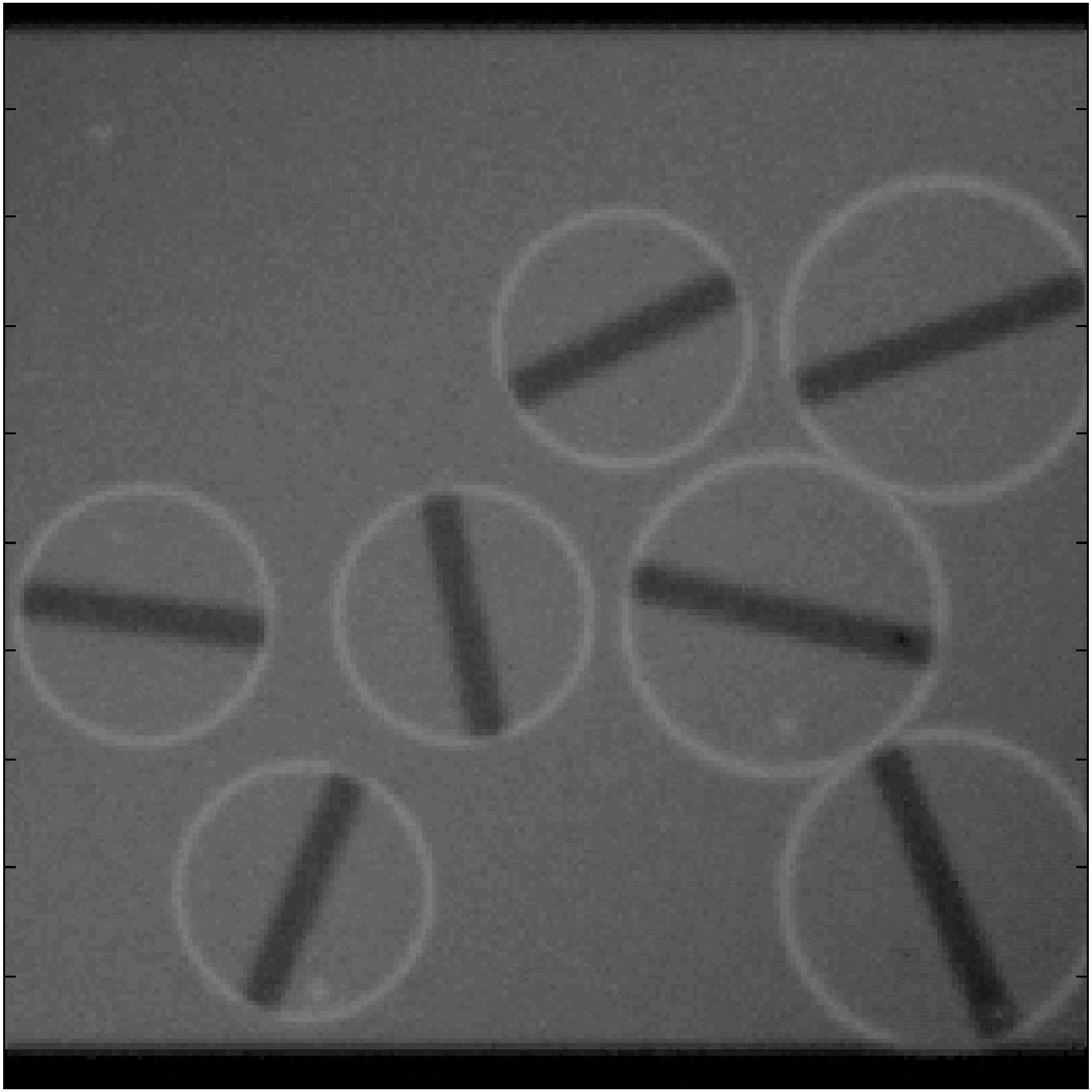
Distinguishing features of granular meida: athermal, dissipative, driven

Jammed = mechanically stable (MS) configuration with extremely small particle overlaps; net forces (and torques) are zero on each particle; stable to small perturbations

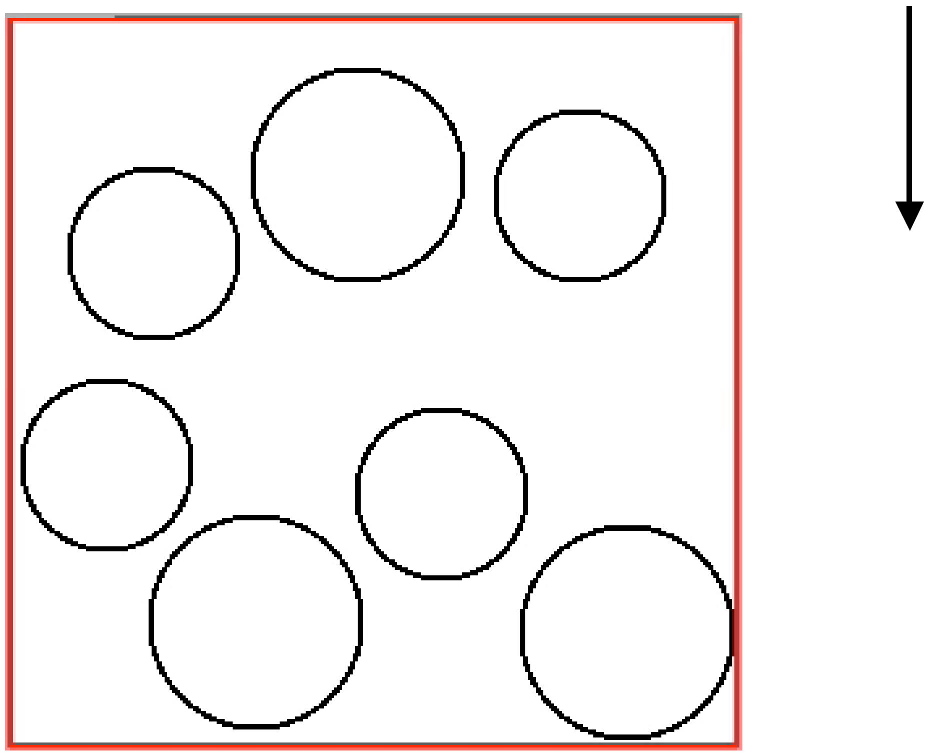
Disorder versus Order



Are jammed packings points in configuration space?



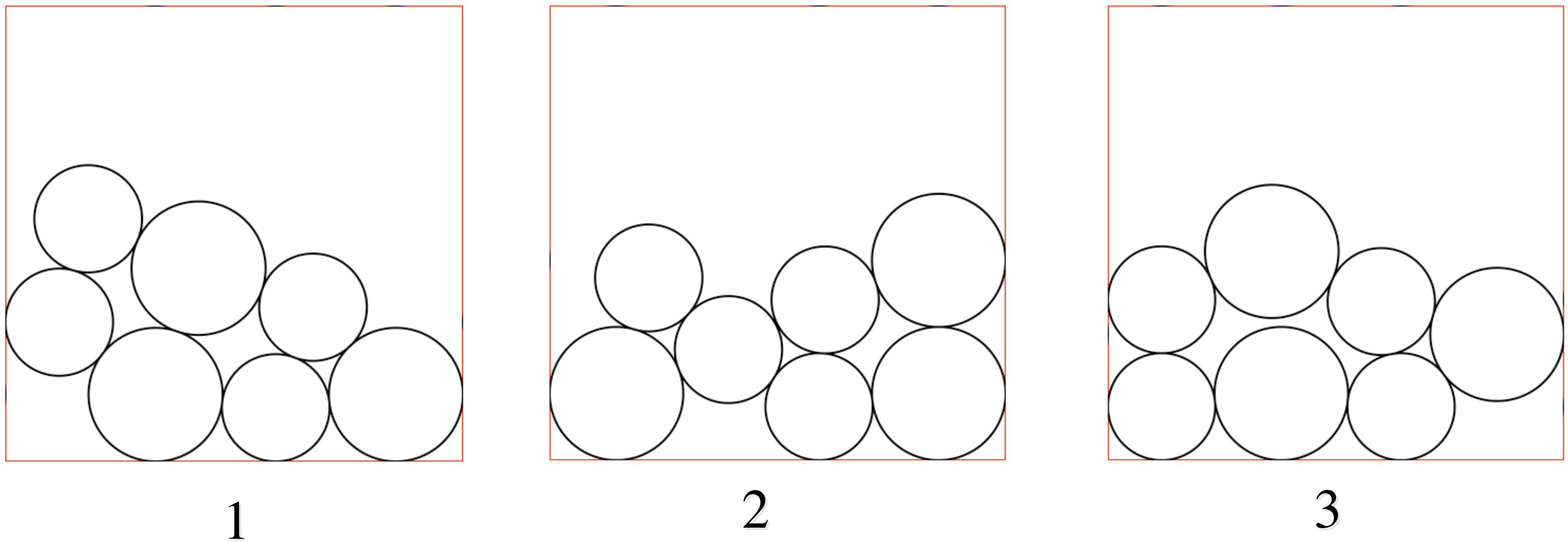
Deposition Algorithm in Simulations



$$\bar{g} = \frac{m_s g}{k\sigma_s}$$

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

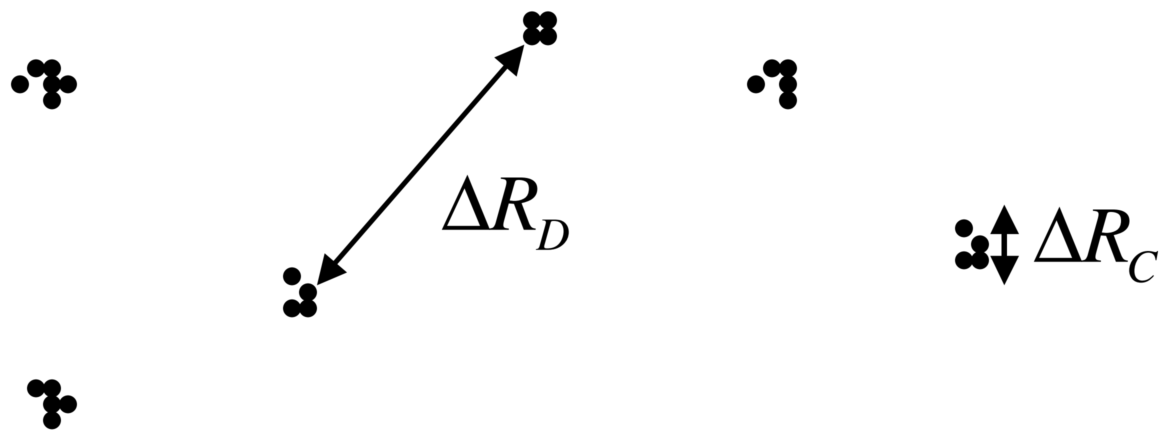
Mechanically Stable Frictionless Packings



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

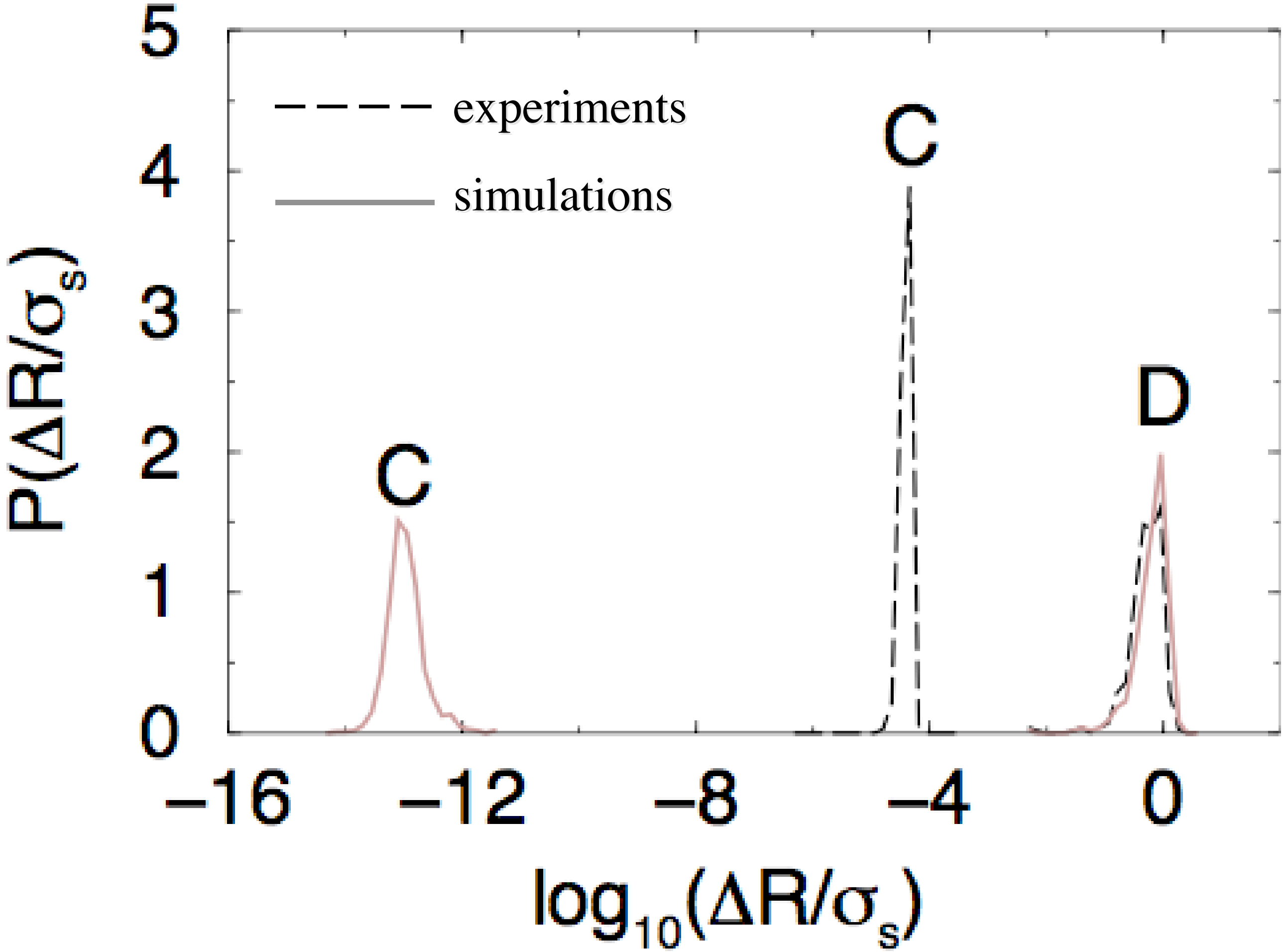
Configuration Space of Mechanically Stable Packings

$$R = \{\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\}$$



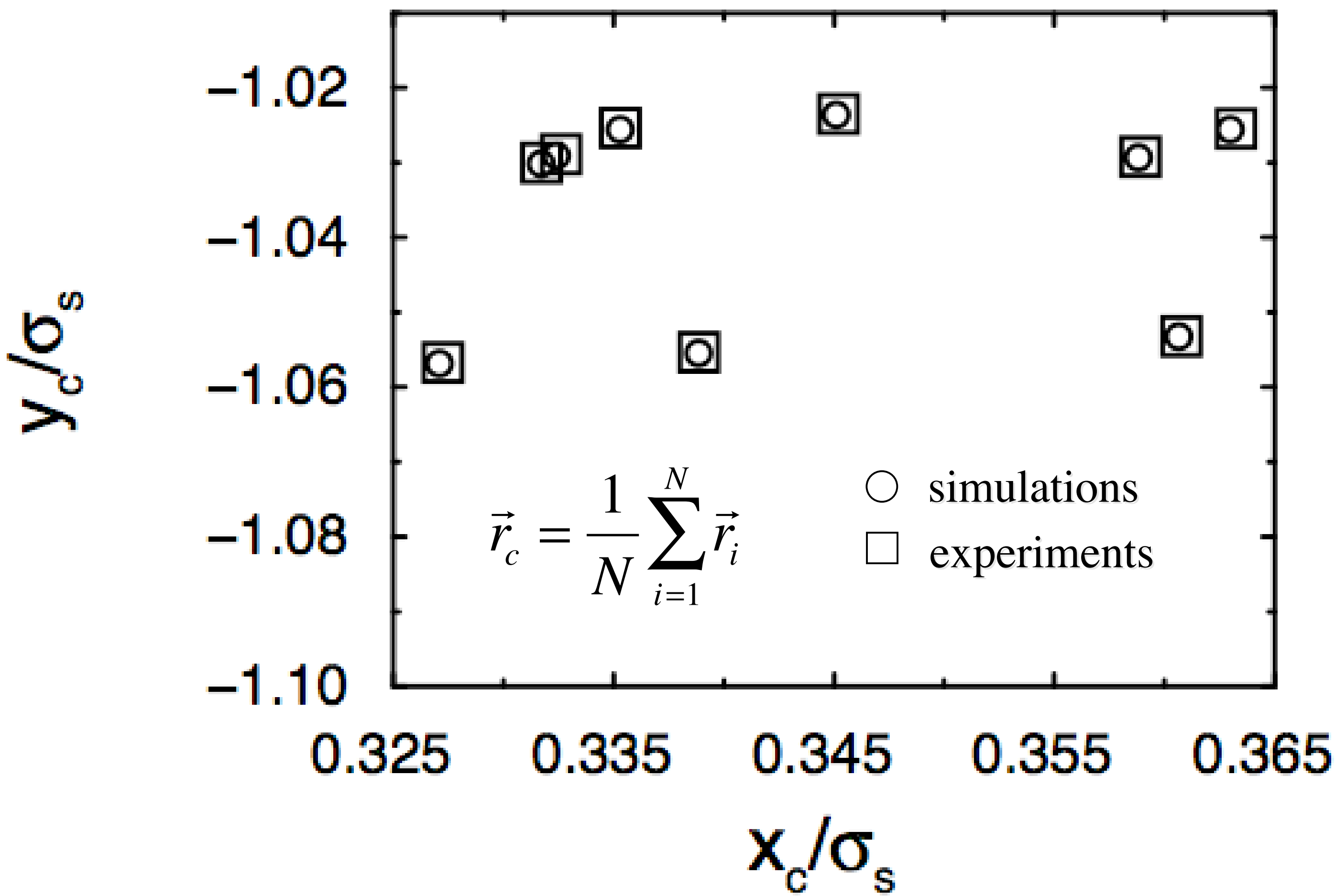
- ΔR_D= distance in configuration space between distinct MS packings
- ΔR_C= error in measuring distinct MS packings

Separation in Configuration Space

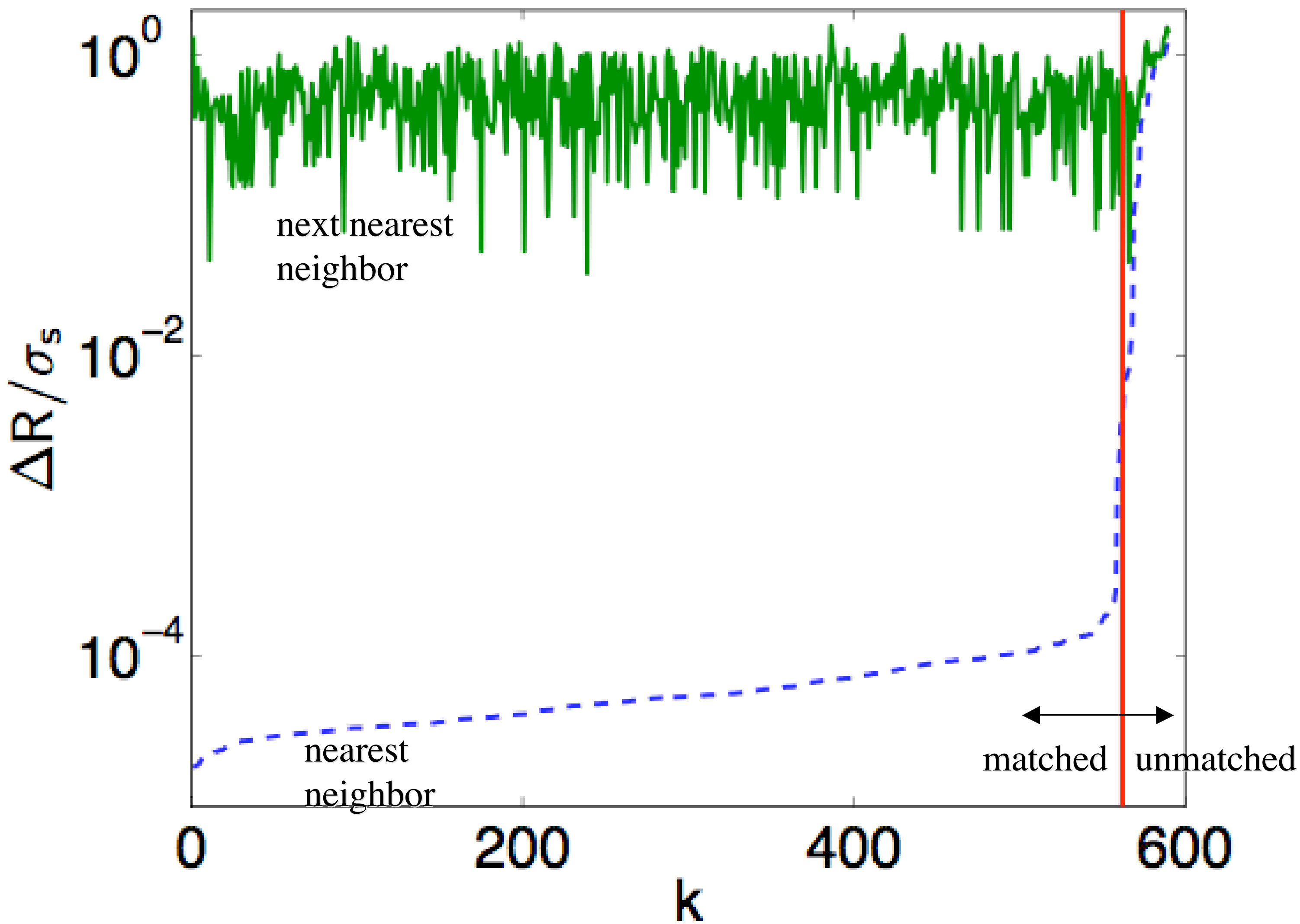


- MS frictionless packings are discrete points in configuration space

Discrete MS Packings



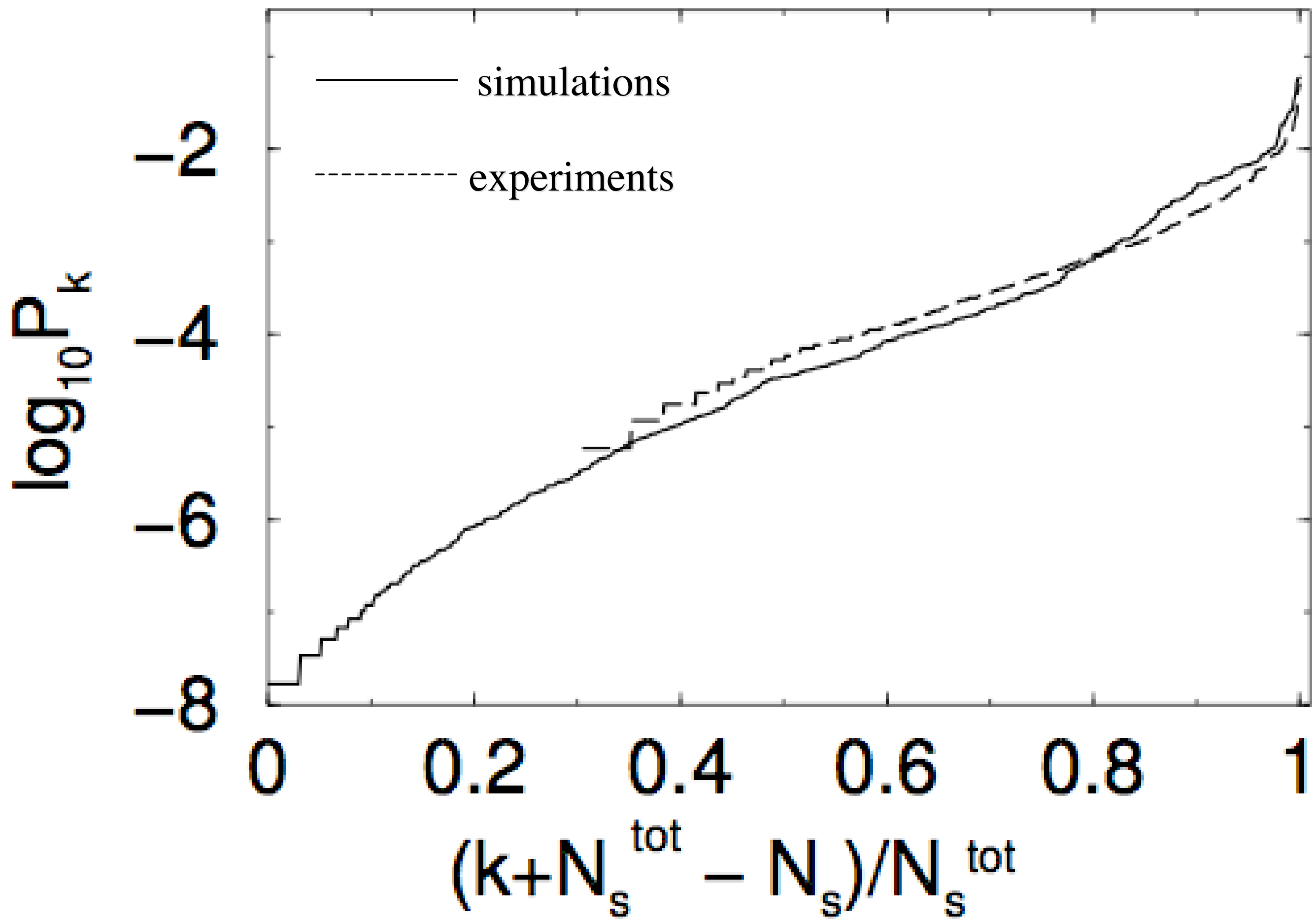
How is the quantitative agreement between sims and exps?



- 95% of distinct MS packing match; others are unstable in sims

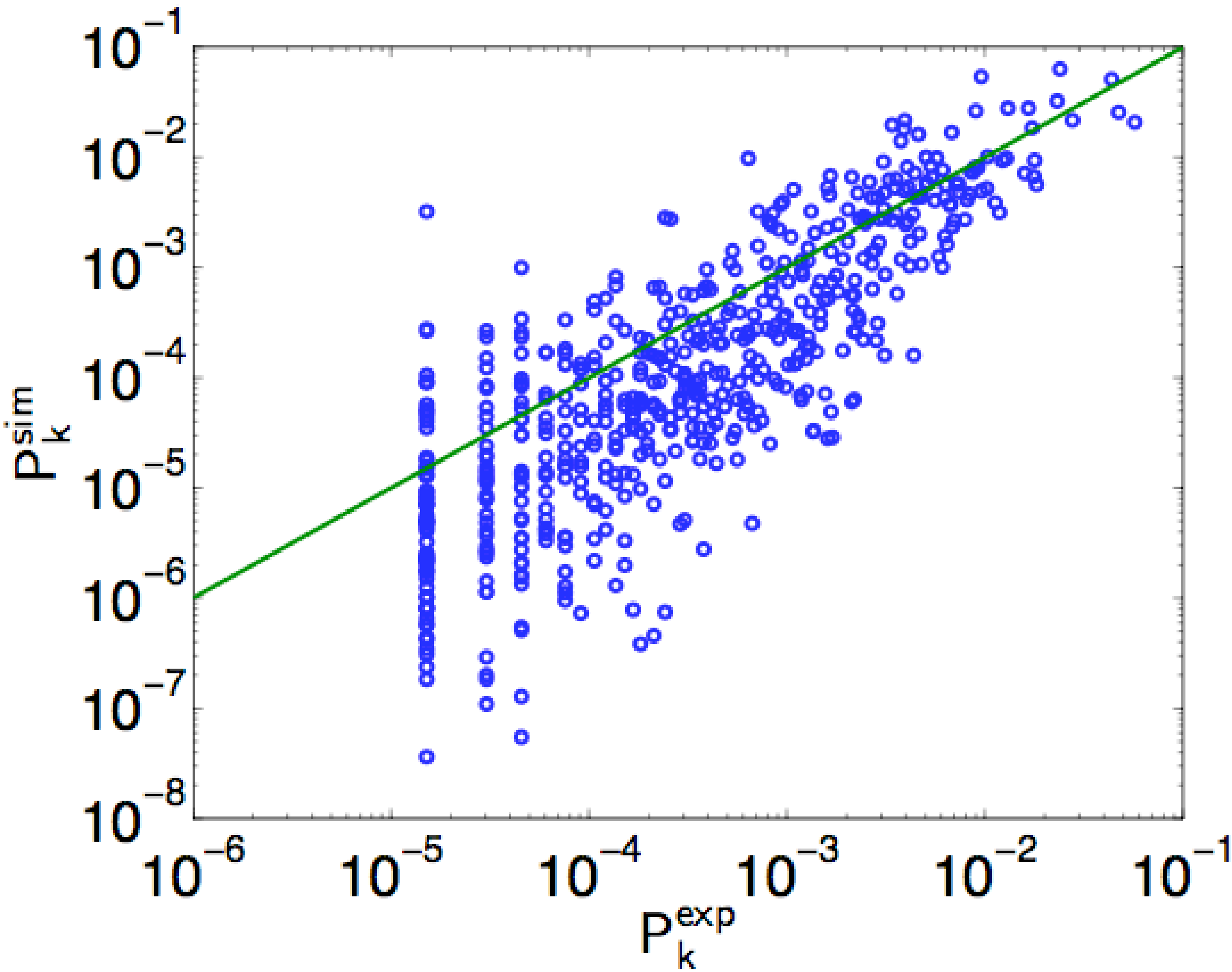
Are jammed packings equally probable?

Sorted Probabilities



- 7 (4) orders of magnitude variation in probabilities in simulations (experiments)

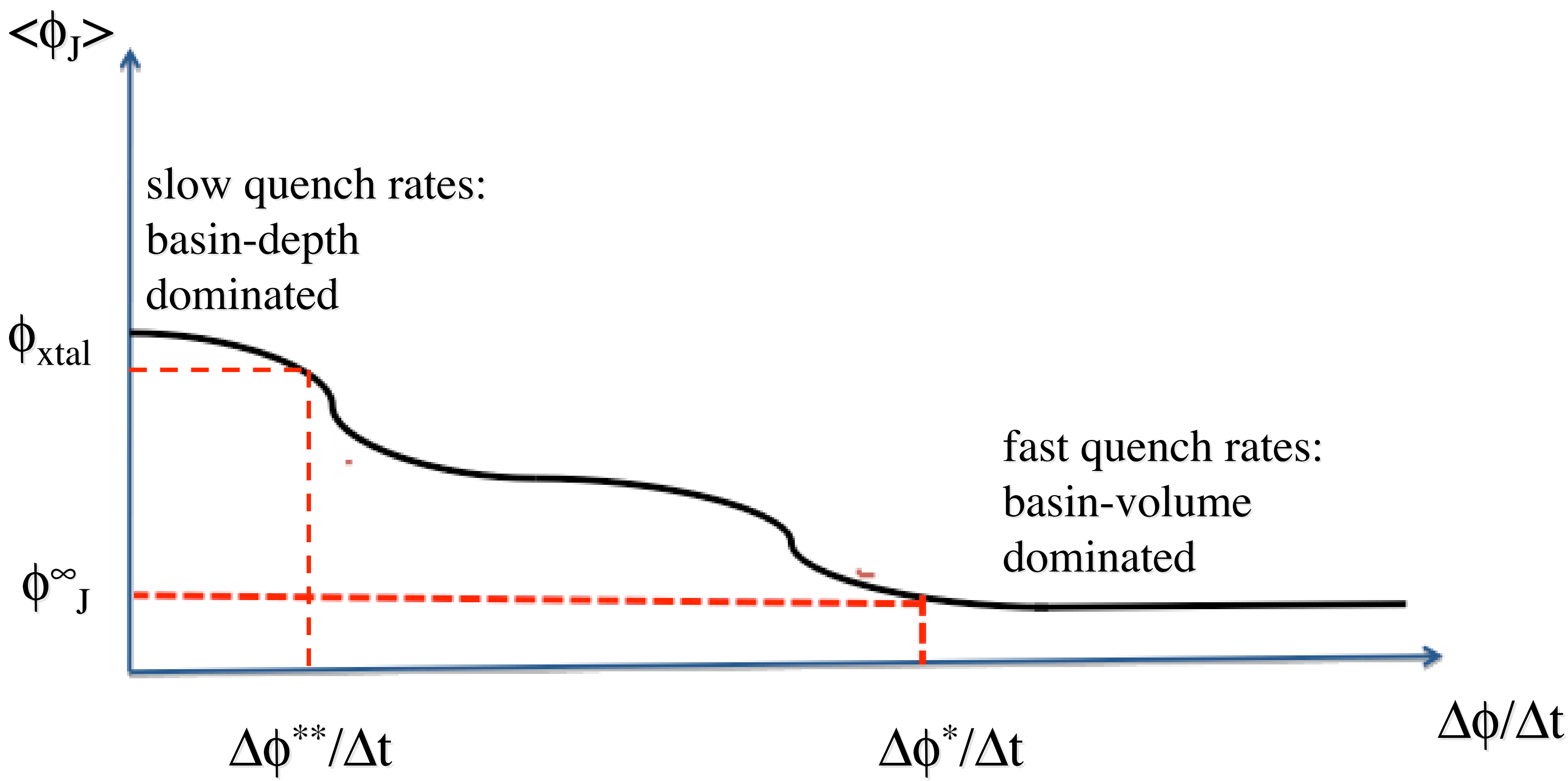
MS Packing Probabilities Are Robust



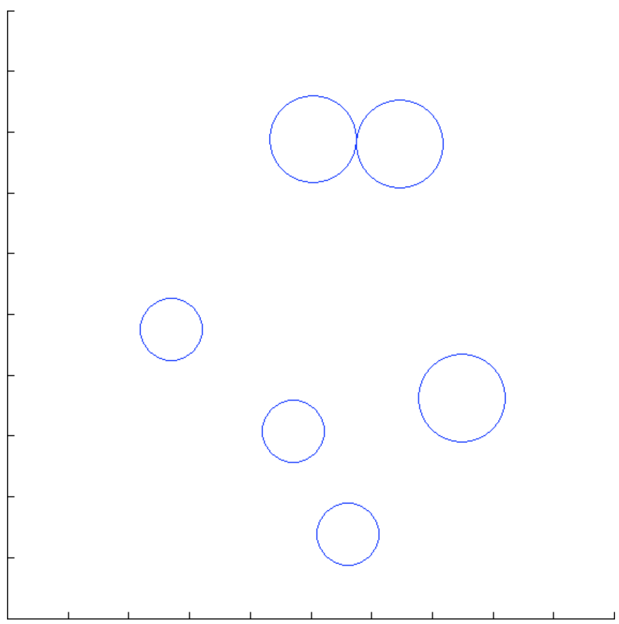
- Rare MS packings in exps are rare in sims; frequent MS packings in exps are frequent in sims

What determines the packing probabilities?

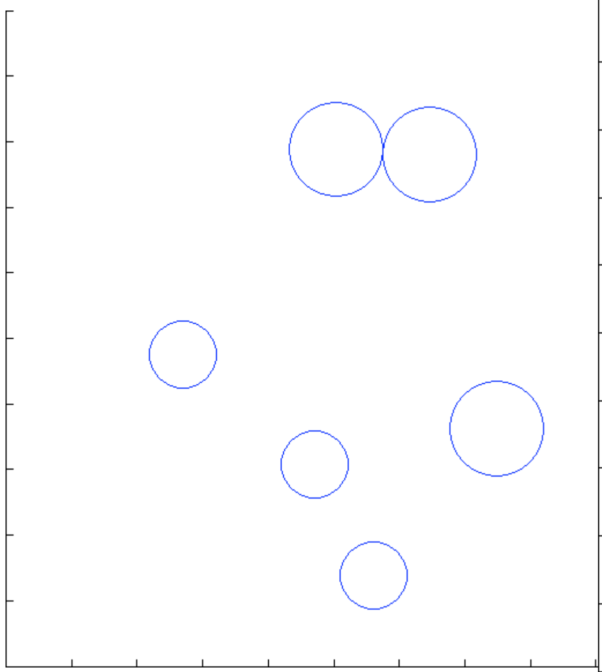
Protocol Dependence of Granular Packings



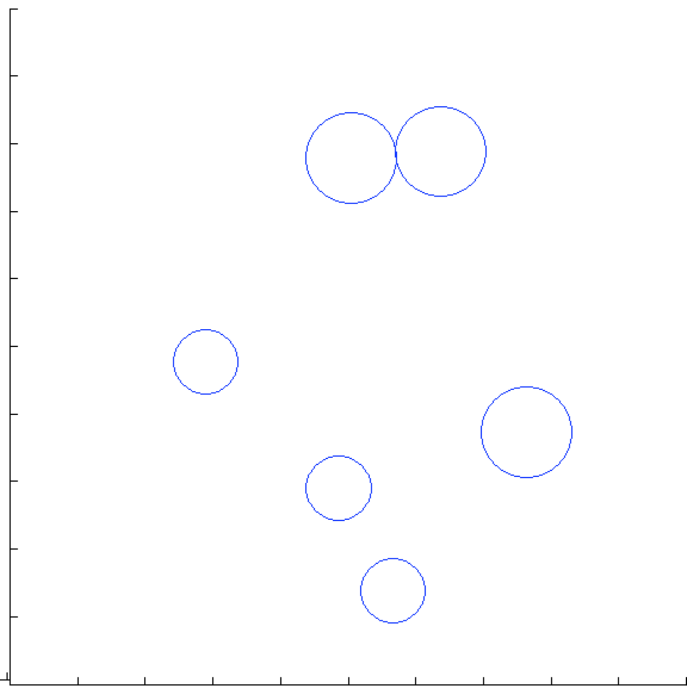
Rate dependence and basin volume



fast rate; ϕ_f=0.622

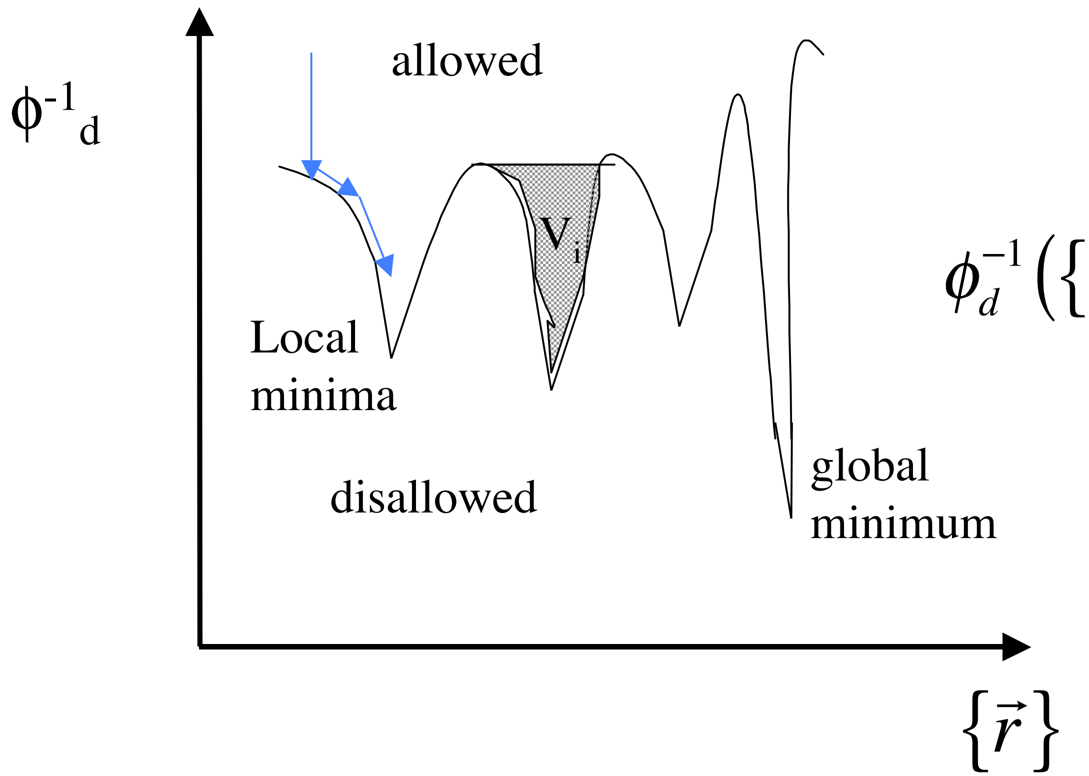


slow rate; ϕ_f=0.730



fast rate; different IC; ϕ_f=0.730

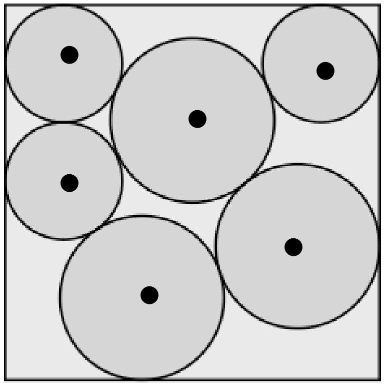
Density landscape for hard spheres



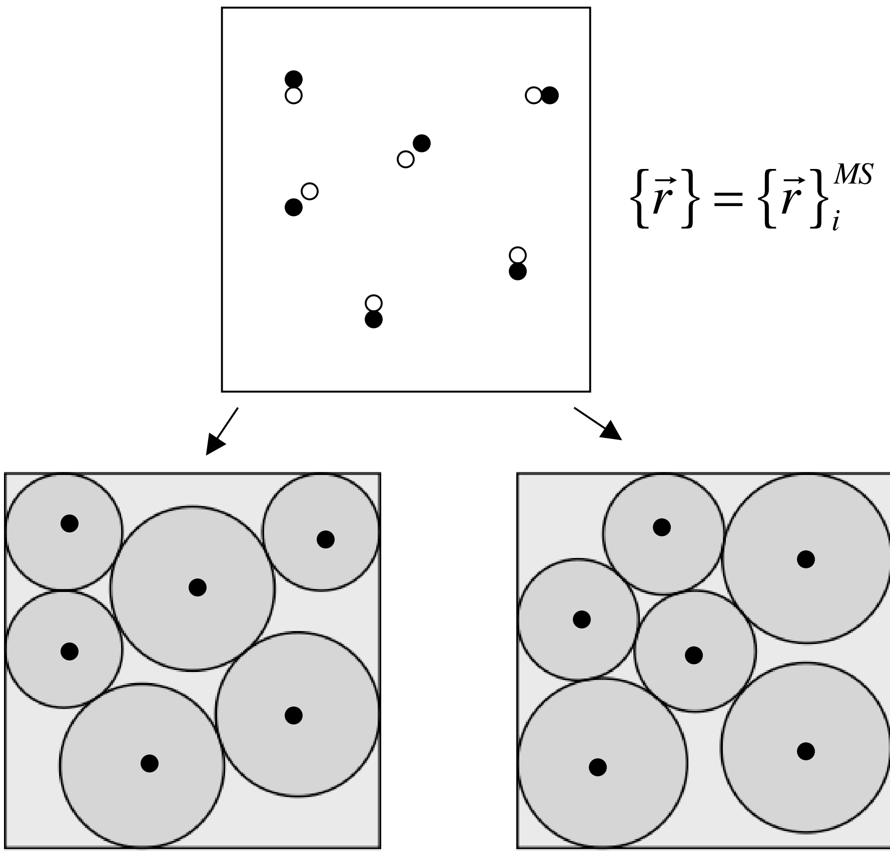
$$\phi_d^{-1}\left(\{\vec{r}\}\right) = \frac{6V}{\pi N \min_{mn}\left|\vec{r}_m - \vec{r}_n\right|^3}$$

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

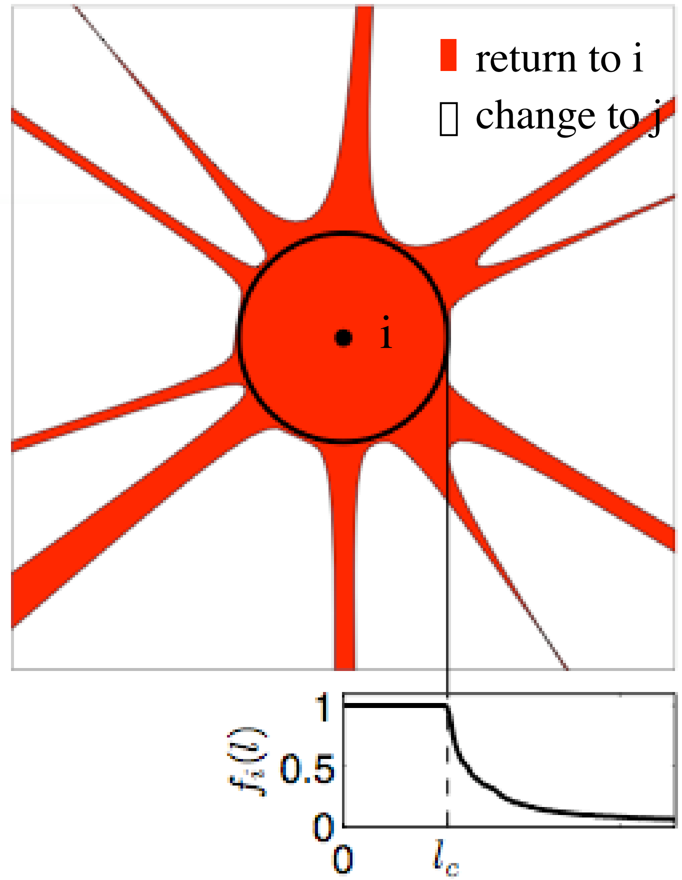


$$\phi_i^{MS}, \{\vec{r}\}_i^{MS}$$



$$\{\vec{r}\} = \{\vec{r}\}_i^{MS} + l\hat{e}_r$$

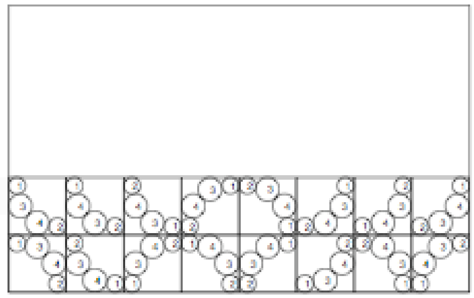
$$f_i(l) = \frac{M_i}{M}$$



$$l = \sqrt{(x_{1f}-x_{10})^2 + (x_{2f}-x_{20})^2 + \cdots + (x_{Nf}-x_{N0})^2 + (y_{1f}-y_{10})^2 + (y_{2f}-y_{20})^2 + \cdots + (y_{Nf}-y_{N0})^2}$$

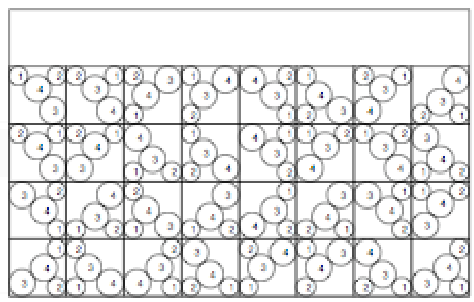
Distance in config. space

Prob=0.413250%

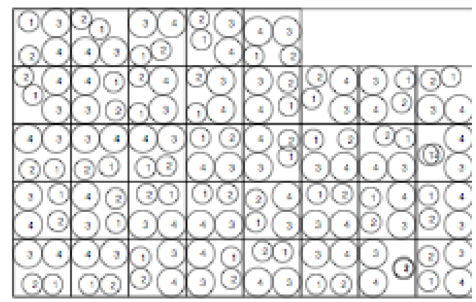


Prob=0.000050%

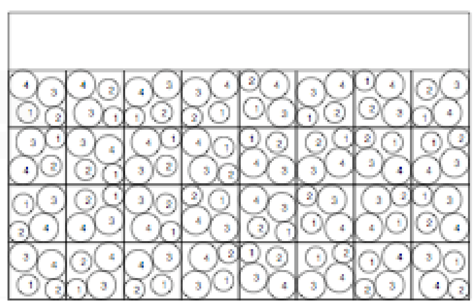
Prob=6.065950%



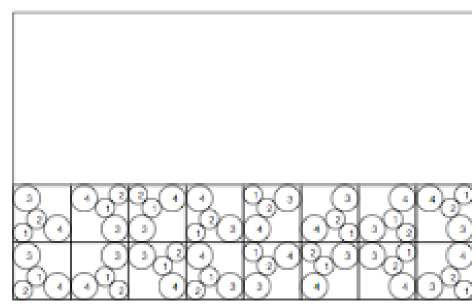
Prob=0.187150%



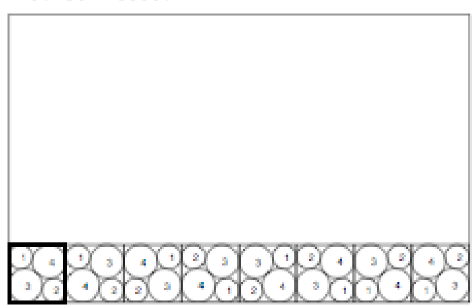
Prob=26.197200%



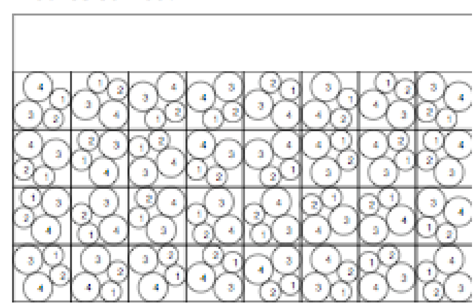
Prob=2.868100%



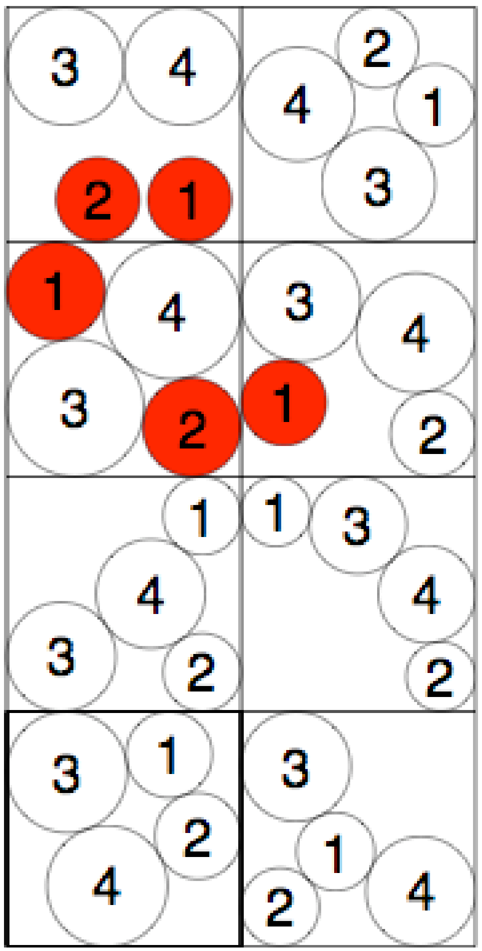
Prob=30.415850%

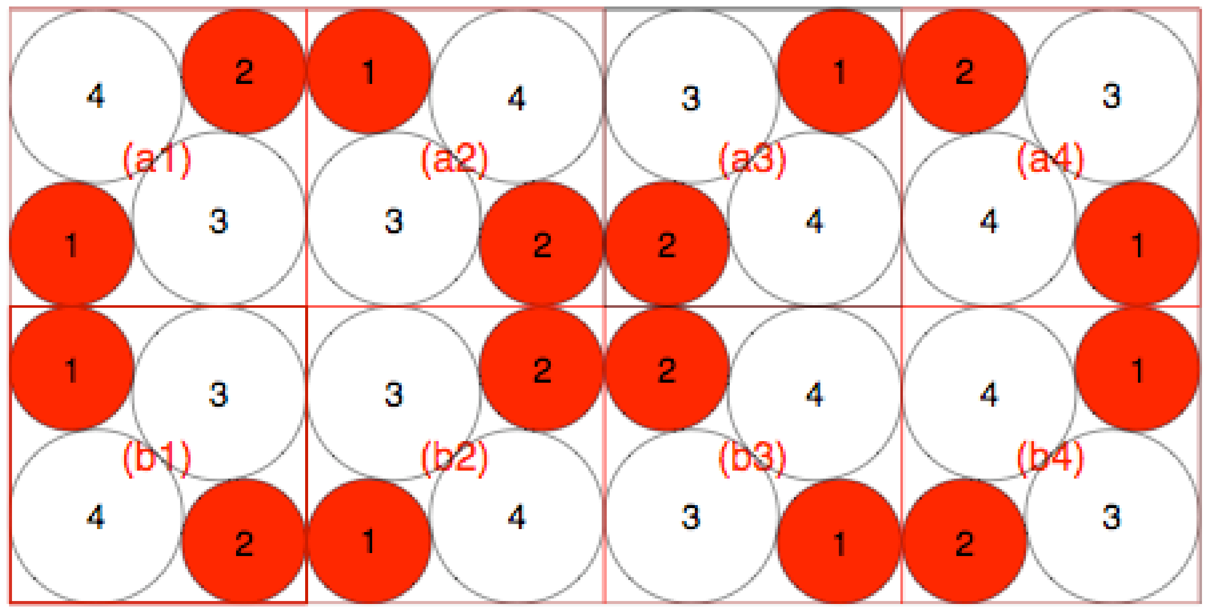


Prob=33.852450%



Distinct N=4 Packings

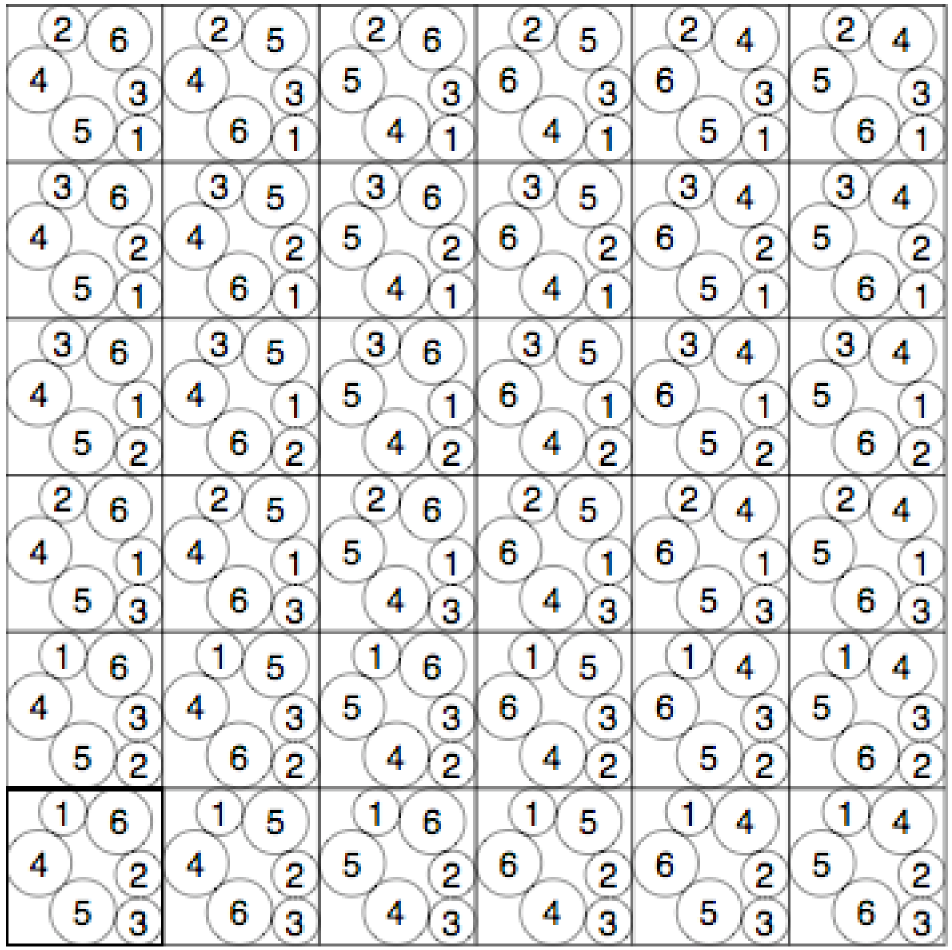




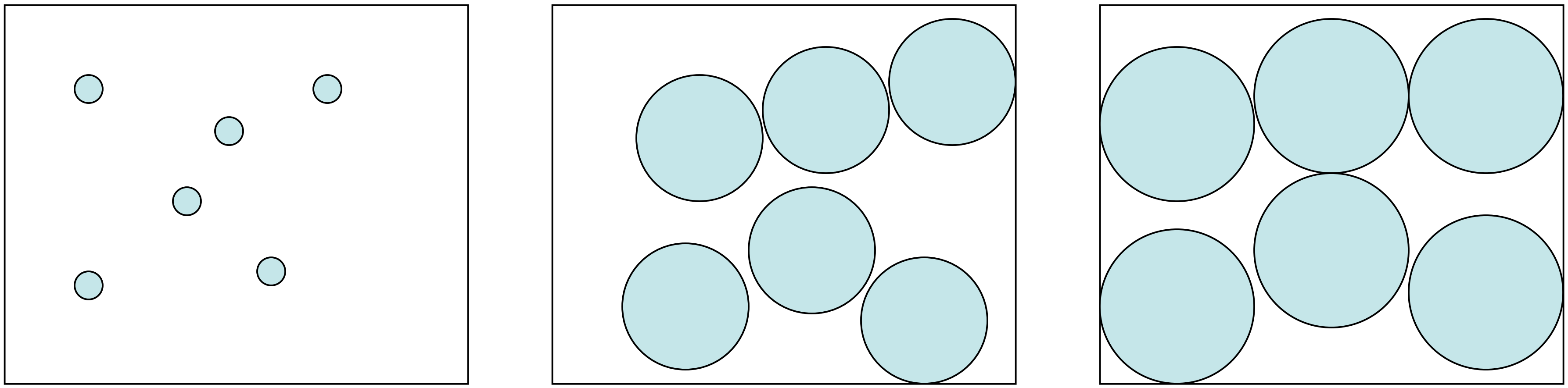
Polarizations

floater

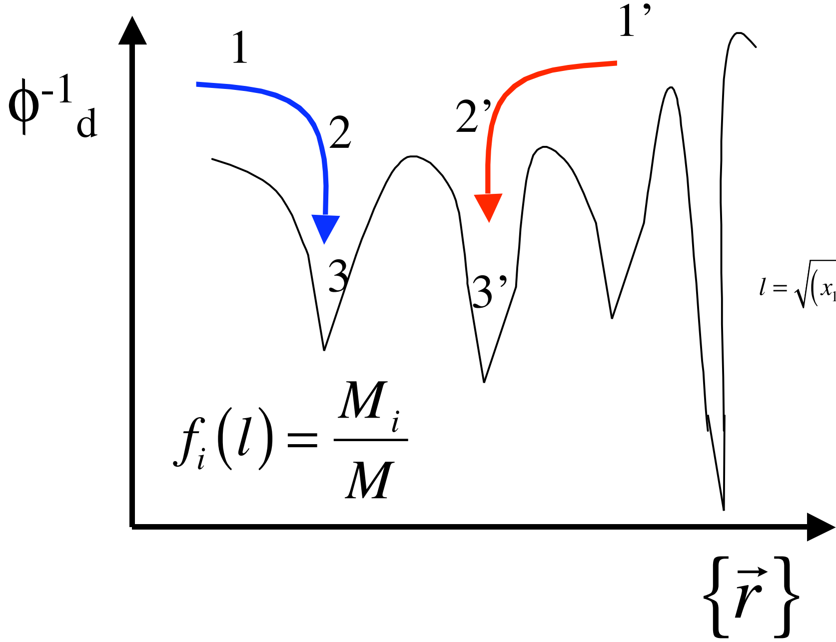
Particle-label permutations



Method 2 (large l): Random initial conditions



$\phi_1, \{\vec{r}\}_1$ $\phi_2, \{\vec{r}\}_2$ $\phi_3, \{\vec{r}\}_3$



Distance in config. space

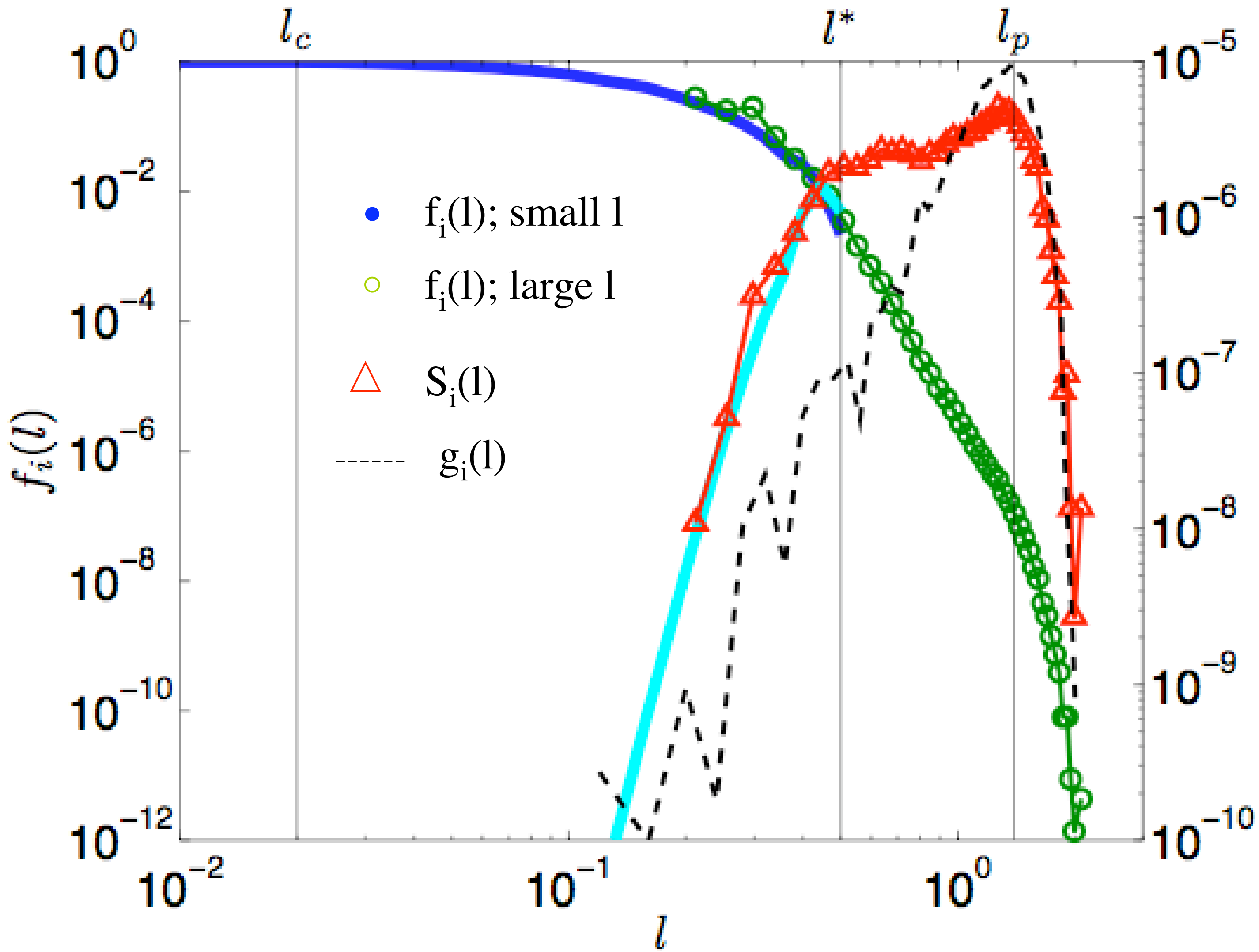
$$l = \sqrt{(x_{1f} - x_{10})^2 + (x_{2f} - x_{20})^2 + \cdots + (x_{Nf} - x_{N0})^2 + (y_{1f} - y_{10})^2 + (y_{2f} - y_{20})^2 + \cdots + (y_{Nf} - y_{N0})^2}$$

Basin Volumes

$$P_i = \frac{V_i}{L^{dN}} \qquad\qquad V_i = \int_0^{\sqrt{dN}} S_i(l)\,dl$$

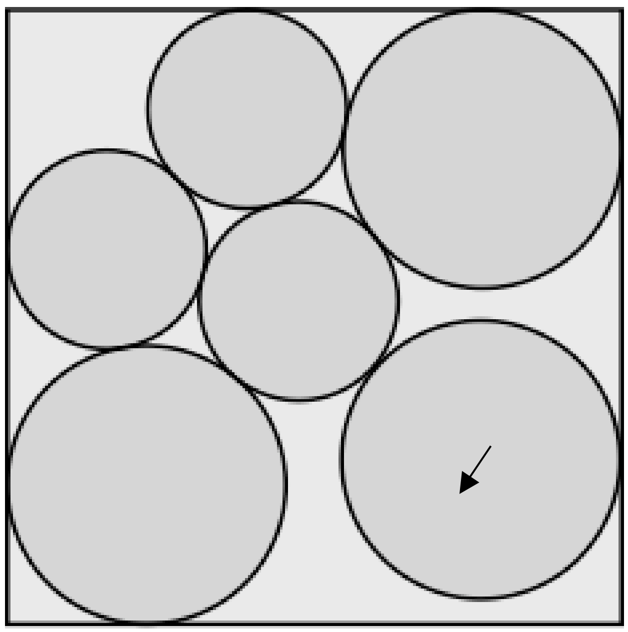
$$S_i(l) = A_{dN} f_i(l)\, l^{dN-1} \mathrm{P}_i N_s! N_l!$$

Weighted/Unweighted basin profile functions

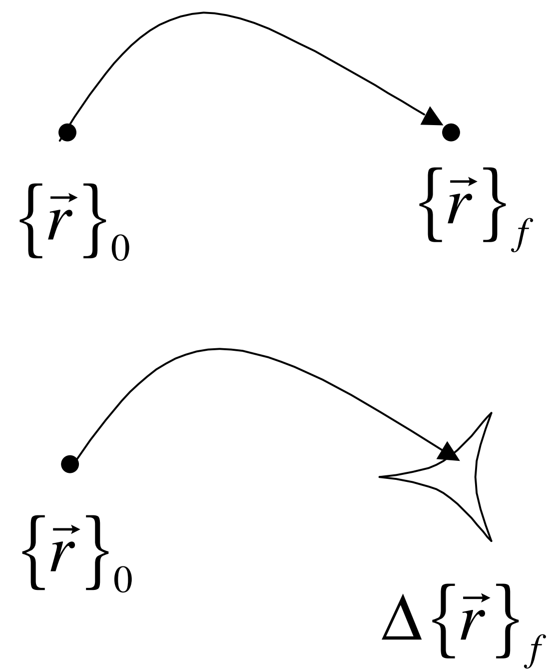


- Probability of MS packing determined by large l, not core region l_c
- Large probability near peak in MS packing separation distribution

Floaters

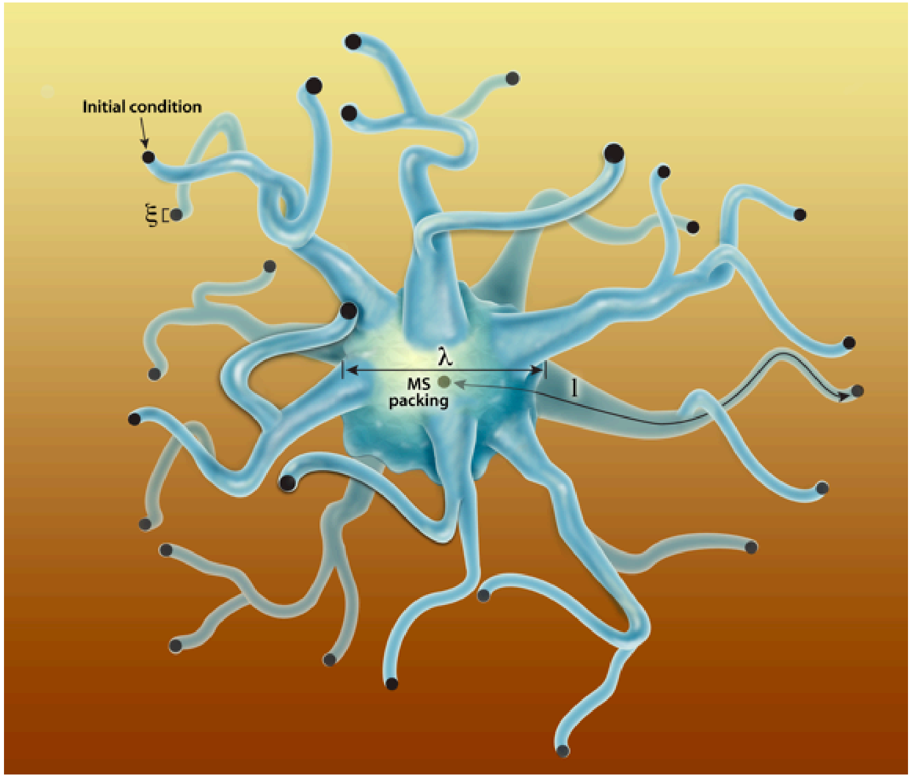


Particles with fewer than 3 contacts



Future Directions

- Probability for MS packings determined by large l, not nearby regions of configuration space
- Study ϕ_i and quench rate dependence of probabilities



Vibrational Response in Granular Media

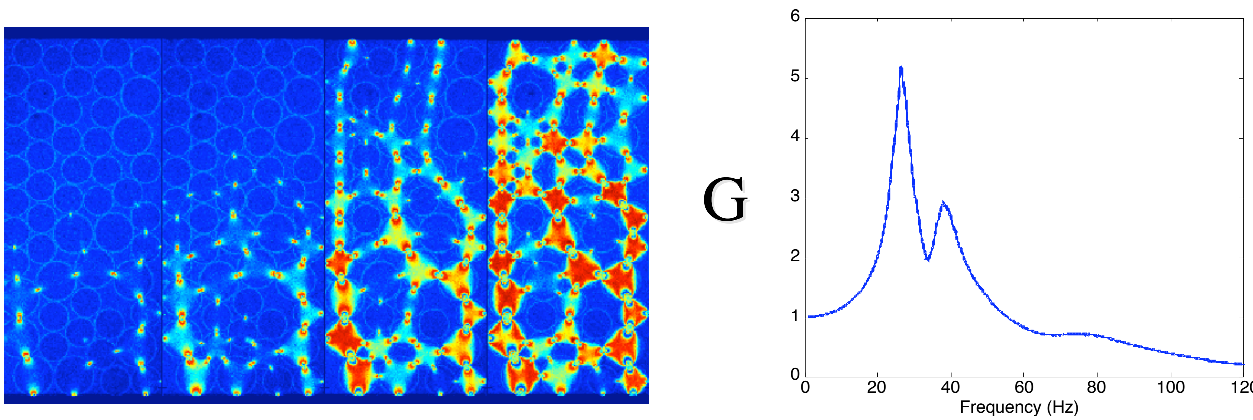
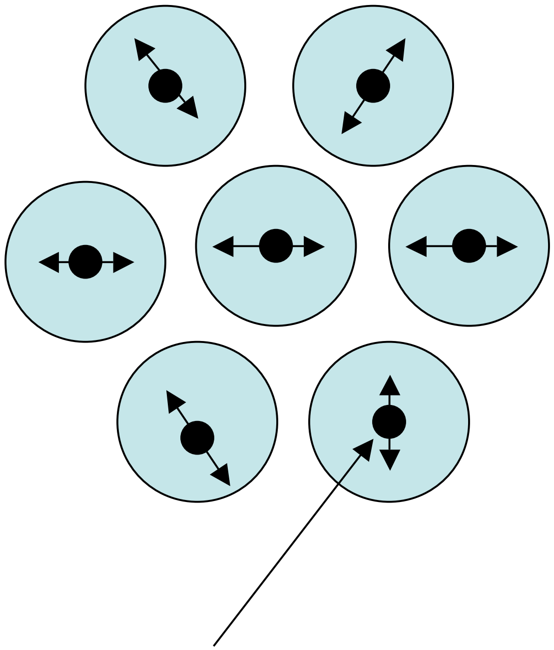
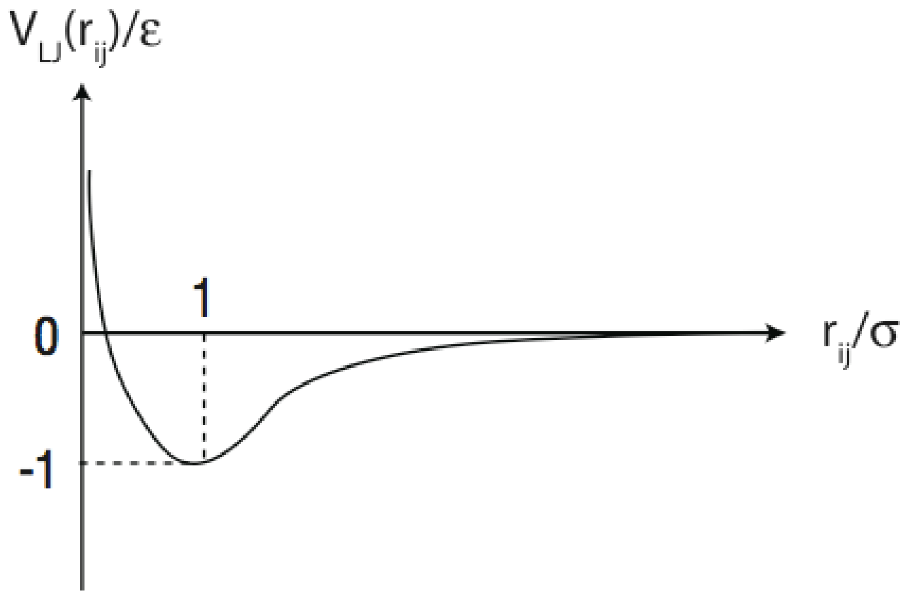


Figure 1: [left] Sound (force) propagation at 4 times and [right] frequency response to a sinusoidal vertical compression of a packed composite material under constant pressure.

Harmonic Solids



$$\vec{r}_0^{\,i} = \left\langle \vec{r}^{\,i}(t) \right\rangle_t$$



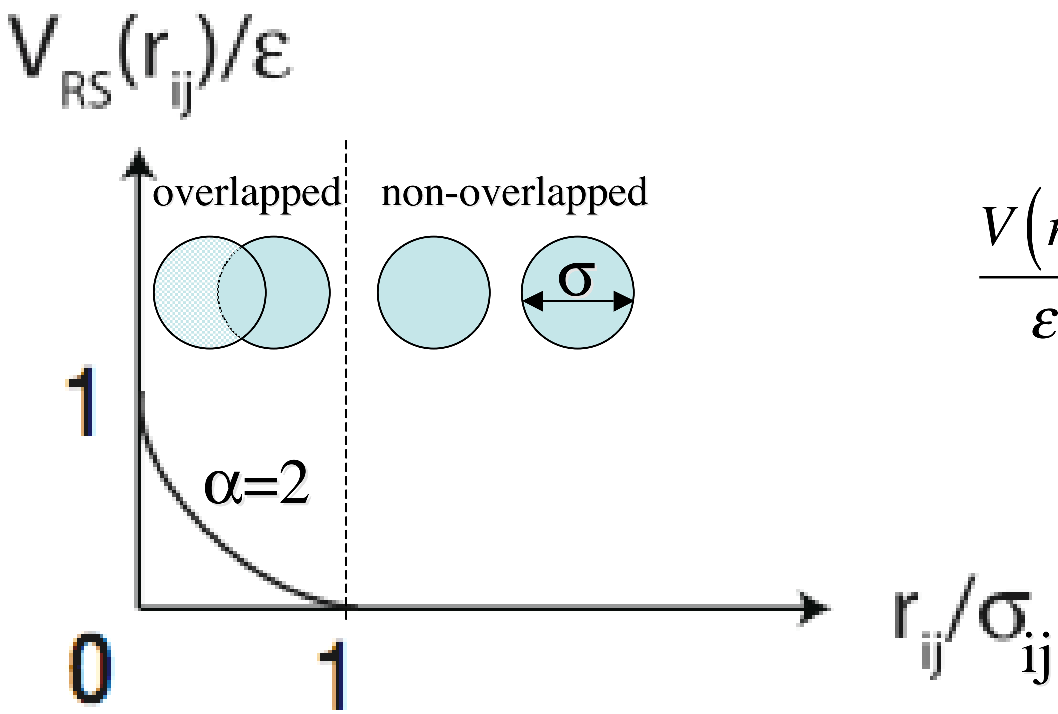
- Atomic and molecular systems
- Pair potentials have `double-sided' minimum and are long-ranged
- Equilibrium positions are well-defined
- Vibrations at low T captured using harmonic approximation

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



$$\frac{V(r_{ij})}{\varepsilon} = \begin{cases} \alpha^{-1}\left(1-\frac{r_{ij}}{\sigma_{ij}}\right)^{\alpha} & r_{ij} \le \sigma_{ij} \\ 0 & r_{ij} > \sigma_{ij} \end{cases}$$

α=2 linear

α=5/2 Hertzian

Total potential energy $V = \sum_{\langle i,j \rangle} V(r_{ij})$

Harmonic approximation: Normal Modes from Dynamical Matrix

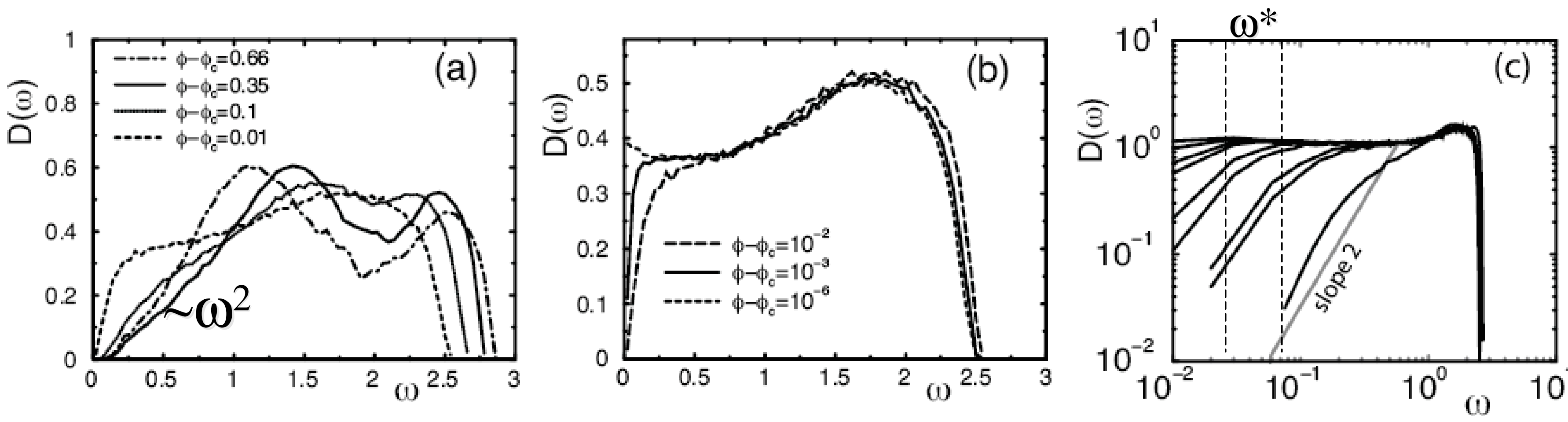
$$M_{\alpha,\beta} = \left. \frac{\partial^2 V(\vec{r})}{\partial r_\alpha \partial r_\beta} \right|_{\vec{r}=\vec{r}_0}$$

α,β=x, y, z, particle index

$\vec{r}_0$ = positions of MS packing

Calculate d N- d eigenvalues; $m_i = \omega^2_i > 0$.

Density of Vibrational Modes via Dynamical Matrix



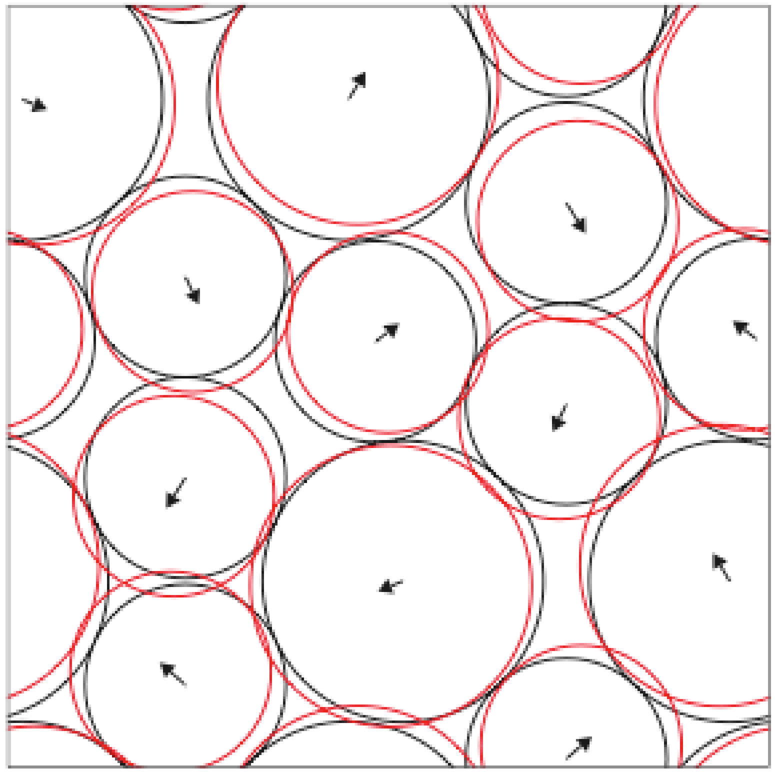
$$D(\omega)d\omega = N(\omega + d\omega) - N(\omega)$$

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

A. J. Liu, S. R. Nagel, W. van Saarloos, and M. Wyart, “The jamming scenario--an introdcution and outlook,” Soft Matter (2010).

Are jammed particulate systems harmonic?

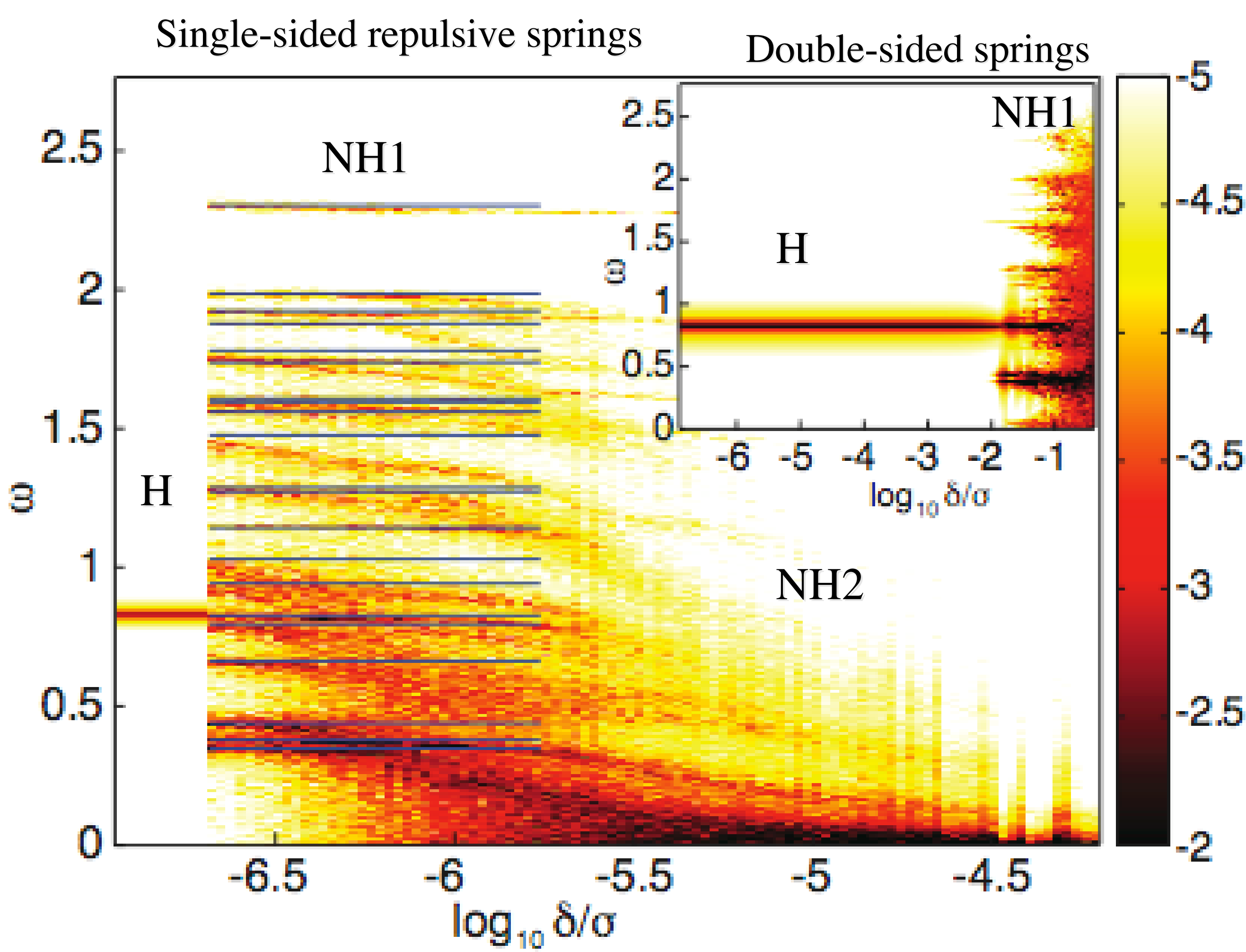
$$\vec{r}_i^{\,'} = \vec{r}_i + \delta \hat{e}_6$$



- Deform system along each ‘eigenmode’ ω_i
- Run at constant NVE, measure power spectrum of grain displacements
- Does system oscillate at frequency ω_i from dynamical matrix?

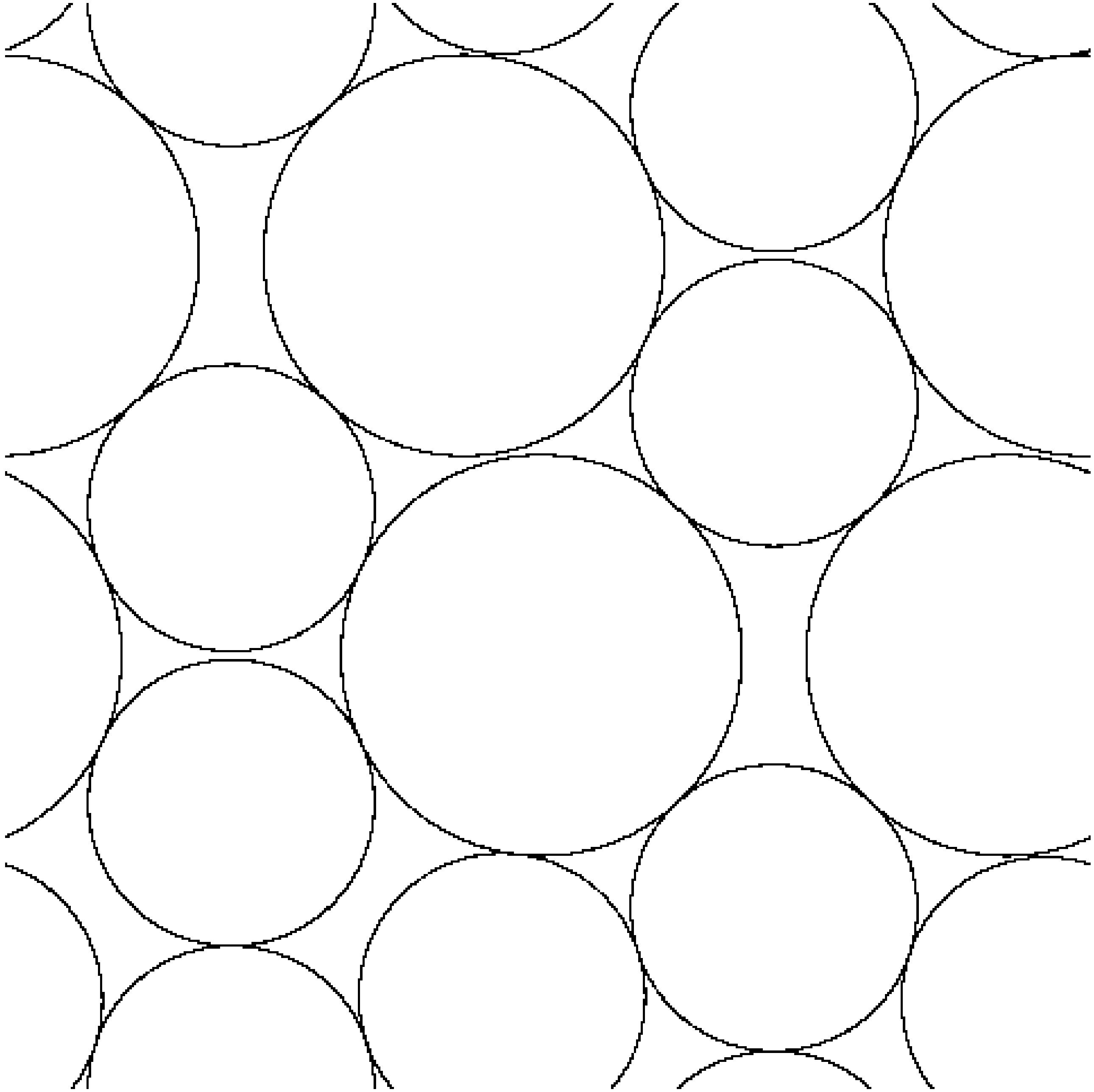
Power-spectrum of particle displacements

N=12
$\Delta\phi=10^{-5}$
Mode=6
Steady-state

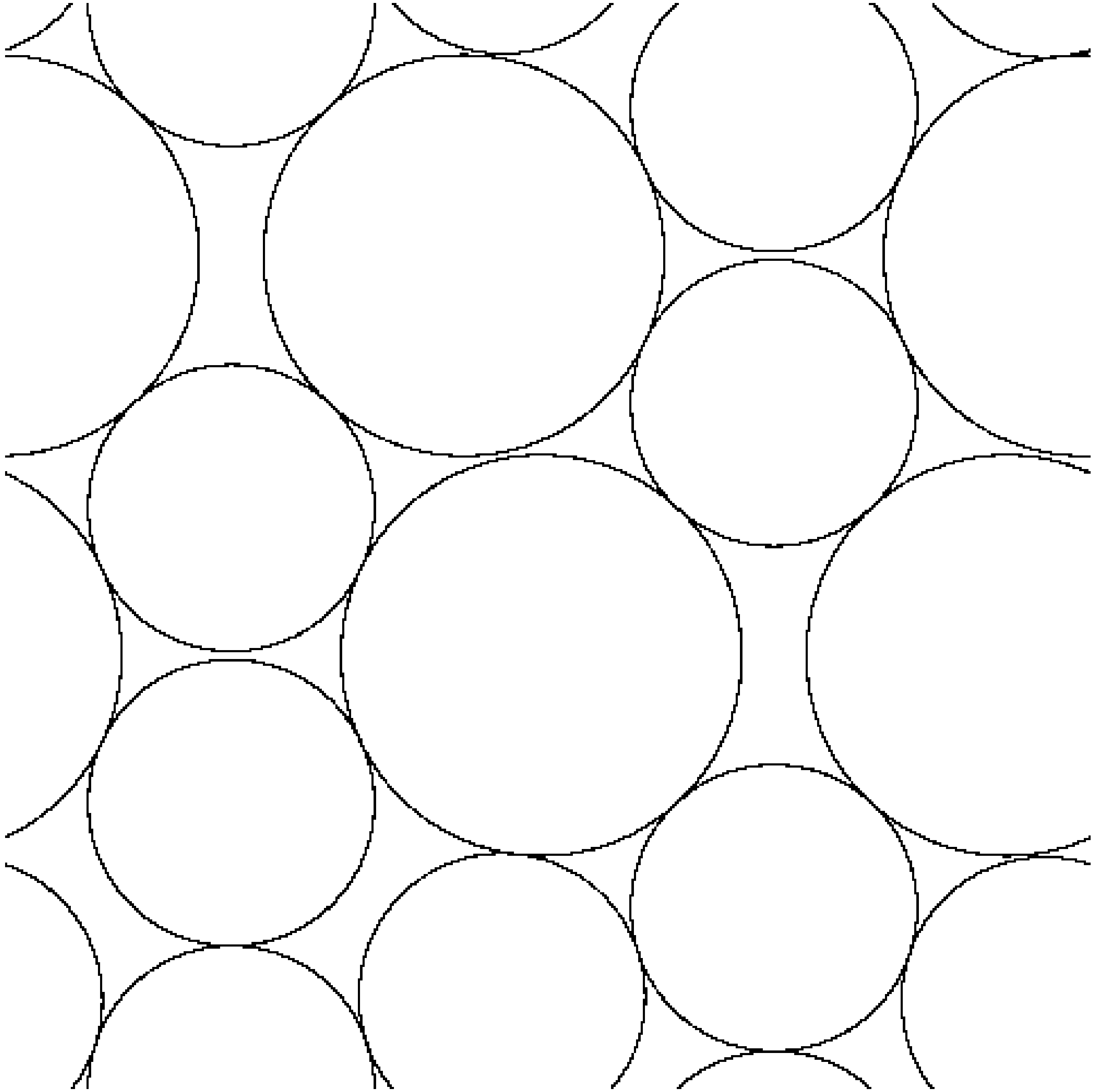


- System becomes strongly nonharmonic at extremely small δ
- First spreads to `harmonic' set of ω (NH1); then continuum of ω (NH2)

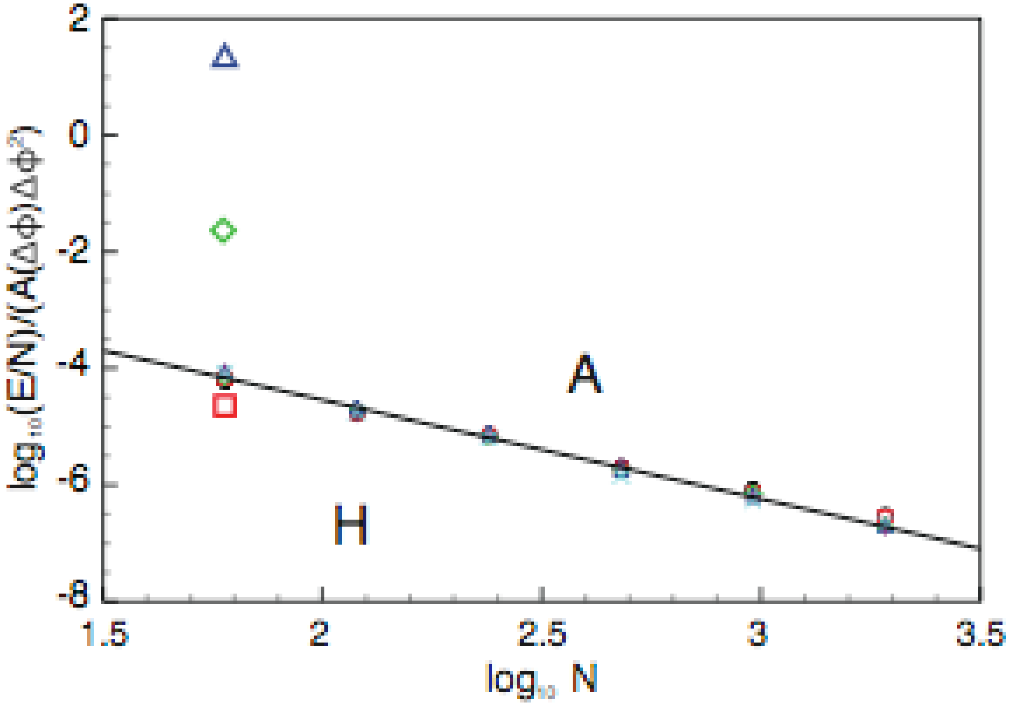
N=12
$\Delta\phi=10^{-5}$
Mode=6
$\delta/\sigma=10^{-5}$

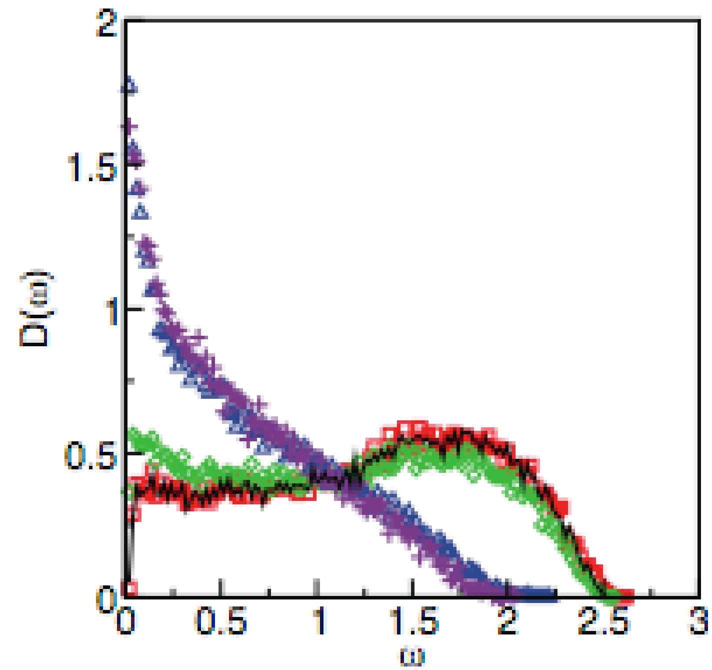


N=12
$\Delta\phi=10^{-5}$
Mode=6
$\delta/\sigma=10^{-3}$

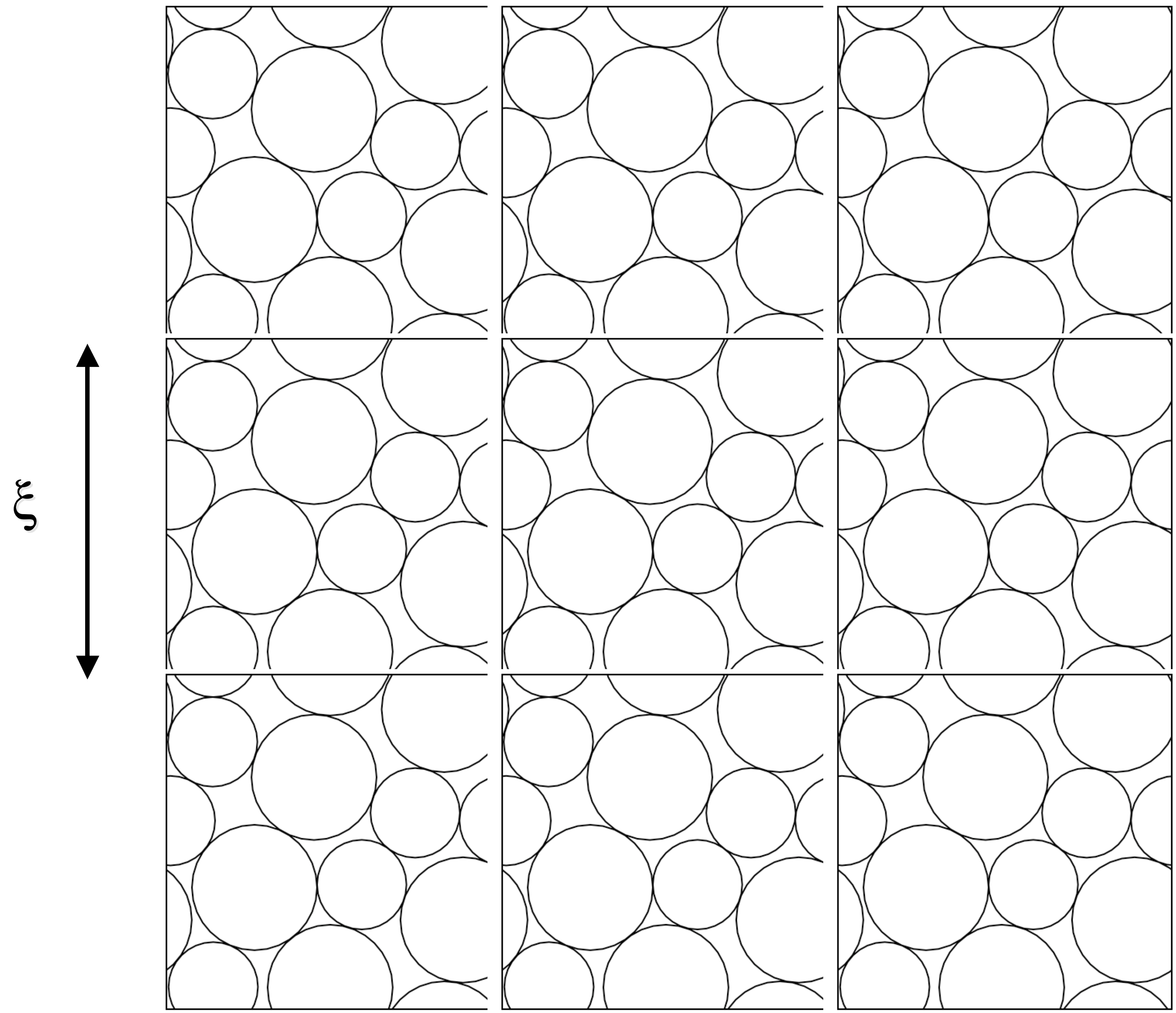


Strongly Anharmonic Behavior

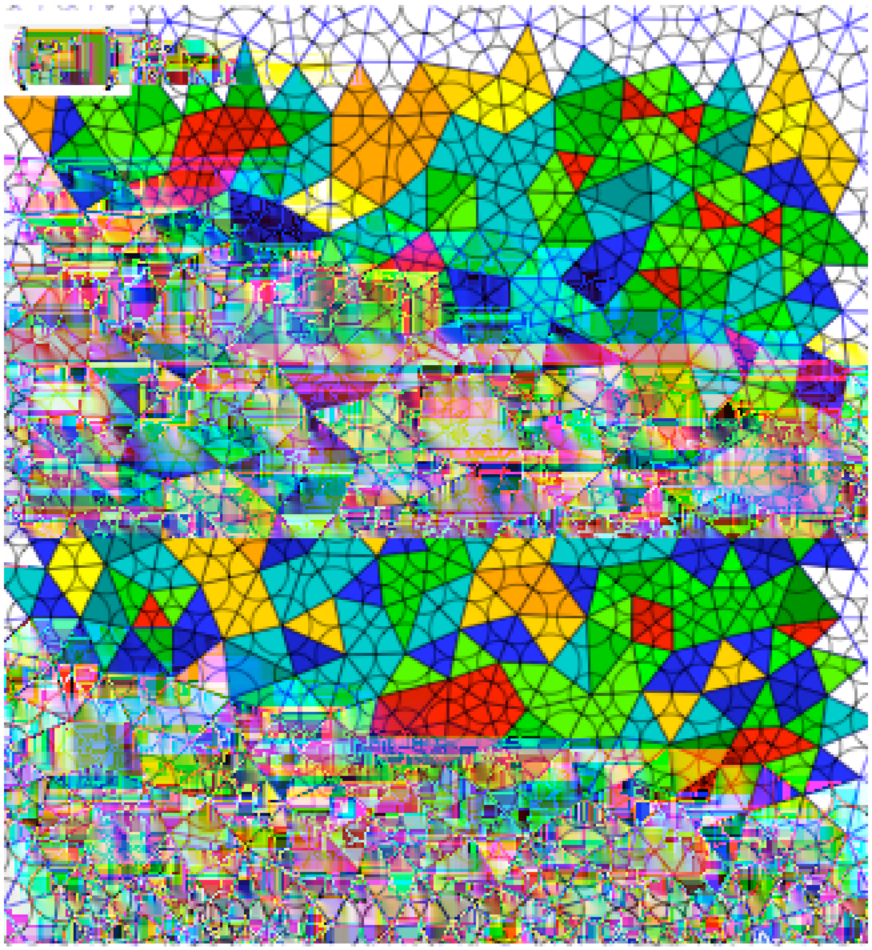


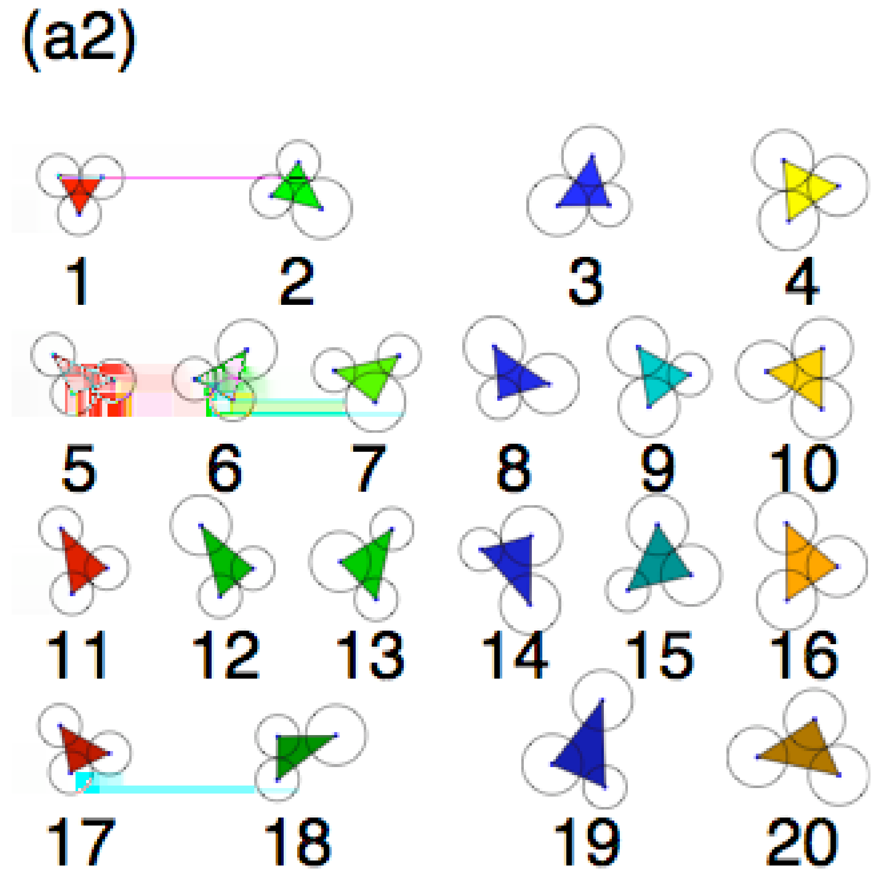


Are large jammed packings composed of highly probable sub-systems?

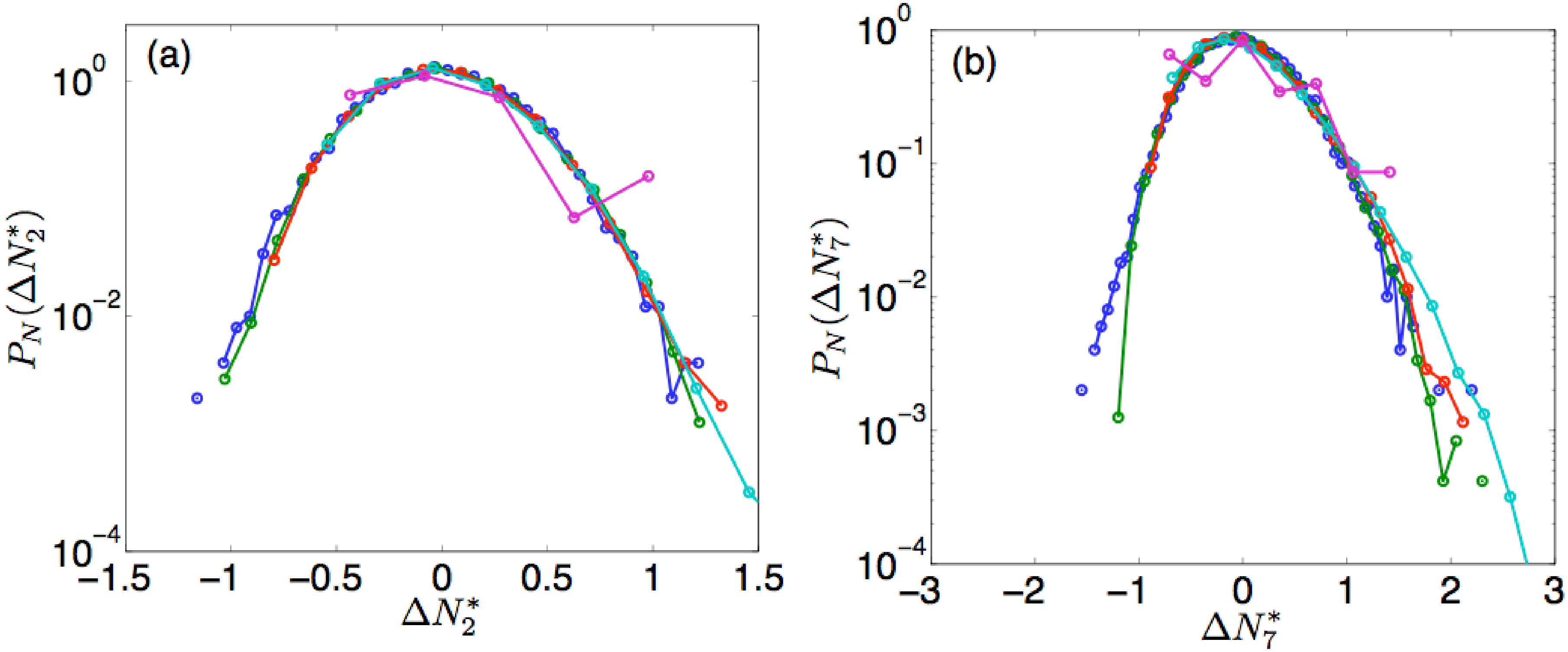


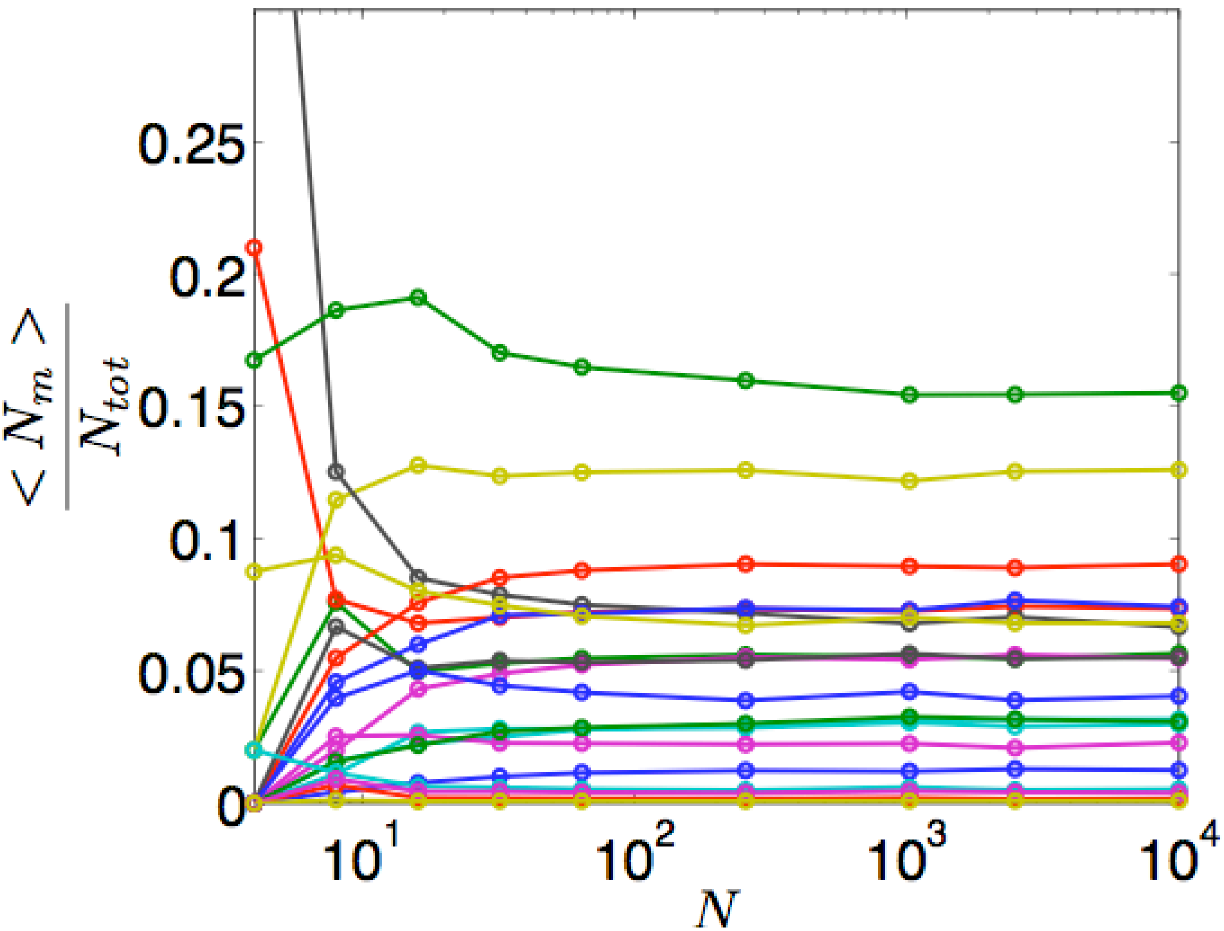
Delaunay triangle packings





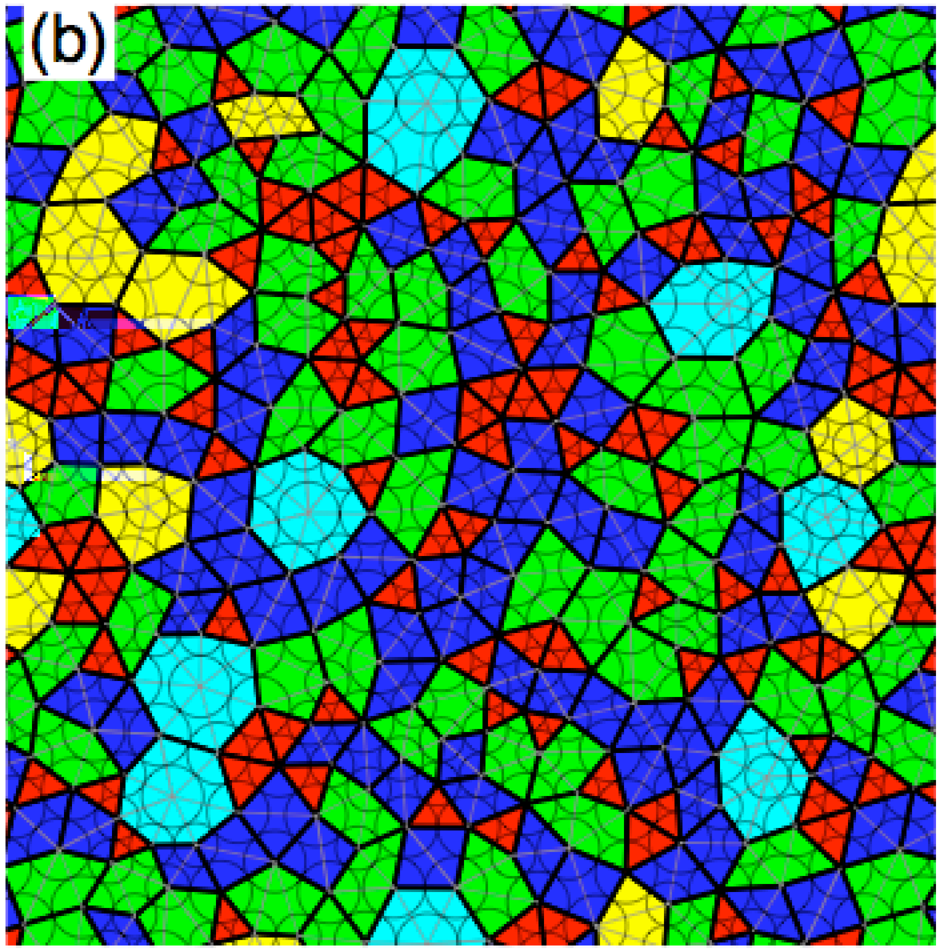
Distribution of tile numbers





- Average values converge quickly with N
- `Compatibility' rules determine large N values

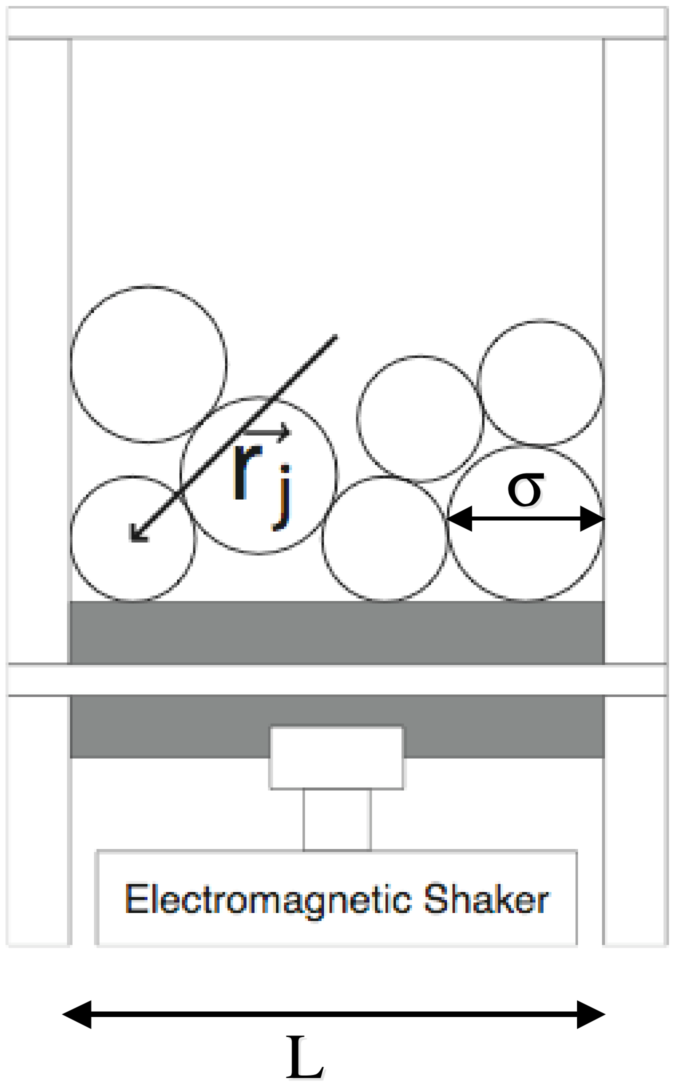
Future Directions

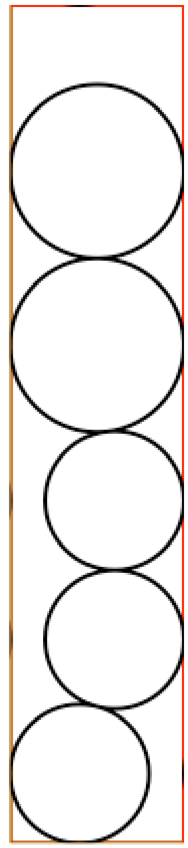


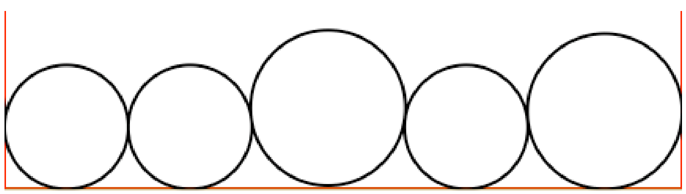
- Form triangles, quadrilaterals, pentagons,… out of all links (from Delanauy triangulation) that surround particles.

When do jammed packings form continuous geometrical families?

Continuous Range of Boundary Conditions, L

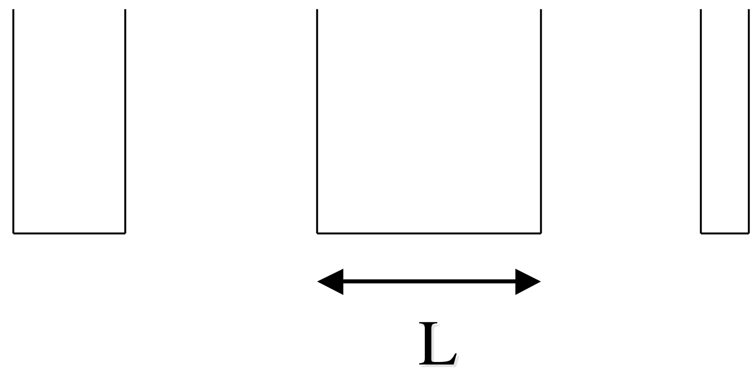




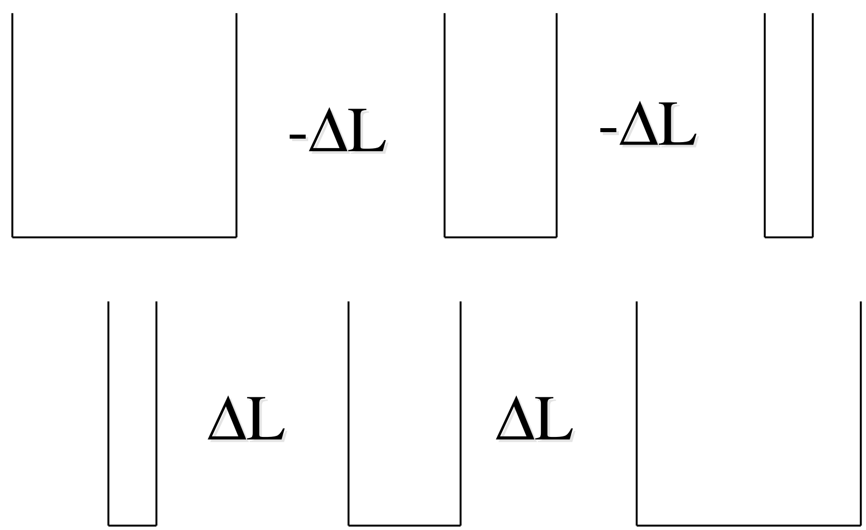


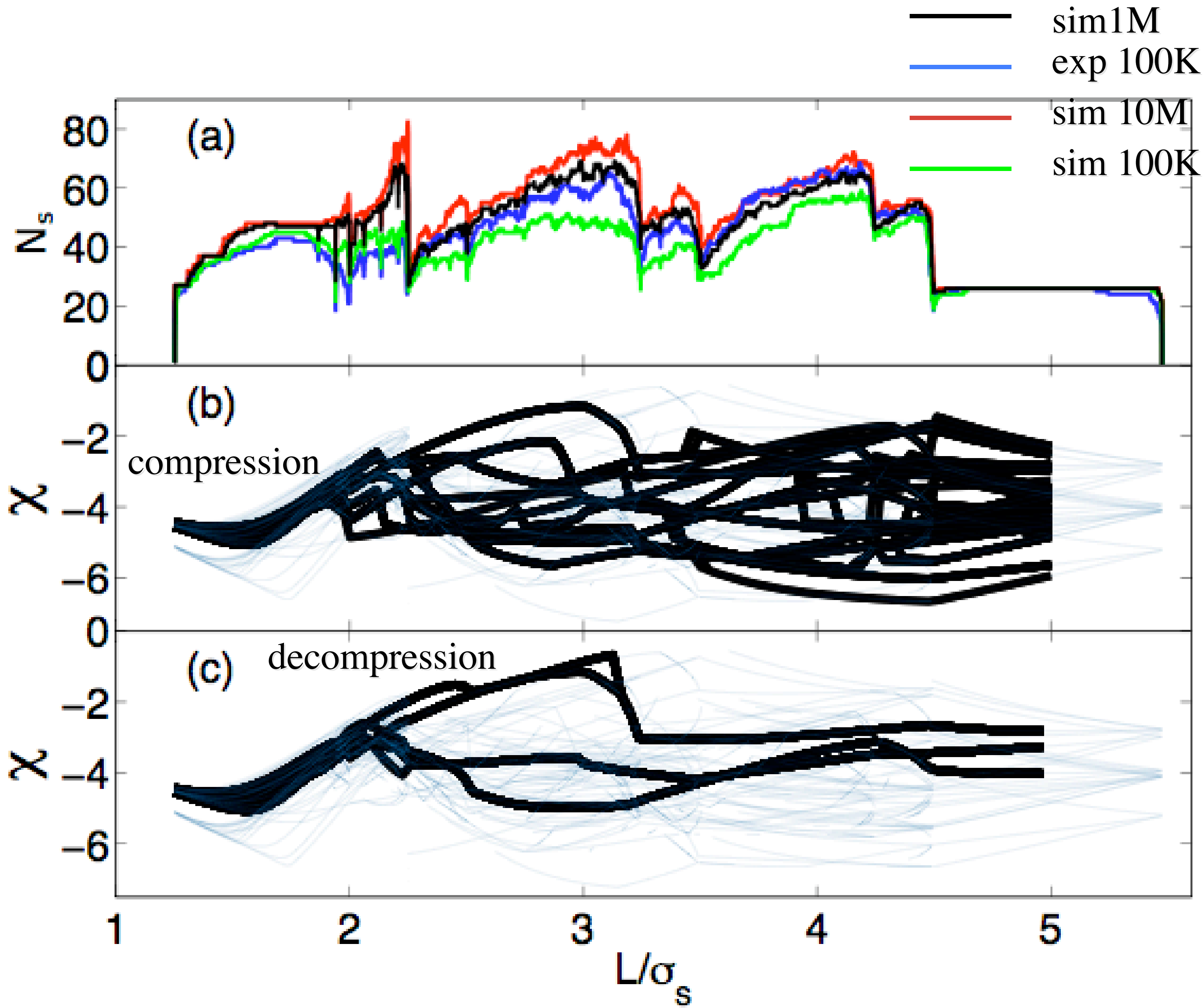
Continuous Range of Boundary Conditions, L_{min} to L_{max}

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

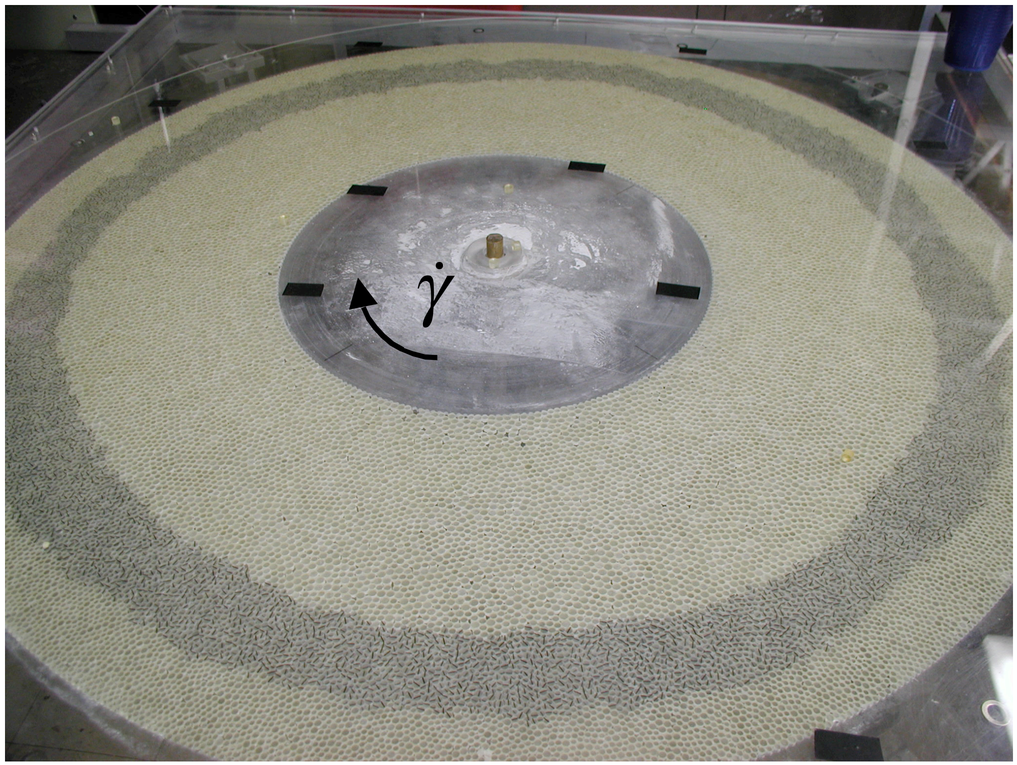


2. Dynamics: Quasistatic compression/ decompression (sim,exp)




sim1M
exp 100K
sim 10M
sim 100K
(a)
N_s
(b)
compression
χ
(c)
decompression
χ
L/σ_s

How do slow, dense shear flows sample MS packings…with equal probability?

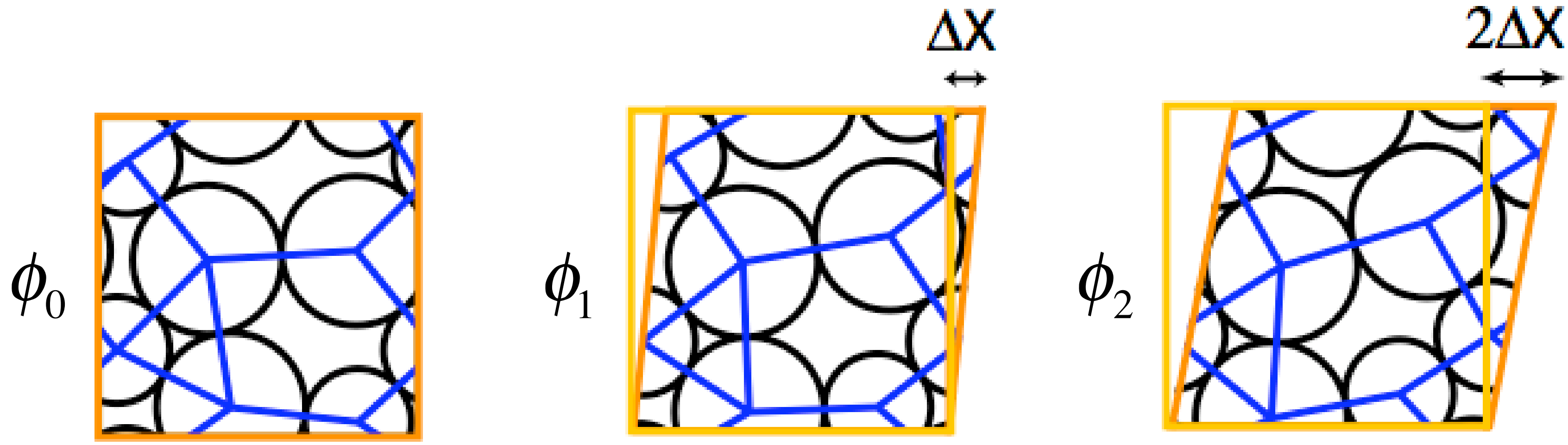


Quasi-static Couette Shear Flow $\dot{\gamma} \rightarrow 0$

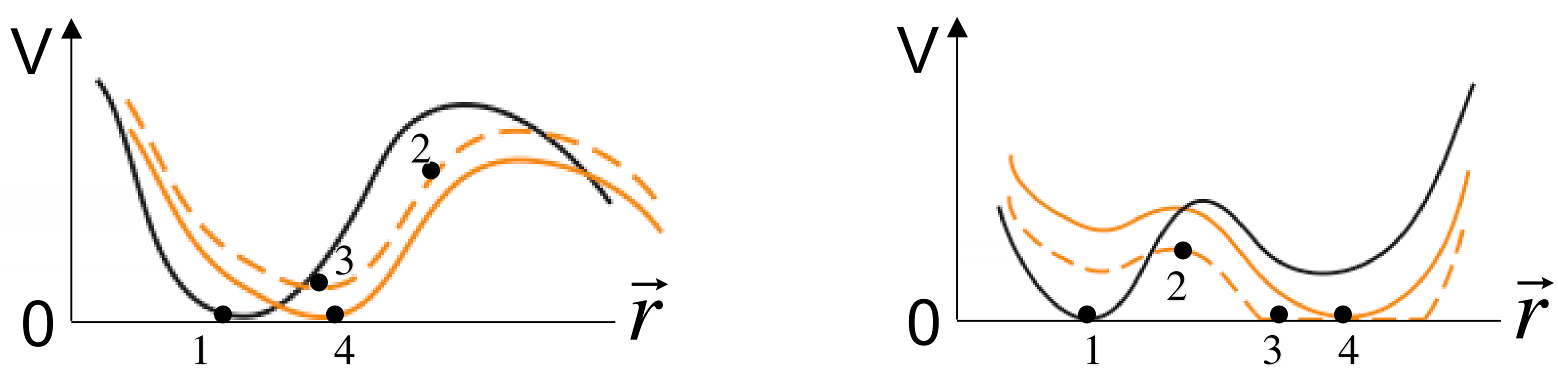
B. Utter and R. P. Behringer Phys. Rev. Lett. 100 (2008) 203302

H. A. Makse and J. Kurchan Nature 415 (2001) 614

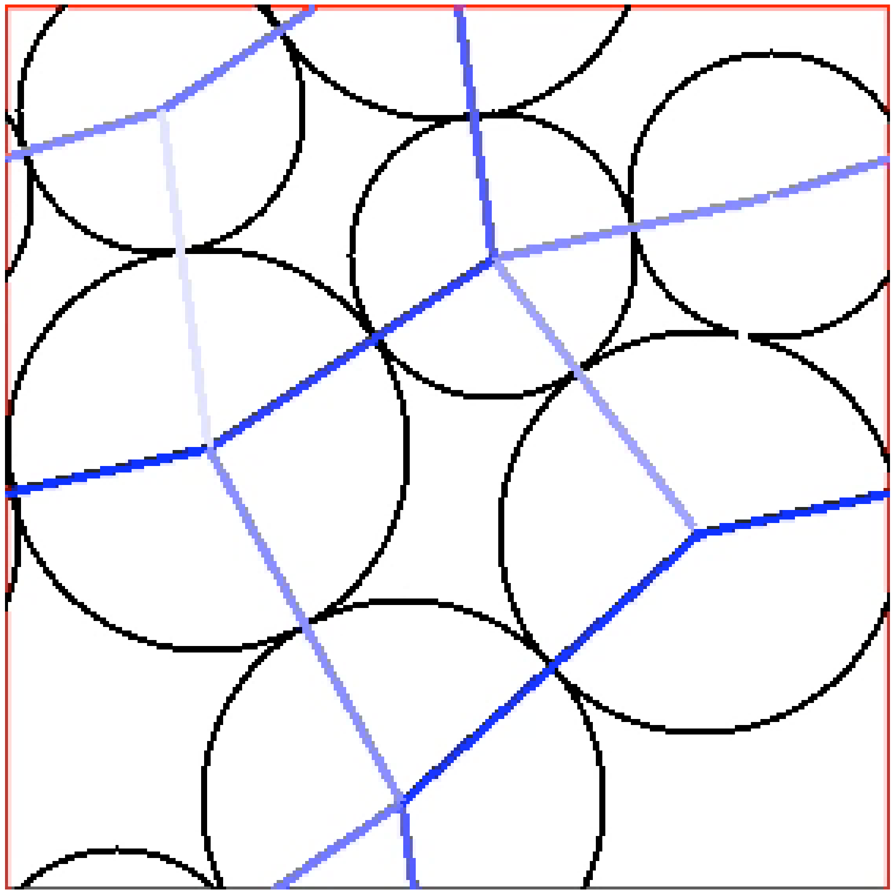
Quasi-static shear flow at zero pressure



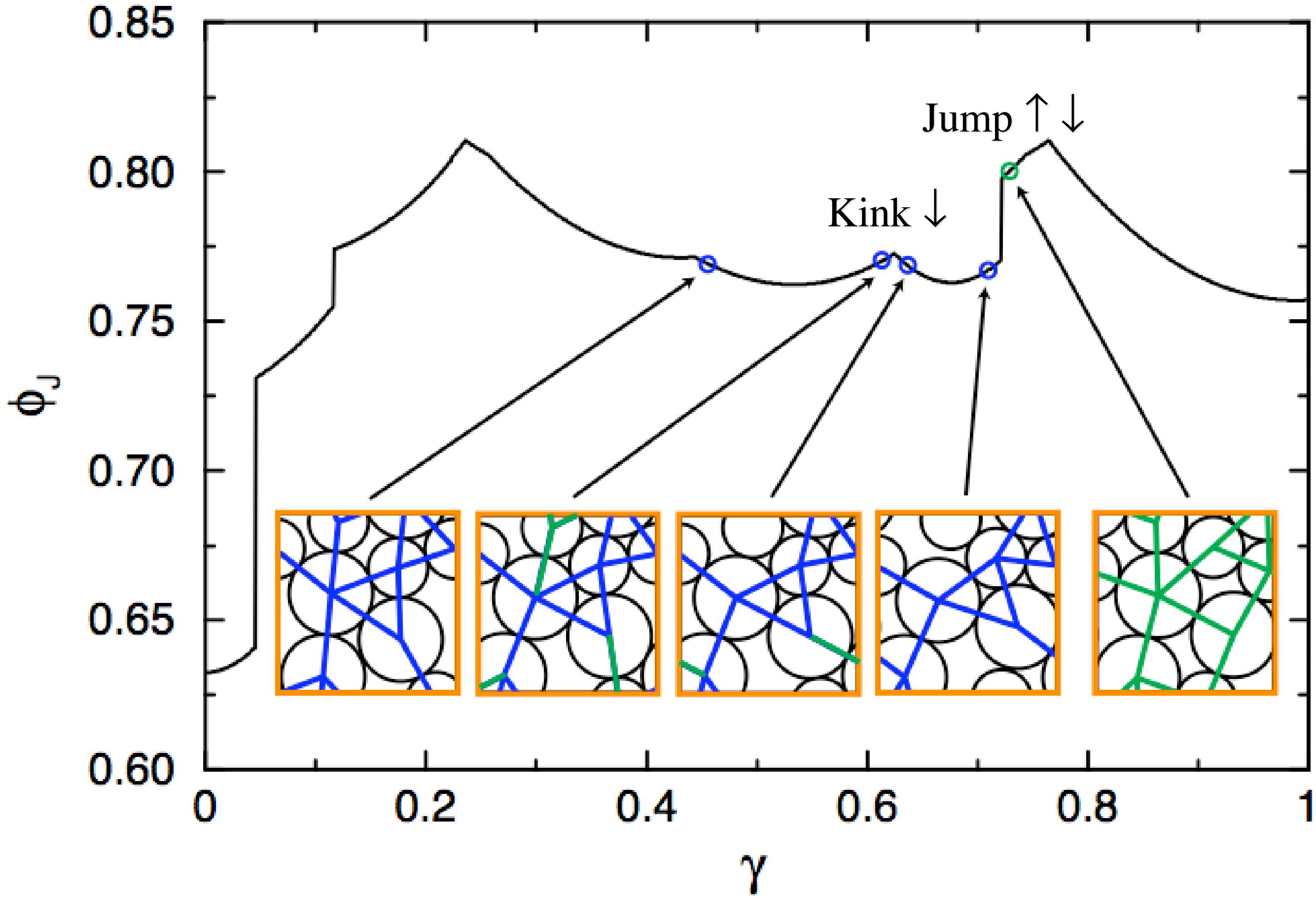
1. Initialize MS packing at zero shear strain
2. Take small step shear strain $x_i' = x_i + \Delta\gamma\, y_i$
3. Minimize energy
4. Find nearest MS packing at P=0 using growth/shrink procedure
5. Repeat steps 2, 3, 4



Quasistatic Shear Flow at Zero Pressure

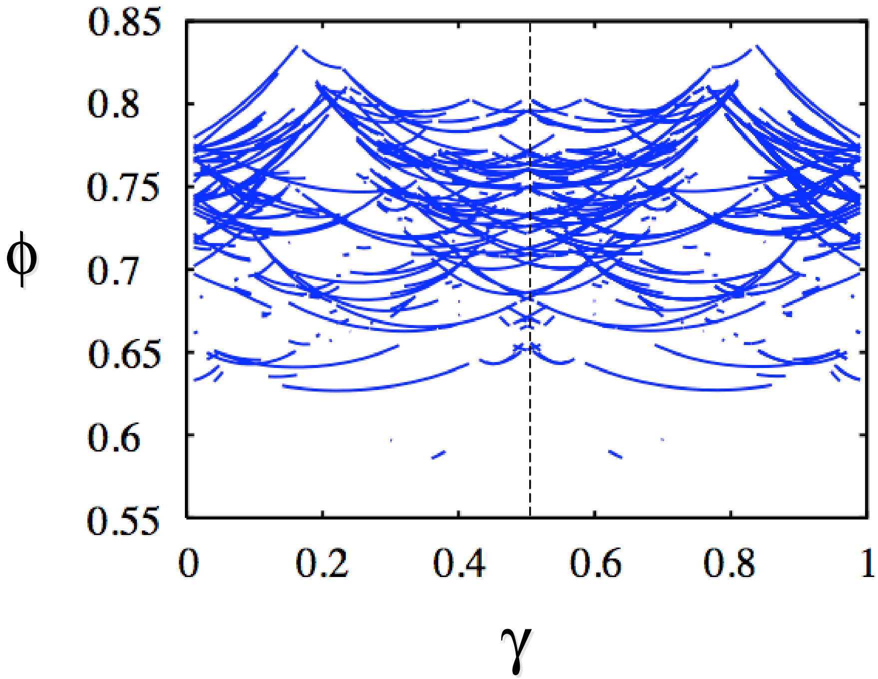


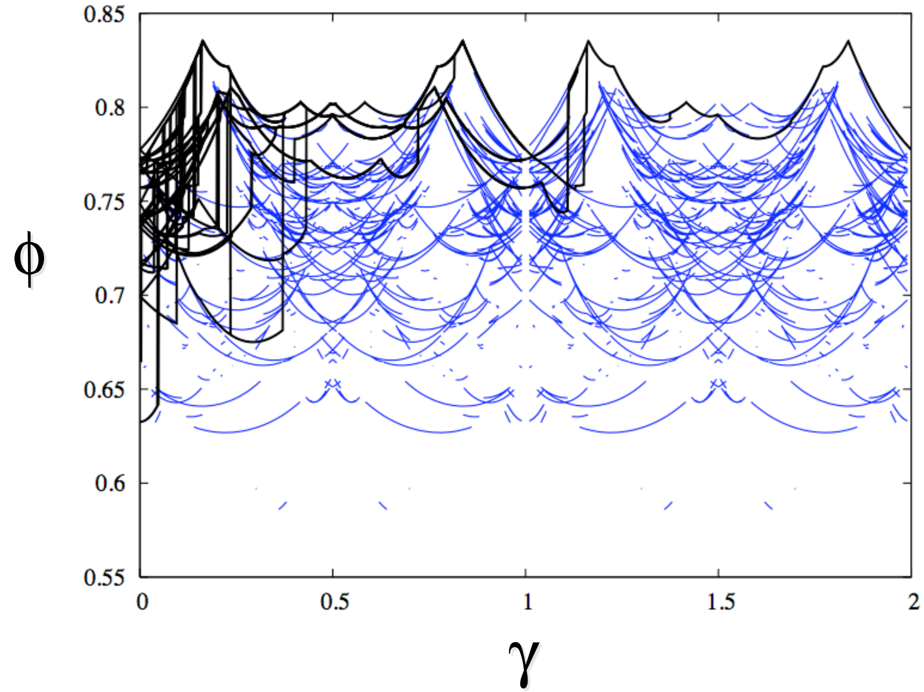
Geometric Families Exist over Continuous Range of γ



- Rearrangement events cause system to switch geometric families

Complete Family Tree



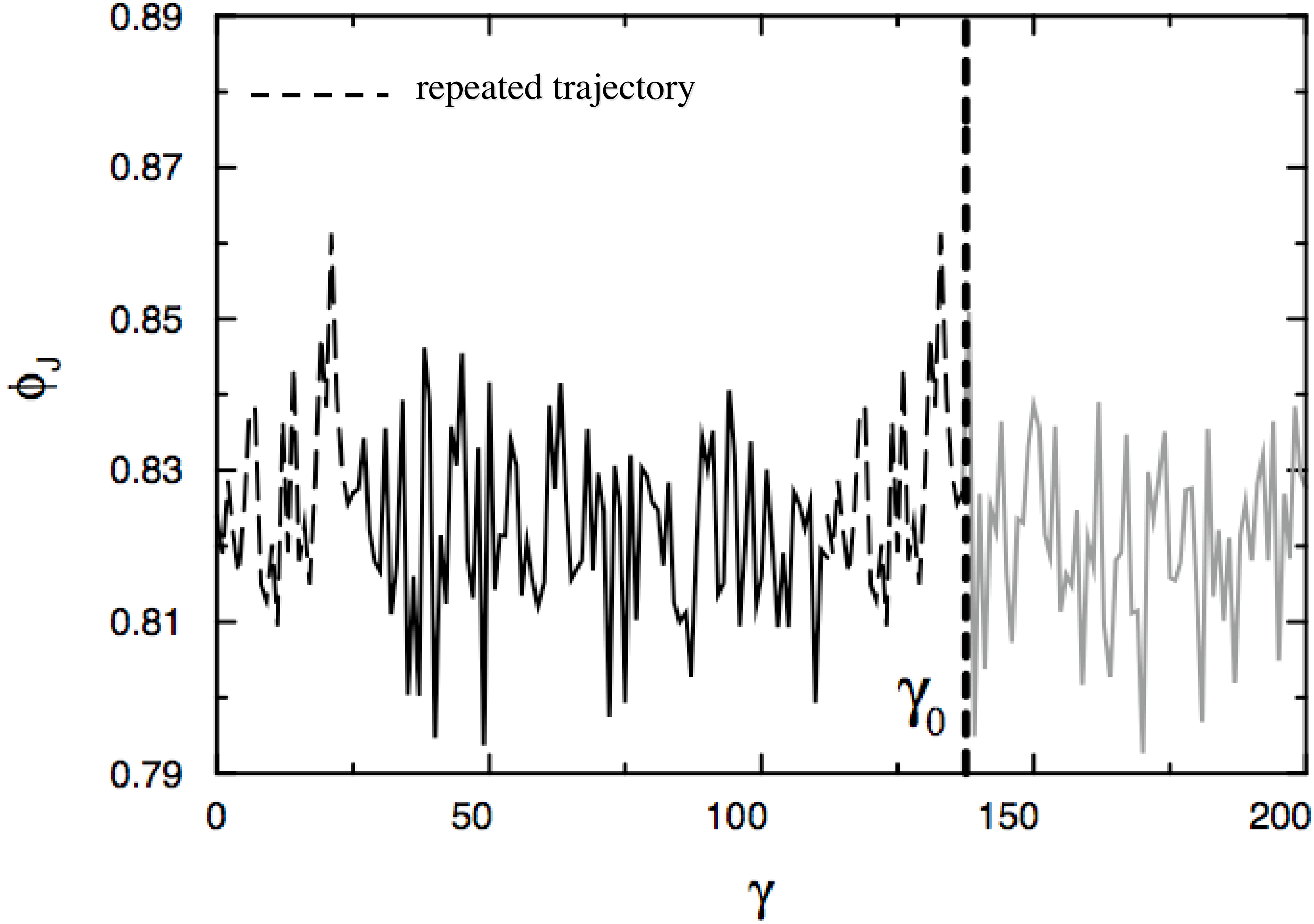


complete family tree

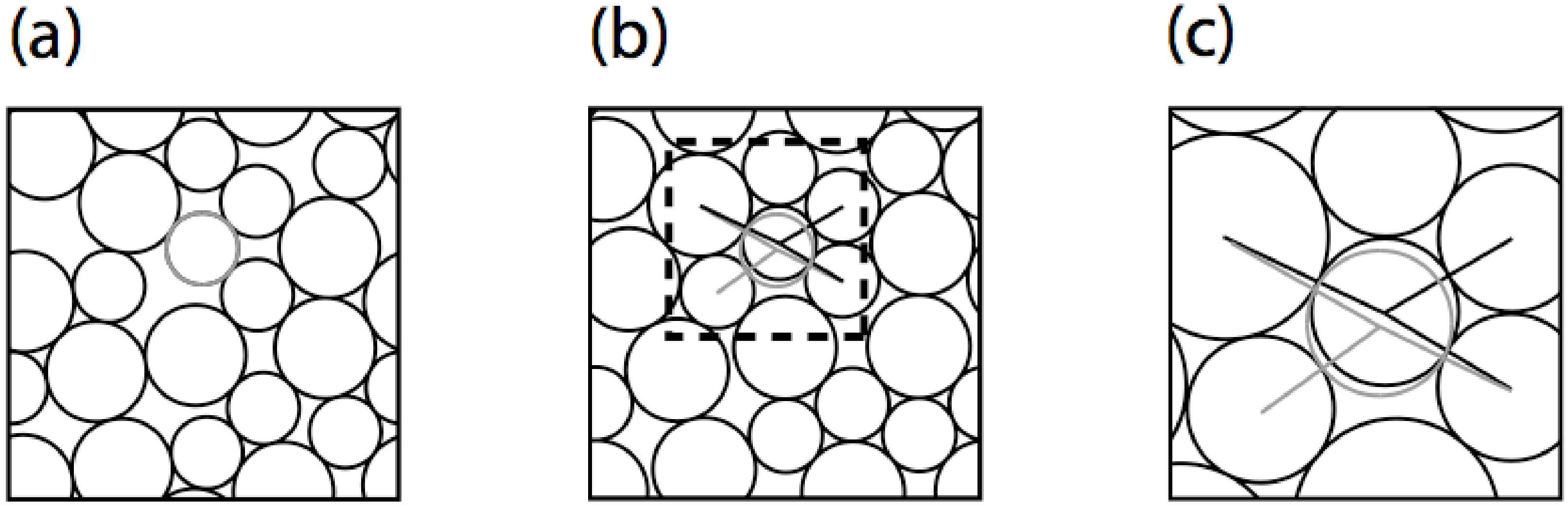
deterministic evolution of all $\gamma=0$ packings

Small systems sample only negligible fraction of available geometric families!

Sensitivity to Initial Conditions: N≥12

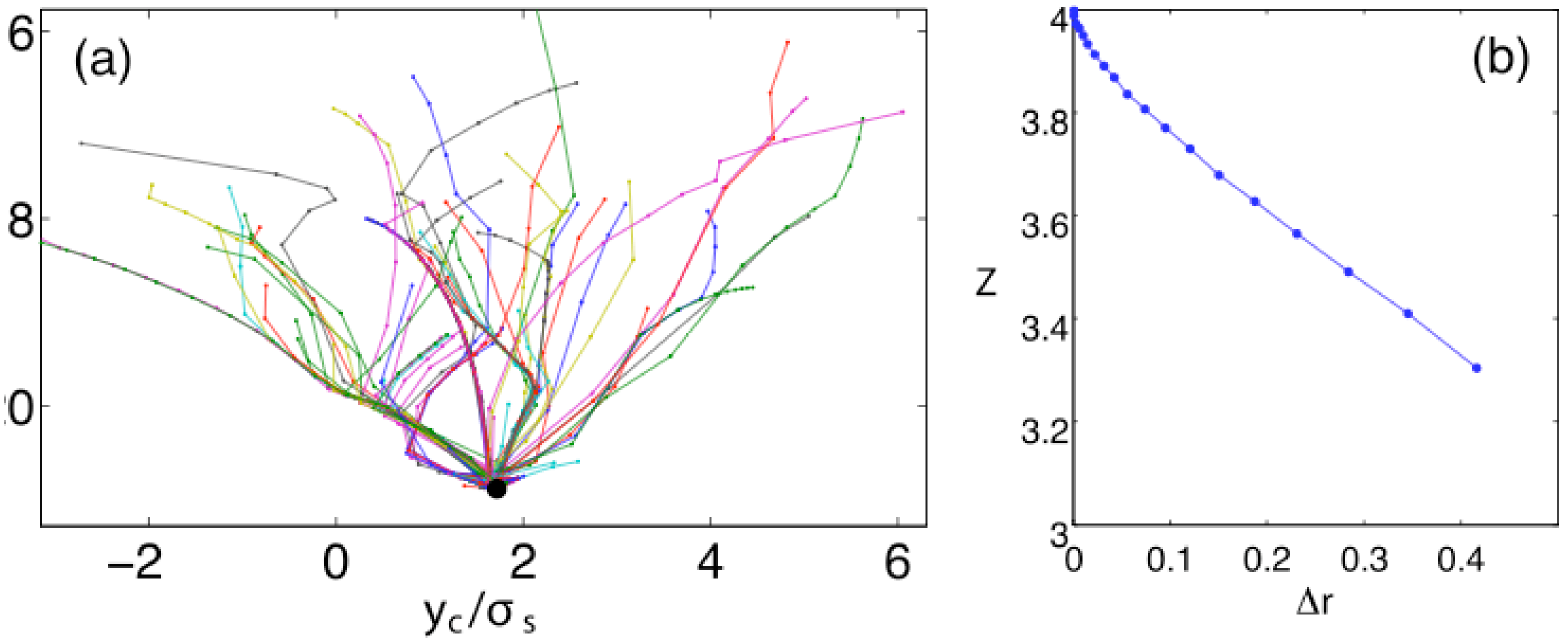


Noise-generation Mechanism: Collinear Particles

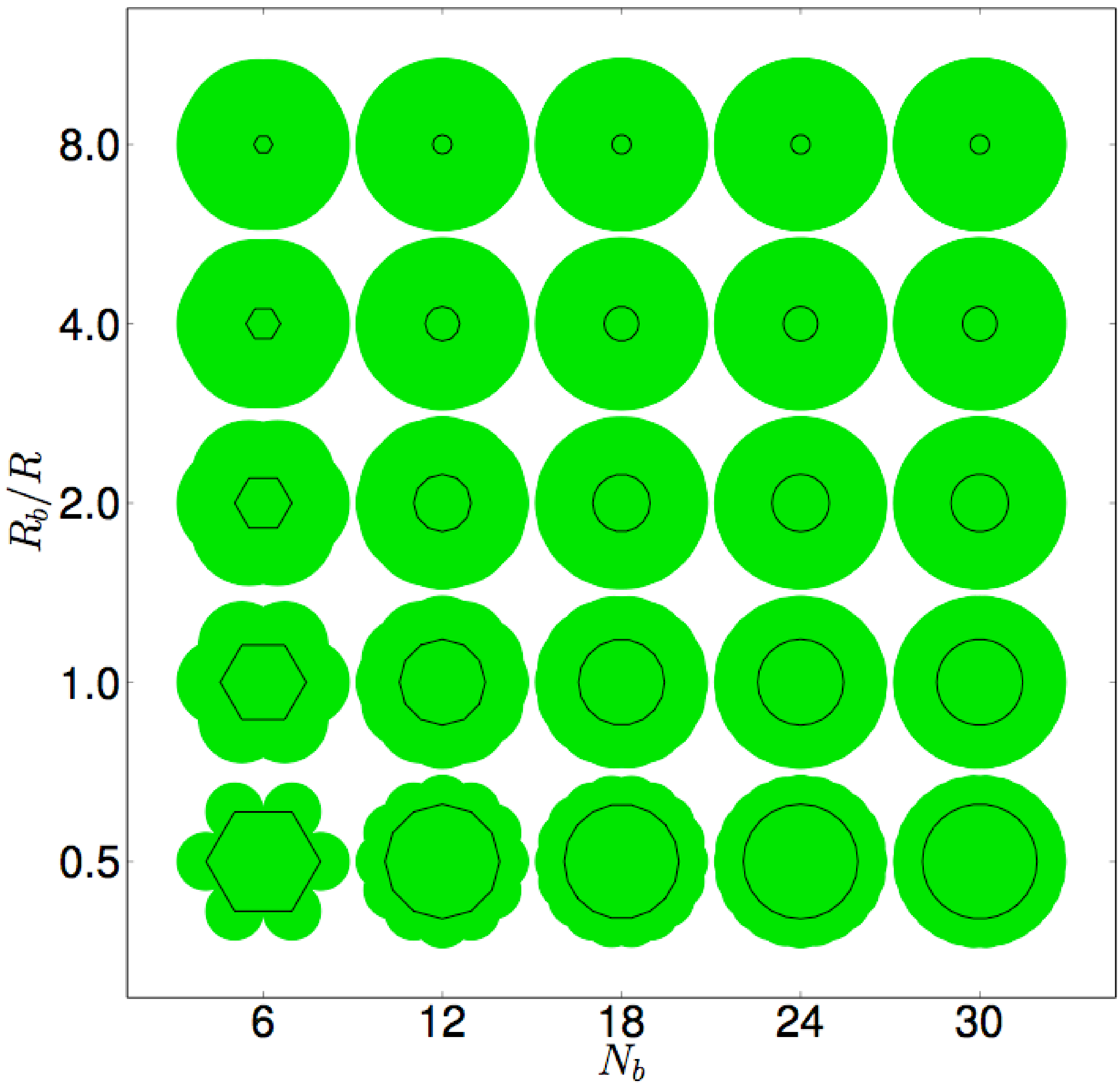


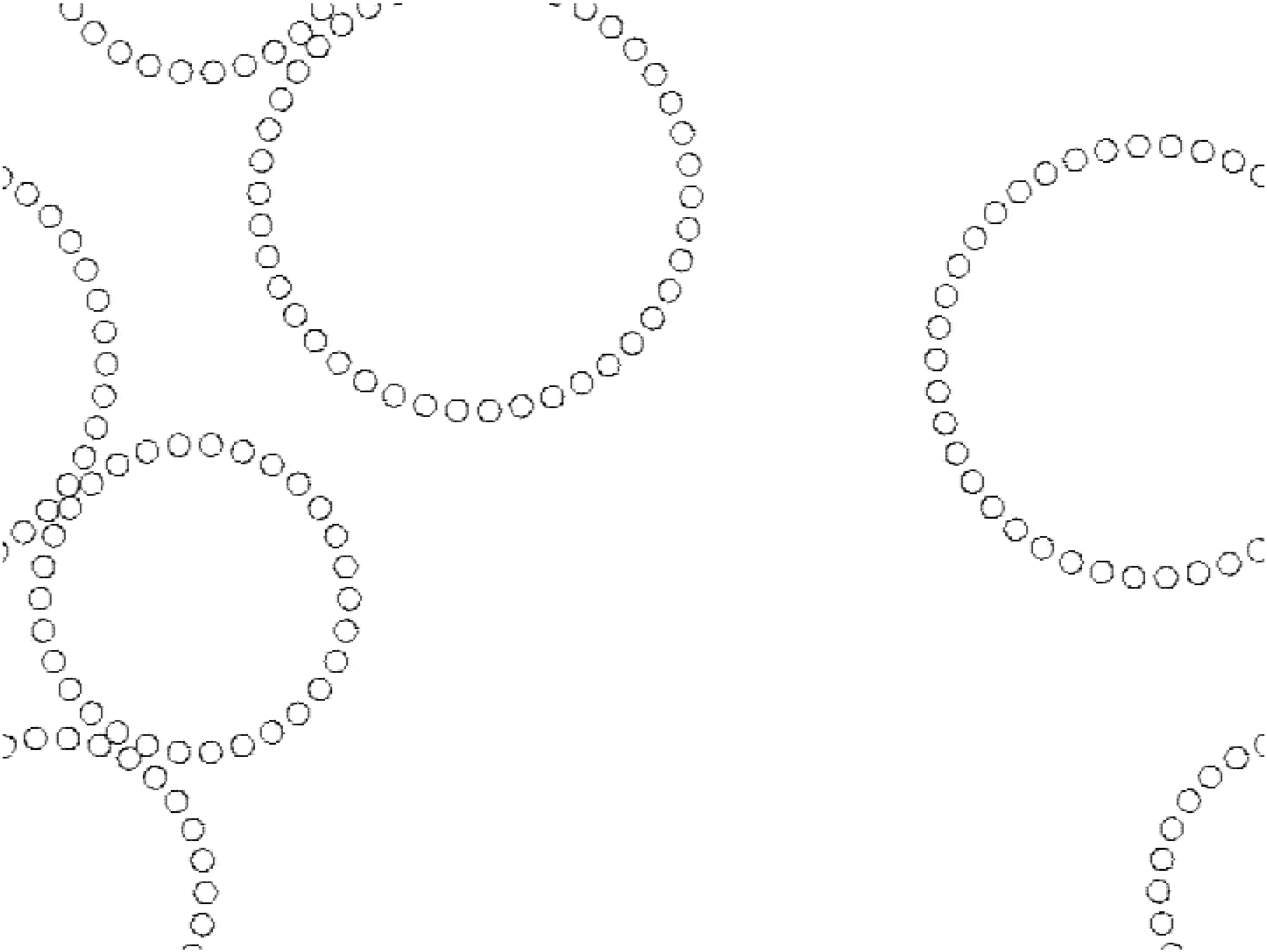
$\gamma = \gamma_0 - \Delta\gamma$ $\qquad$ $\gamma = \gamma_0$

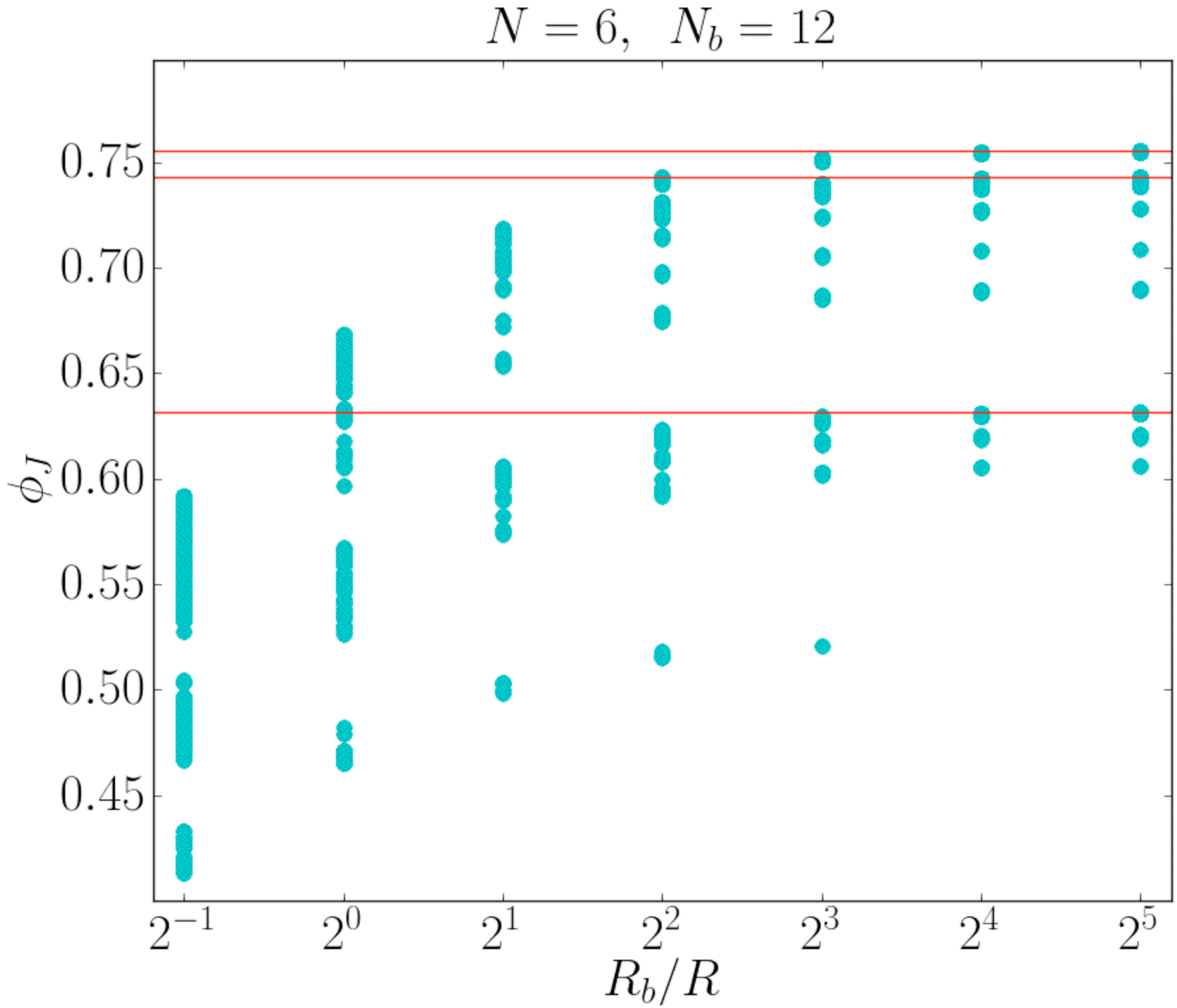
Frictional Geometric Families



Bumpy Particles

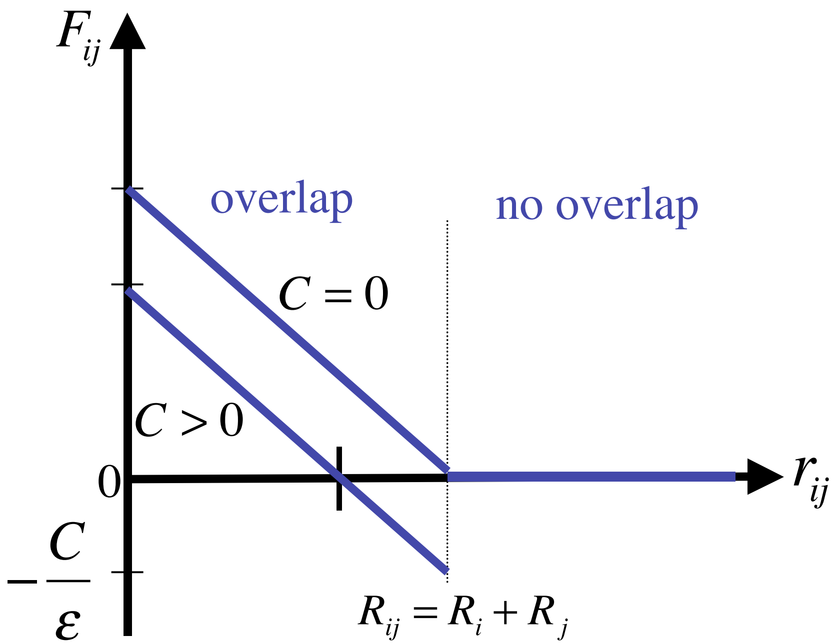


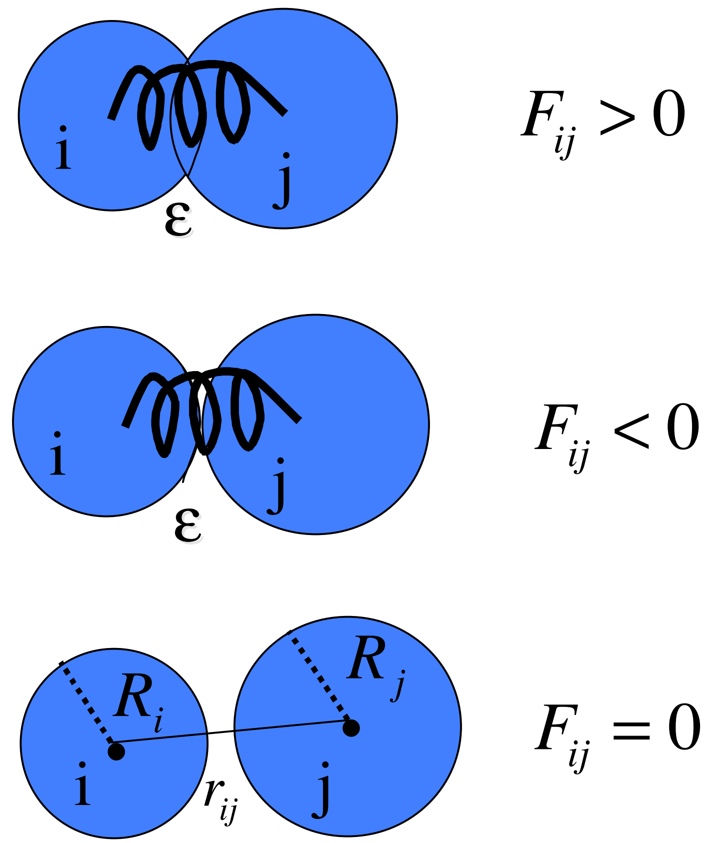




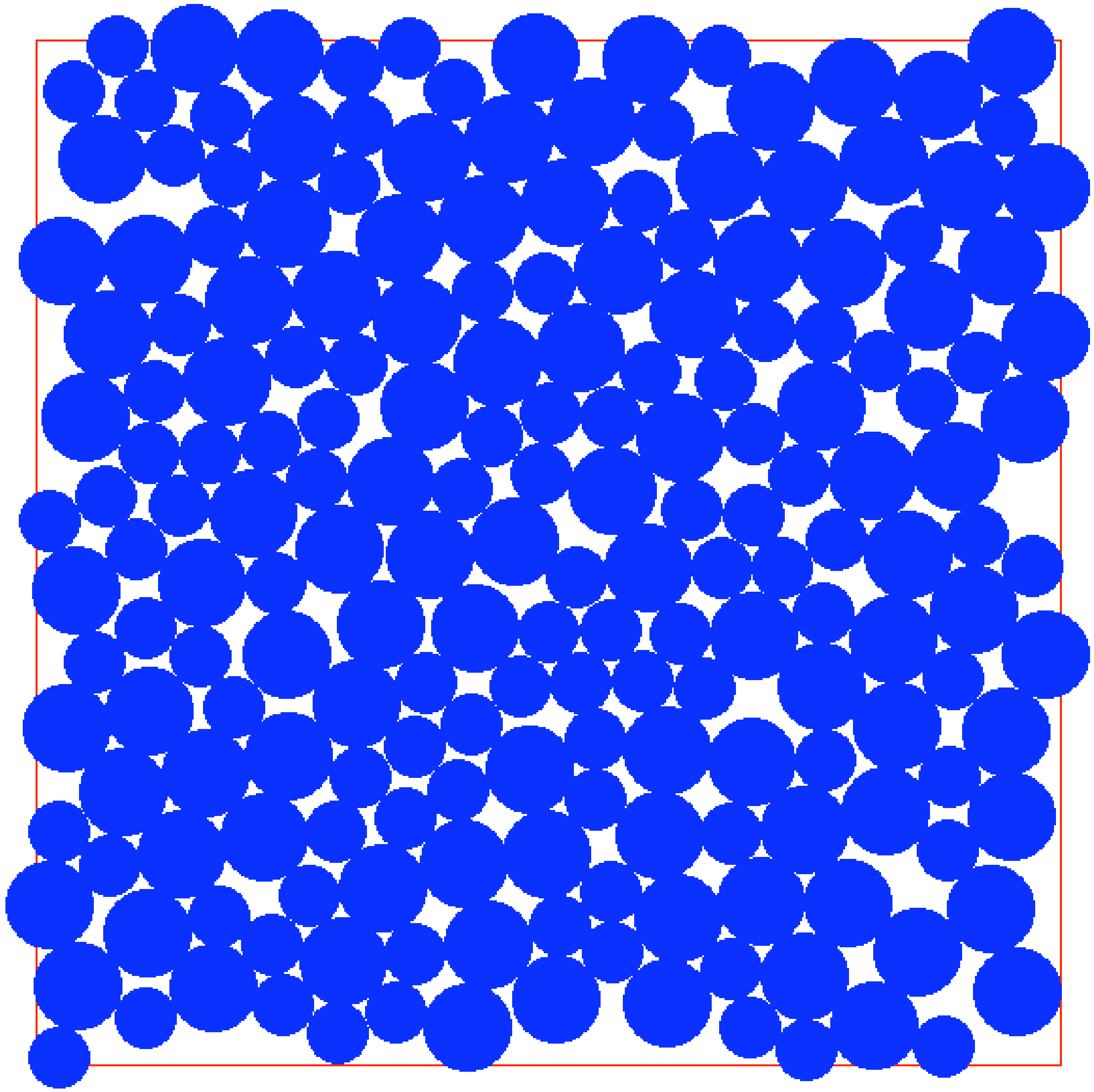
$N = 6, \quad N_b = 12$
0.75
0.70
0.65
0.60
0.55
0.50
0.45
ϕ_J
2^{-1}
2^0
2^1
2^2
2^3
2^4
2^5
R_b/R

Sticky Disks

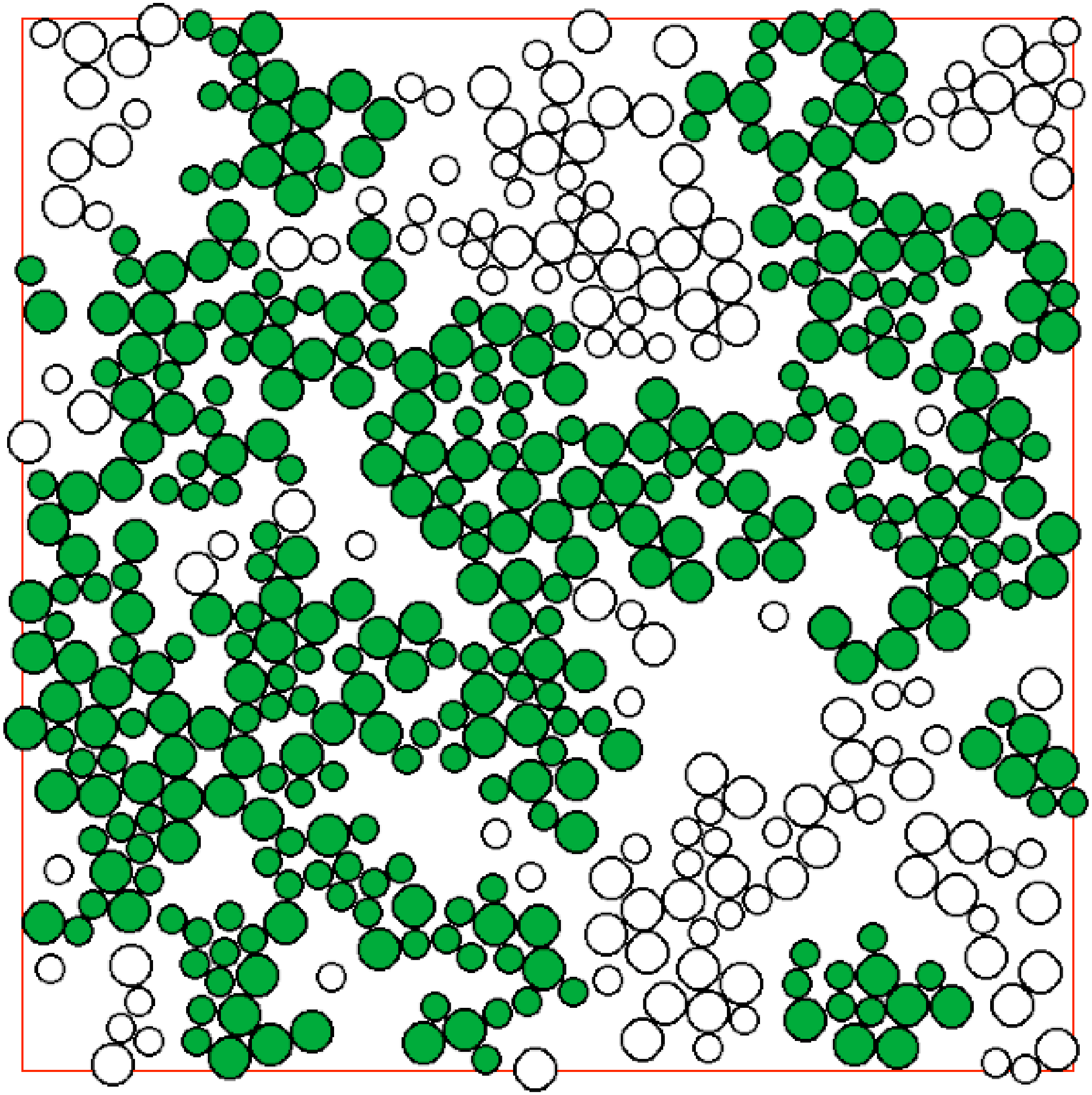




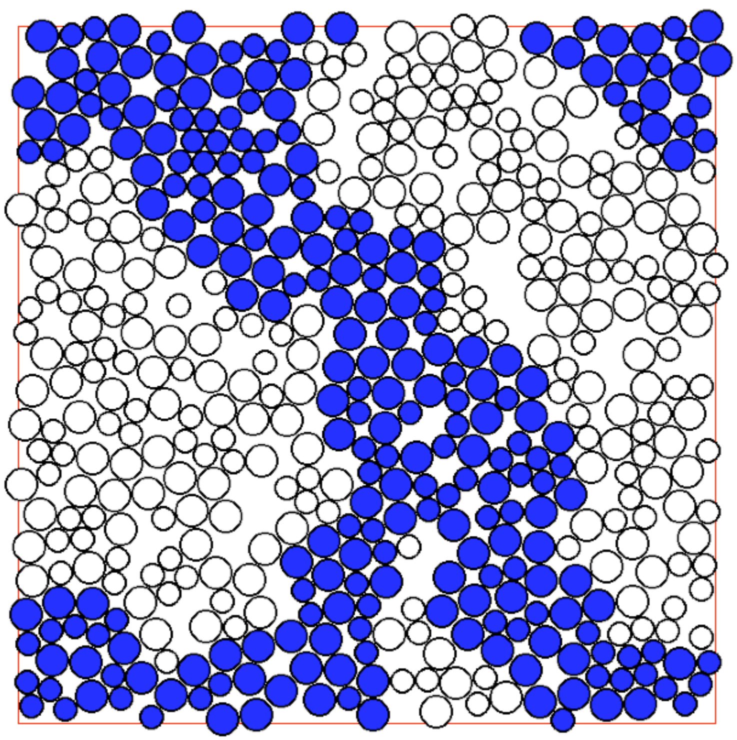
- Study $C/\varepsilon \to 0$ limit
- 50 - 50 binary mixtures of disks with $R_2/R_1=1.4$

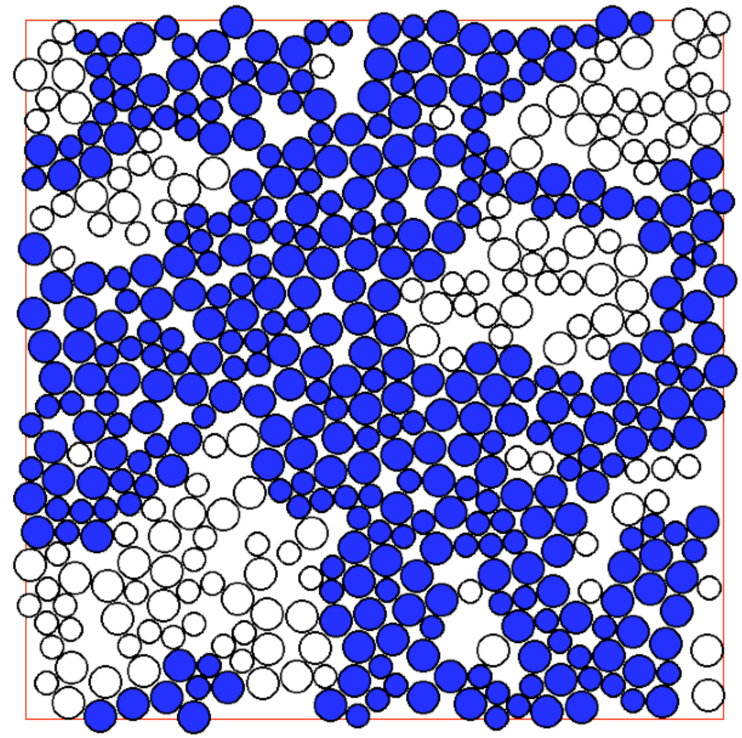


Bond Percolation

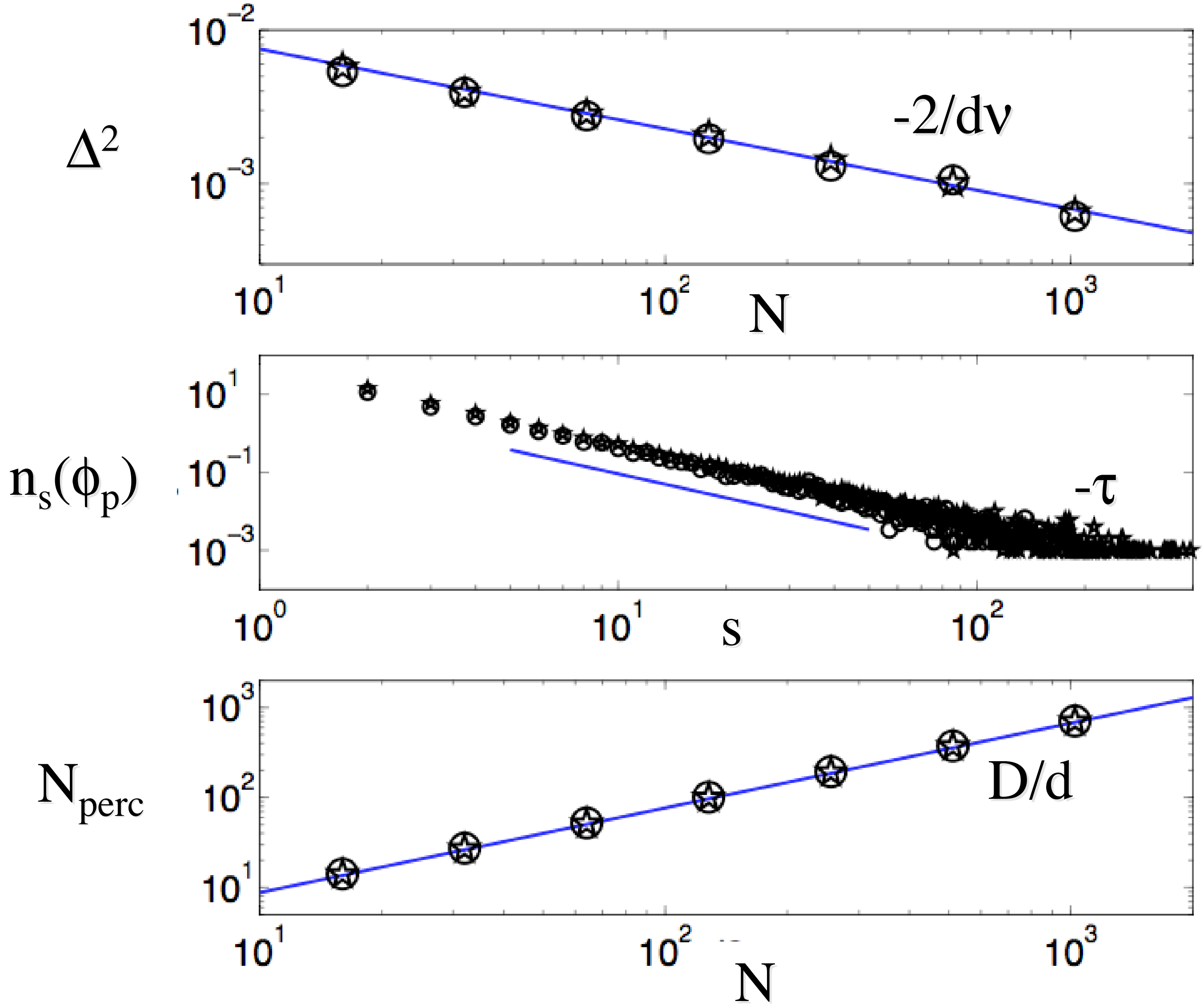


Rigidity Percolation





Rigidity Percolation Exponents

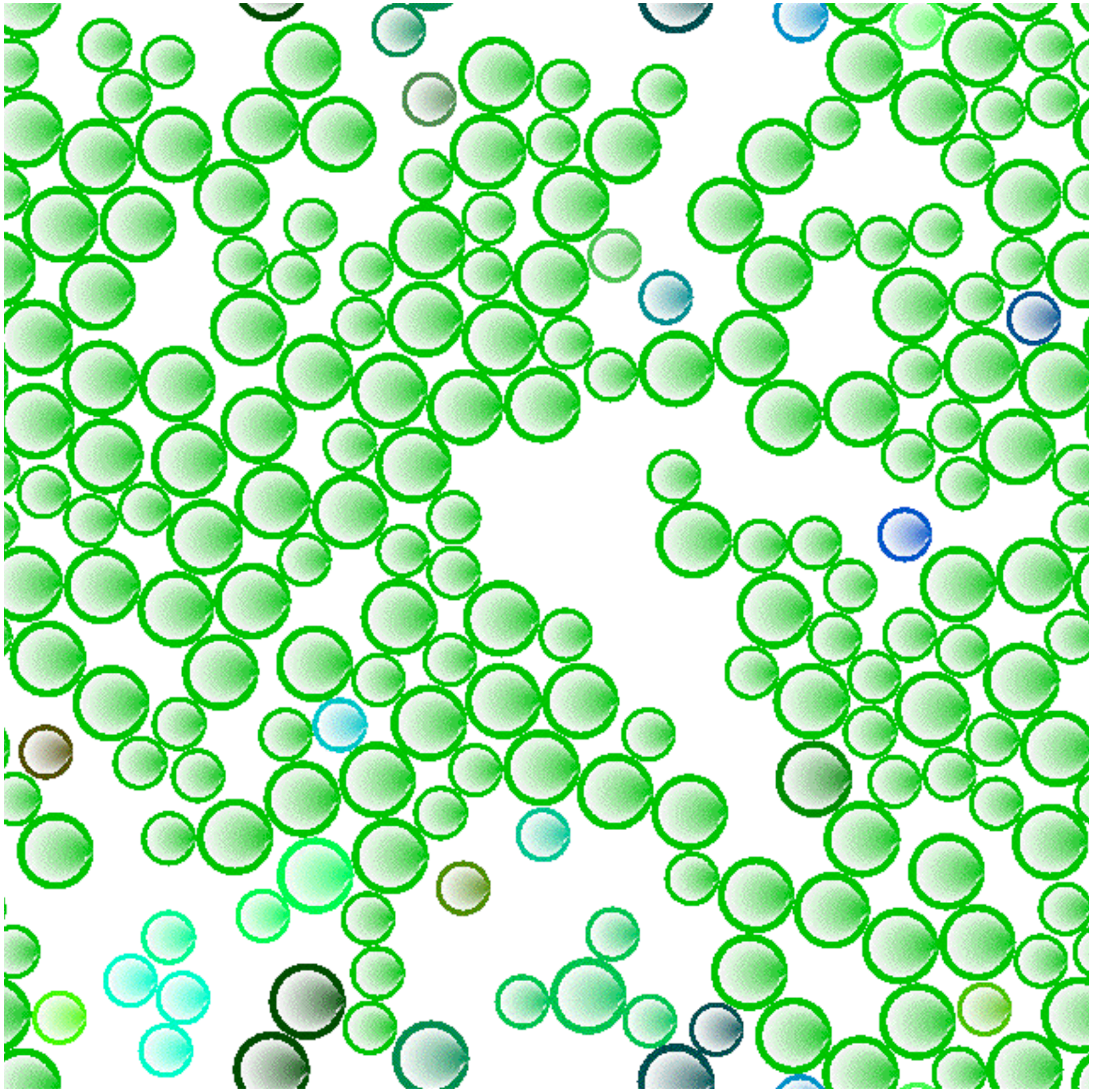


ν=1.92

D=1.88

τ=2.04

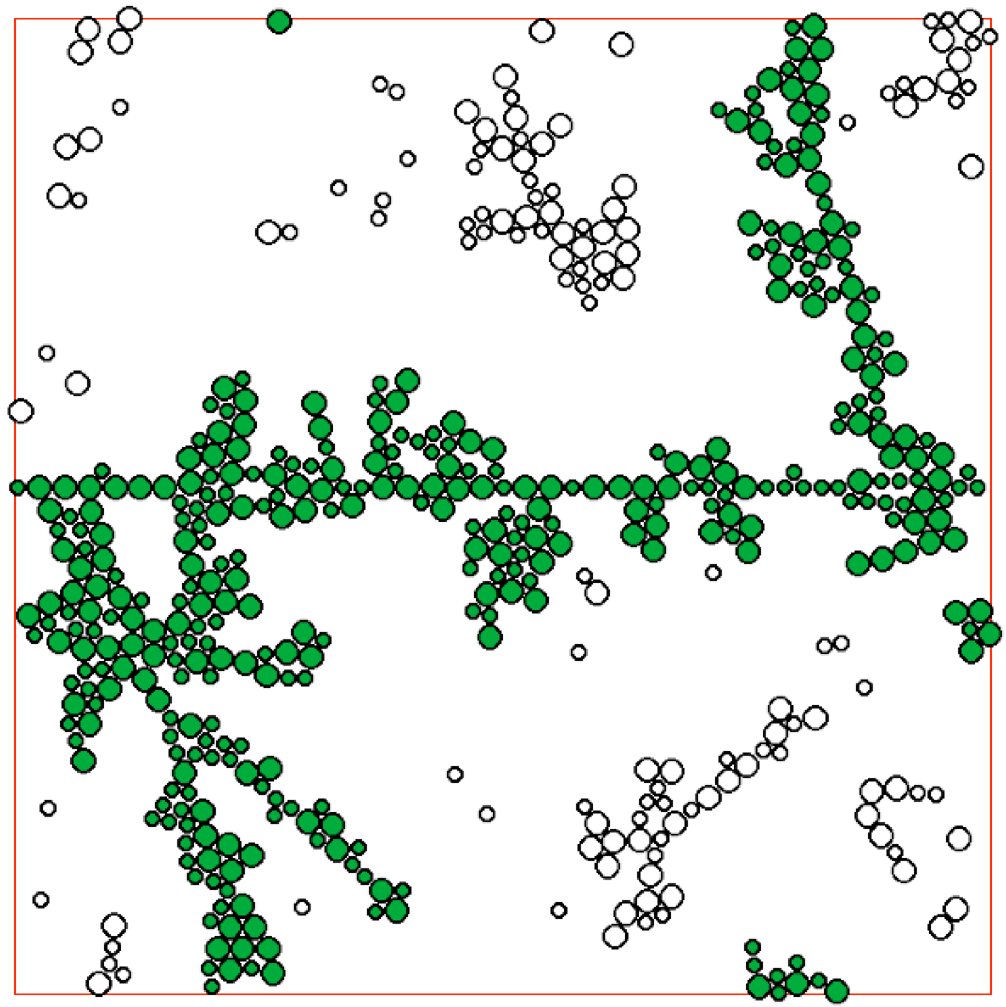
Contact Percolation in Repulsive Disks



Percolation Critical Exponents

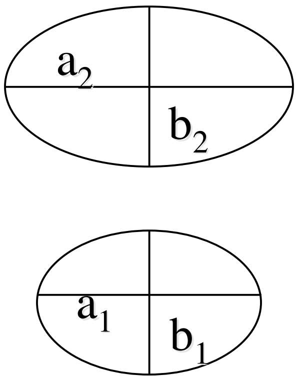
	Nature	sticky	repulsive disks	Rod (a=3)	Rod (a=6)
η			1.127	0.734	0.479
ϕ_c		0.558	0.676	0.520	0.381
D	1.89	1.88±0.04	1.907±0.013	1.900±0.004	1.908±0.018
τ	2.06±0.02	2.04±0.04	2.01±0.03	1.99±0.03	1.97±0.03
ν	1.6±0.1	1.92±0.03	1.376±0.065	1.404±0.055	1.420±0.044

Cyclic Compression and Decompression



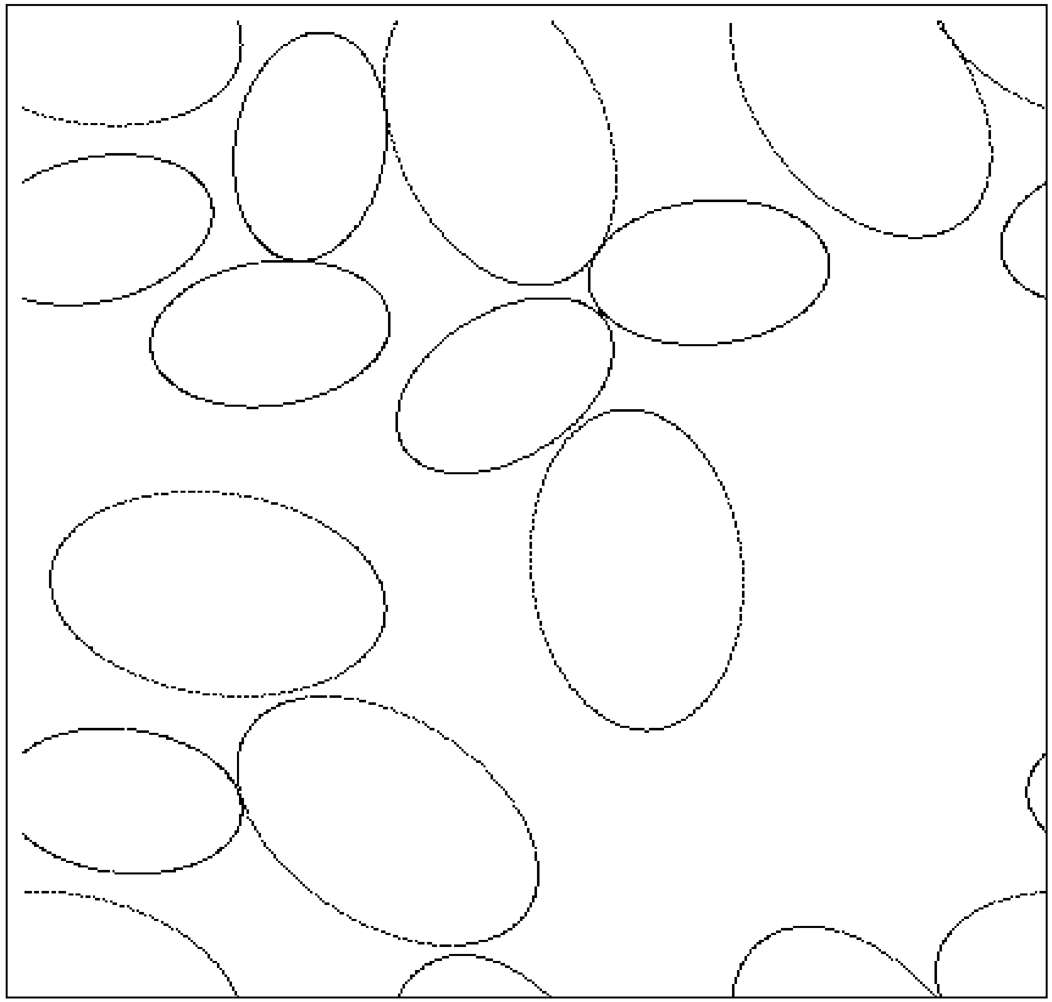
Packings of ellipse-shaped particles

bidisperse



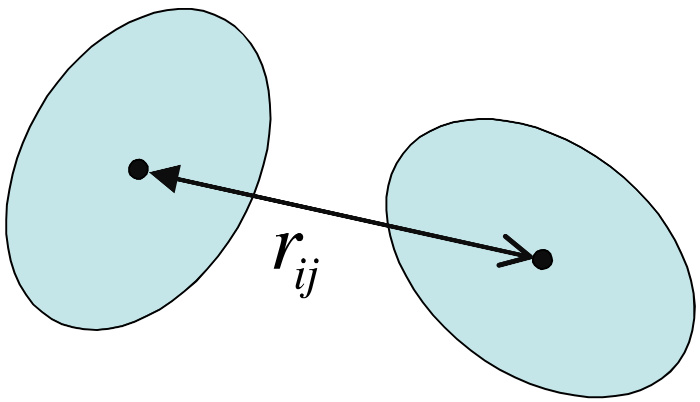
$$\frac{a_1}{b_1} = \frac{a_2}{b_2} = \alpha$$

$$\frac{a_1}{a_2} = 1.4$$

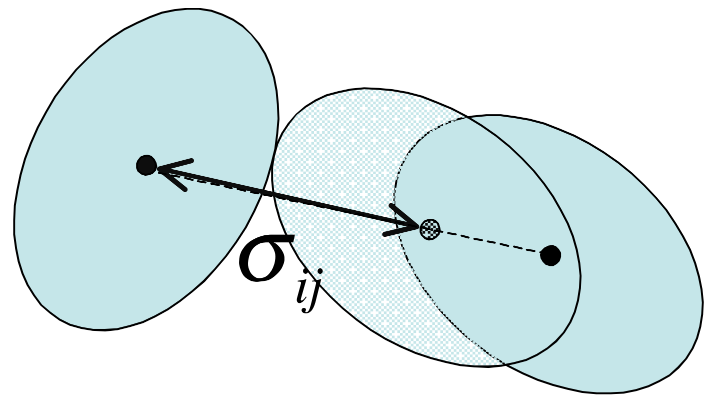


compression method-fixed aspect ratio α

Pairwise Repulsive Interactions: True Contact Distance



$$V(r_{ij}) = 0$$

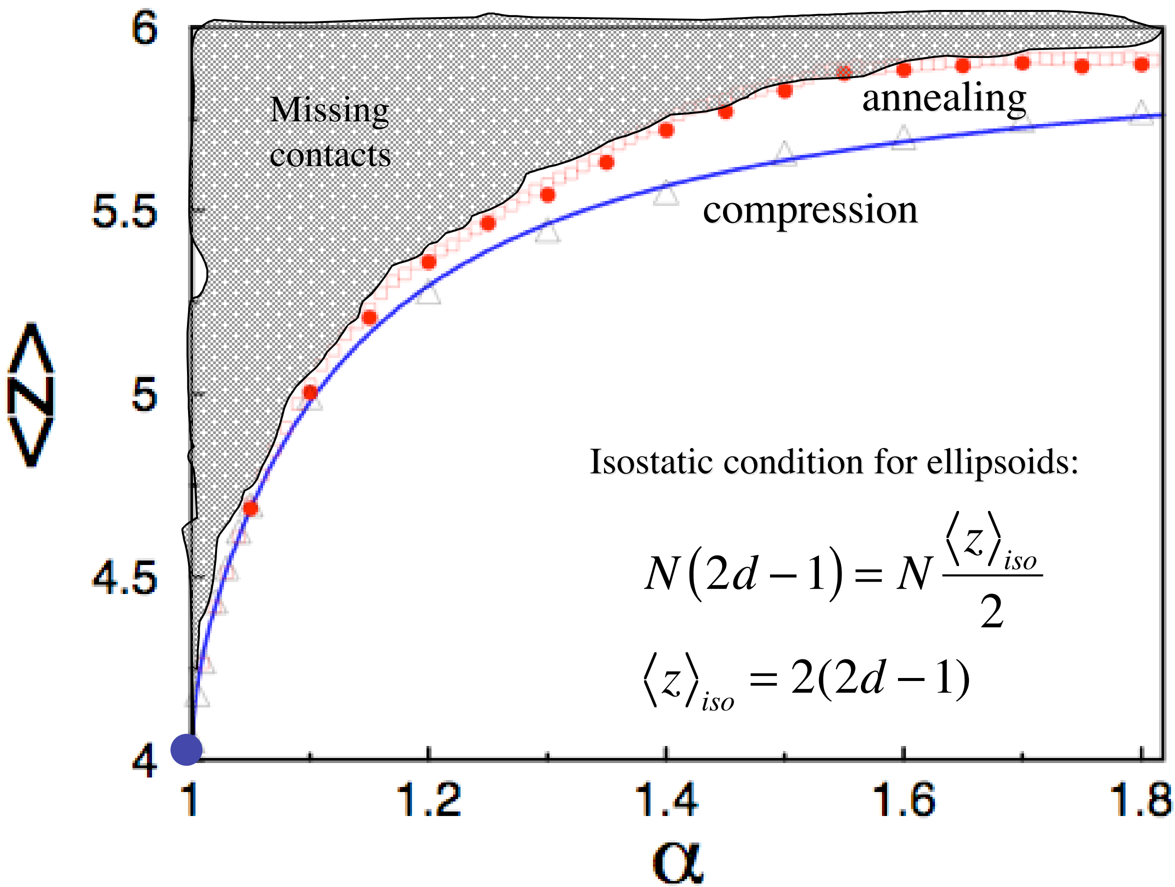


$$V(r_{ij}) > 0$$

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

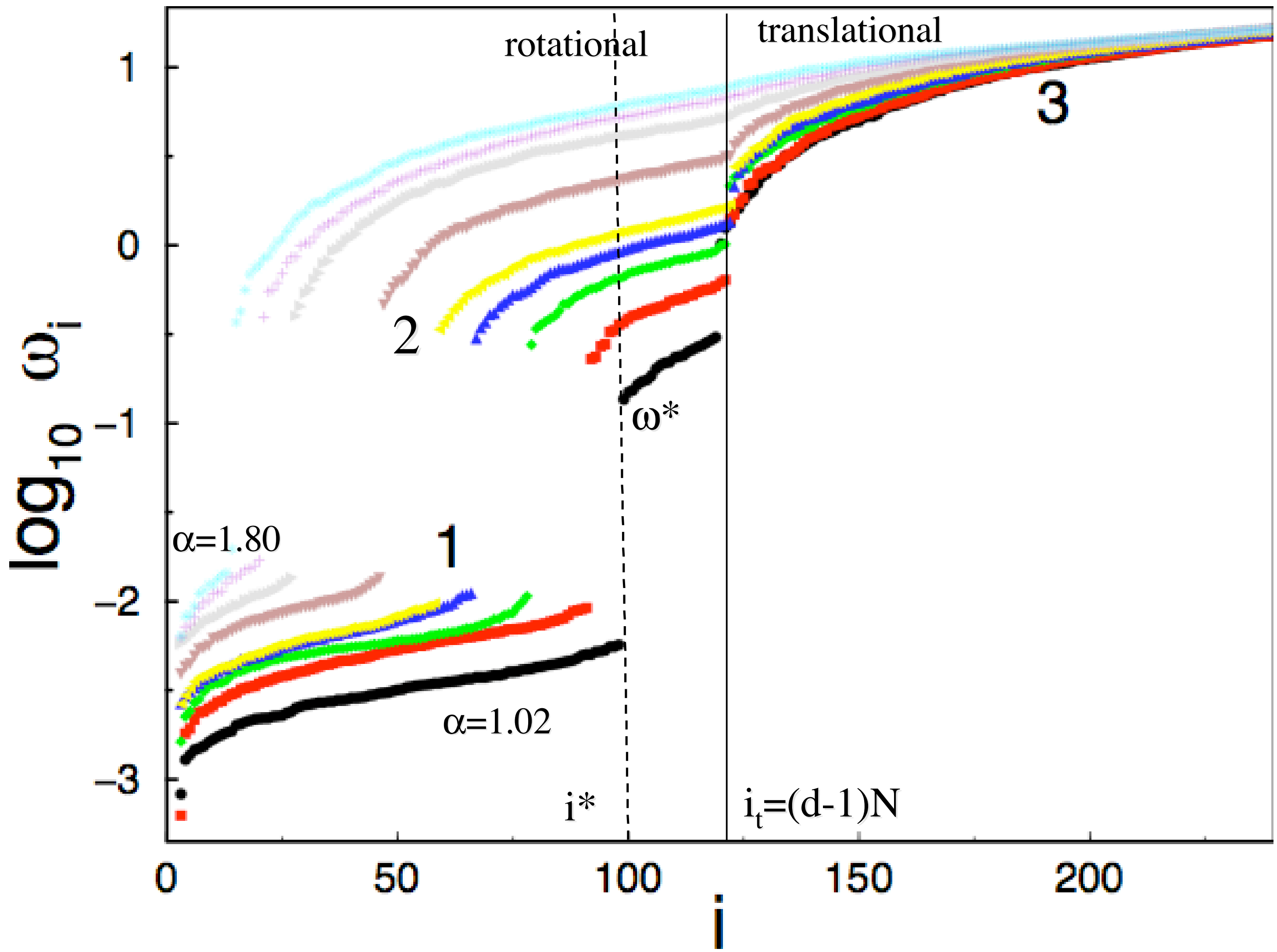
α=2; linear springs

Average Contact Number



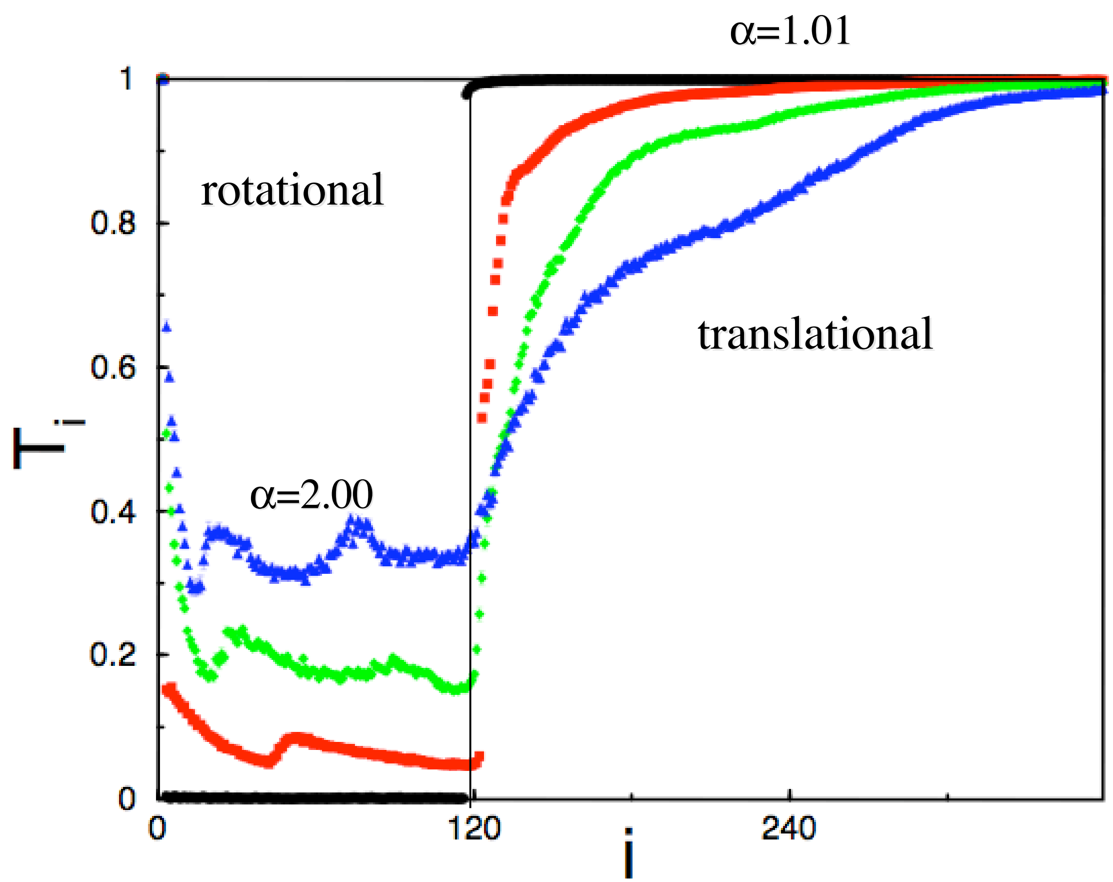
- Not a discontinuous jump from <z> = 4 to 6.
- Quartic modes to the rescue!

Eigenfrequency Spectra



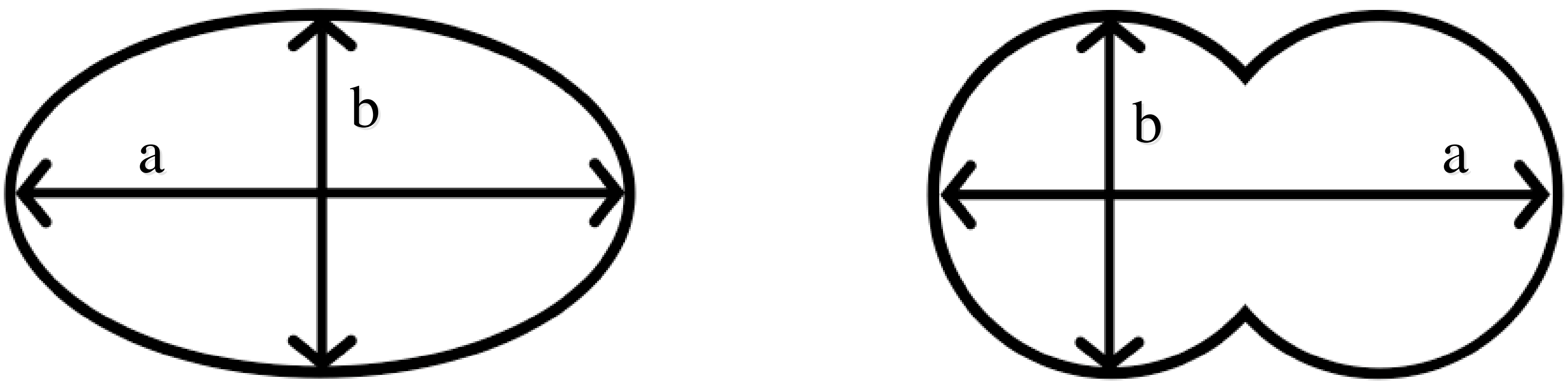
- Two gaps in spectrum over range of aspect ratios
- Onset of first gap depends on aspect ratio
- Second gap closes at large aspect ratios

Rotational/Translational Character of Eigenmodes



$$T_i = \sum_{j=1}^{N}\left[\left(e_{xi}^{j}\right)^2 + \left(e_{yi}^{j}\right)^2\right] \qquad T_i = 1 - R_i$$

What is the difference between between a dimer and an ellipse?



$\alpha = a/b$

Structural Properties