Random Close Packing Revisited:

Counting the ways to pack frictionless disks

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Questions:

- What does random close packing mean? Most dense random jammed state? Most likely random jammed state? Does RCP depend on algorithm used to create jammed states?

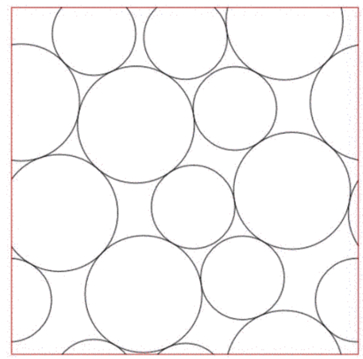
- Is there a way to define random close packing that does not depend on protocol?

Plan of attack:

- Enumerate 'all' collectively jammed states in small 2D bidisperse (50-50; diameter ratio=1.4) systems

- Define RCP via an ensemble of jammed states with $P(\phi)$

- Decompose $P(\phi)$ into density of jammed packing fractions and the frequency distribution



jammed packing

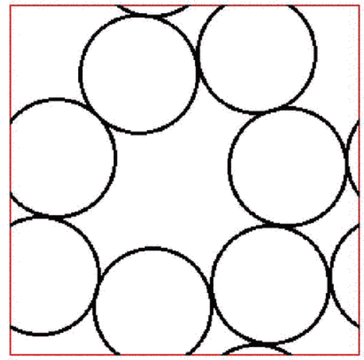
Why study random close packing?

- Simple question, complicated answer

- Study of static packings important for understanding many jammed systems, e.g. granular materials and colloidal glasses

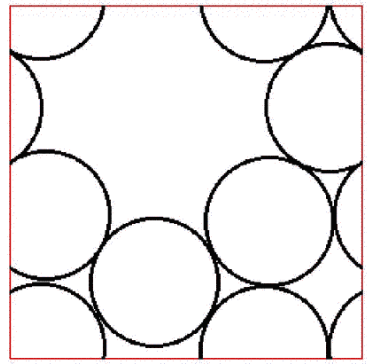
1. Different jammed states can have same ϕ, but possess very different mechanical properties
2. Unjammed states can jam when sheared
3. Different nearly jammed states at same ϕ can unjam on drastically different timescales
4. Can we better understand link between configuration space and slow dynamics?

Locally versus Collectively Jammed States



Locally Jammed

- Each particle unable to move when other particles held fixed; N_c=3
- Collective motions are possible
- Unjams when collision dynamics turned on
- Infinite number LJ states



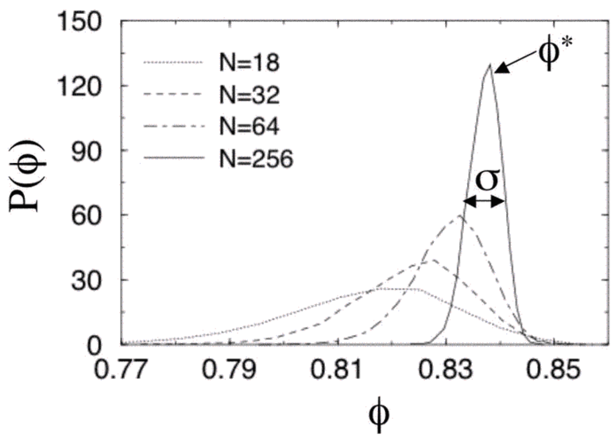
Collectively Jammed

- No single or group of particles allowed to move when others held fixed; N_c=4
- No collective motions allowed
- Stable when collision dynamics turned on
- Discrete; finite number of CJ states for finite N

S. Torquato and F. H. Stillinger, *J. Phys. Chem. B* **105**, 11849 (2001)

Probability to obtain CJ state at ϕ

$$P(\phi) = \frac{\text{number of trials that jam at } \phi}{\text{total number of trials}}$$



50-50 mixture with d_2/d_1=1.4

1. $P(\phi)$ becomes δ-function located at $\phi^* \rightarrow \phi_0$=0.842 in infinite system size limit
2. Why does $P(\phi)$ become so sharply peaked as $N \rightarrow \infty$? (a) Few CJ states with $\phi \neq \phi_0$ exist or (b) CJ states exist over range of ϕ, but only those with $\phi = \phi_0$ are highly probable
3. Does location of peak in $P(\phi)$ when $N \rightarrow \infty$ depend on protocol? Study $P(\phi)$ for many different protocols or …

O'Hern, Silbert, Liu, Nagel *Phys. Rev. E* **68** 011306 (2003)

Decompose P(ϕ)

$$P(\phi) = \rho(\phi)\beta(\phi)$$

Probability to obtain CJ state at ϕ — Density of CJ packing fractions — Frequency distribution

- $\rho(\phi)d\phi$=number of unique CJ states within $d\phi$; *protocol independent*
- $\beta(\phi)$=frequency with which CJ state at ϕ occurs; *protocol dependent*
- Does $\rho(\phi)$ control shape of $P(\phi)$ in $N\rightarrow\infty$ limit? If so, location of peak in $P(\phi)$ when $N\rightarrow\infty$ is protocol-independent definition of RCP.

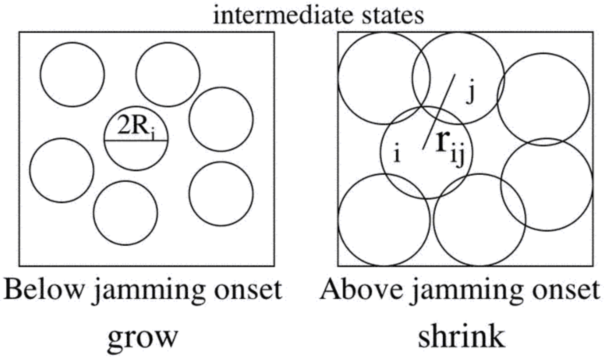
How do we create jammed states?

Grow and shrink soft repulsive particles followed by relaxation via energy minimization

Protocol:

- Begin with random collection of disks at $\phi_i << \phi^*$
- Minimize total potential energy until $V_{n+1}<V_{min}$ or $(V_{n+1}-V_n)/V_n=10^{-16}$
- If $V_{n+1}<V_{min}$, grow each disk by ΔR
- If $(V_{n+1}-V_n)/V_n=10^{-16}$, shrink each disk by ΔR
- Minimize total potential energy until $V_{n+1}<V_{min}$ or $(V_{n+1}-V_n)/V_n=10^{-16}$
- $\Delta R\rightarrow\Delta R/2$ when switching from compression to expansion or vice-versa
- Repeat until $V_{min} < V_{n+1} < 2V_{min}$; save final particle positions and ϕ; final states have small overlaps

intermediate states



Soft, repulsive potential

$$\frac{V^*(r_{ij})}{\varepsilon} = \begin{cases} \frac{1}{2}\left(1-\frac{r_{ij}}{R_{ij}}\right)^2 & r_{ij} < R_{ij} \\ 0 & r_{ij} \geq R_{ij} \end{cases}$$

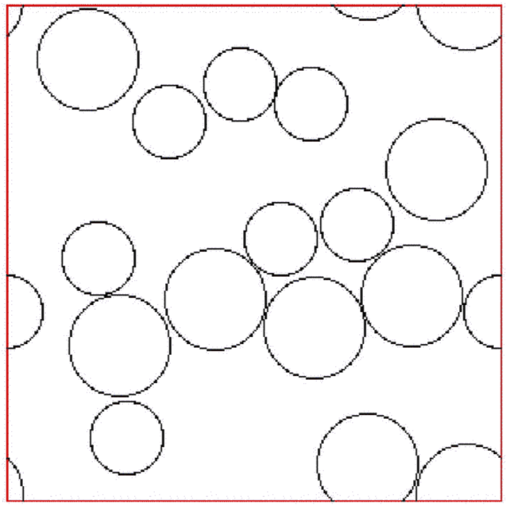
$$V = \sum_{i>j} \frac{V^*(r_{ij})}{\varepsilon} \qquad R_{ij} = R_i + R_j$$

Jamming protocol from start to finish

N=16

50-50 bidisperse mixture with $R_2/R_1=1.4$

periodic boundary conditions(1X1)



$\phi_i=0.400$
$\phi_f=0.805$

- Vary random initial conditions and conduct $N_{trials} = 10^{10}$ to find ' all' CJ states for small systems from N=6 to N=18
- $P(\phi)$ will depend on ΔR and minimization procedure, but $\rho(\phi)$ WILL NOT

How do we determine whether final states are collectively jammed?

1. Collectively jammed state = mechanically stable state

Is dynamical matrix positive definite?

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

i,j=particle index
α,β=spatial index
$\vec{r}_0$ = positions of jammed state

all dN-d eigenvalues $\kappa_i > 0$

2. number of constraints = number of degrees of freedom

$$N_c^* = dN - d + 1$$

d=spatial dimension

number of contacts (N_c^*); Translational invariance (d)

$$N_c \geq N_c^*$$

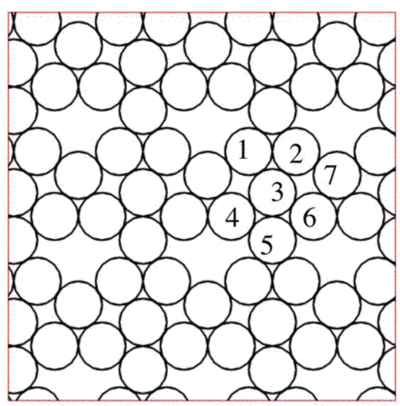
How do we determine whether two CJ states are distinct?

Compare sorted lists of eigenvalues of dynamical matrix; CJ states distinct if $\kappa_i^1 \neq \kappa_i^2$ for any i

(also compare topologies)

- CJ states at different ϕ are distinct
- CJ states at same ϕ may or may not be distinct

What is a topology?

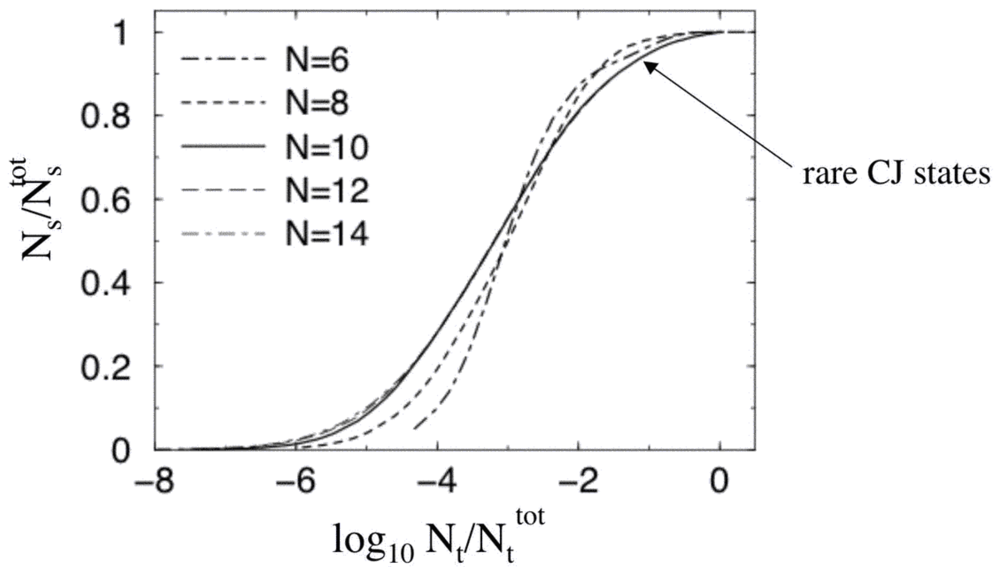


Particle #	
1	2, 3, 5, 7
2	1, 3, 5, 7
3	1, 2, 4, 5, 6
4	3, 5, 6, 7
5	1, 2, 3, 4, 6
6	3, 4, 5, 7
7	1, 2, 4, 6

Adjacency matrix $A=A^T$

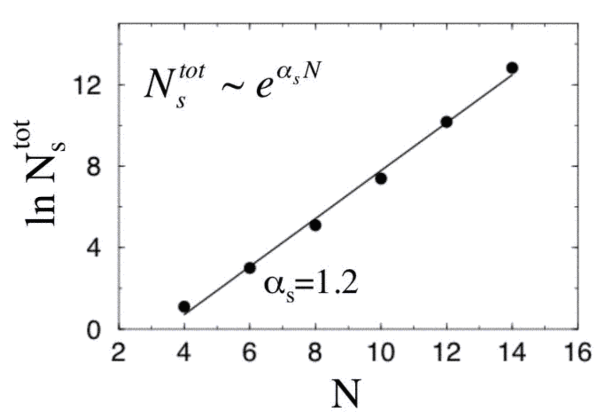
$$\begin{matrix} 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 \end{matrix}$$

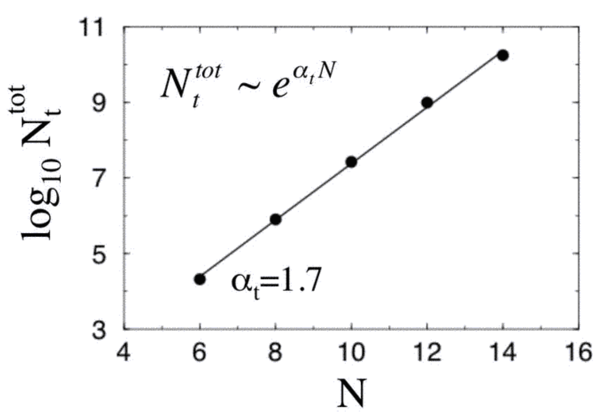
Can we find 'all' CJ states?



- Master curve for N>8; allows extrapolation of N_s^{tot}
- No new CJ states for number of trials = $10N_t^{tot}$
- No new CJ states for different protocol (molecular dynamics with dissipation and dynamic friction)

Can we find 'all' CJ states for large systems?



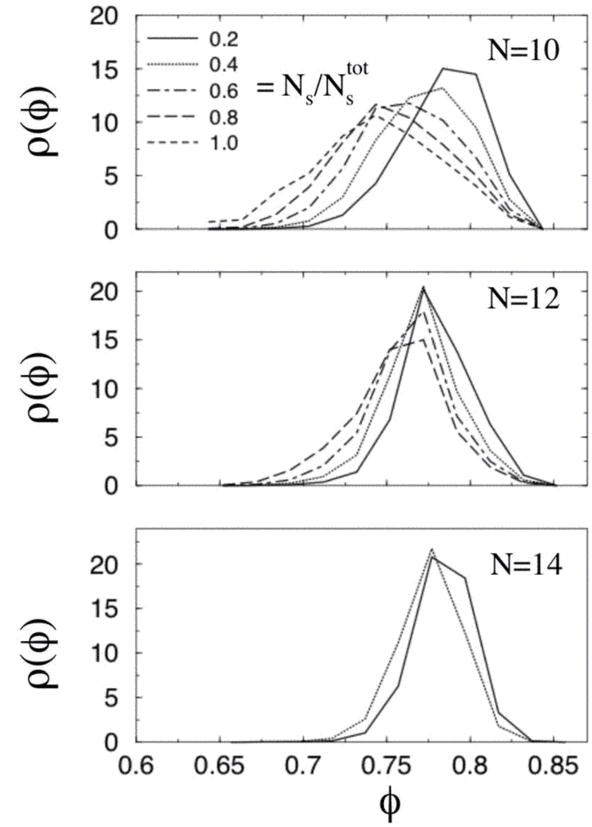


- Exponential growth of total number of states N_s^{tot}
- Exponential growth of number of trials required to find N_s^{tot}; large number of rare CJ states; feature of phase space *not algorithm*
- Are rare CJ states important?

How does density of CJ packing fractions depend on fraction of CJ states obtained?

- $\rho(\phi)$ evolves with N_s/N_s^{tot}
- Large-ϕ side decreases, small-ϕ side increases; rare states occur at small ϕ
- 'Gaussian' shape with width comparable to that for $P(\phi)$

$$\rho(\phi)d\phi = \frac{N_s(\phi + d\phi) - N_s(\phi)}{N_s}$$



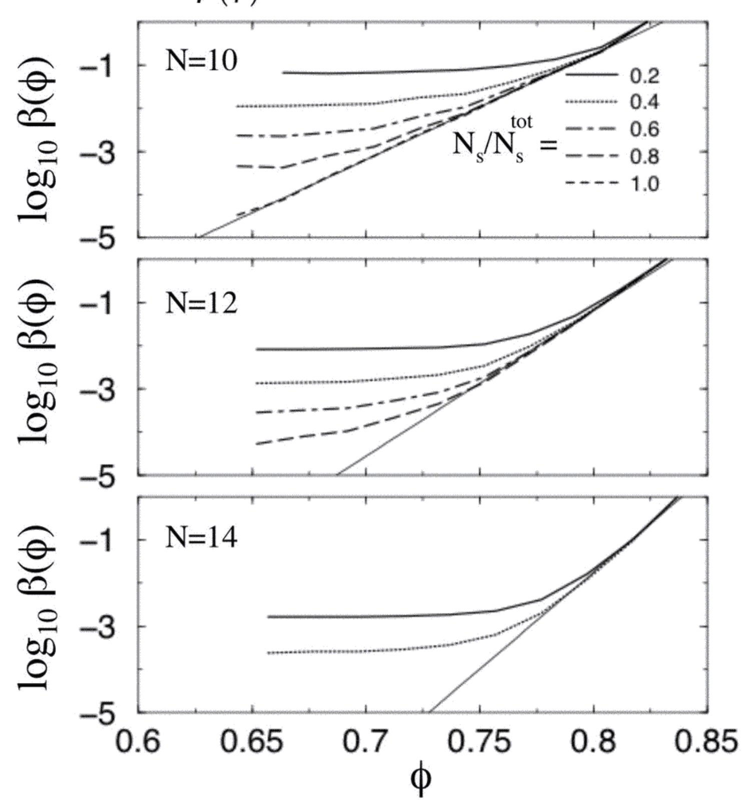
How does frequency distribution depend on ϕ?

- Frequency distribution is not uniform
- $\beta(\phi)$ increases exponentially with ϕ in $N_s/N_s^{tot} \to 1$ limit

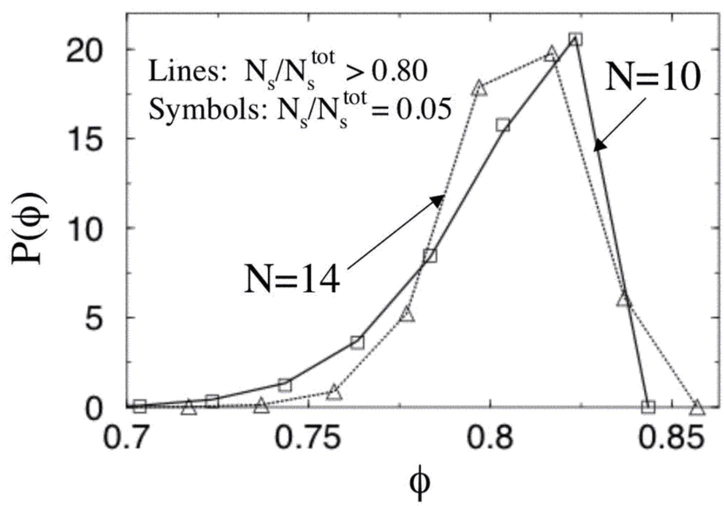
$$\beta(\phi) \sim e^{\lambda\phi}$$

- exponent λ increases with N

$$\beta(\phi) = \frac{P(\phi)}{\rho(\phi)} = \text{frequency with which CJ state at } \phi \text{ occurs}$$

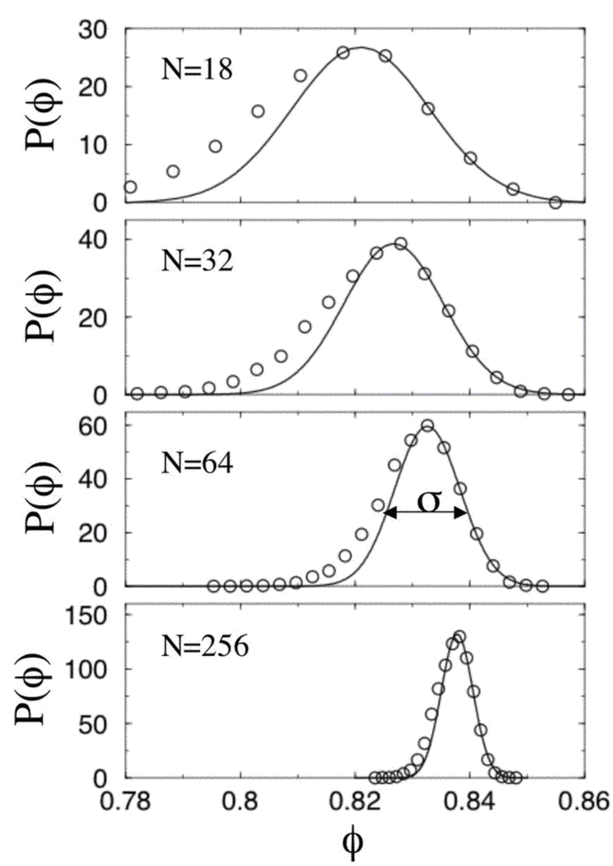


Is $P(\phi)$ sensitive to rare CJ states?



- $P(\phi)$ does not depend sensitively on fraction of CJ states obtained N_s/N_s^{tot}
- $P(\phi)$ can be calculated accurately even in large systems

What is the shape of $P(\phi)$ in the large system limit?



- Independent of number of trials
- Gaussian in large N limit
- Width decreases with increasing N

$\sigma \sim N^{-\Omega}$, with $\Omega \sim 0.55$

Phys. Rev. E **68** 011306 (2003)

$$P(\phi) = \rho(\phi)\beta(\phi)$$

$$e^{-\frac{(\phi-\phi^*)^2}{2\sigma^2}} \qquad e^{-\frac{(\phi-\phi_\rho)^2}{2\sigma^2}} \qquad e^{\lambda\phi}$$

- P(ϕ) is Gaussian in large N limit
- β(ϕ) is exponential in large N limit
- ρ(ϕ) is Gaussian and controls width of P(ϕ)

$$\phi^*(N) = \phi_\rho(N) + \sigma^2(N)\lambda(N)$$

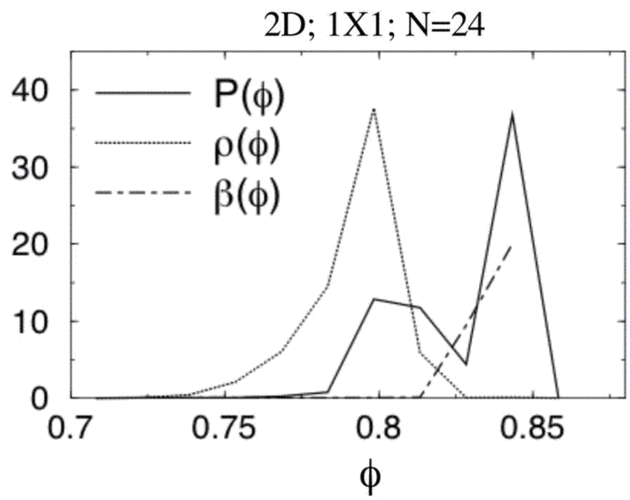
If λ has weaker N dependence than $\lambda \sim N^{2\Omega}$,
$\sigma^2(N)\lambda(N) \to 0$ and location of peak in P(ϕ) controlled by ρ(ϕ).

$\phi^*(N\to\infty)$ is *protocol-independent* definition of random close packing.

Future Directions I: Monodisperse Systems

Is there a protocol-independent definition of random close packing in monodisperse systems?

What is the shape of P(ϕ) in the large N limit?

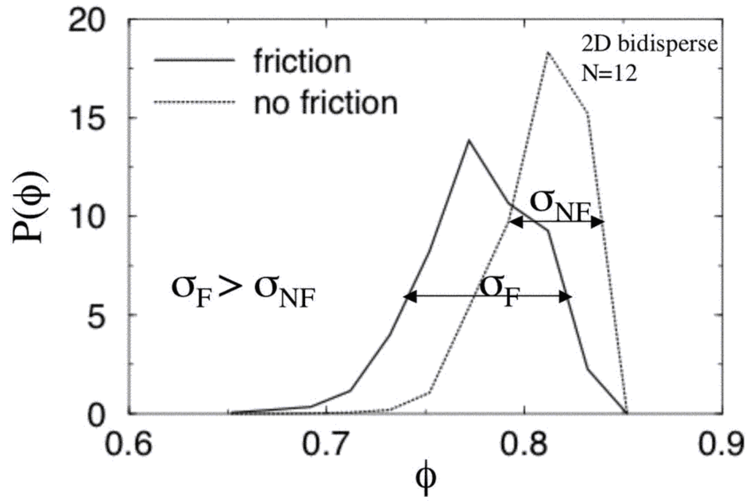


Differences between 2D monodisperse and bidisperse systems:

- Two peaks in P(ϕ); $\phi_1 \approx 0.80$ ↔ amorphous, $\phi_2 \approx 0.84$ ↔ partially ordered
- β(ϕ) falls off rapidly, largest peak in P(ϕ) does ***not*** correspond to peak in ρ(ϕ)
- Protocol-dependent frequency distribution plays important role in determining P(ϕ)
- No protocol-independent definition of RCP in 2D monodisperse systems?

Future Directions II: Static Friction

- Can we understand *random loose packing* by studying distribution of jammed states in systems with static friction?
- $P(\phi)$ for static friction is wider and shifted to lower ϕ.
- Where is peak in $P(\phi)$ in large N limit?



Conclusions

- Decomposed probability distribution $P(\phi)$ of CJ states into protocol-independent $\rho(\phi)$ and protocol-dependent $\beta(\phi)$

- $\rho(\phi)$ is Gaussian and controls width of $P(\phi)$; $\beta(\phi)$ increases exponentially with ϕ

- If $\sigma^2(N)\lambda(N)\to 0$, location of peak in $P(\phi)$ controlled by $\rho(\phi)$; better understand $\beta(\phi)$ by measuring amount of phase space associated with each CJ state

- Protocol independent definition of RCP, location of peak in $P(\phi)$ in $N\to\infty$ limit.

- Many *rare* CJ states; are they important for understanding slow dynamics in glassy systems?

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