2254-9

Workshop on Sphere Packing and Amorphous Materials

25 - 29 July 2011

Calculations of the Probabilities of Jammed Packings

Corey S. O'Hern

Dept.of Mech. Eng. & Mat. Sci.
Dept.of Physics, Yale University
P.O. Box 208286, New Haven, CT 06520
U.S.A.

Strada Costiera 11, 34151 Trieste, Italy - Tel.+39 040 2240 111; Fax +39 040 224 163 - sci_info@ictp.it

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Corey S. O'Hern
Department of Mechanical Engineering & Materials Science
Department of Physics
Yale University

What is the ***best*** packing?

What is the ***most probable*** packing (given a protocol)?

Outline

1. Jammed packings do not occur with equal probability.
2. Basins of attraction for jammed packings.
3. Contact percolation critical point(s).

Important Point #1

To accurately measure packing probabilities, one must identify all possible packings…

…first studies must be performed on small systems.

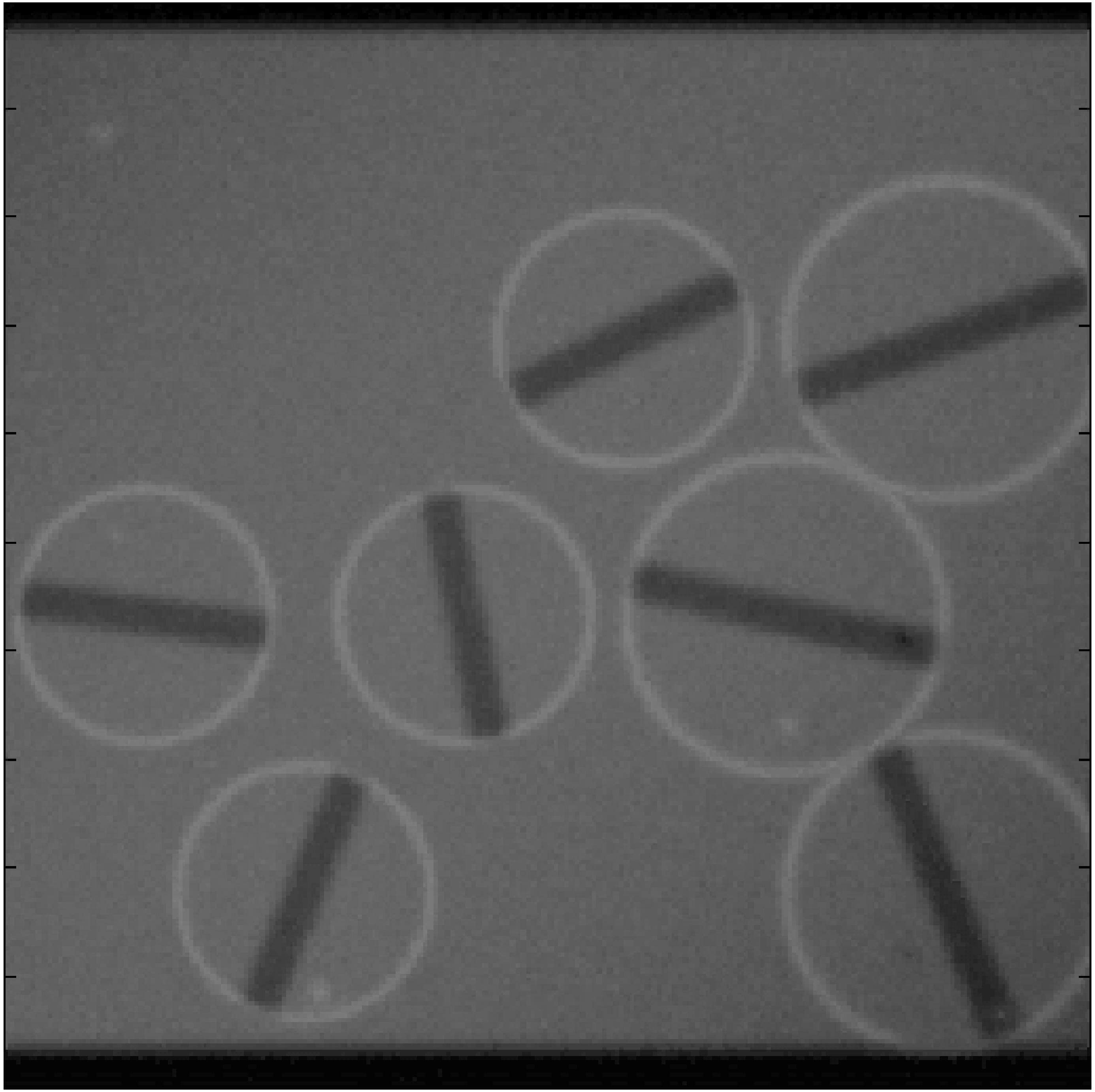
Motivation

- In small systems, we can show that jammed packings occur with very different probabilities.   So what?

- In large systems, it appears that packings occur with equal probability, *i.e.* each packing occurs once, but within a narrow set of structural properties (for a given protocol).

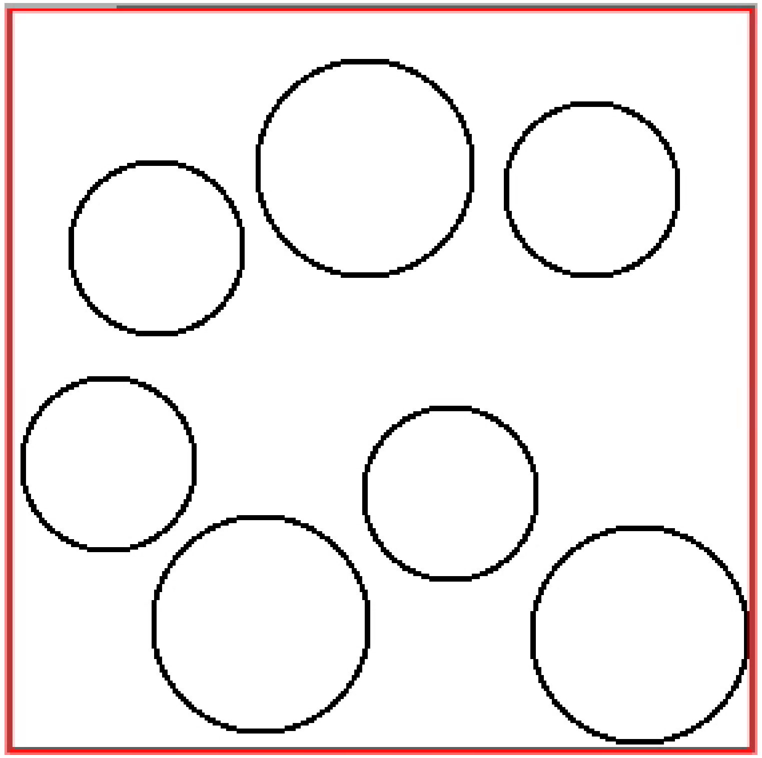
- But if the protocol is changed, a different narrow set of packings will occur.

- The problem of understanding packing probabilities in small systems is similar to understanding protocol dependence of packings in large systems.



GG, JB, CSO, MS,
Phys. Rev. E 80
(2009) 061304.

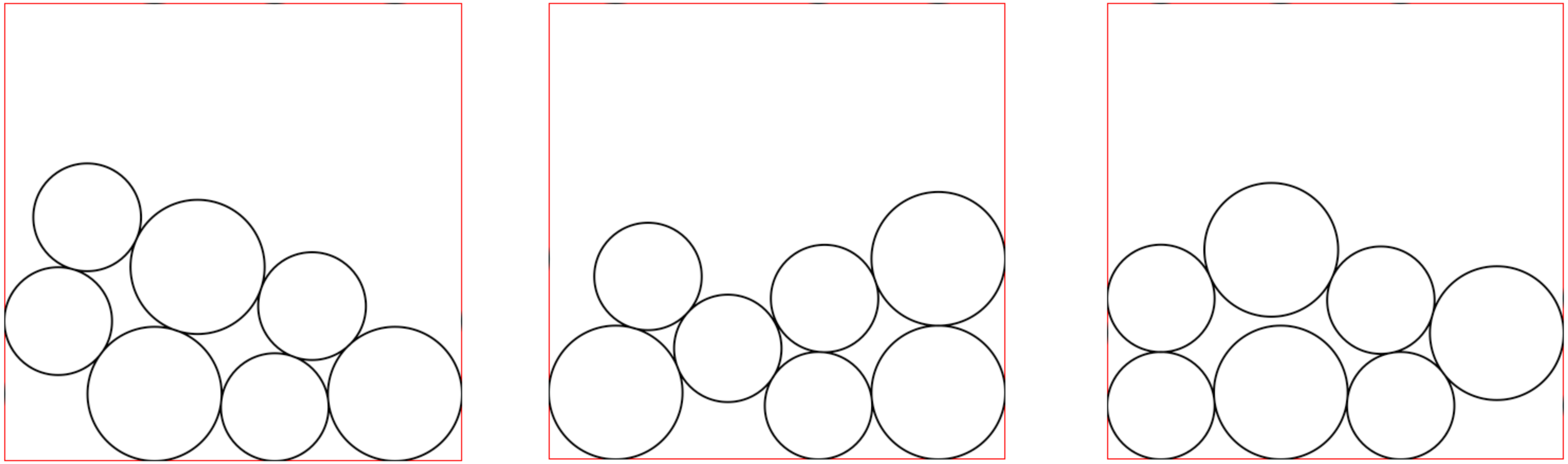
Deposition Algorithm in Simulations



$$\bar{g} = \frac{m_S g}{k \sigma_S}$$

- 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



1 2 3

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

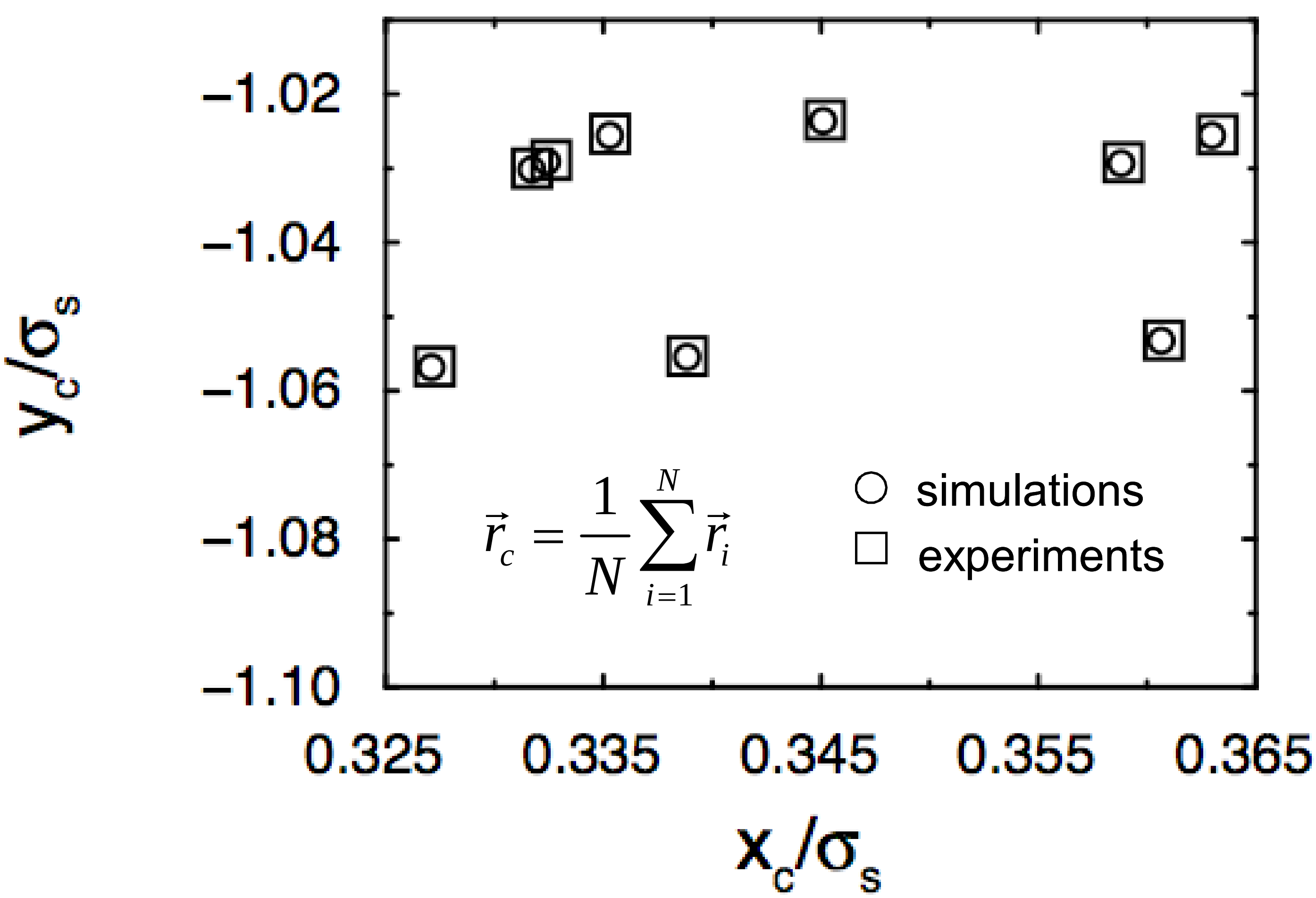
Mechanical Stability and Distinguishability

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

α,β=x, y, z, particle index

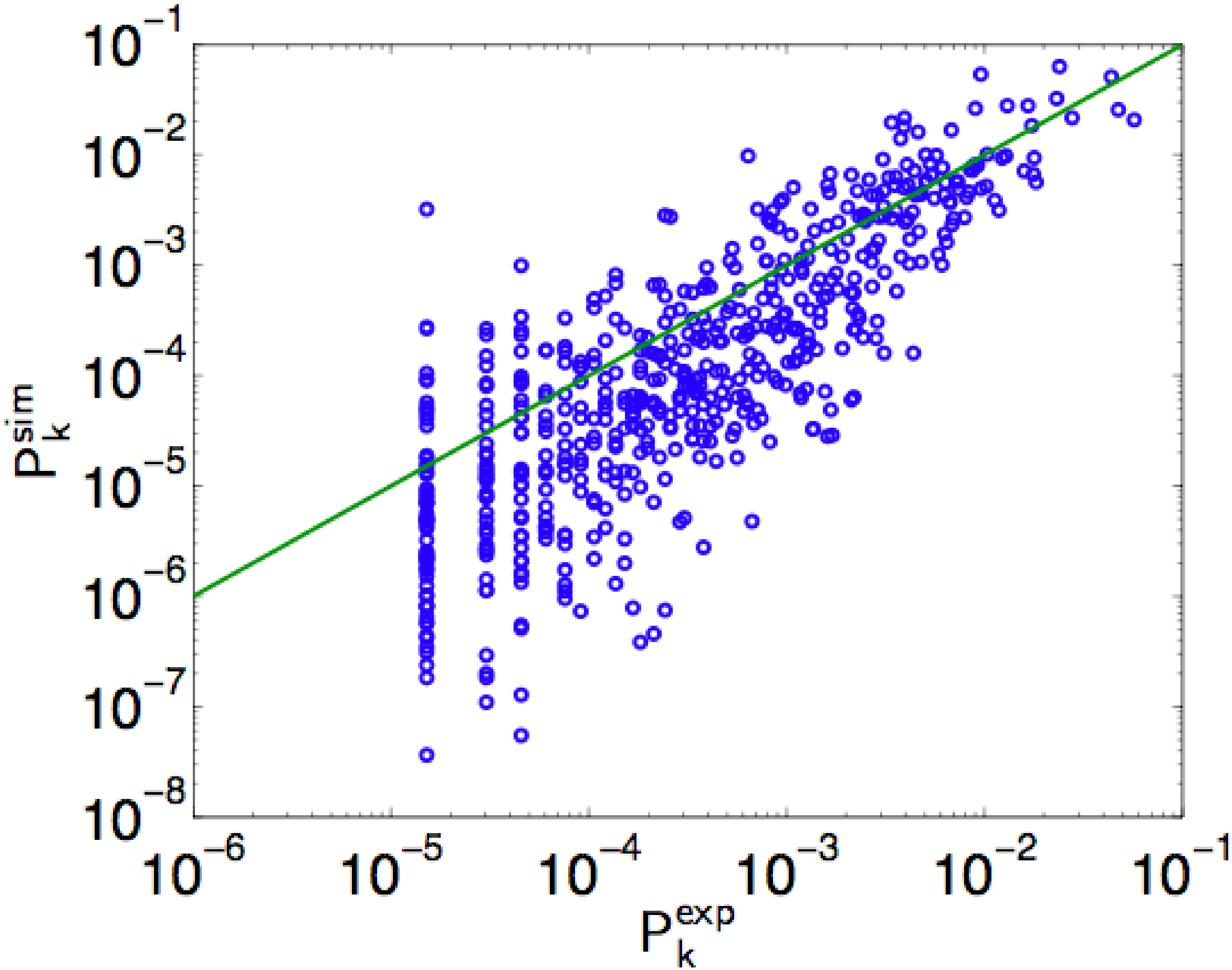
$\vec{r}_0$ = positions of MS packing

Calculate d N- d eigenvalues



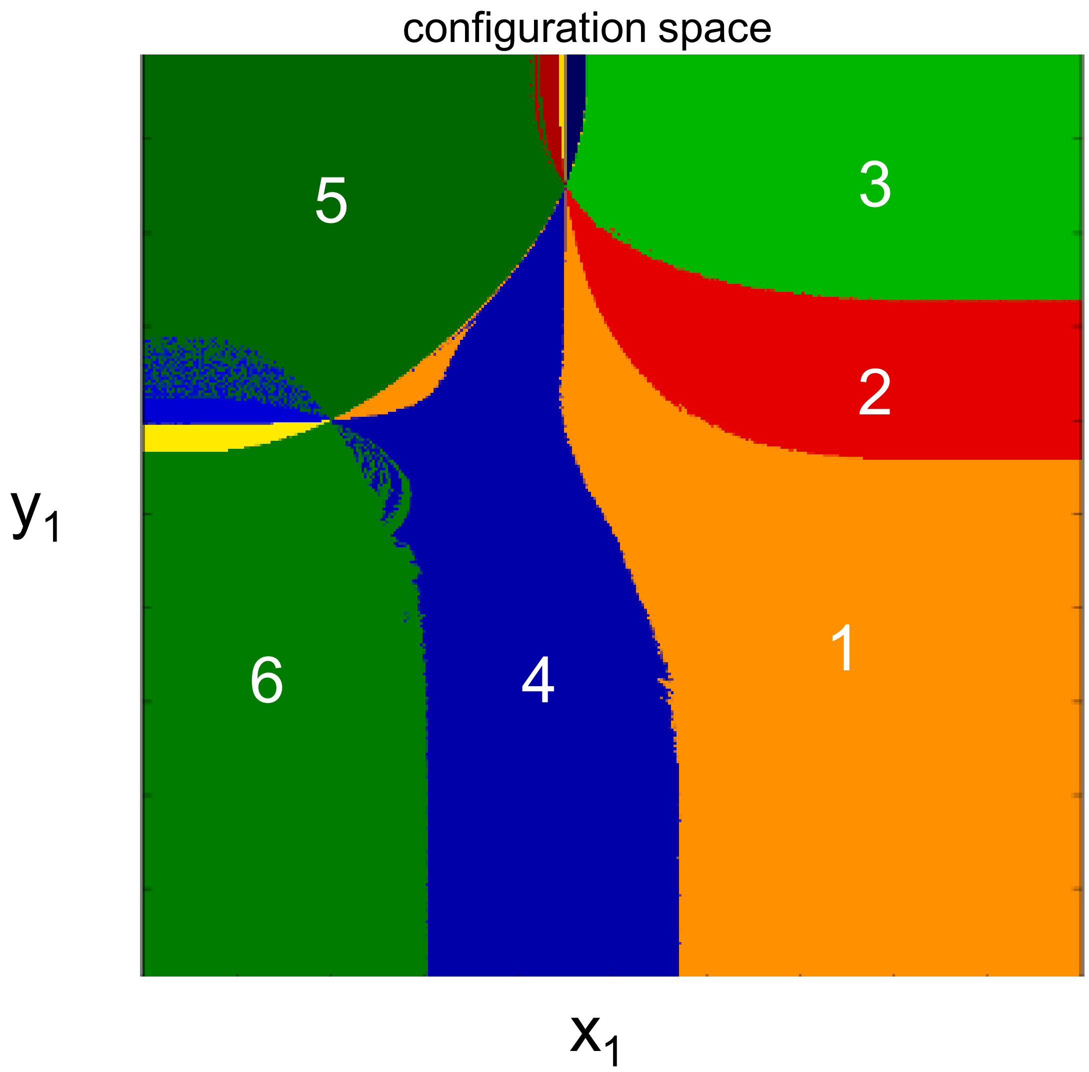
−1.02
−1.04
−1.06
−1.08
−1.10
0.325
0.335
0.345
0.355
0.365
x_c/σ_s
y_c/σ_s
$\vec{r}_c = \frac{1}{N}\sum_{i=1}^{N}\vec{r}_i$
simulations
experiments

Packing Probabilities Are Robust*



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

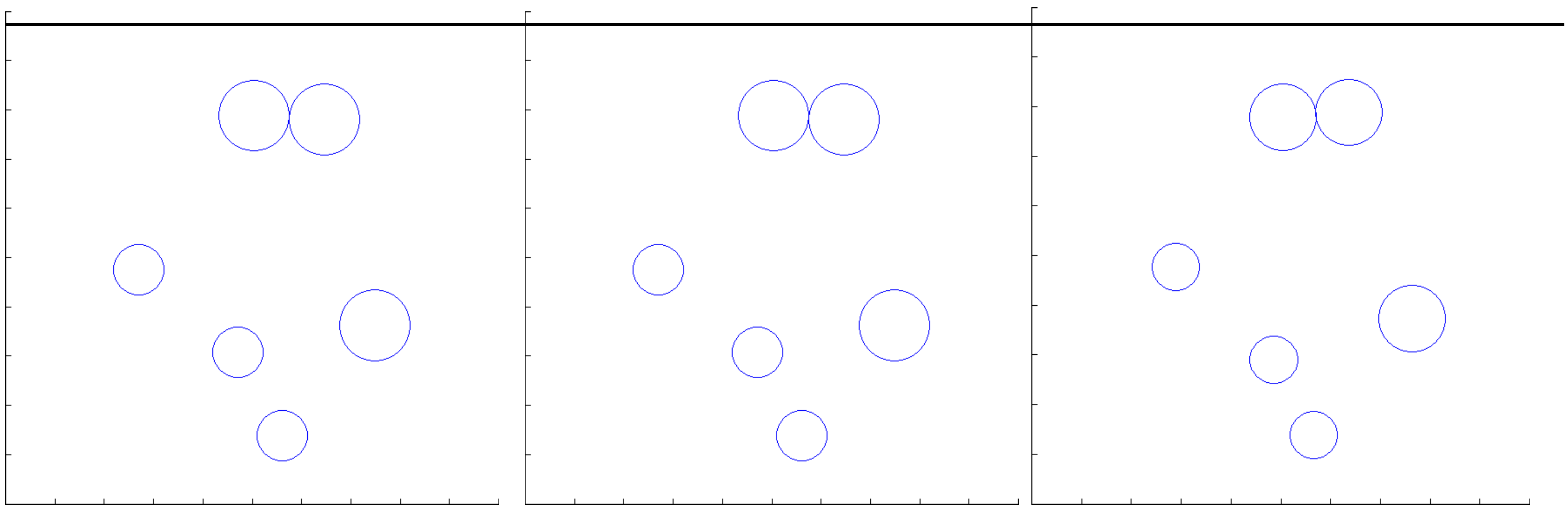
Calculations of Basin Volumes



$P_i = V_i / L^{dN}$

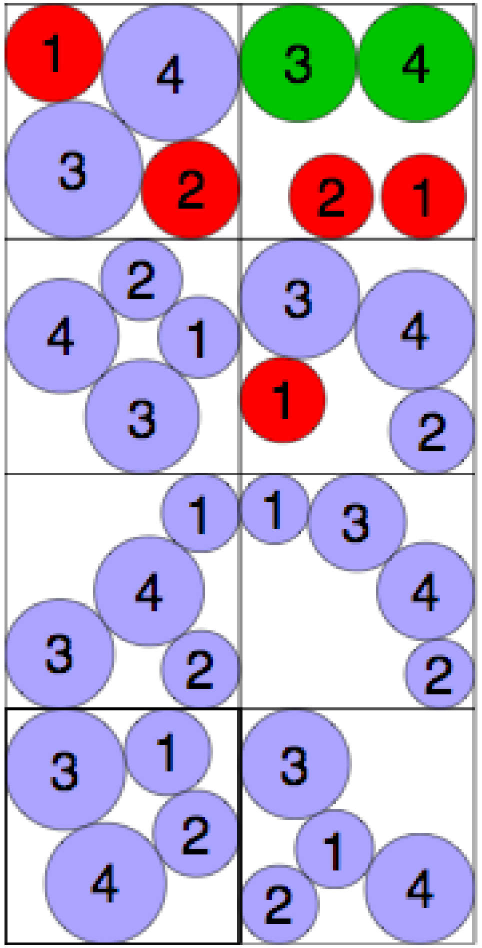
$\phi_0 = 0$

(Dissipation) rate dependence and basin volume

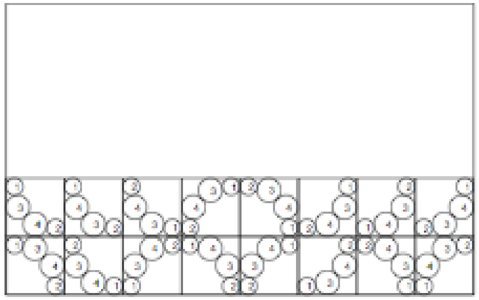


fast rate; ϕ_f=0.622   slow rate; ϕ_f=0.730   fast rate; different IC; ϕ_f=0.730

N=4 packings

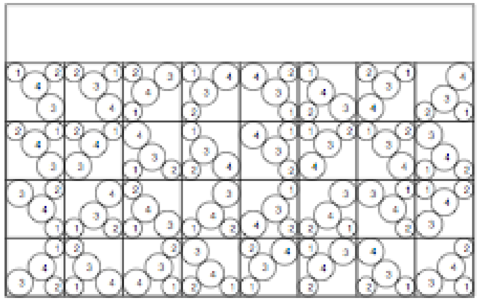


Prob=0.413250%

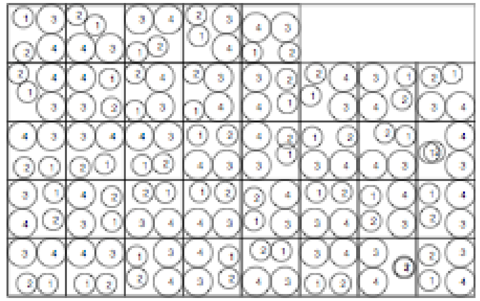


Prob=0.000050%

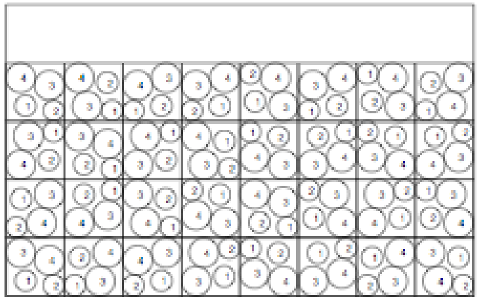
Prob=6.065950%



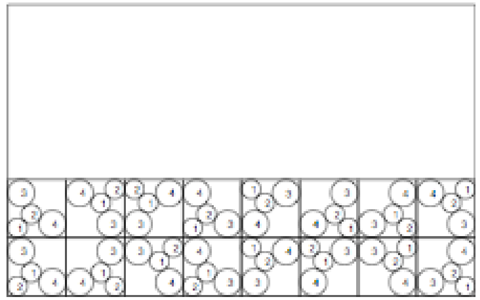
Prob=0.187150%



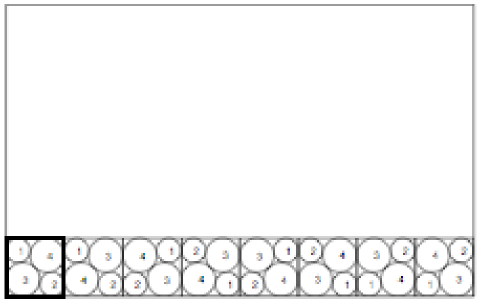
Prob=26.197200%



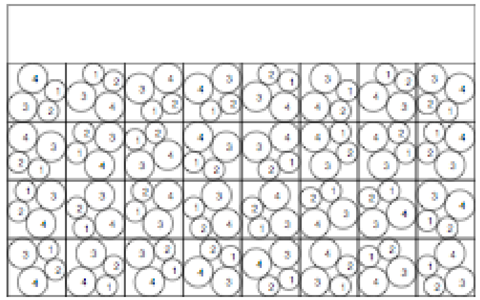
Prob=2.868100%



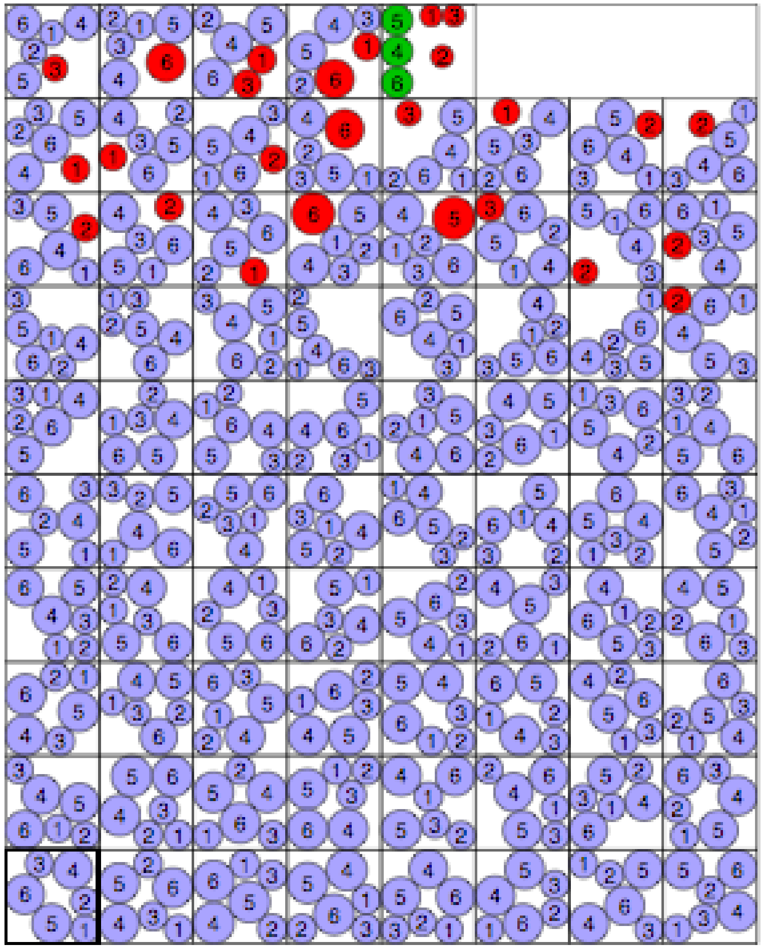
Prob=30.415850%



Prob=33.852450%

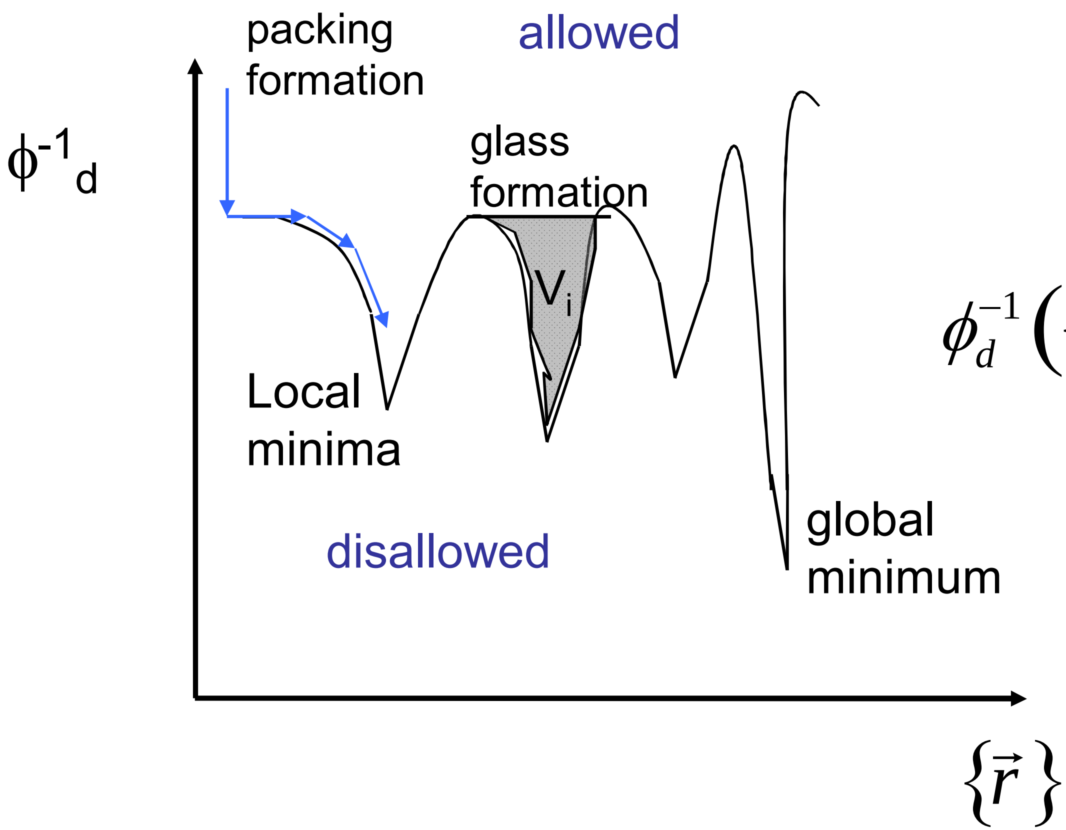


N=6



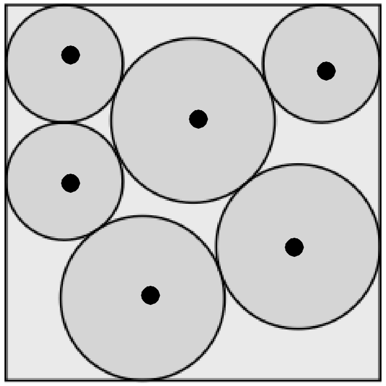
N	N_s
4	7*
6	75*
8	500
10	3983
12	16935

What determines MS packing probabilities: Density landscape for hard spheres

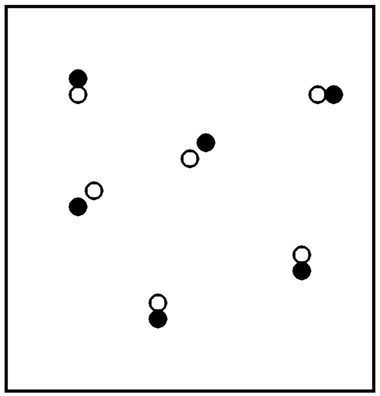


$$\phi_d^{-1}(\{\vec{r}\}) = \frac{6V}{\pi N \min_{mn} \left| \vec{r}_m - \vec{r}_n \right|^3}$$

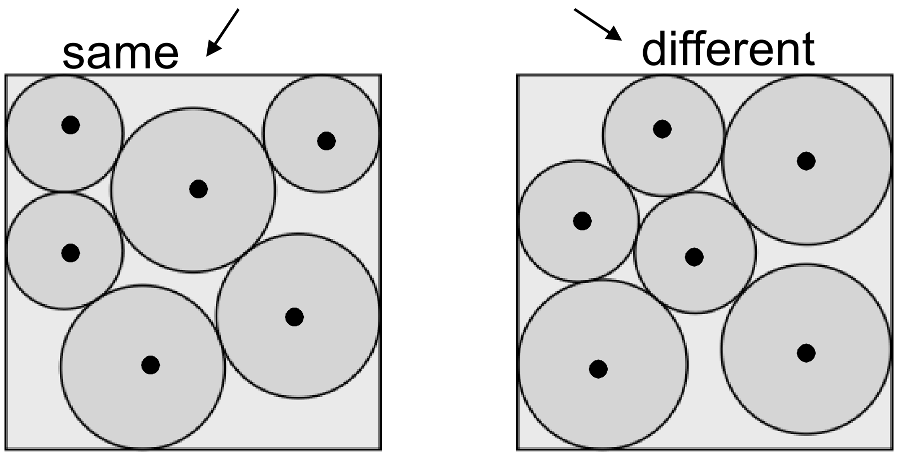
Method 1 (small l): Probability to return to a given MS packing



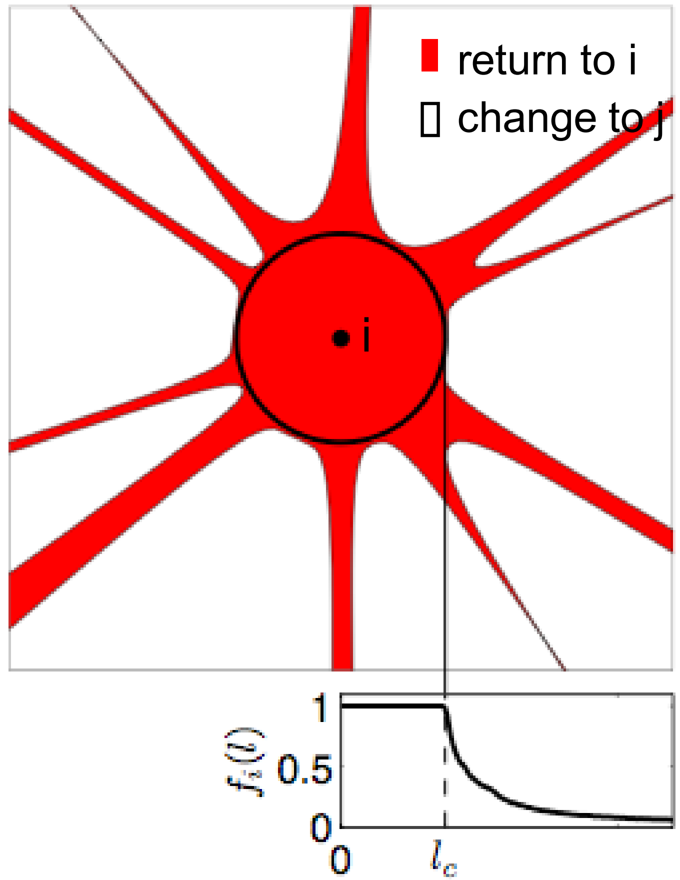
$$\phi_i^{MS}, \{\vec{r}\}_i^{MS}$$



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

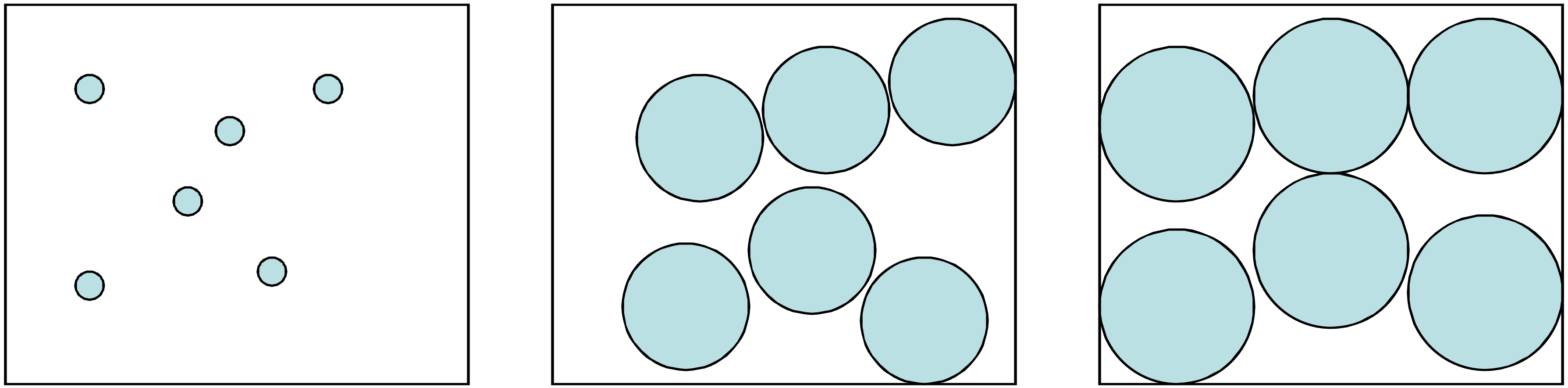


$$f_i(l) = \frac{M_i}{M}$$

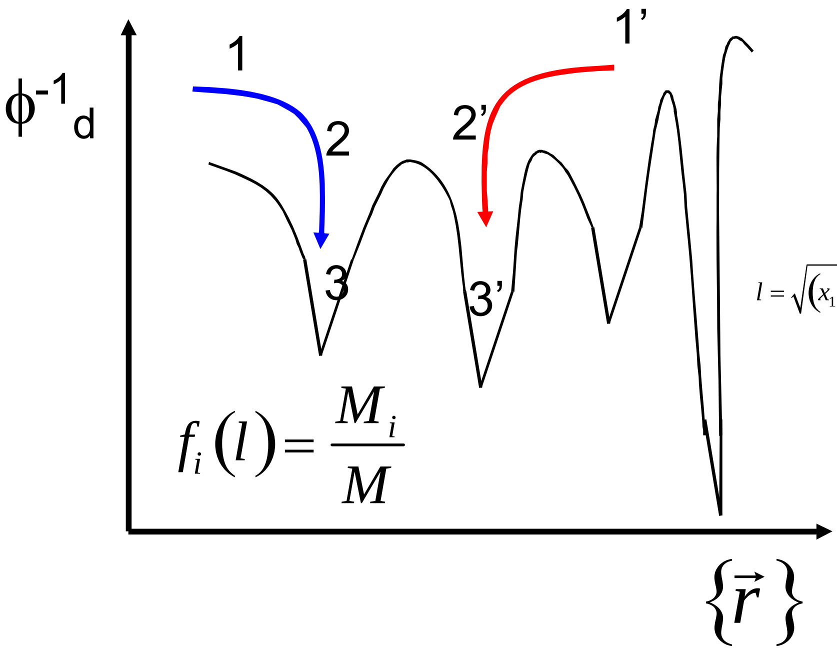


$$l = \sqrt{(x_{1f} - x_{10})^2 + (x_{2f} - x_{20})^2 + \cdots + (x_{Nf} - x_{N0})^2 + (y_{1f} - y_{10})^2 + (y_{2f} - y_{20})^2 + \cdots + (y_{Nf} - y_{N0})^2}$$

Method 2 (large l): Random initial conditions



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



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

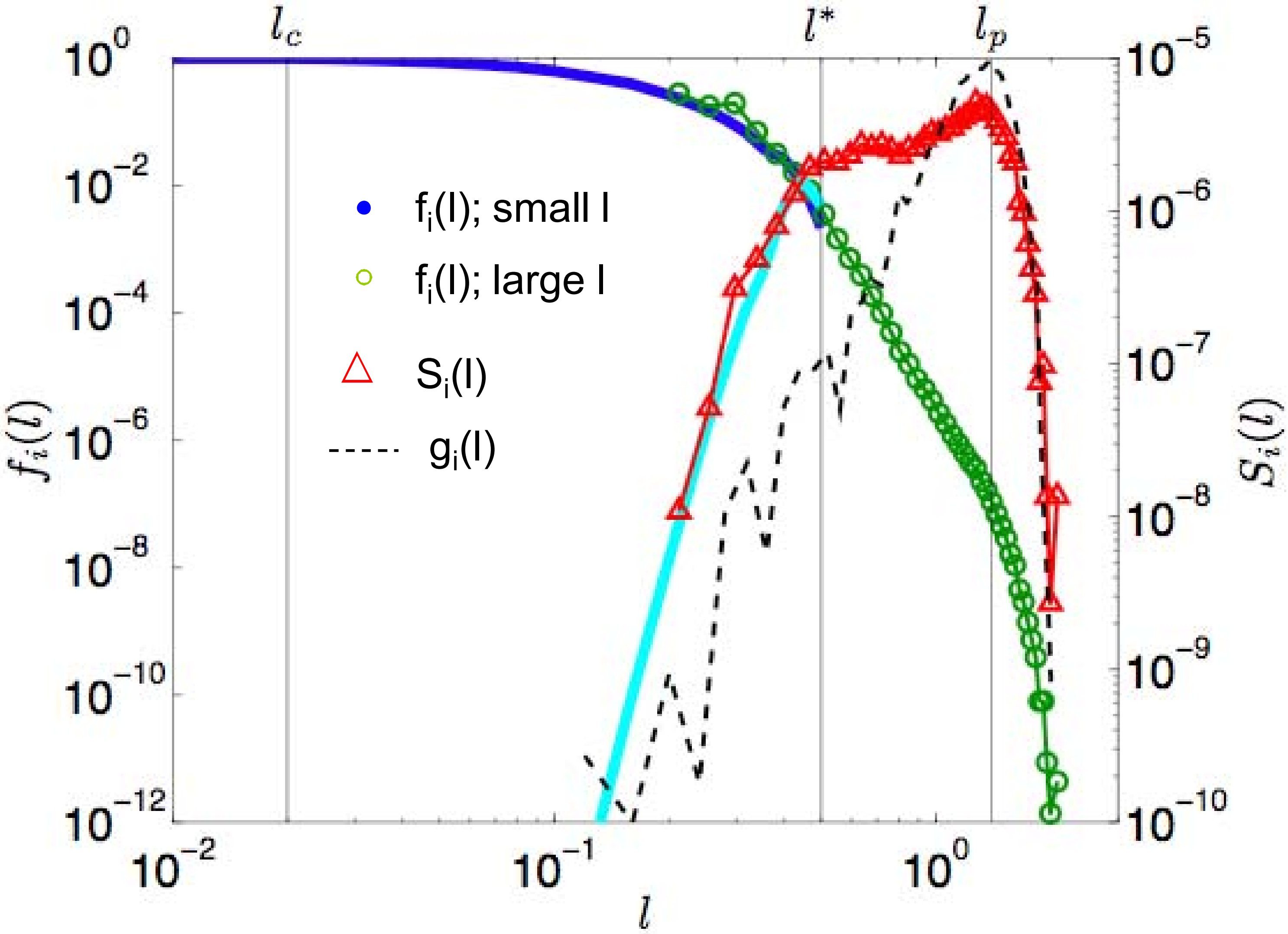
Basin Volumes

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

$$S_i(l) = A_{dN} f_i(l) l^{dN-1} \rho_i N_s! N_l!$$ weighted basin profile function

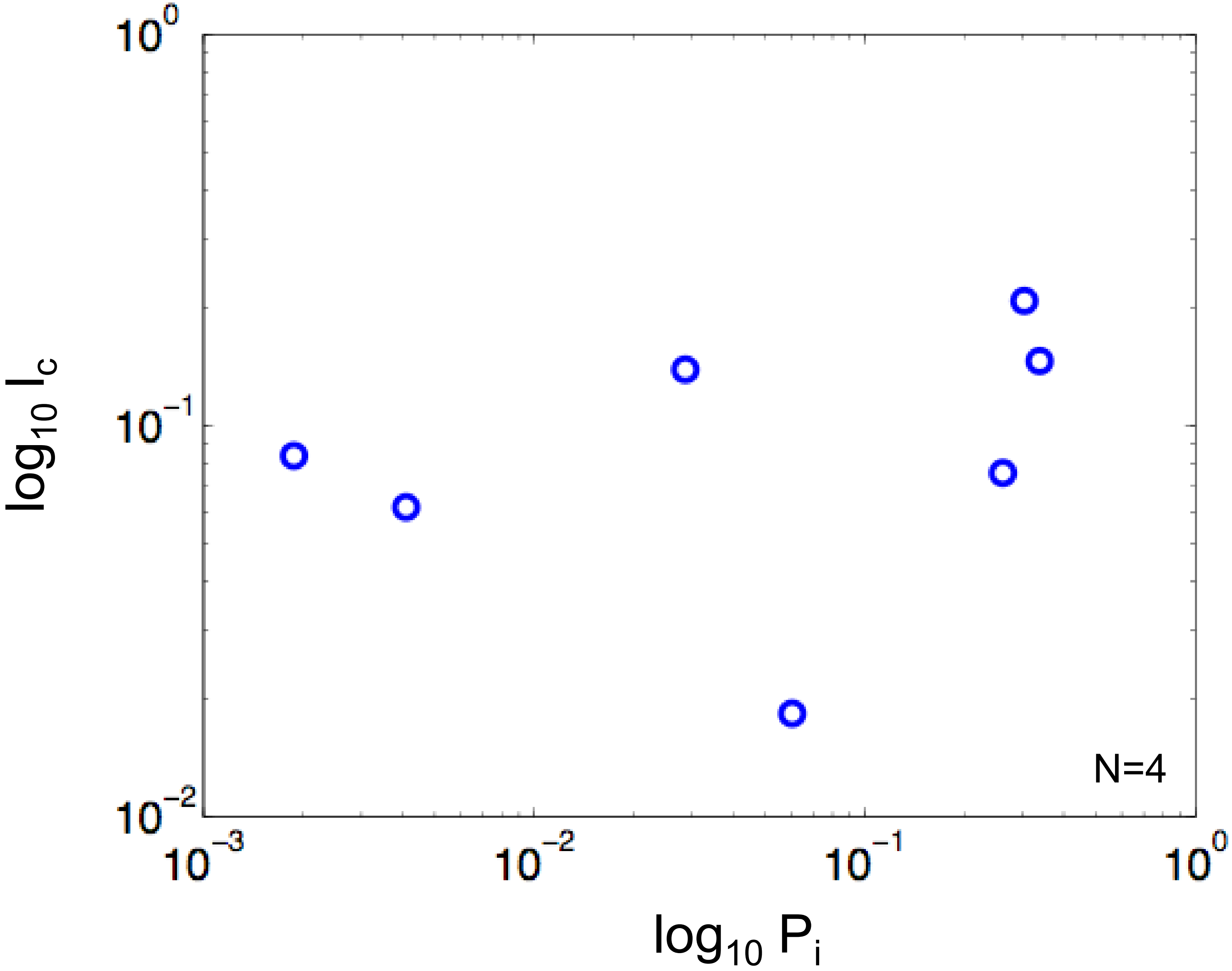
$f_i(l)$ unweighted basin profile function

Weighted/Unweighted basin profile functions

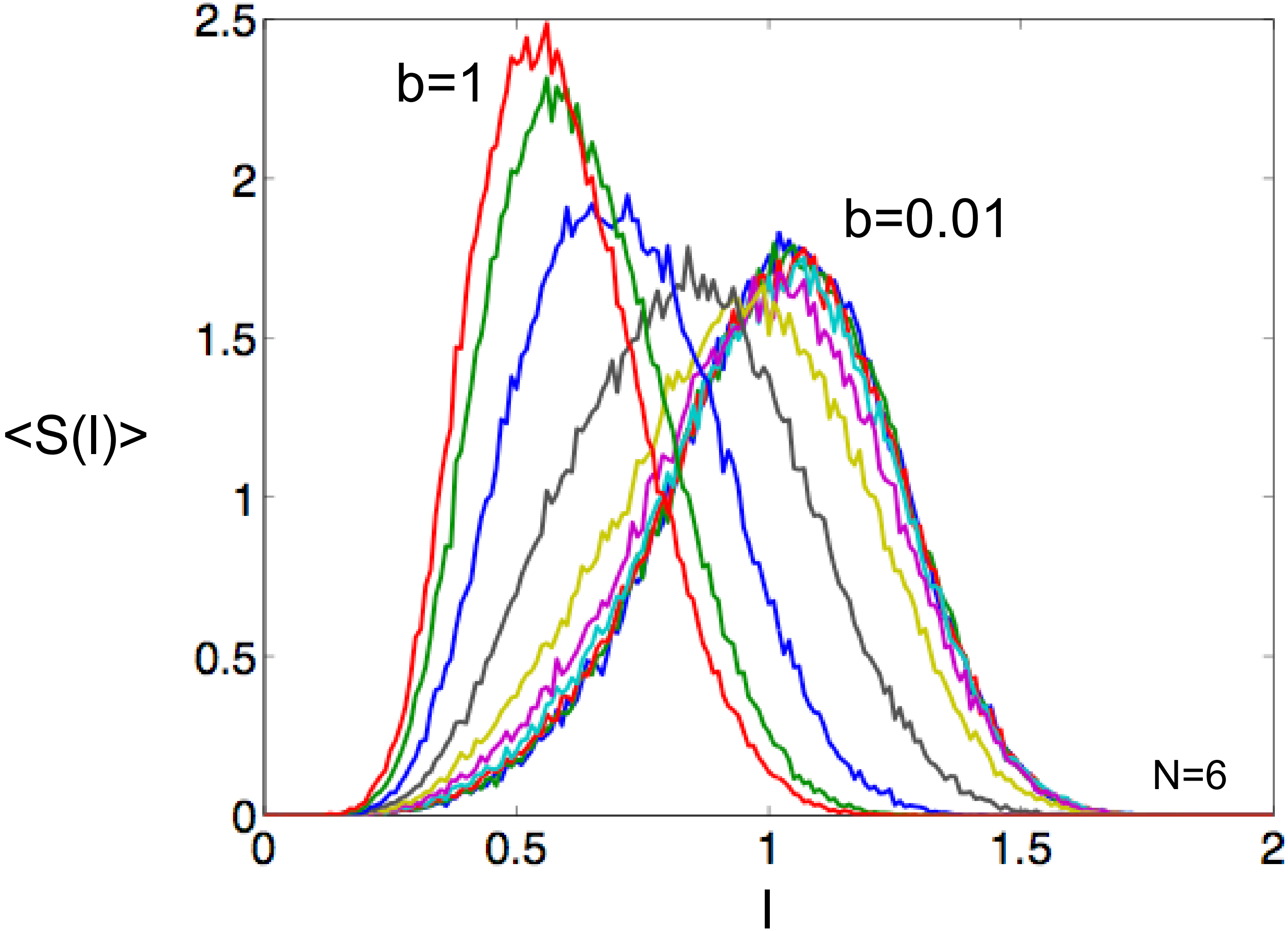


- Probability of MS packing determined by large l, not core region l_c

Do local properties determine probability?

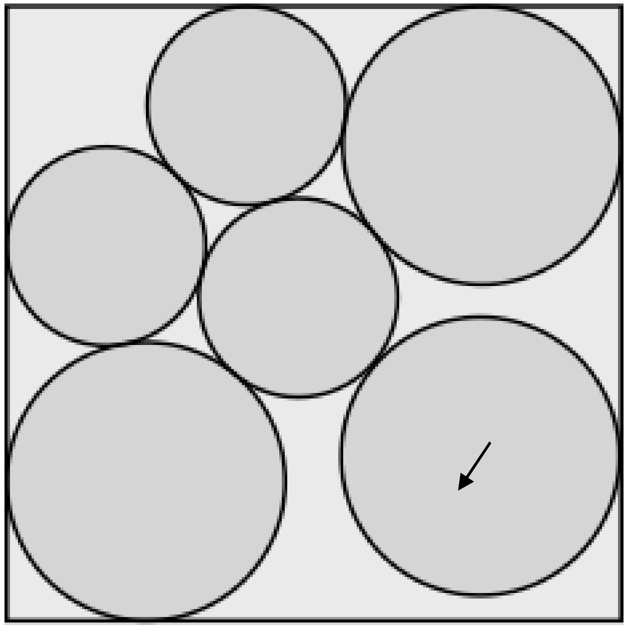


Thermal Quench Rate Dependence

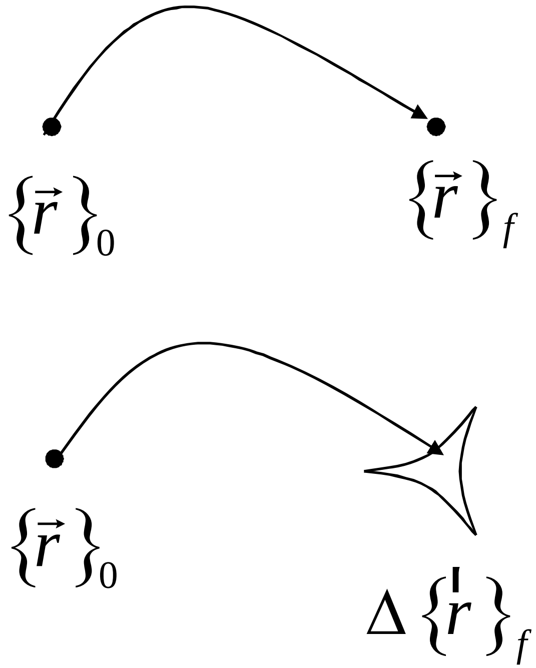


Future Directions

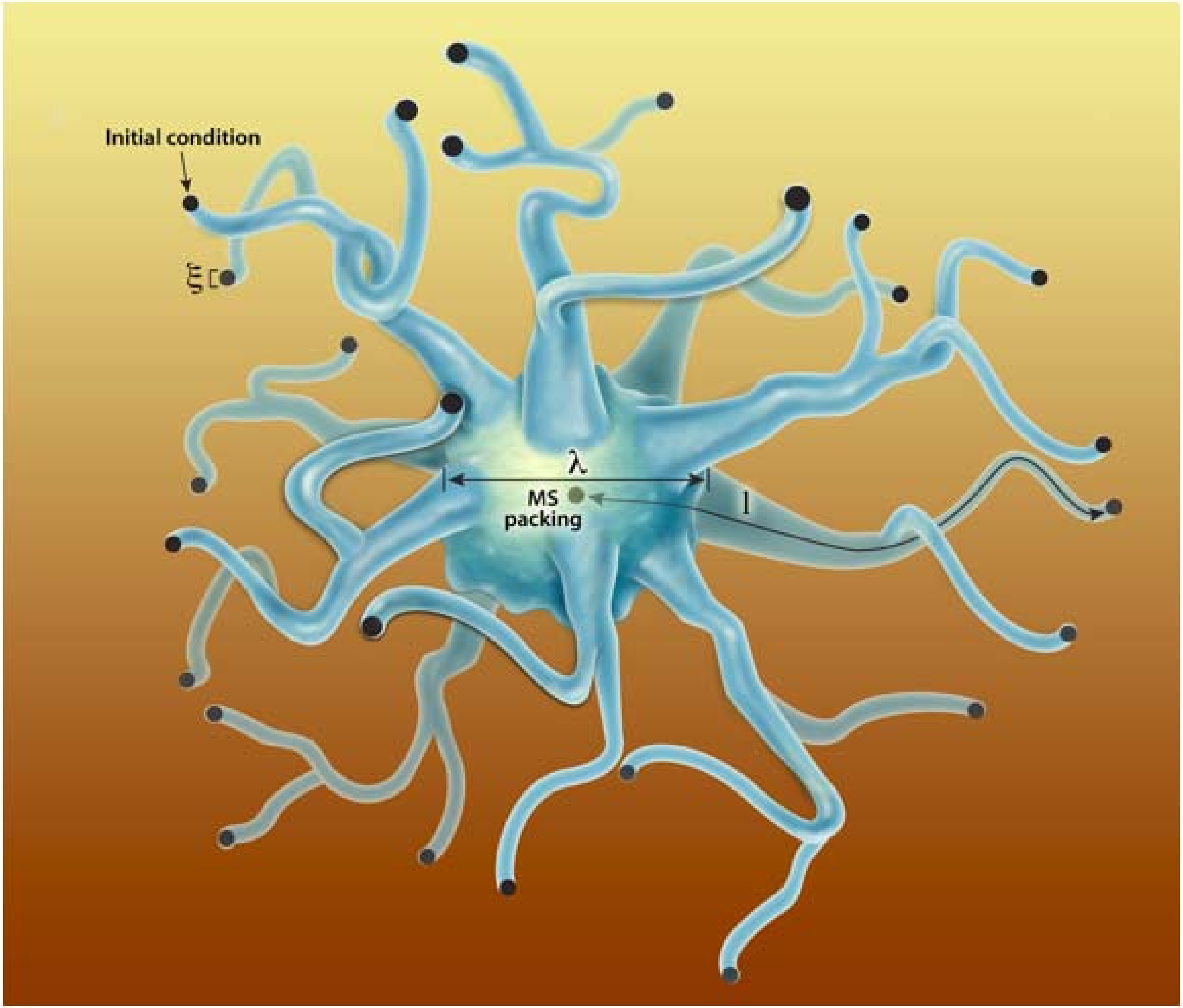
- Rattlers



Particles with fewer than 3 contacts

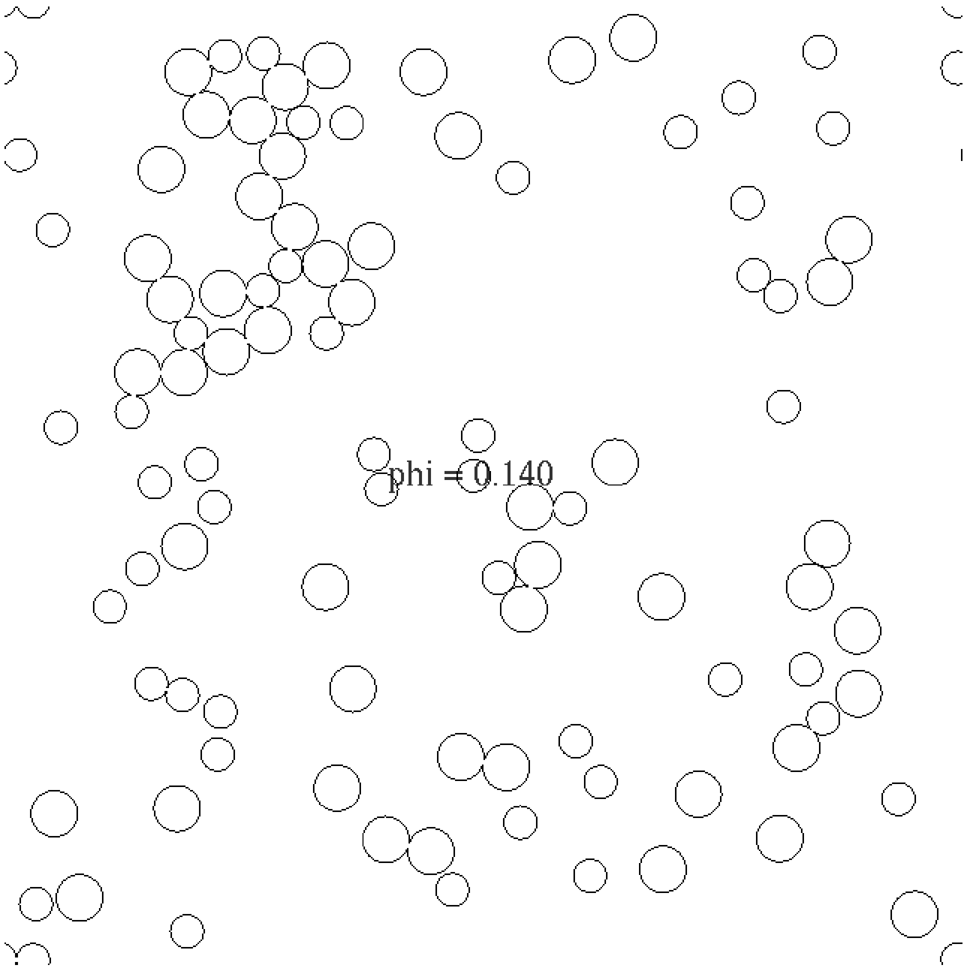


- Study ϕ_i and quench rate dependence of probabilities

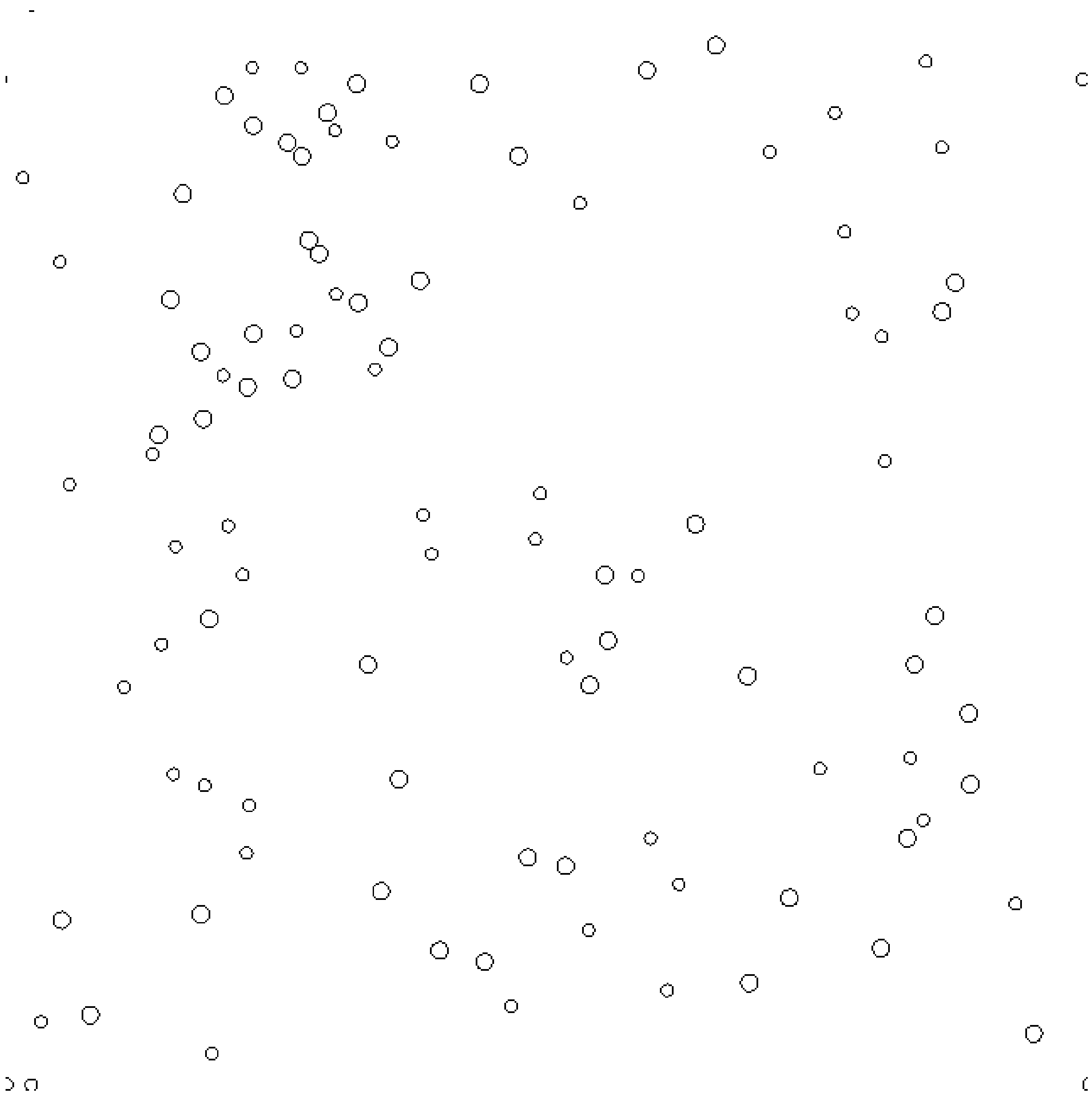

Initial condition
ξ
λ
MS
packing
l

What important processes signal jamming and determine packing probabilities?

Contact Percolation

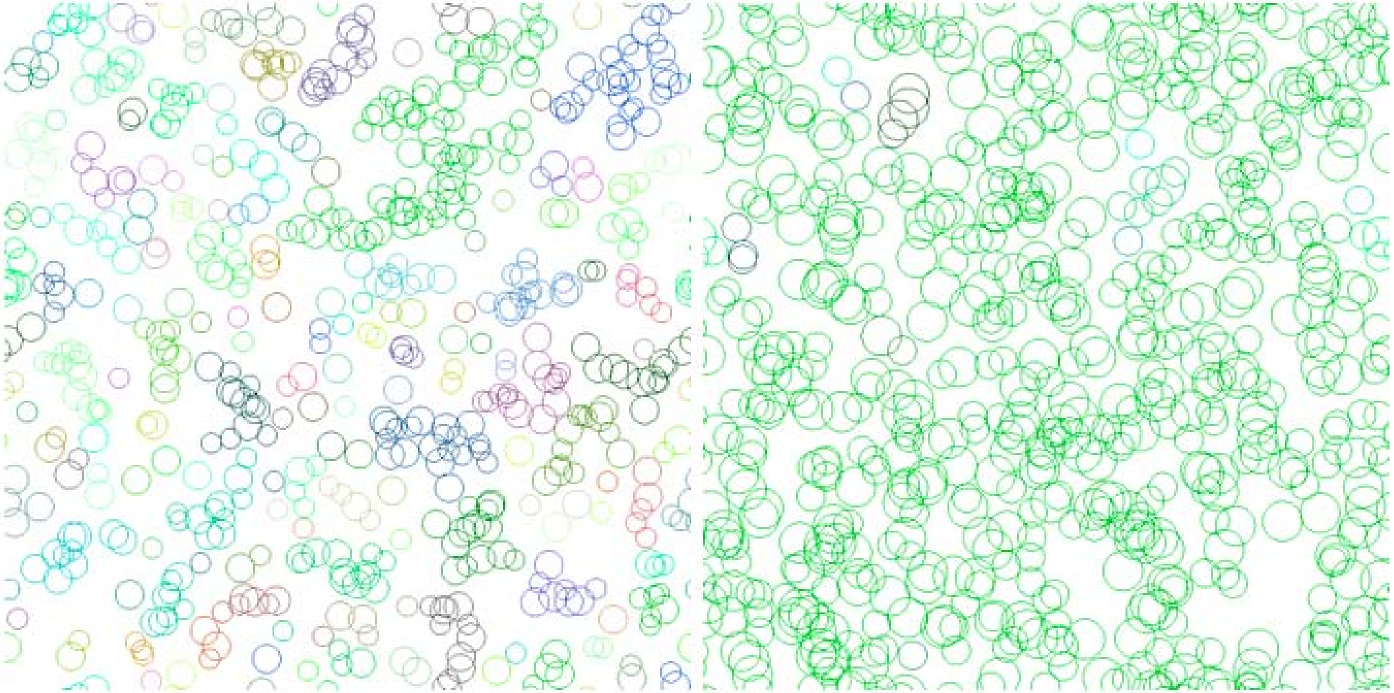


Cooperative Motion



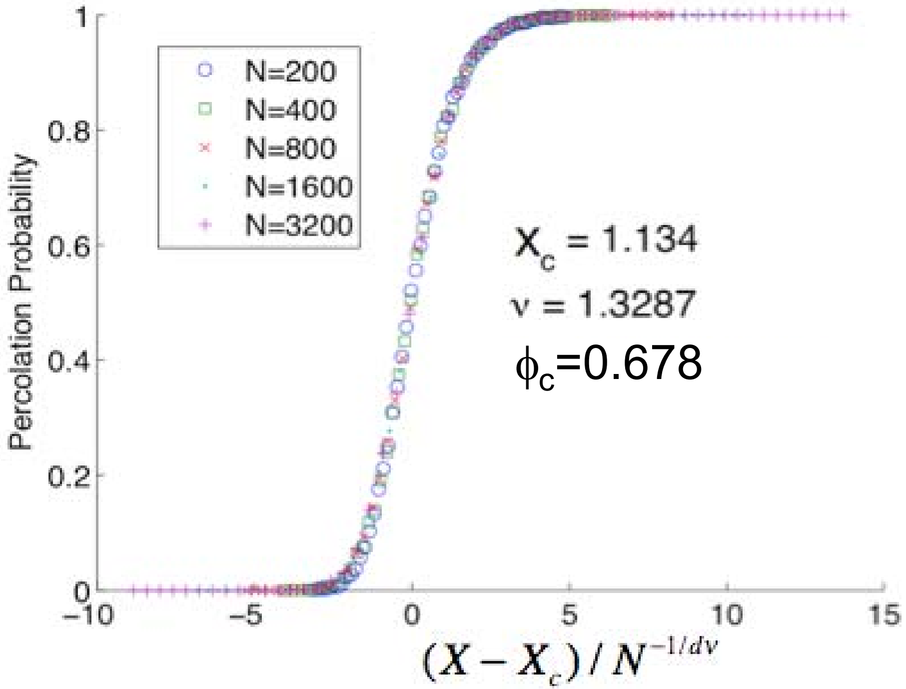
'Random' Continuum Percolation

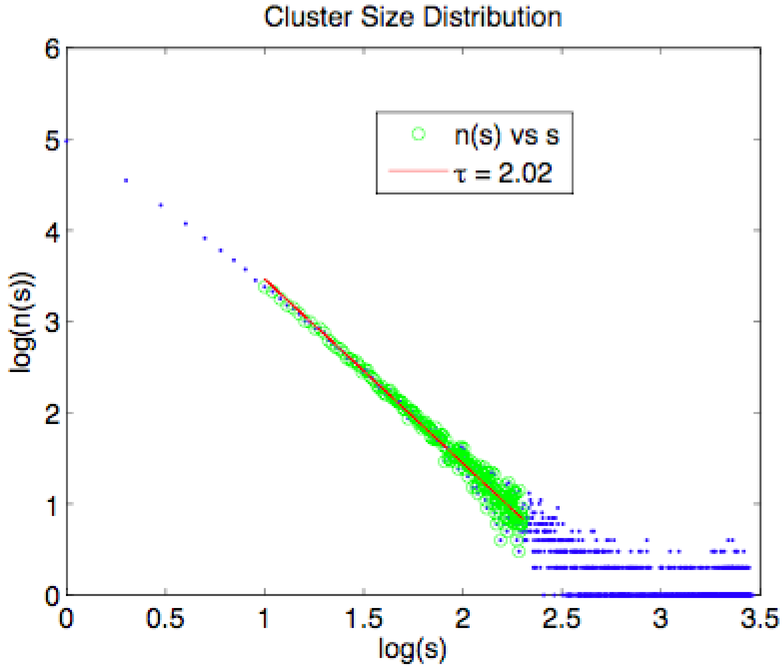
unpercolated percolated

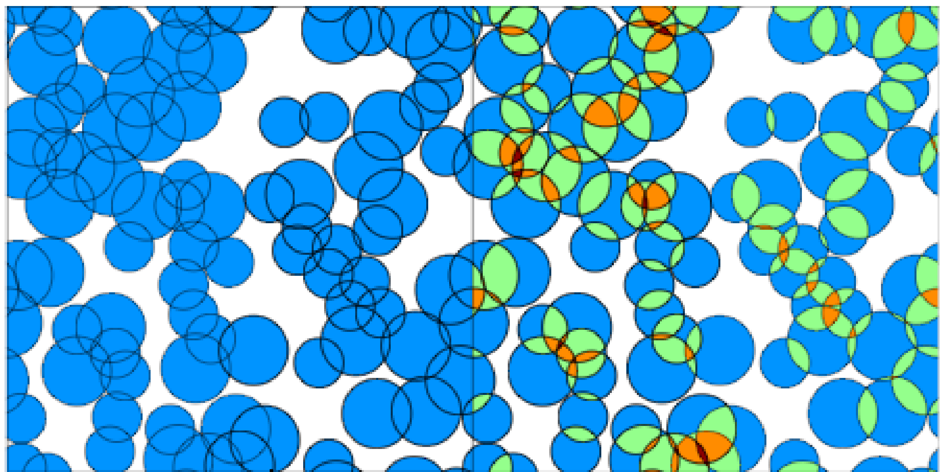


$$X_p = N\pi R_p^2 / L^2$$

Critical Scaling Exponents





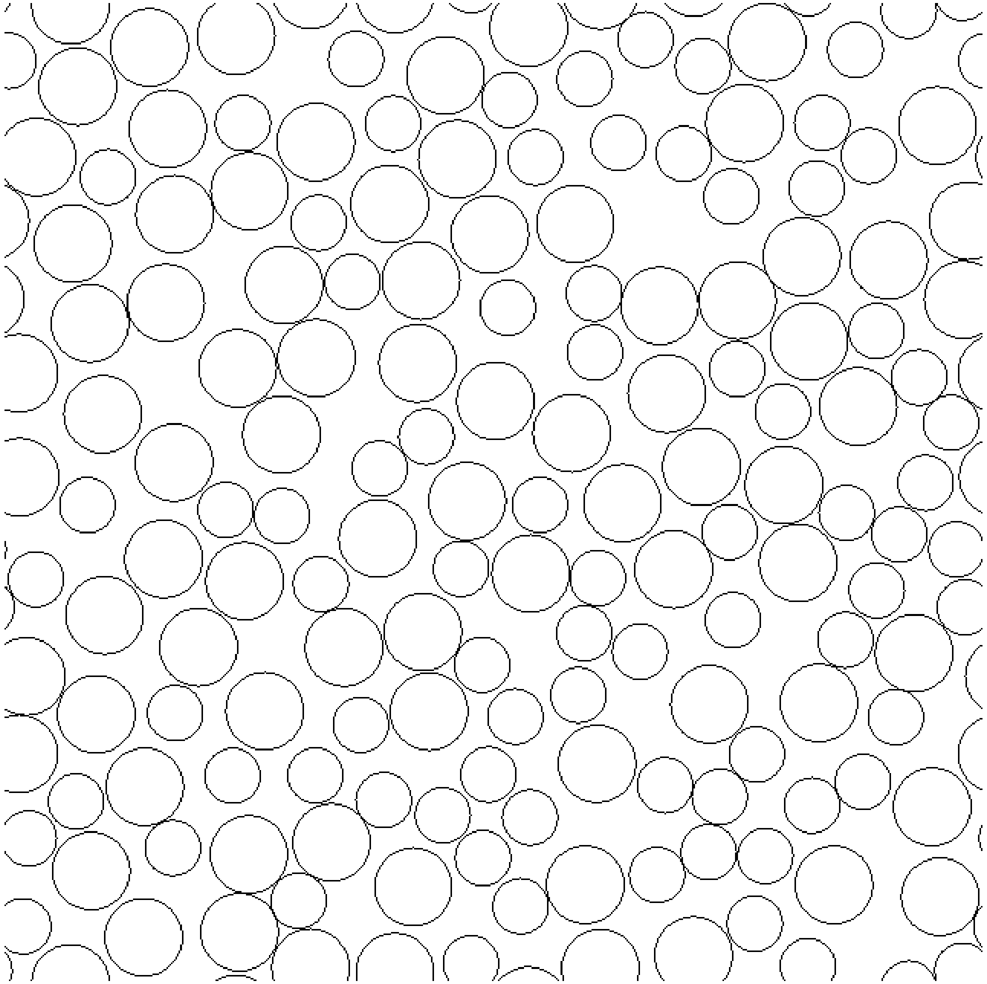


ϕ X

X_c	1.13
ϕ_c	0.678
D	1.91
τ	2.02
ν	1.33

How is the percolation transition influenced by spatial correlations?

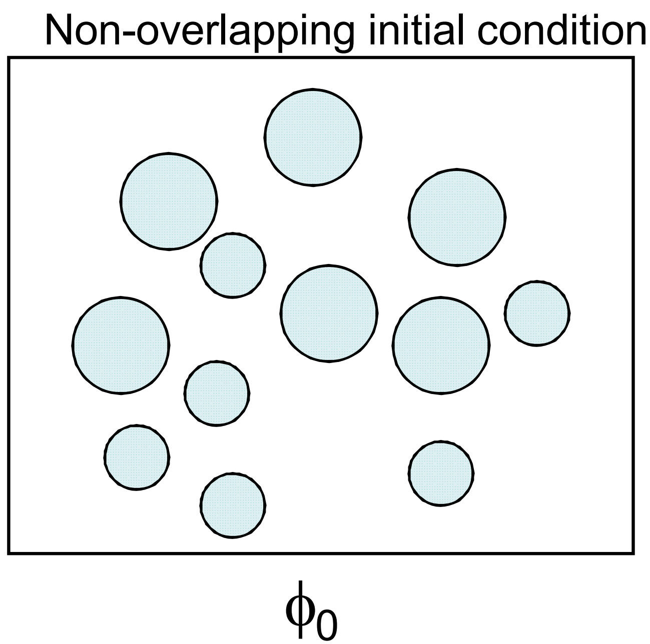
ϕ_0=0.6

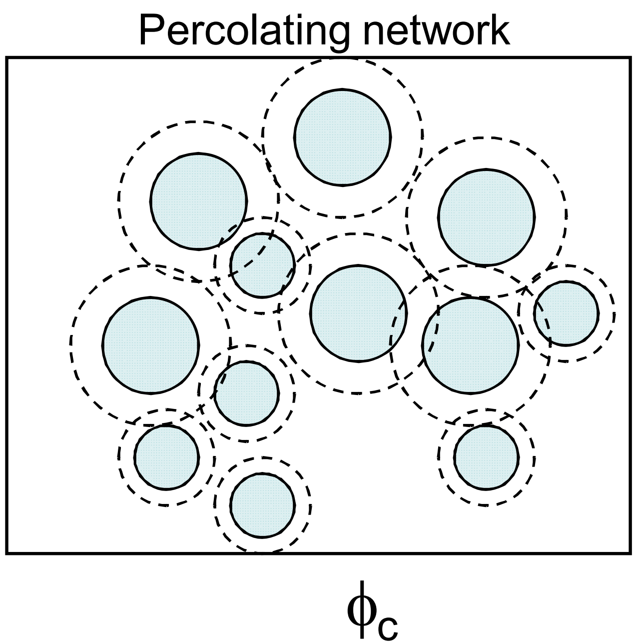


Constant NVE Hard Sphere Dynamics

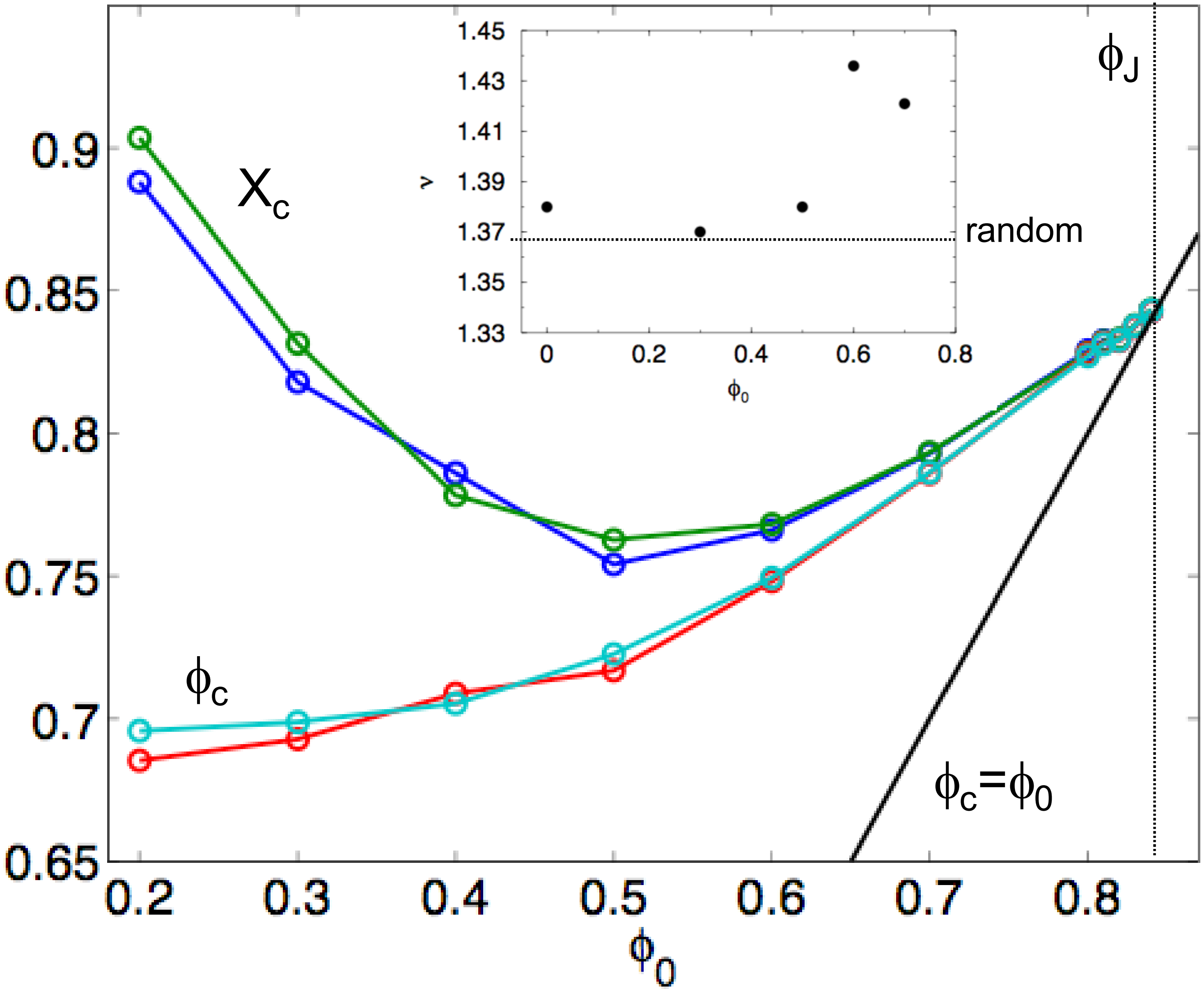
"Porosity for the penetrable-concentric-shell model of two-phase disordered media: Computer simulation results", S. B. Lee & S. Torquato, J. Chem. Phys. 89 (1988) 3258.

ϕ_0-dependent Percolation

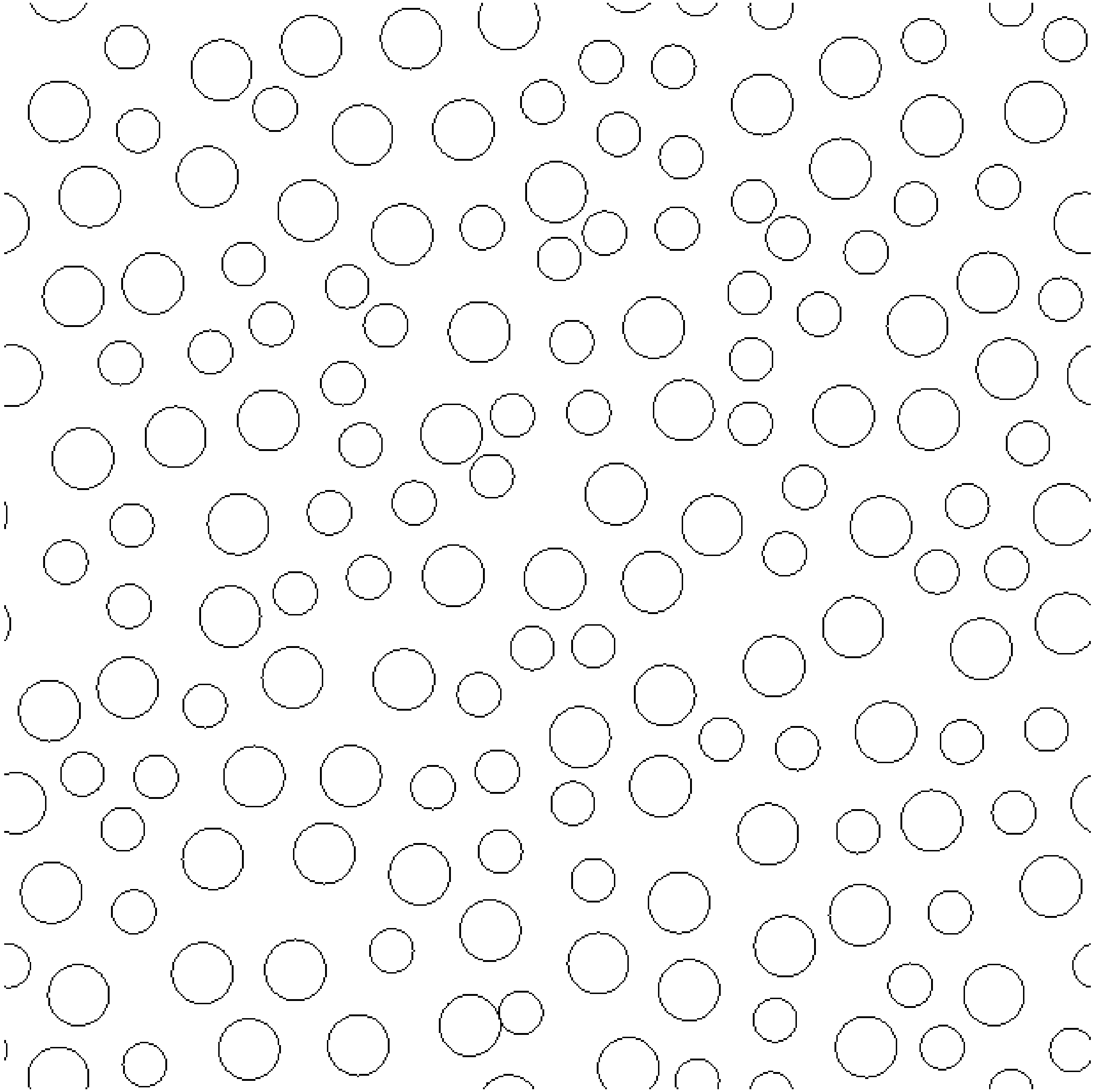




Percolation Transitions

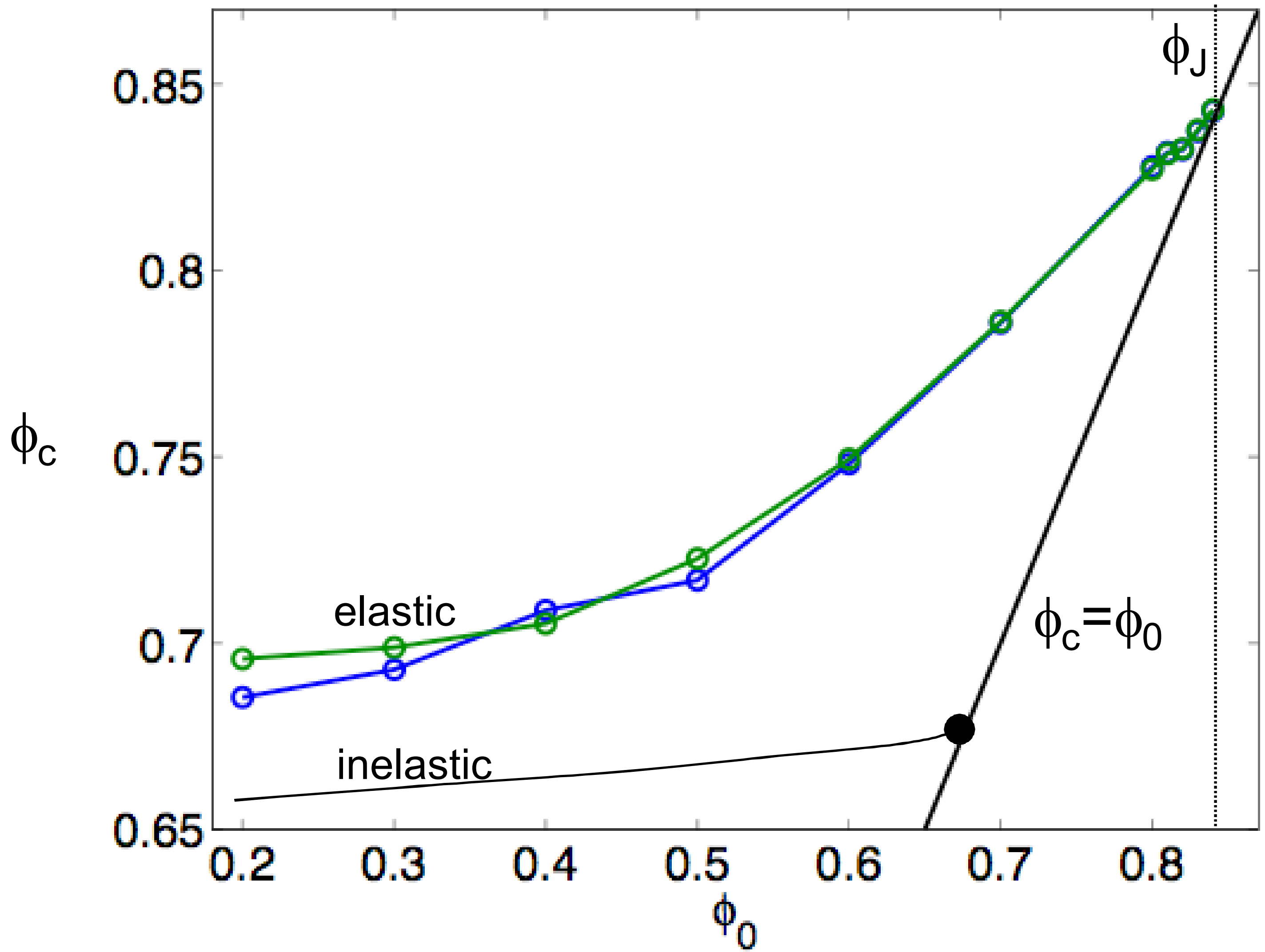


Inelastic Hard Sphere Dynamics

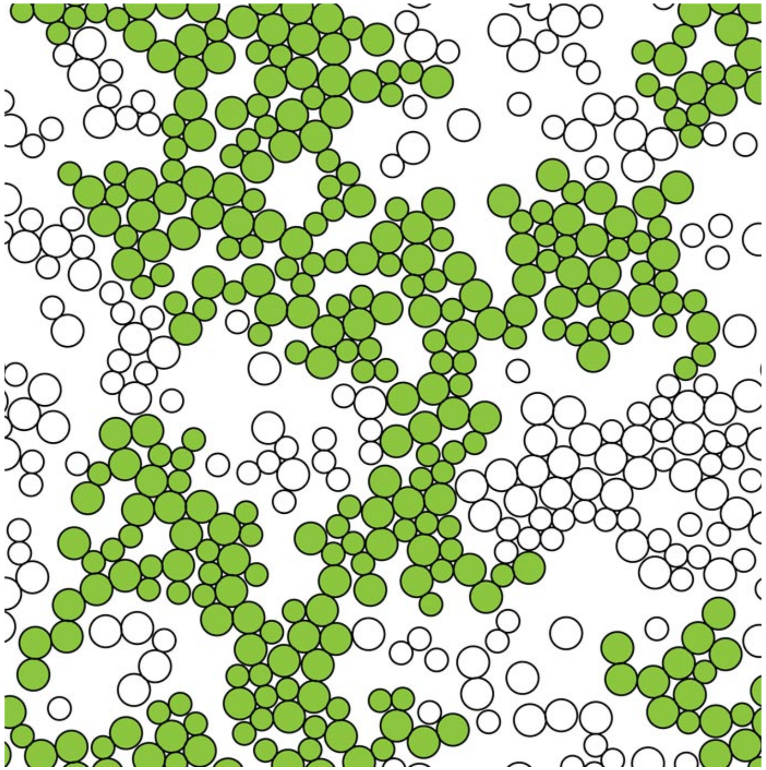


ϕ_0=0.3

Inelastic Dynamics



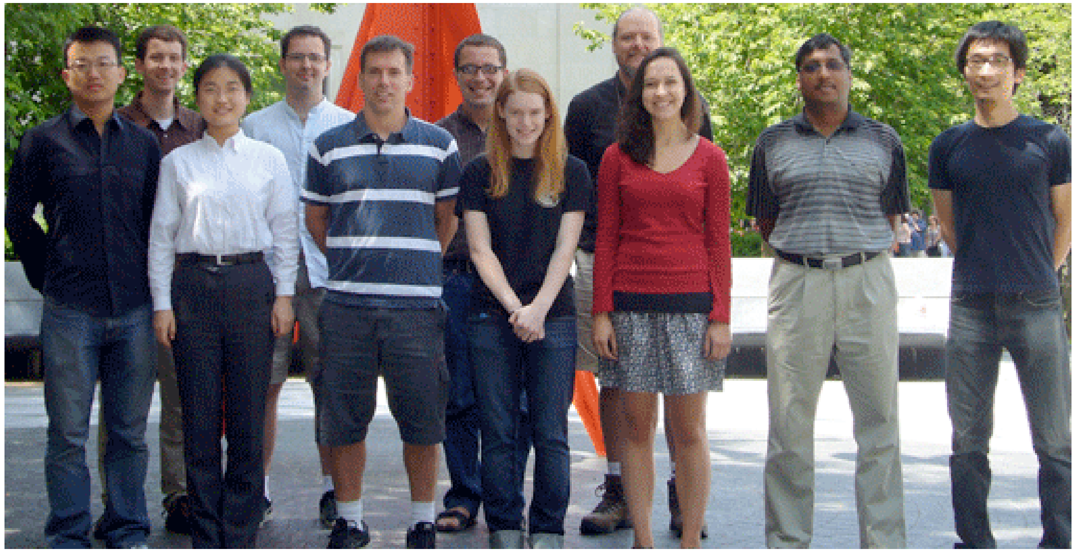
Sticky Disks



	elastic disks	sticky disks
D	1.91	1.88
τ	2.02	2.04
ν	1.38	1.92

Study cooperative motion/correlation lengths below jamming?

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
NSF-PHY-1019147, Duration: 7-1-10 to 6-30-15
NSF-DMR-1006537, Duration: 9-1-10 to 8-31-13