Disentangling the role of structure formation and friction in shear jamming

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Avalanches, plasticity and nonlinear response in nonequilibrium solids

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In Collaboration with:

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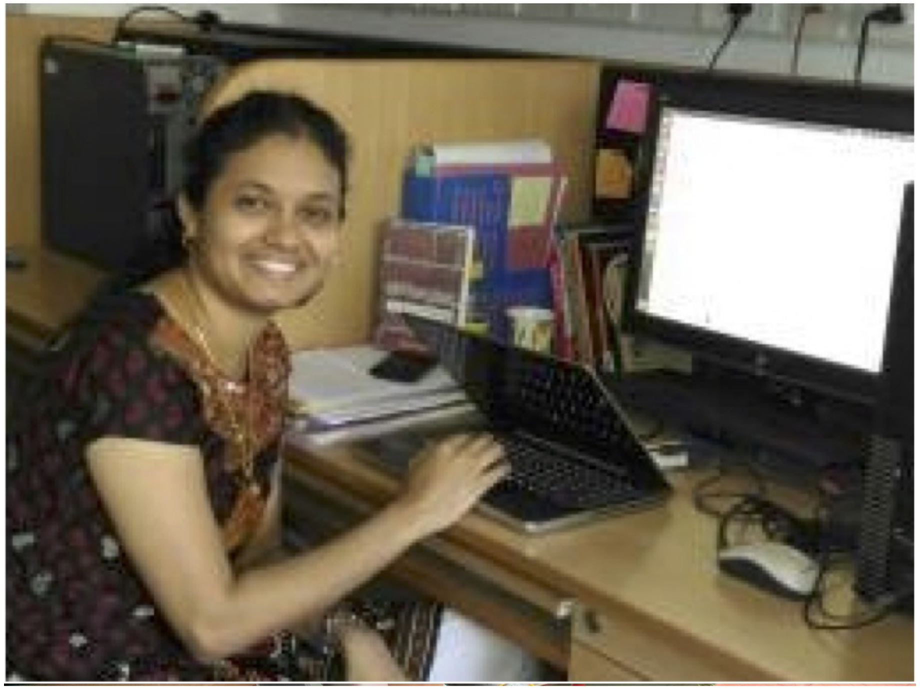
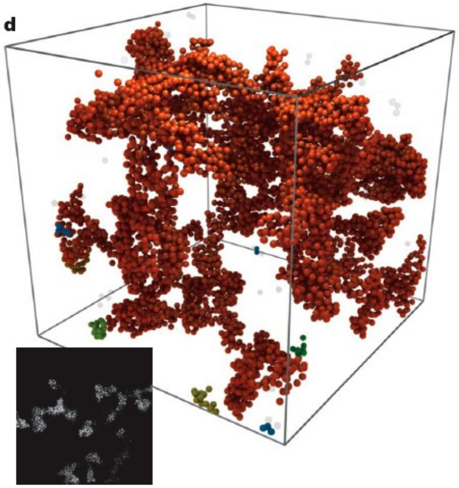


Vinutha and Sastry, Nature Physics (2016)
(in preparation)

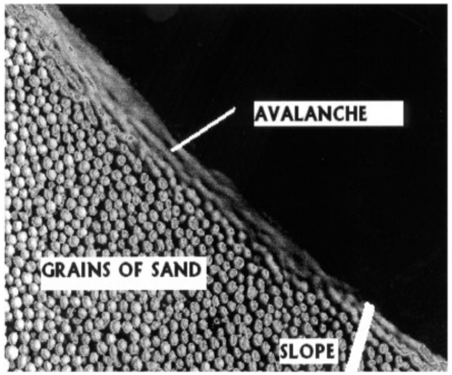
Structurally Arrested States

Many substances exist in long lived states other than the equilibrium state – structurally arrested states.

Glasses, gels, jammed granular matter are some examples.



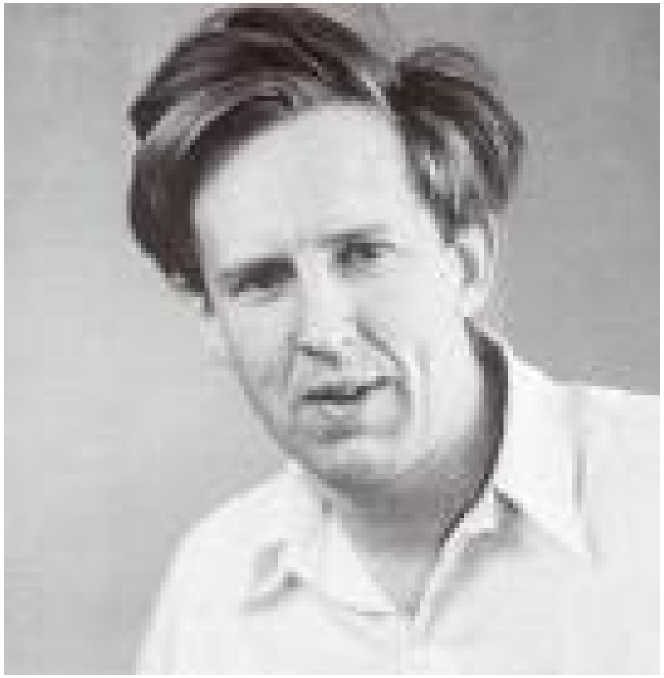
Jammed Granular Matter



Granular matter: Composed of meso- to macroscopic particles, whose assemblies are *athermal*, possess interesting properties not typical of thermal condensed phases.

Many intriguing properties relate to the transition between flowing and arrested states.

Jammed packings, random close packing..



J D Bernal

Bernal's pioneering work explored amorphous packings of spheres (1960s).

The goal was to understand the structure of liquids.

Models used included packings of ball bearings, which were "shaken and compressed" to obtain close packed arrangements.

"Random close packing" of particles at volume fraction ~ 0.64

But also "random loose packing" ~ 0.58

Value of packing fraction obtained in a variety of ways leading to expectation of universality of this value, but no common understanding of origin.

Use of hard sphere packings as model system.

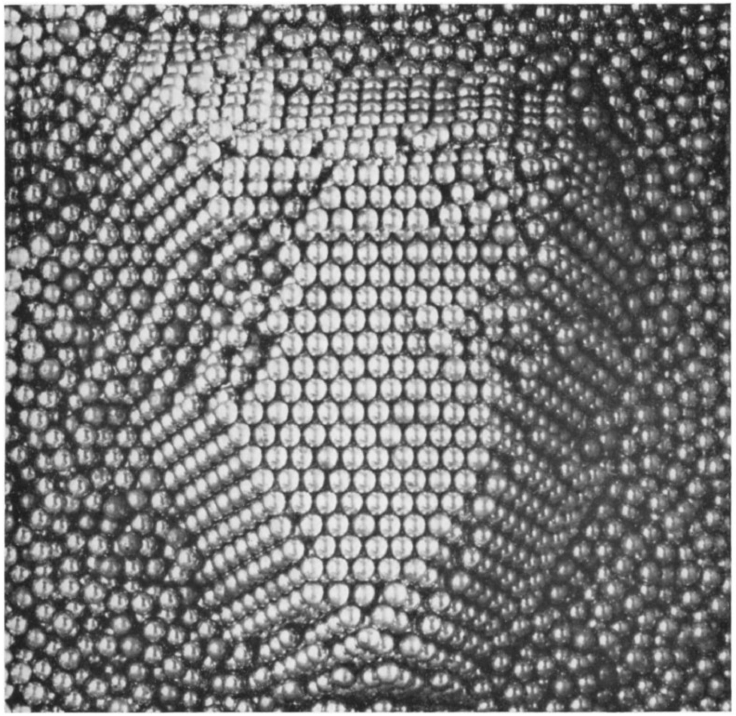
Hard Sphere Phase diagram

Fluid below packing fraction of ~ 0.545 (equilibrium 0.494)

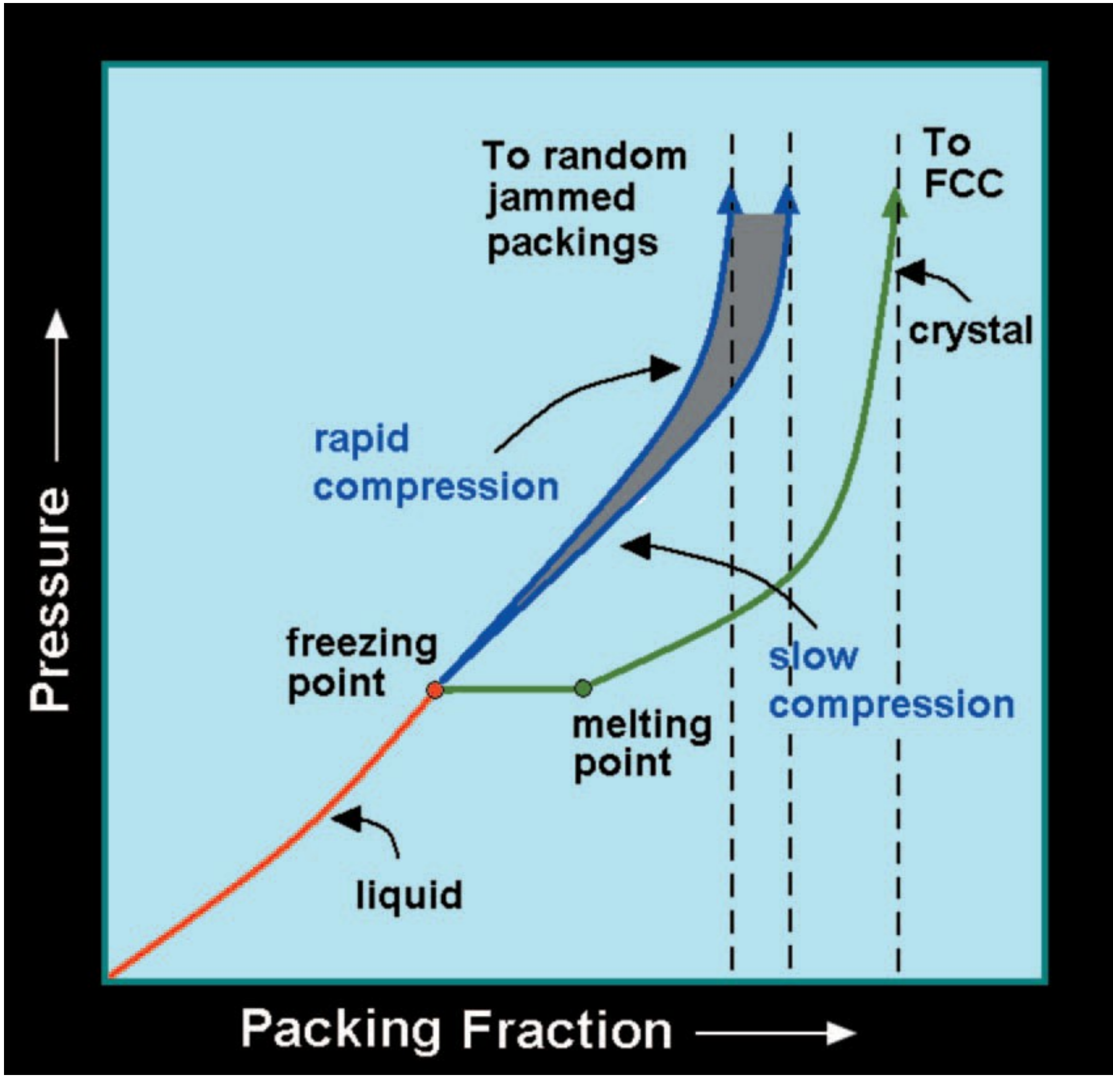
Glass transition ~ 0.58

Random close packing ~ 0.64

Close packing ~ 0.74

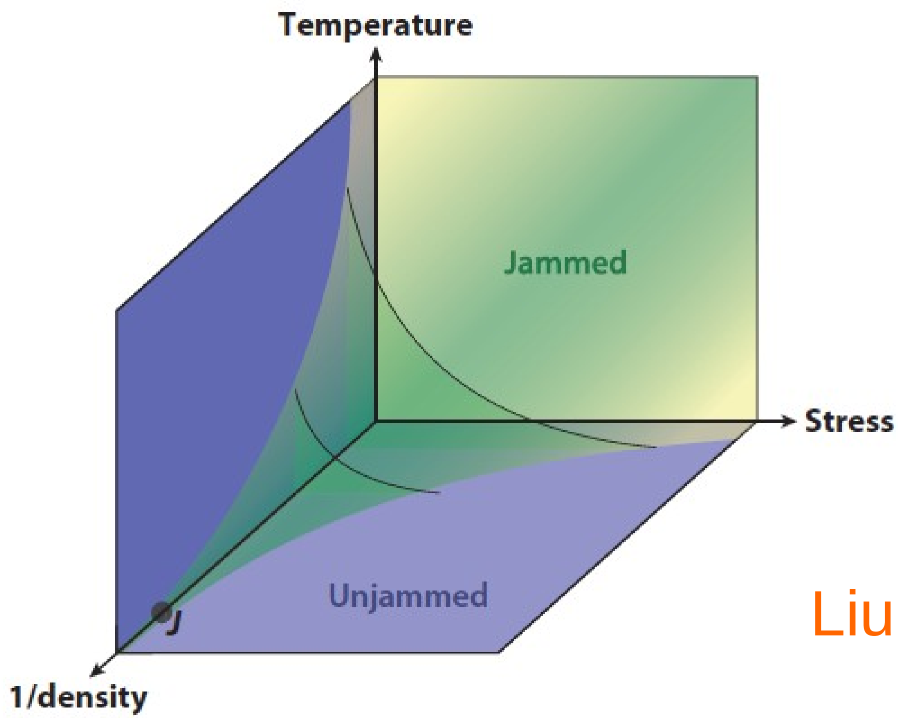


Bernal Proc. Roy. Soc. A, volume 280, 1964



From: Torquato Stillinger RMP 2010

Jamming Phase Diagram



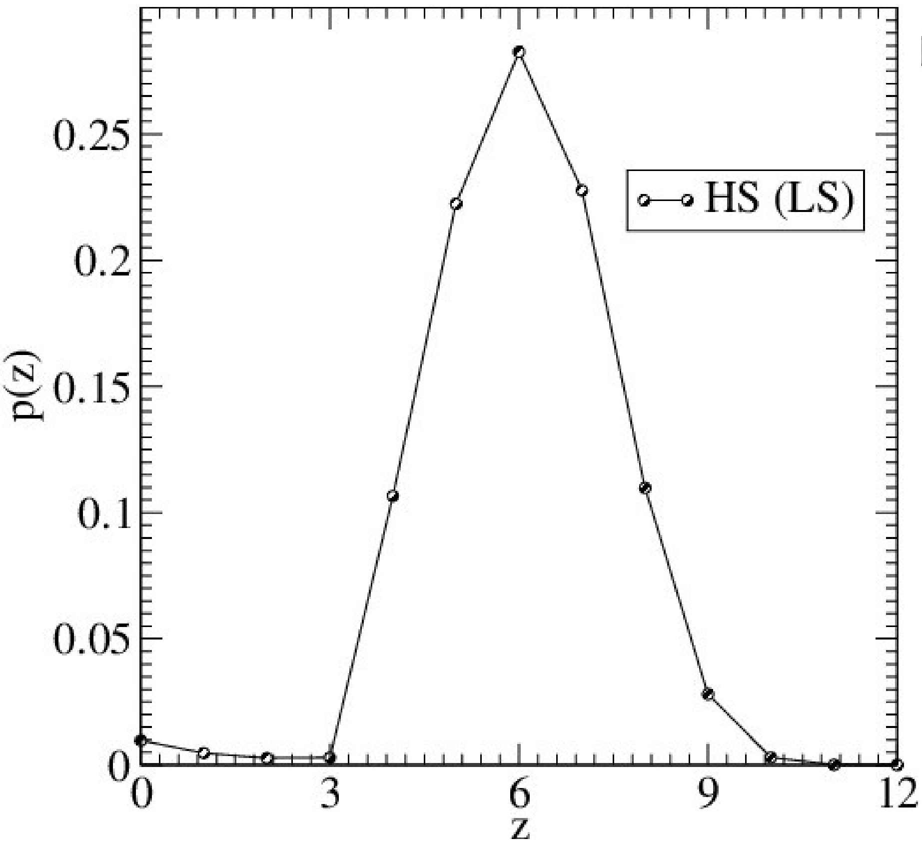
Liu, Nagel (1998)

The jamming phase diagram proposed as a unified view of the transition from jammed to unjammed or fluid states, when temperature, density or applied stress is changed.

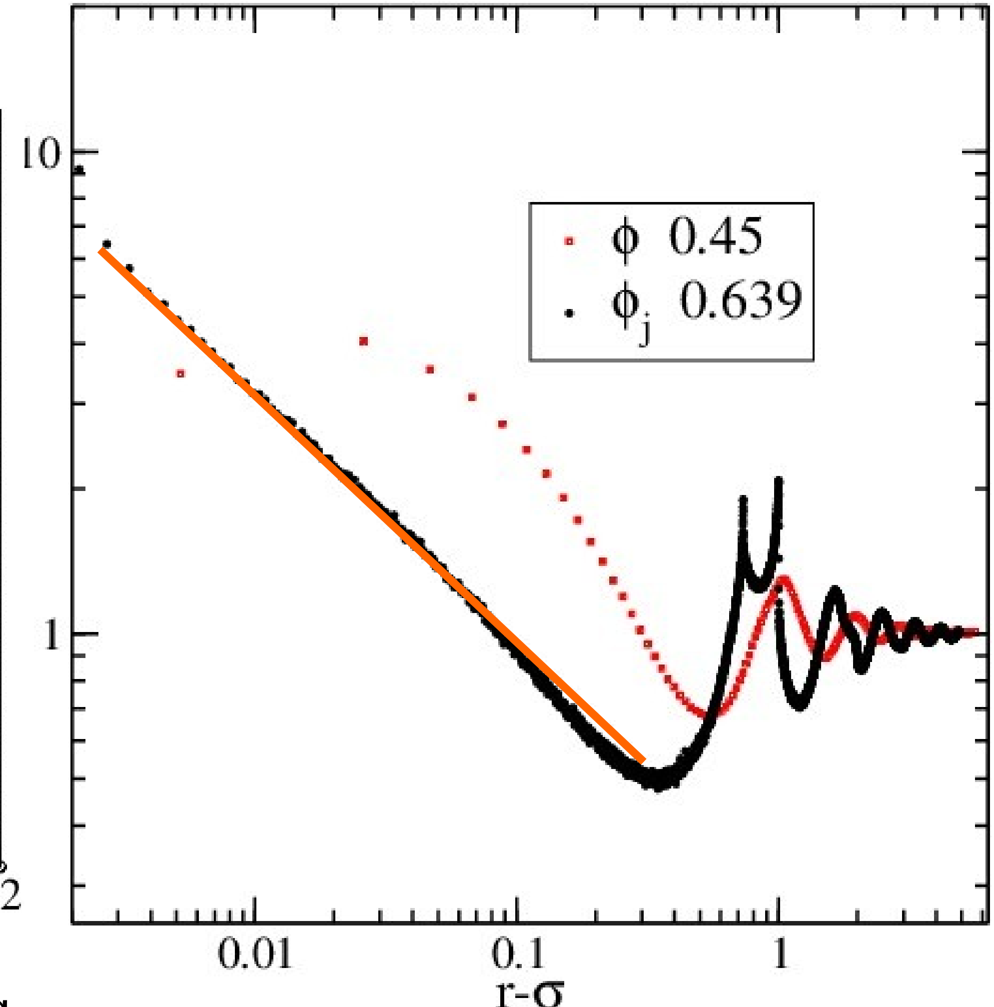
Focus on point J as a way of unraveling the nature of the transition between jammed and un-jammed states.

Computational studies using hard and soft sphere models to understand the nature of the J point.

Structure at RCP



Mechanical stability of jammed packing implies coordination number of **six** (and **four** with friction present) – Isostaticity.



Delta function at contact.

Power law singularity near contact.

Discontinuity in first and second peak.

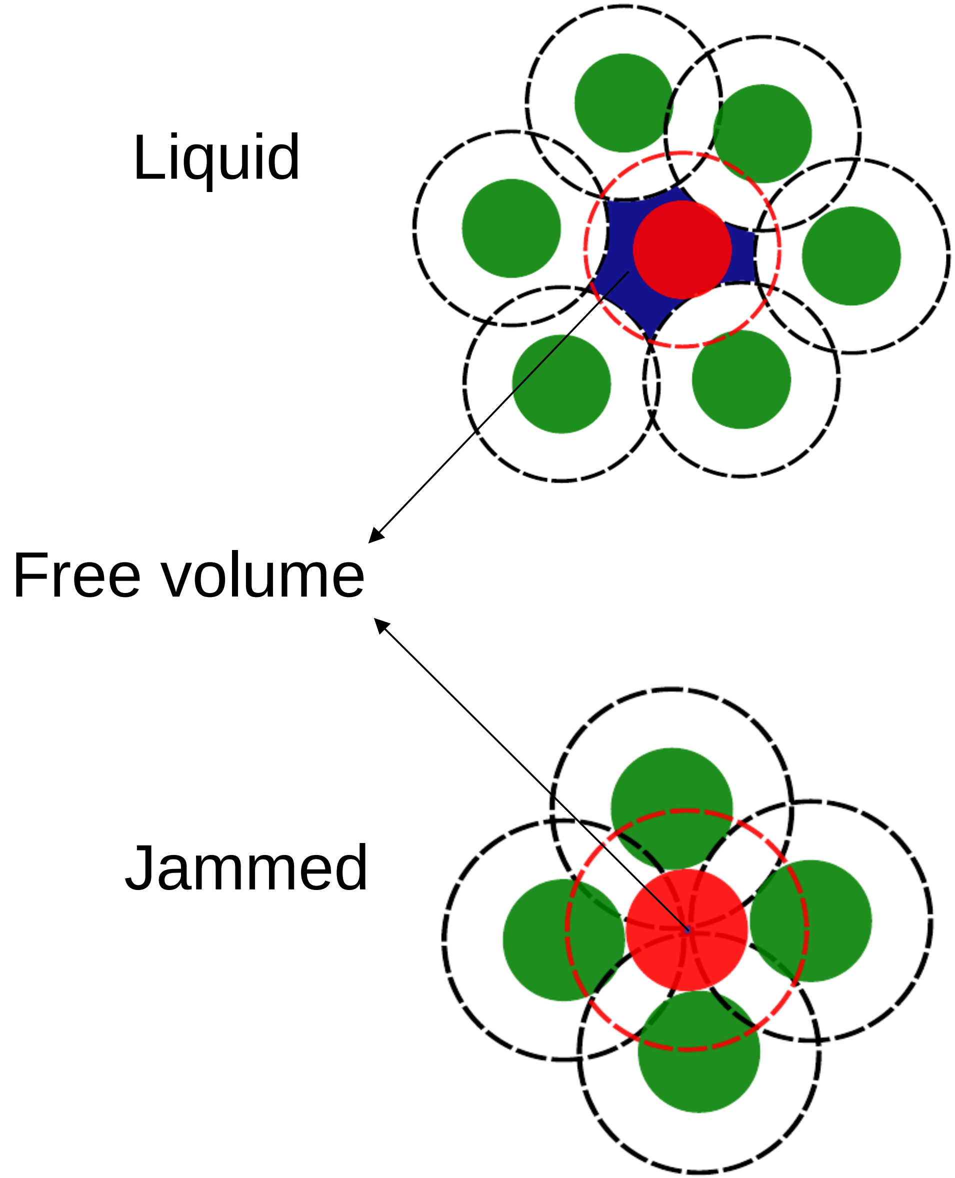
Free Volume

Free volume is the volume over which the centre of a given sphere can translate given that the other N-1 spheres are fixed.

Free volume vanishes at the jamming point.

Can be evaluated precisely using an efficient algorithm.

[Sastry et al 1997/1998]

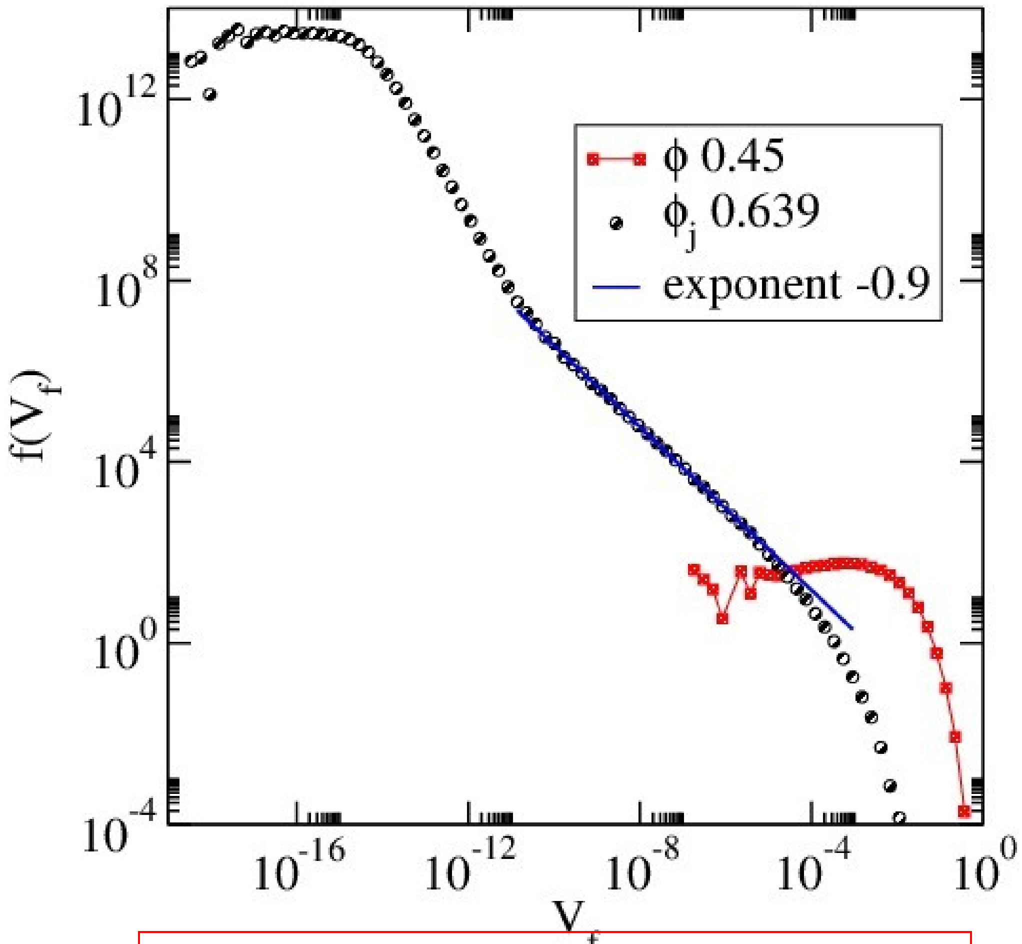


Free volume distributions near jamming

For jammed configurations, free volume is zero. We expect a narrow peak for slightly unjammed configurations.

But – we find a distribution with a power law tail with exponent ~ -0.9

Maiti and Sastry JCP 2014



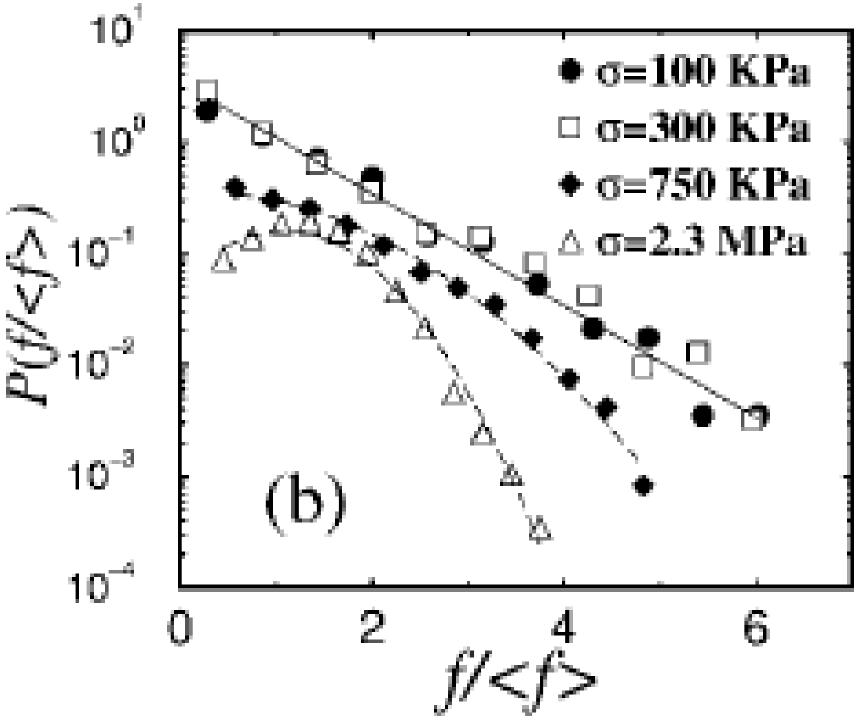
Free volumes over 20 decades!

Power law tail in the free volume distribution! A distinct signature of jamming!

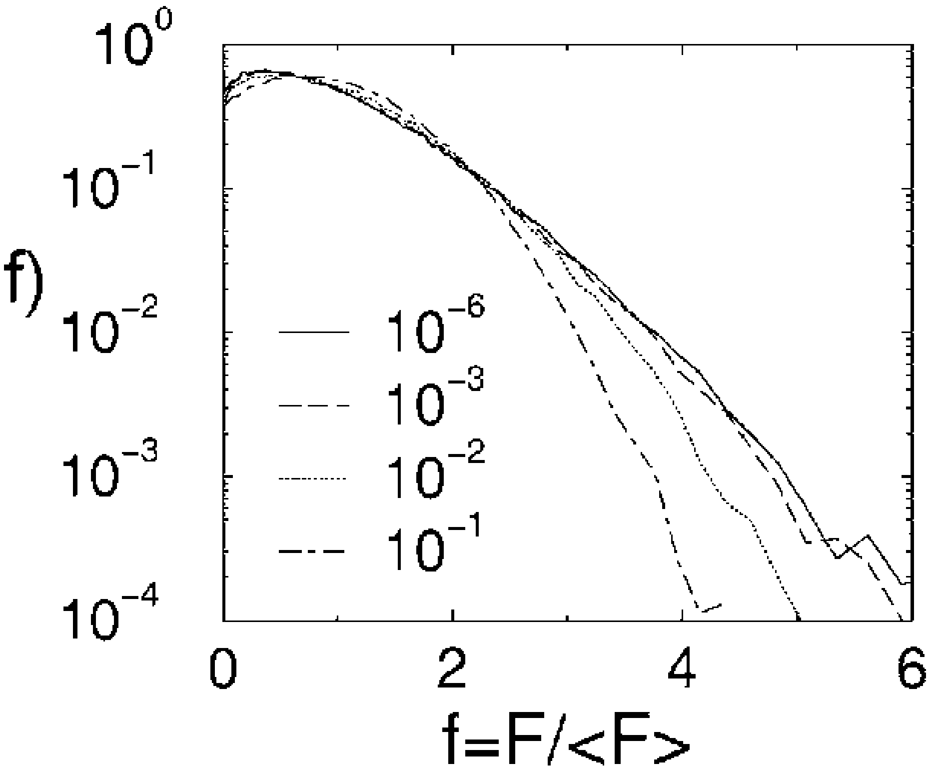
Valid for jammed configurations in other conditions (and vice versa)?

Force Distributions

Presence of a finite force peak in contact force distributions an indication of jamming.



Makse et al PRL 2000

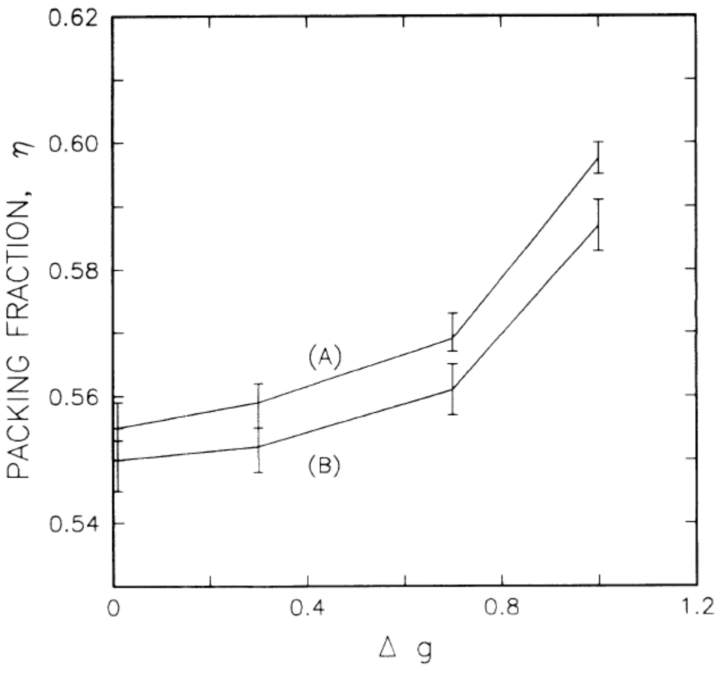


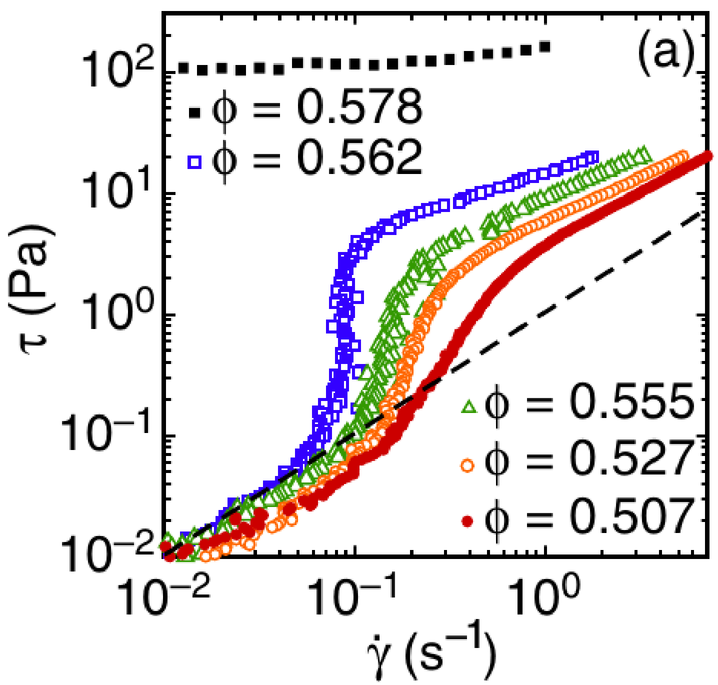
Silbert et al PRE 2006

Random Loose Packing, Dilatancy, Shear Thickening..

Other than the glass transition, other interesting phenomena expected around packing fraction 0.55 -- 0.58.

Structural origins of these phenomena?





Onoda, Liniger PRL 1990

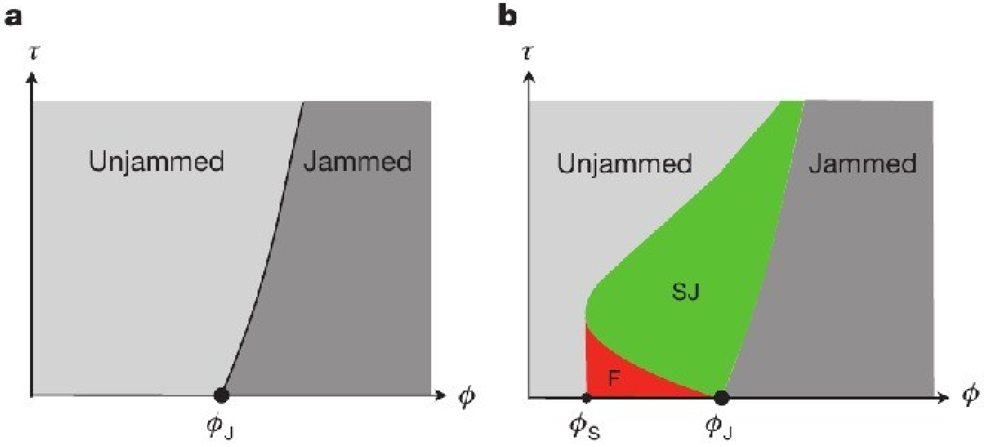
Brown and Jaeger PRL 2009

Shear jamming

Below ϕ_J jamming can be induced by friction

[Many recent studies: Silbert, Makse & co, Hayakawa & co, Coniglio & co et al]

In particular, jamming induced by shear deformation of frictional particle packings have been of interest.



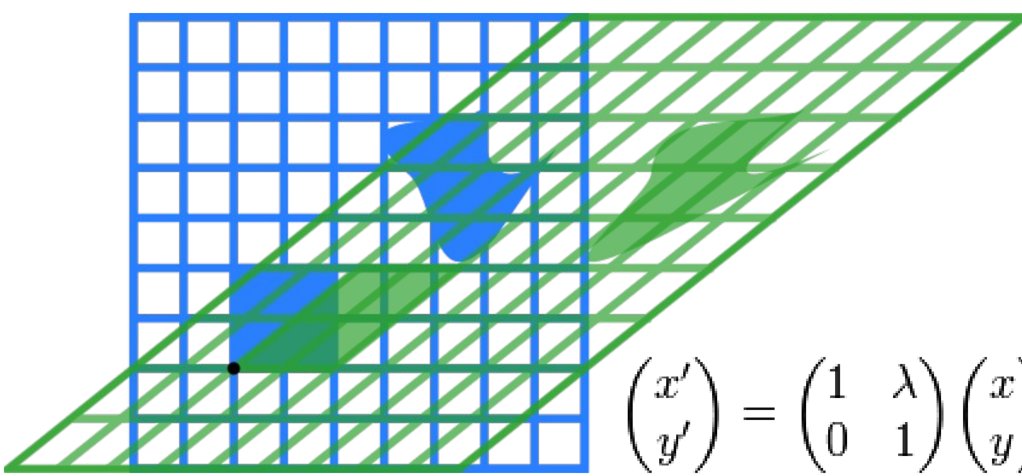
Dapeng Bi, et al., Nature 480, 357(2011)

Does shear deformation induce features of jamming in frictionless packings?

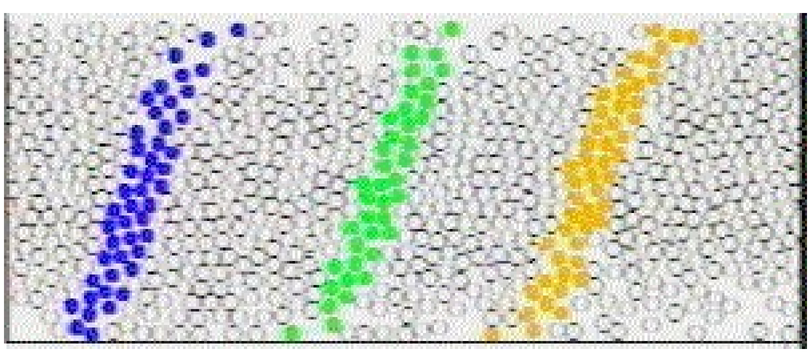
More precisely, what roles do shear and friction play in shear jamming?

Sphere Packings subject to Shear Deformation

1. It is interesting to explore ways other than isotropic compression to generate jammed configurations.
2. Shear deformation is one such possibility.
3. Subject hard sphere configurations to shear deformation.
4. Study geometrical and mechanical features of resulting structures.



$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.$$



Summary of what we do and what we find

*Monodisperse soft spheres (Mainly N = 2000, but system size effects studied for a wide range).

*Compress from fluids at packing fraction 0.45, or decompress from jammed packings at 0.64 to desired density.

*Athermal Quasistatic Strain till steady state is reached. [Deform incrementally, minimize energy at each step].

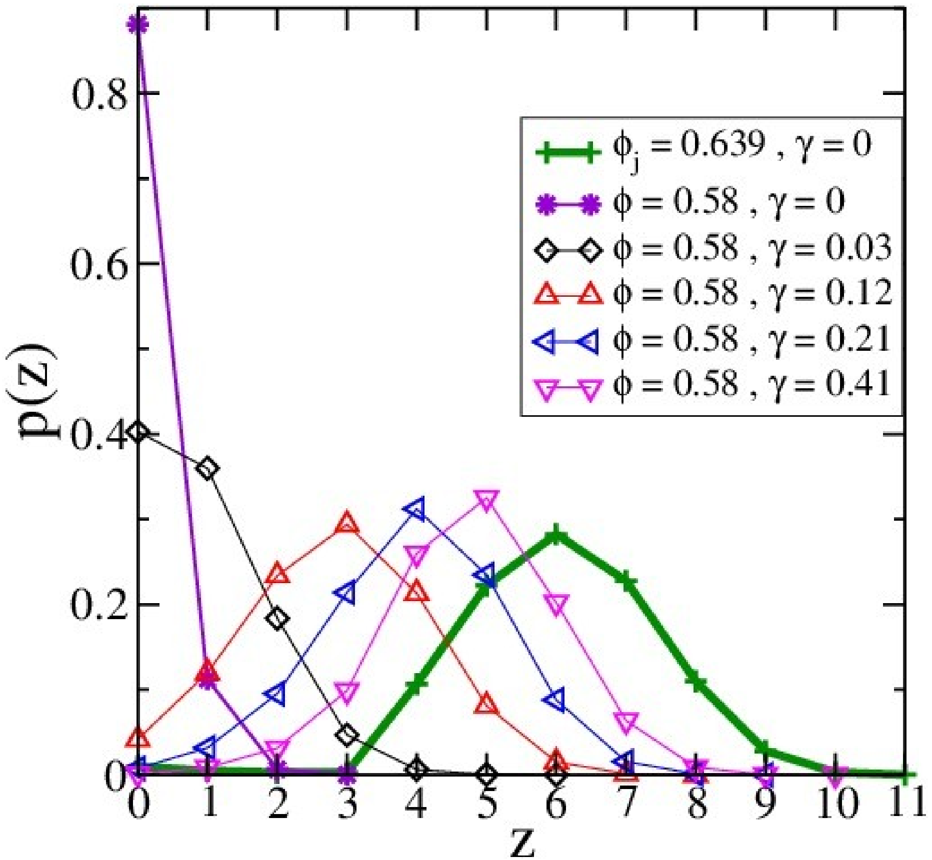
*Analyze geometry, force network,vibrational modes.

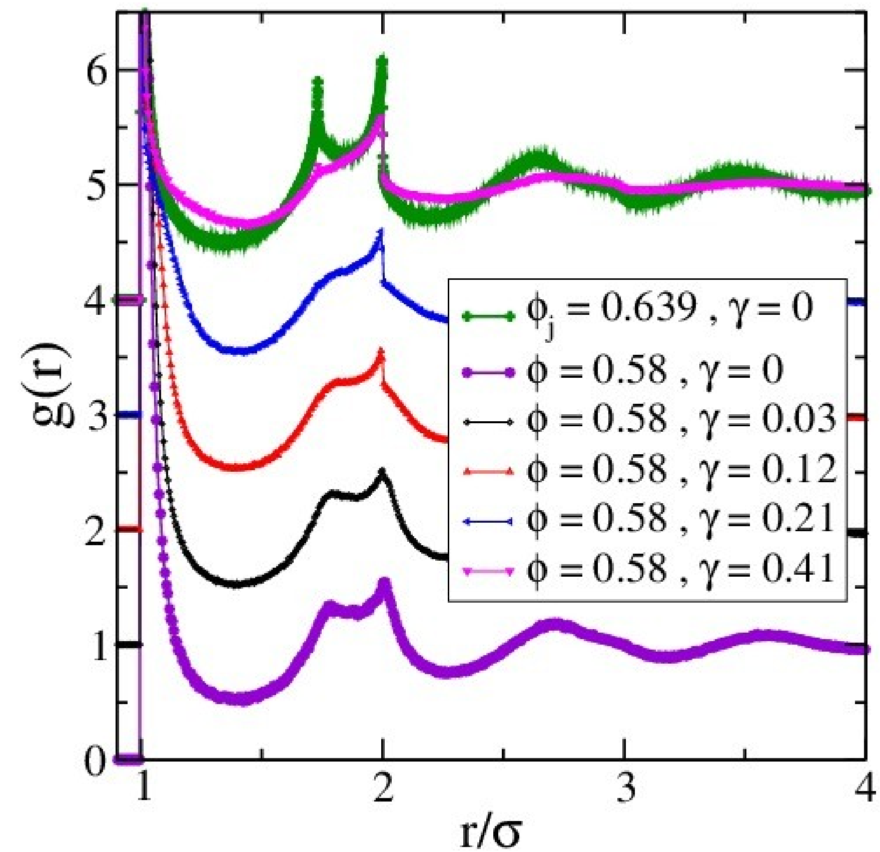
Structure evolves to look like jammed packings.

Threshold density 0.57 above which friction may stabilize sheared configurations.

Can independently verify force balance from geometry of steady state configurations.

Evolution of sphere configurations under shear

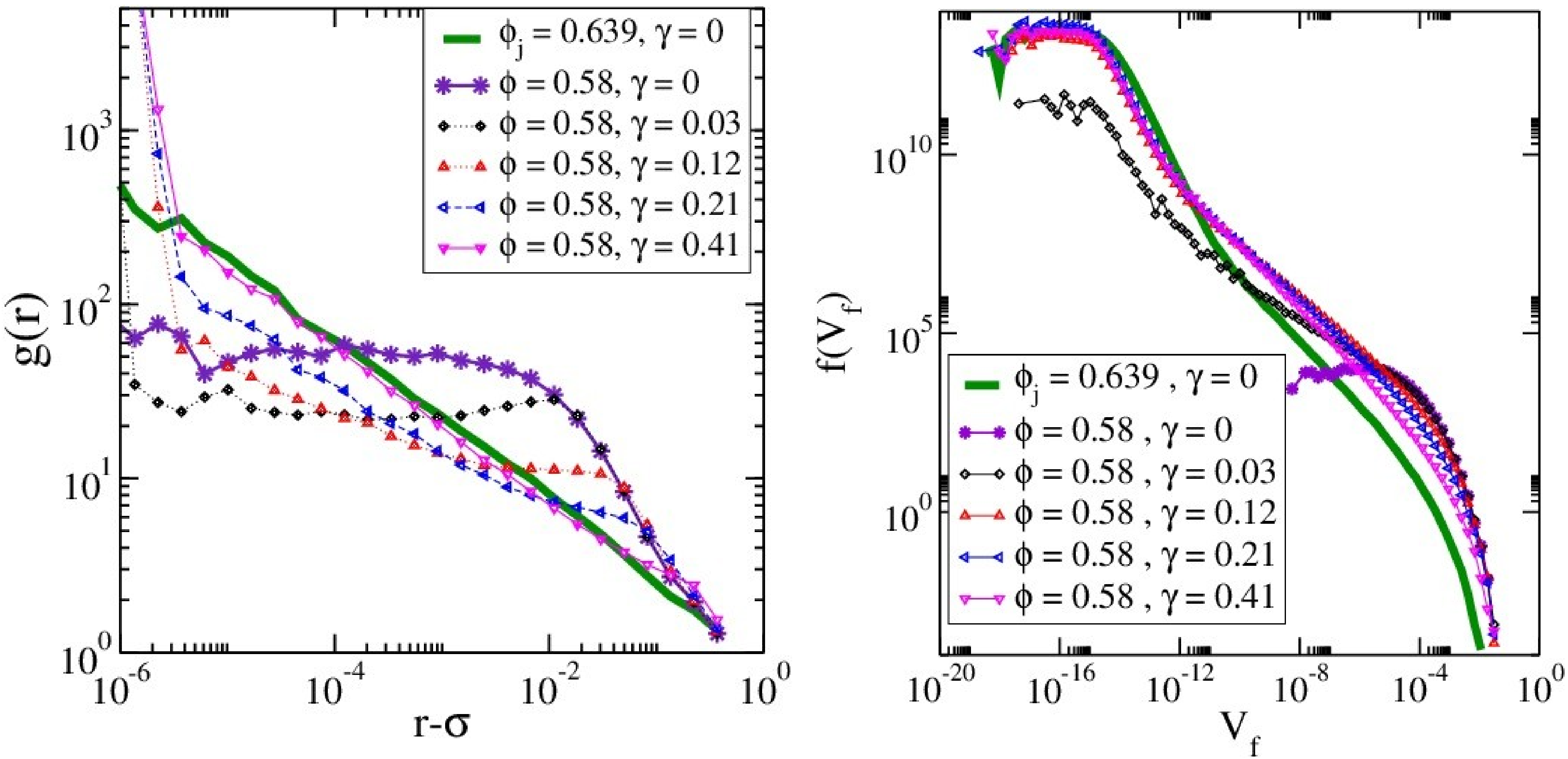




Increase of contact neighbors per particle with shear.

The discontinuity in the second peak of g(r) develops as the packing is sheared.

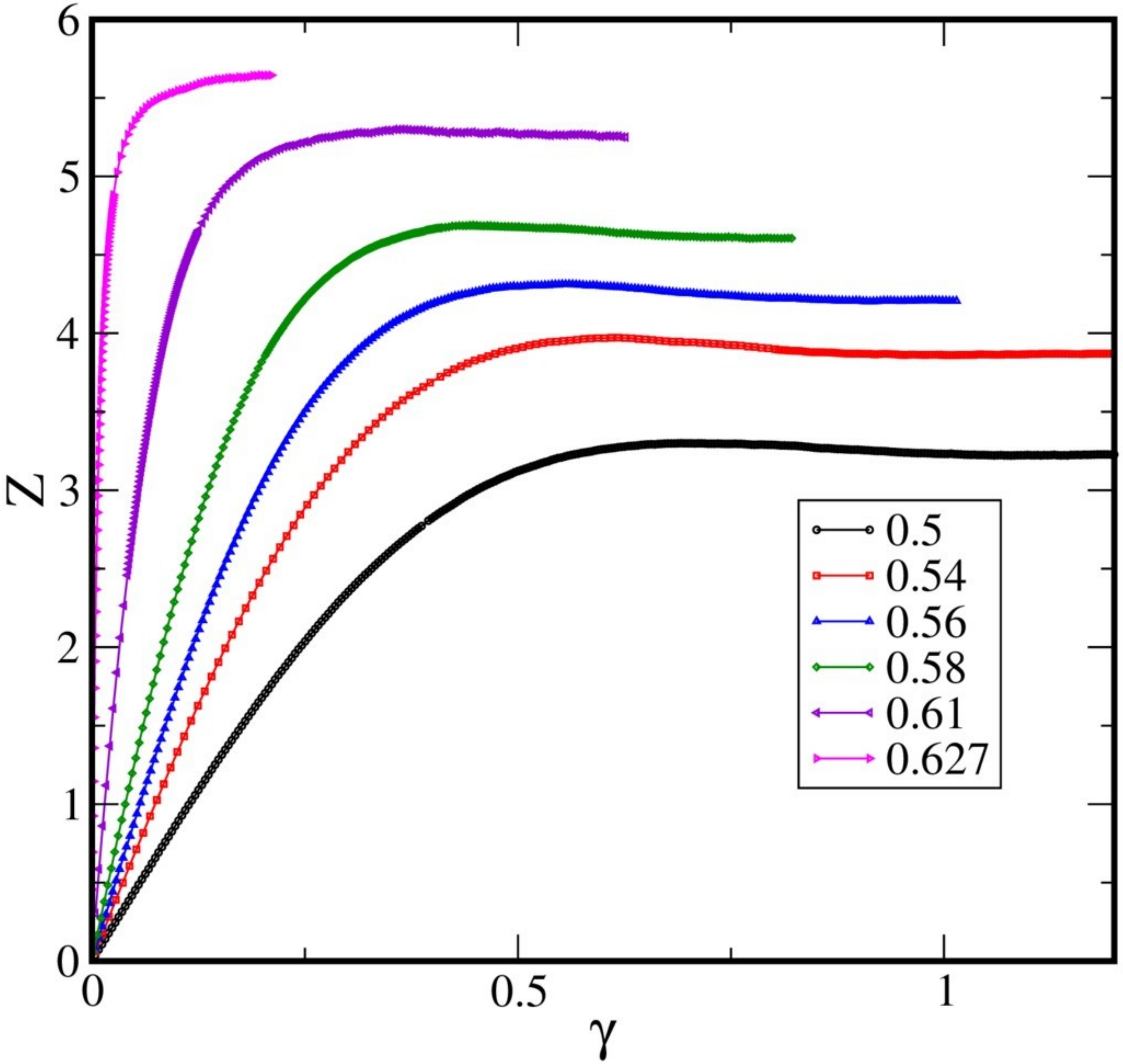
Evolution of free volumes under shear



Particles lose free volumes due to shear and power law tail shows that packing becomes jammed-like with shear.

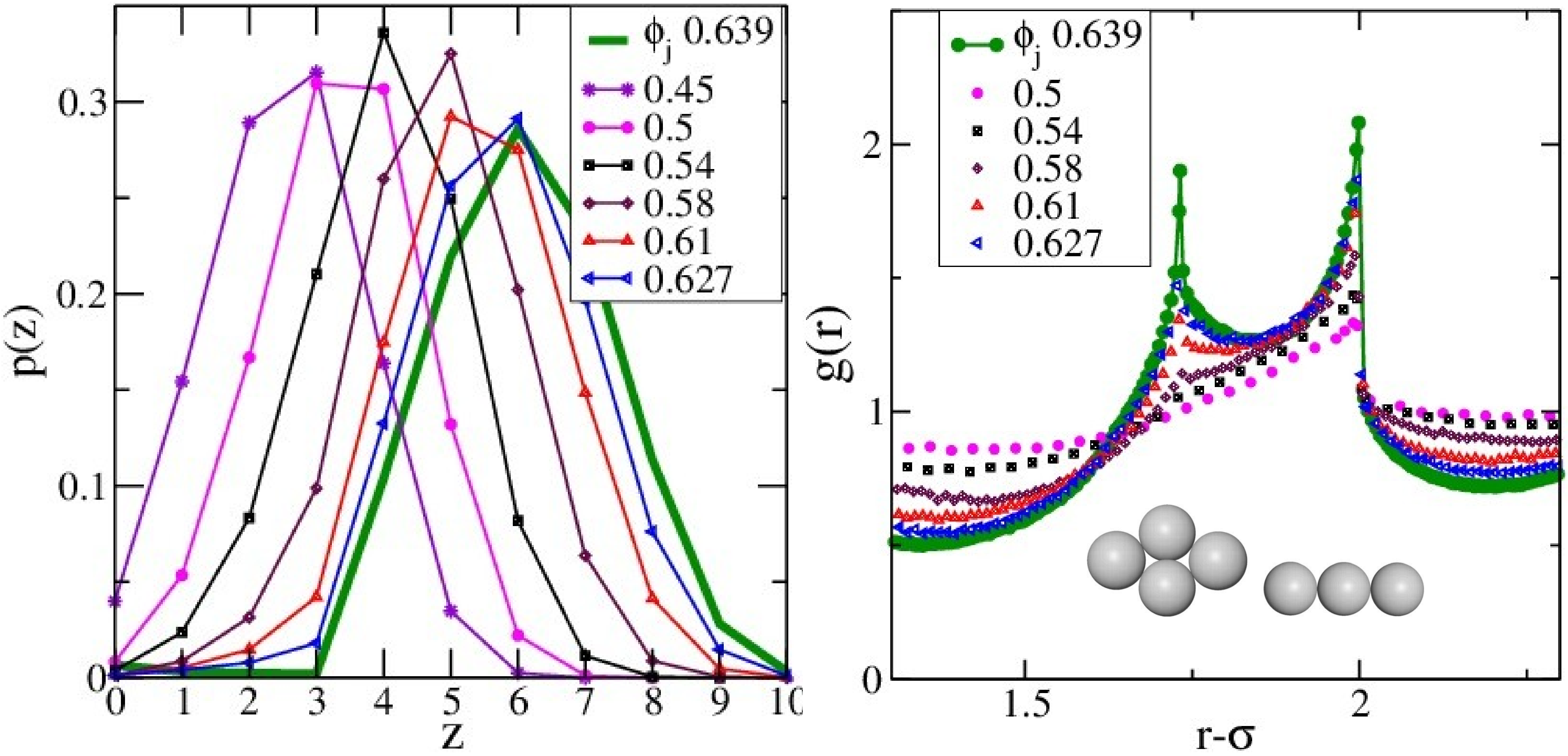
Near contact pair correlation function shows develops power law, a feature associated with jamming.

Steady State: Contact Number



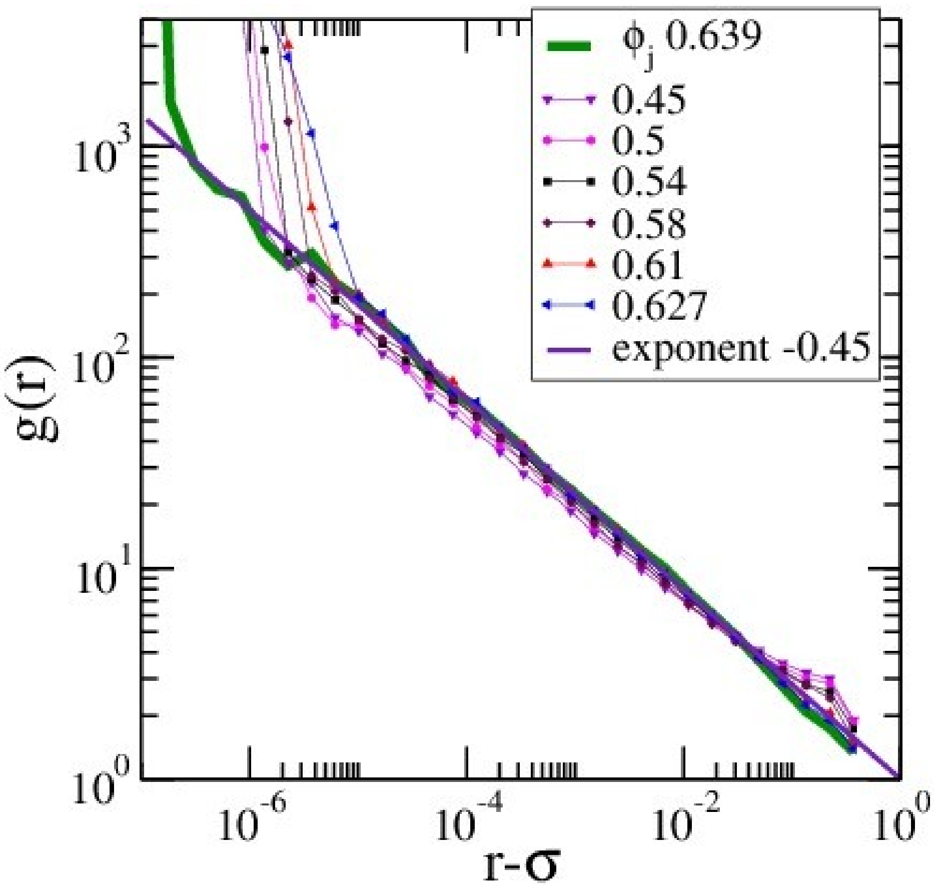
Average number of contacts per particle (Z) as a function of strain for different packing fraction. Saturation of Z indicates the system has reached steady state.

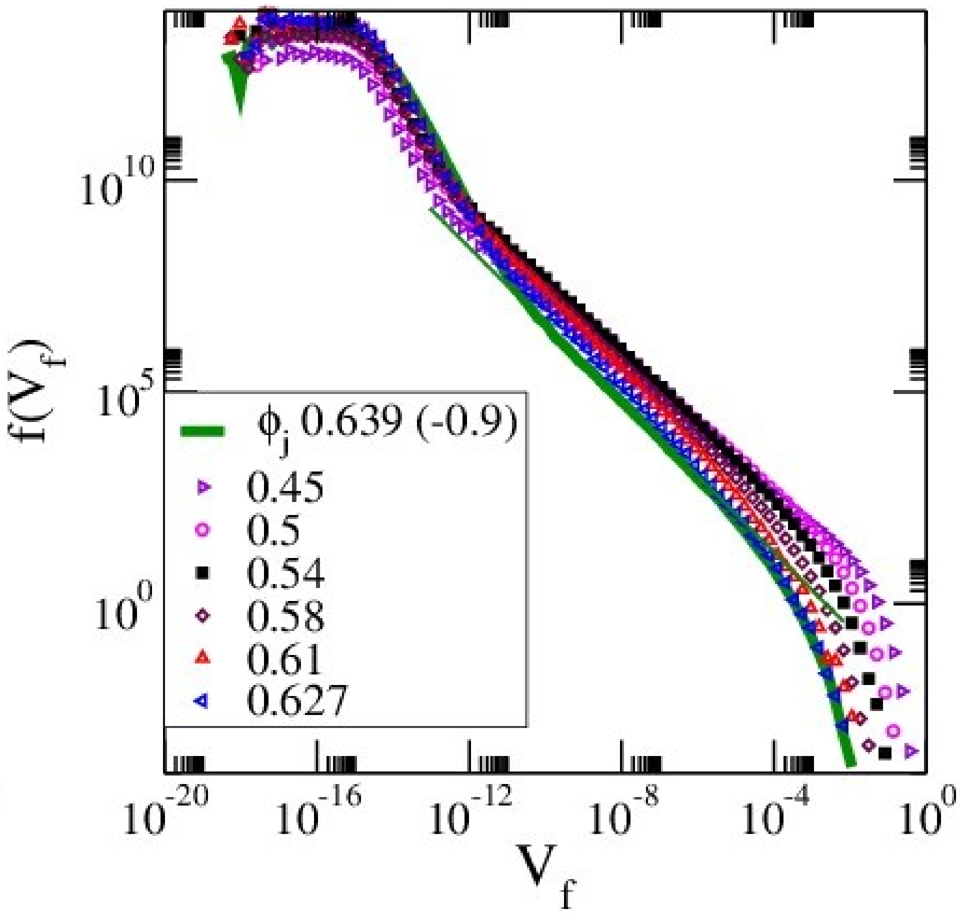
Structure in the steady sate



Coordination number and g(r) in steady state for different packing fraction.

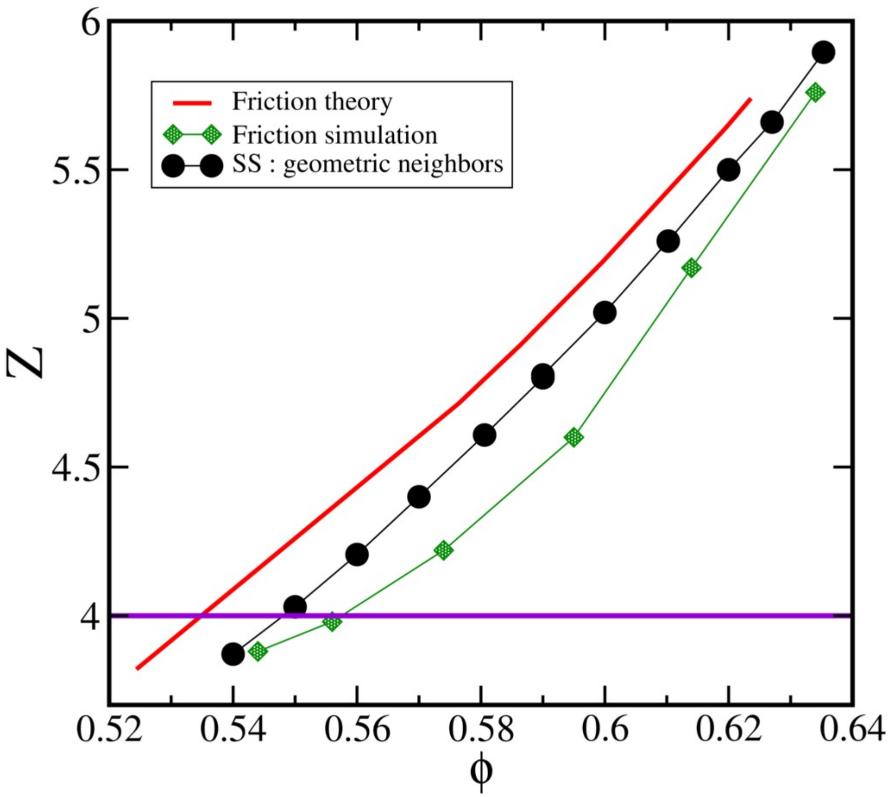
g(r) and free volumes

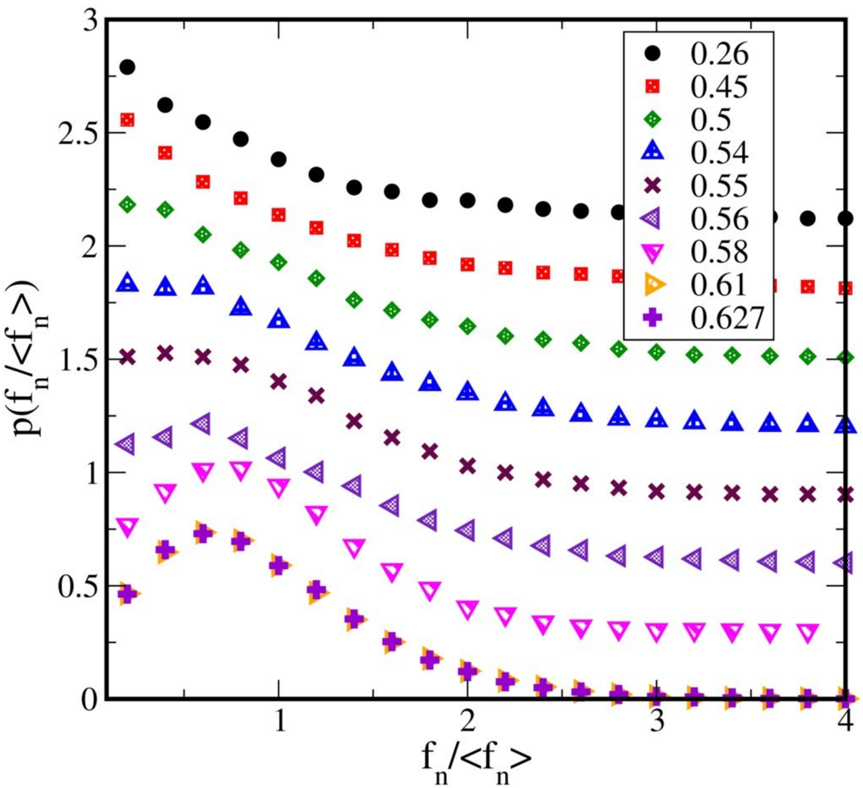




Power law divergence in g(r) and power tail in free volume distribution is seen for all packings in steady state.

Coordination number and force distributions





Steady state sheared packings frictional packings have similar structure.

Sheared packings above $\Phi = 0.55$ have a peak in the force distribution.

1. P.Wang, et al., Physica A 390, 427(2011).

2. L. E. Silbert , Soft Matter 6, 2918 (2010).

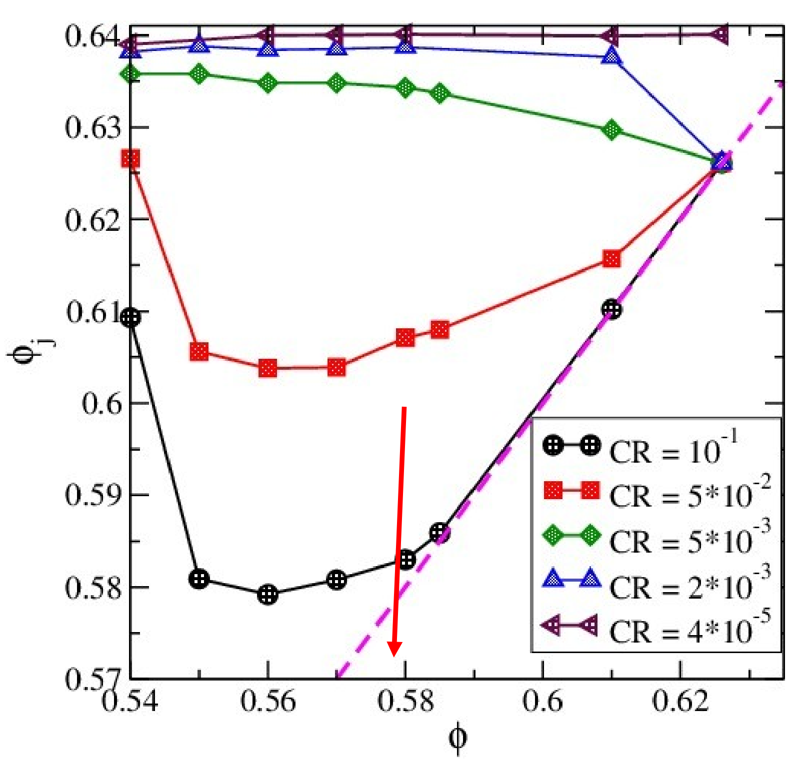
Stability of sheared packings

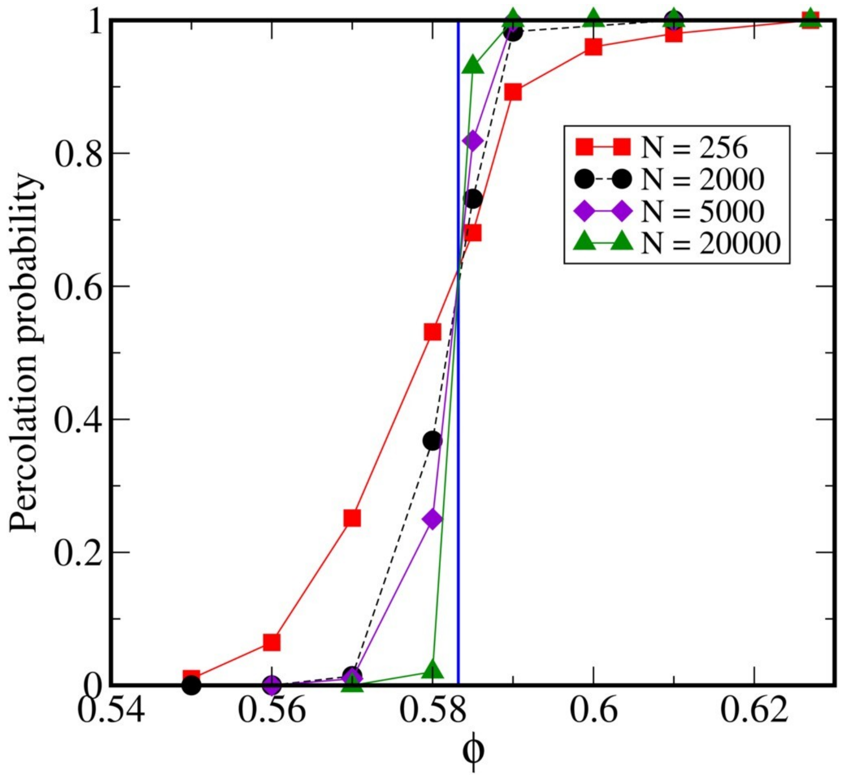
Steady state sheared configurations map to compression rate dependent (Lubachevsky-Stillinger) jammed configurations.

Evidence of crossover at ~ 0.58, for fast compression!!

Percolation of spheres with 2D contacts.

What does it mean? Frictionless spheres will unjam for slow compression.
What about frictional spheres, with the same configurations?





Dynamics with Friction: Discrete Element Method

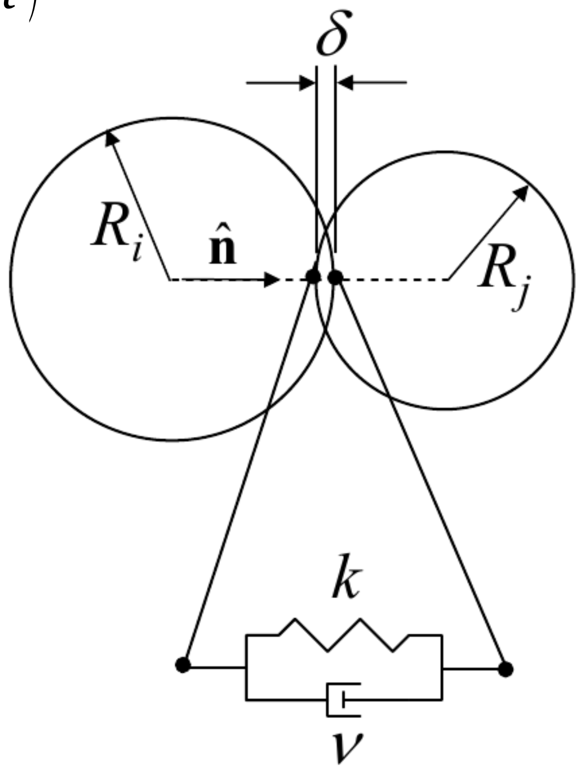
Particles interact when they are in contact

$$F=\left(k_n d\vec{n}_{ij}-mg_n\vec{v}_n\right)-\left(k_t DS_t+mg_t\vec{v}_t\right)$$

Parameters : $k_n=k_t=2$ $g_n=2g_t$

Global damping : $F=-\eta\vec{V}$

Linear spring dashpot model



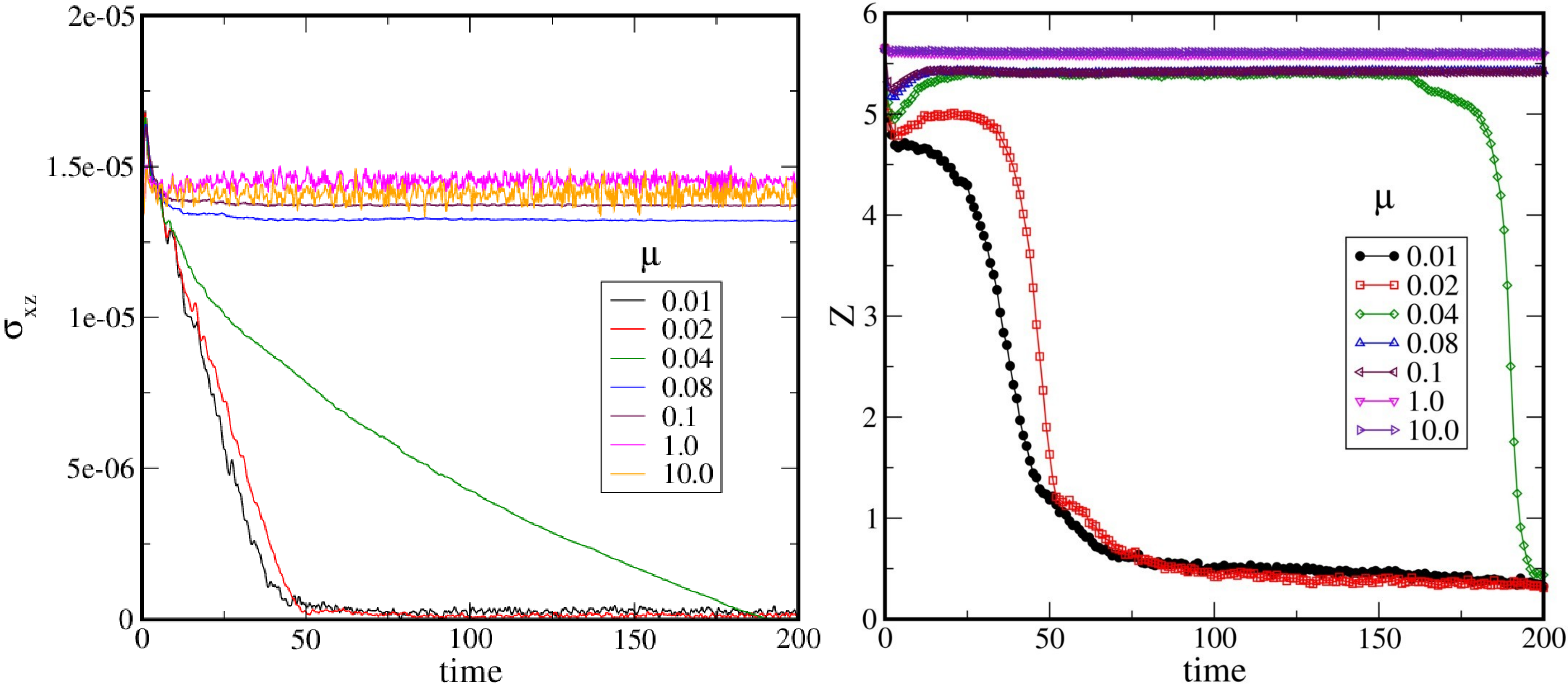
Subject sheared steady configurations to molecular dynamics with friction and damping.

Study threshold friction coefficient beyond which sheared configurations are stable.

DEM: Cundall and Strack 1979.

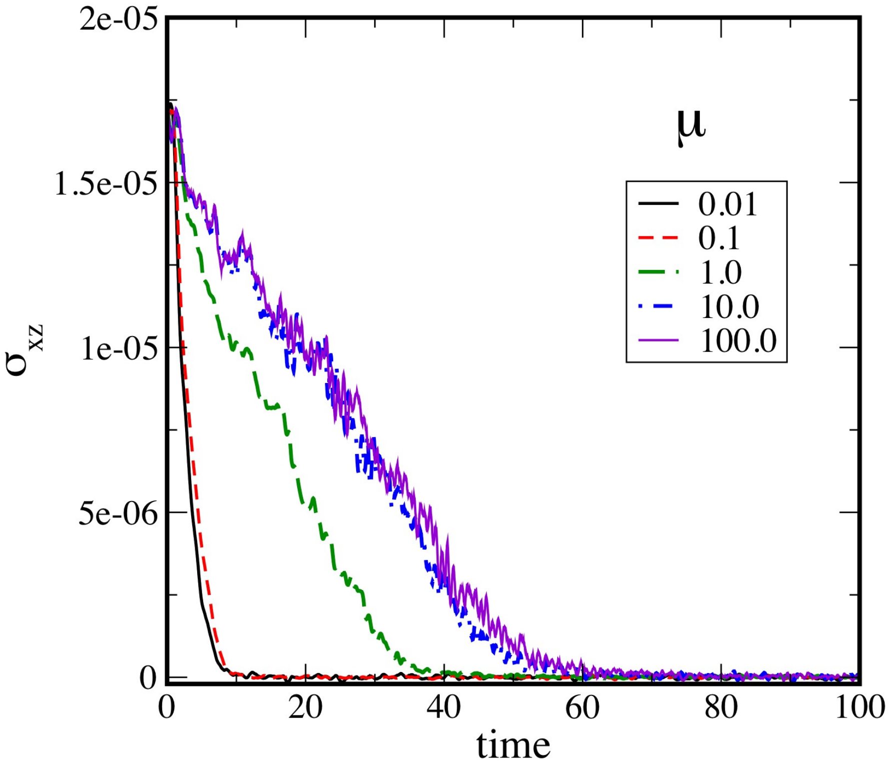
Frictional jamming : L. E. Silbert , Soft Matter 6, 2918 (2010).

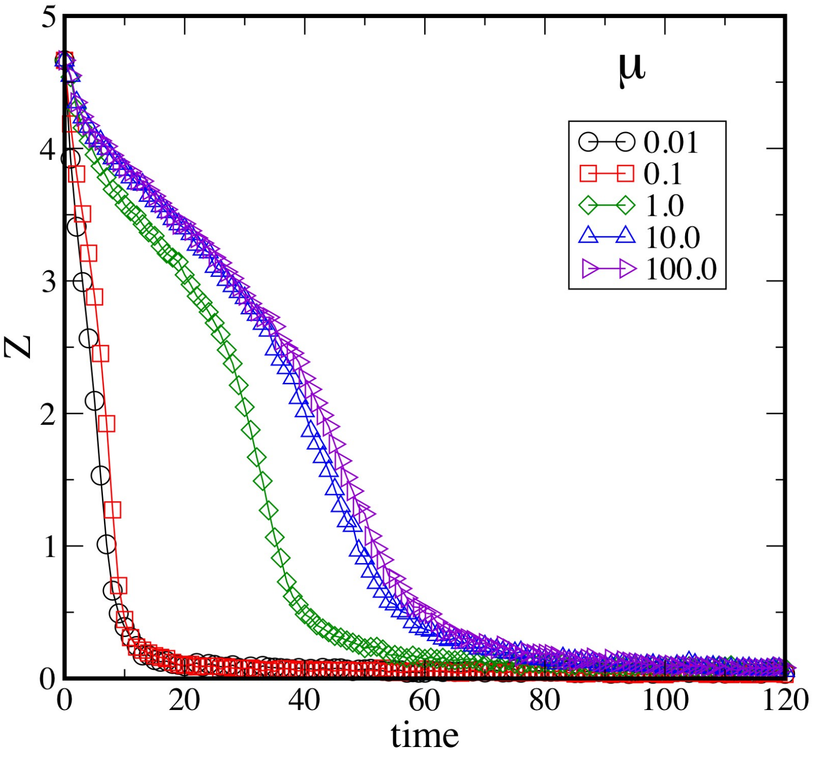
Dynamics with Friction: $\varphi = 0.627$



Stresses and contact number are finite for frictional coefficients leading to jamming above a threshold friction, and zero for unjammed final states.

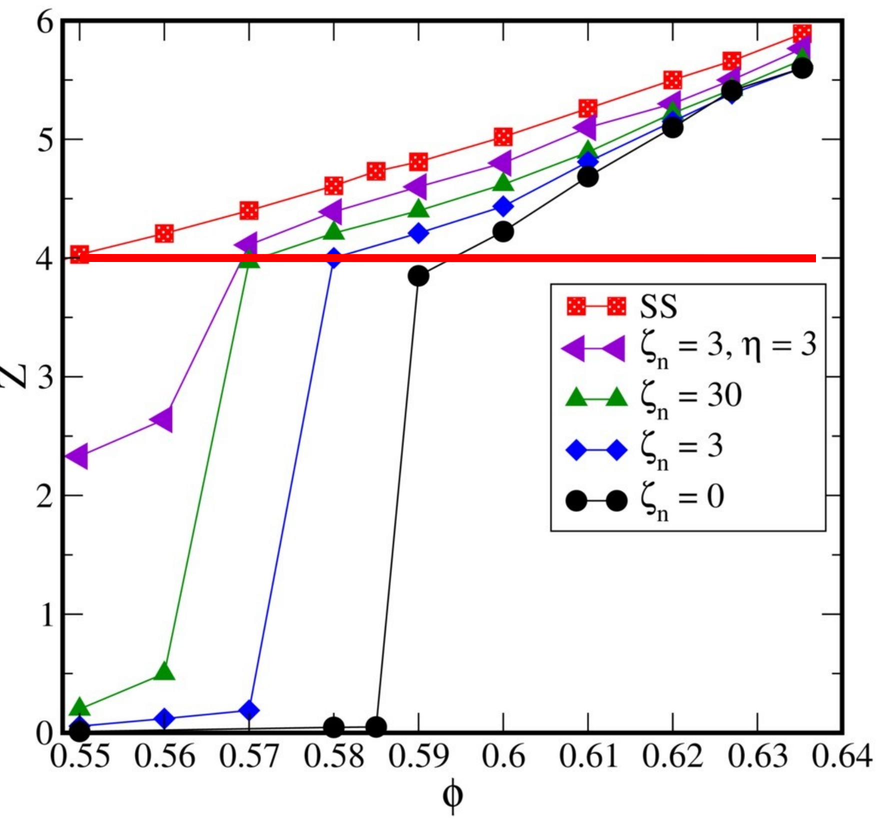
Dynamics with Friction: φ = 0.58

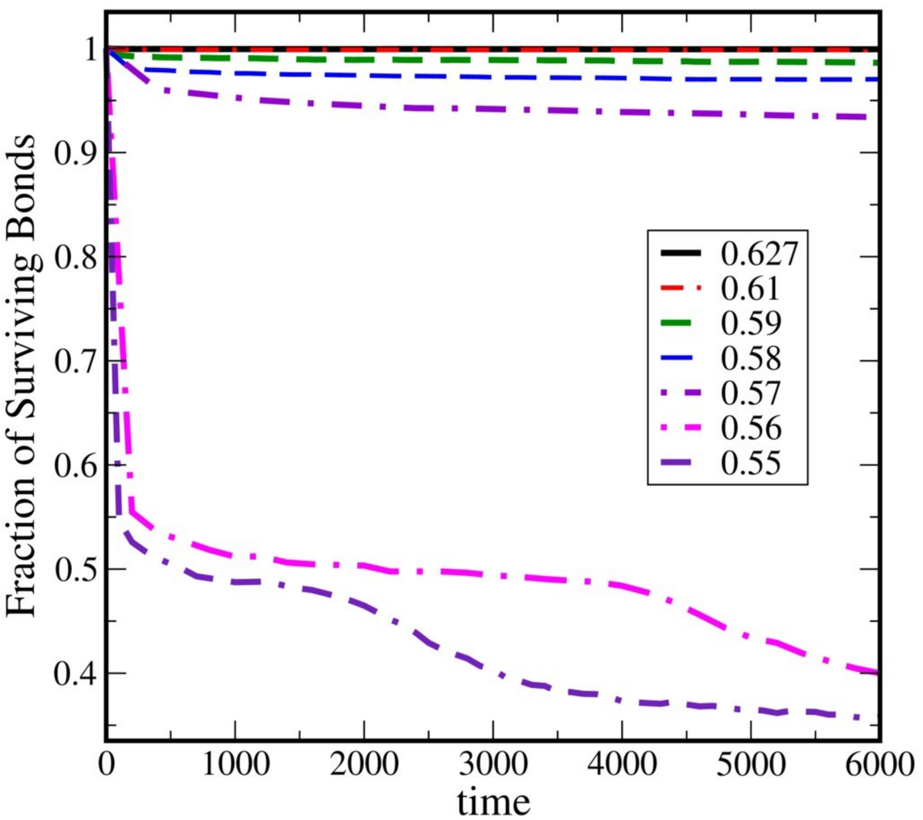




Stresses and contact number always decay implying unjammed final states for all frictional coefficients, with no damping. Damping leads to more stable final structures at low densities.

Frictional dynamics

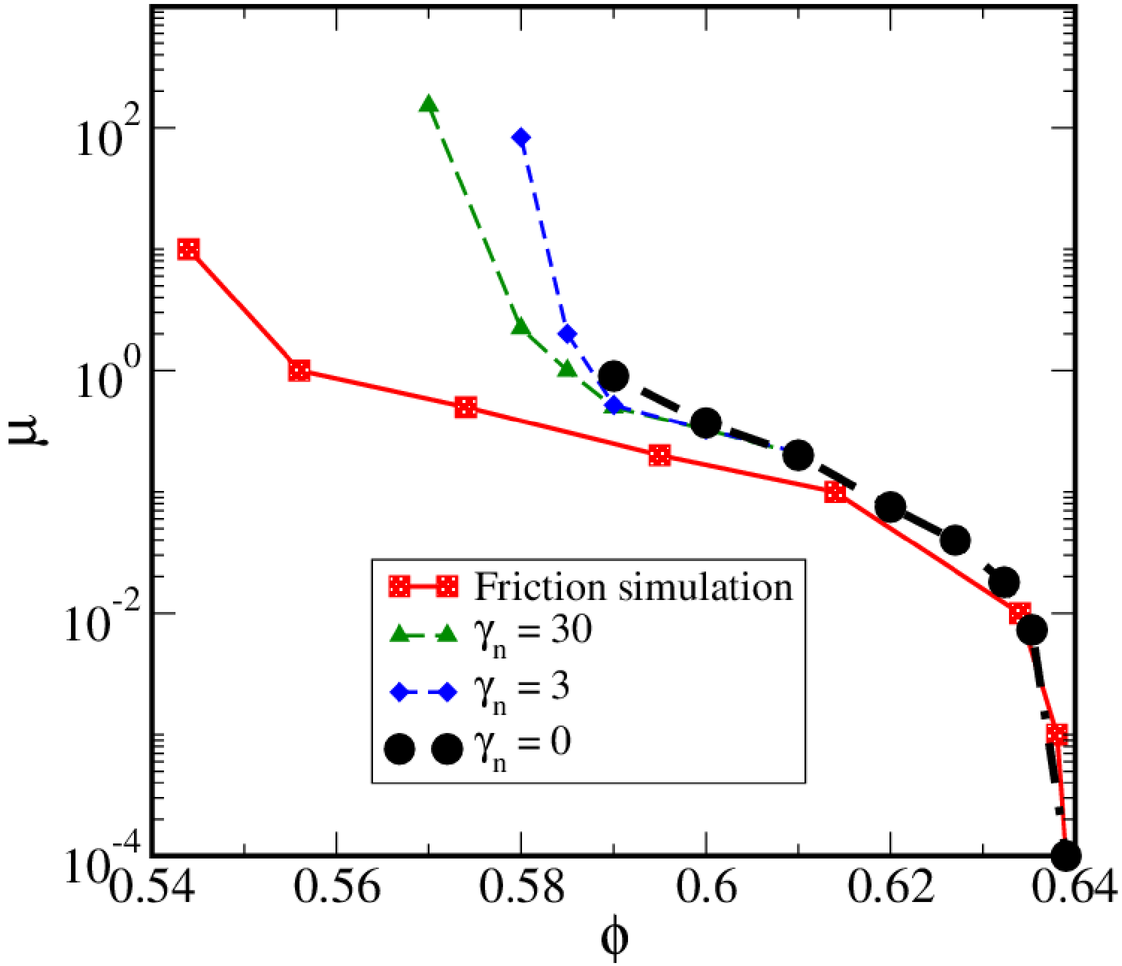




The steady state frictionless packings can be stabilized by inclusion of friction over a range of densities below the isotropic jamming point.

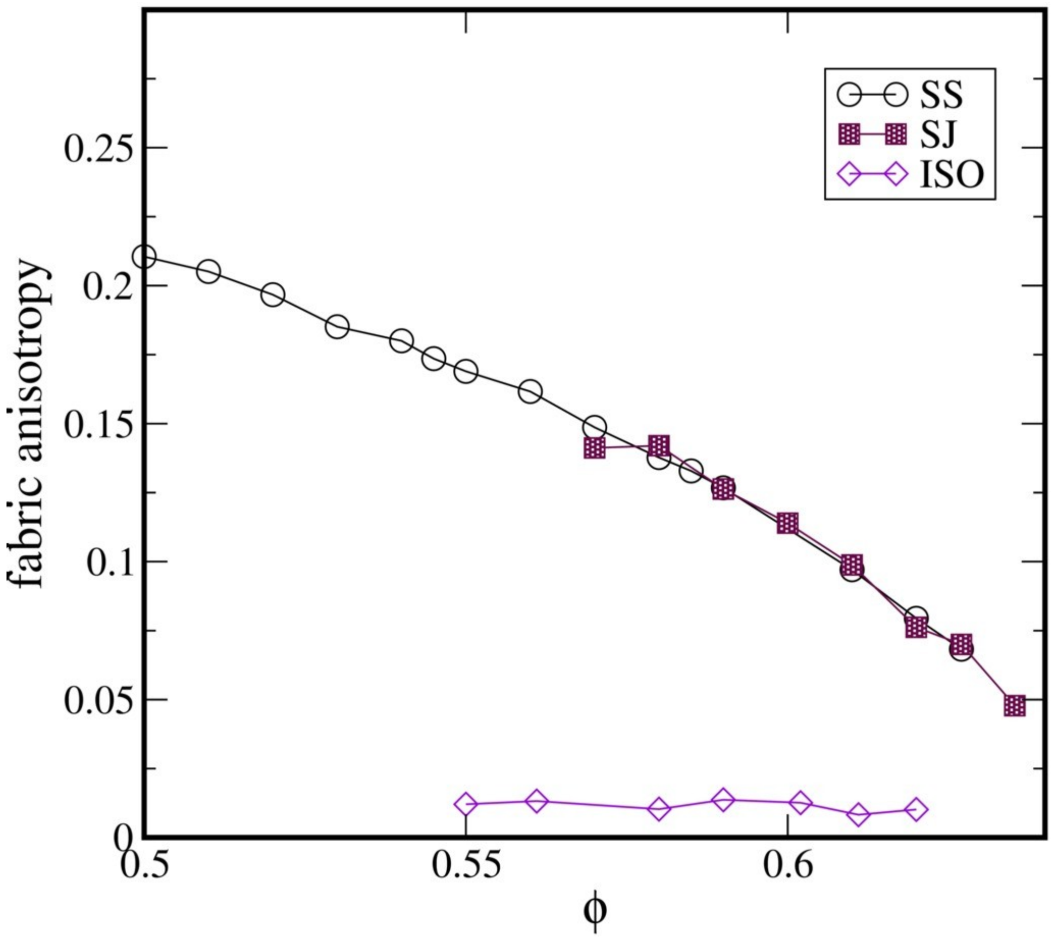
The lower limit on coordination number is **4** and density for shear Jamming is **0.55** (by extrapolation).

Dependence on friction coefficient



Frictional jamming : L. E. Silbert , Soft Matter 6, 2918 (2010).

Anisotropy



Definition of fabric tensor :

$$\hat{R} = \frac{1}{N} \sum_{i \neq j} \frac{\vec{r}_{ij}}{|r_{ij}|} \otimes \frac{\vec{r}_{ij}}{|r_{ij}|}$$

$\vec{r}_{ij}$ is the distance between the pair i and j.

$$C_1 > C_2 > C_3$$

are the eigenvalues of the fabric tensor.

Steady state and shear jammed configurations are anisotropic.

$$FA = \frac{C_1 - C_3}{C_1 + C_2 + C_3}$$

Force Balance from Geometry

But can we infer force balance directly from geometry?

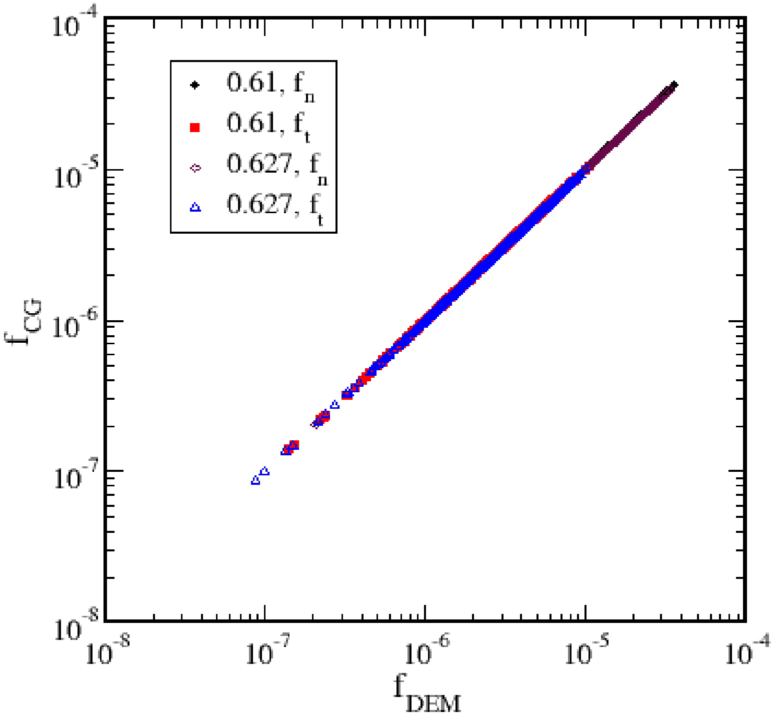
Contact matrix M defined in terms of geometry of steady state configurations.

Force and torque balance equations in terms of contact matrix M:

$$M|f> = 0$$

Minimize the energy function to obtain force configurations:

$$E = <f|M^T M|f>$$



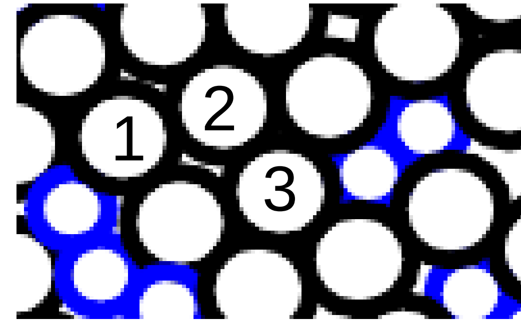
N=256

Estimated forces match those obtained from frictional (DEM) simulations initiated with the same configurations.

Direct evidence that sheared steady states evolve geometry that induces shear jamming.

Constructing the contact matrix

$$M=\begin{pmatrix}
\hat{n}_{12}{}^{x} & \hat{n}_{13}{}^{x} & \dots & \hat{\theta}_{12}{}^{x} & \hat{\theta}_{13}{}^{x} & \dots & \hat{\phi}_{12}{}^{x} & \hat{\phi}_{13}{}^{x} & \dots \\
-\hat{n}_{12}{}^{x} & 0 & \dots & -\hat{\theta}_{12}{}^{x} & 0 & \dots & -\hat{\phi}_{12}{}^{x} & 0 & \dots \\
0 & -\hat{n}_{13}{}^{x} & \dots & 0 & -\hat{\theta}_{13}{}^{x} & \dots & 0 & -\hat{\phi}_{13}{}^{x} & \dots \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\
\hat{n}_{12}{}^{y} & \hat{n}_{13}{}^{y} & \dots & \hat{\theta}_{12}{}^{y} & \hat{\theta}_{13}{}^{y} & \dots & \hat{\phi}_{12}{}^{y} & \hat{\phi}_{13}{}^{y} & \dots \\
-\hat{n}_{12}{}^{y} & 0 & \dots & -\hat{\theta}_{12}{}^{y} & 0 & \dots & -\hat{\phi}_{12}{}^{y} & 0 & \dots \\
0 & -\hat{n}_{13}{}^{y} & \dots & 0 & -\hat{\theta}_{13}{}^{y} & \dots & 0 & -\hat{\phi}_{13}{}^{y} & \dots \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\
\hat{n}_{12}{}^{z} & \hat{n}_{13}{}^{z} & \dots & \hat{\theta}_{12}{}^{z} & \hat{\theta}_{13}{}^{z} & \dots & \hat{\phi}_{12}{}^{z} & \hat{\phi}_{13}{}^{z} & \dots \\
-\hat{n}_{12}{}^{z} & 0 & \dots & -\hat{\theta}_{12}{}^{z} & 0 & \dots & -\hat{\phi}_{12}{}^{z} & 0 & \dots \\
0 & -\hat{n}_{13}{}^{z} & \dots & 0 & -\hat{\theta}_{13}{}^{z} & \dots & 0 & -\hat{\phi}_{13}{}^{z} & \dots \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots &
\end{pmatrix}$$



example

$$\vec{f}_i = \Sigma_j(\hat{n}_{ij} f^n_{ij} + \hat{\theta}_{ij} f^\theta_{ij} + \hat{\phi}_{ij} f^\phi_{ij}) = 0$$

$$\Gamma_i = \Sigma_j \vec{R}_i \times \vec{F}_{ij} = 0$$

$$\Gamma_i = \Sigma_j R_i (f^\theta_{ij} \hat{\phi}_{ij} - f^\phi_{ij} \hat{\theta}_{ij})$$

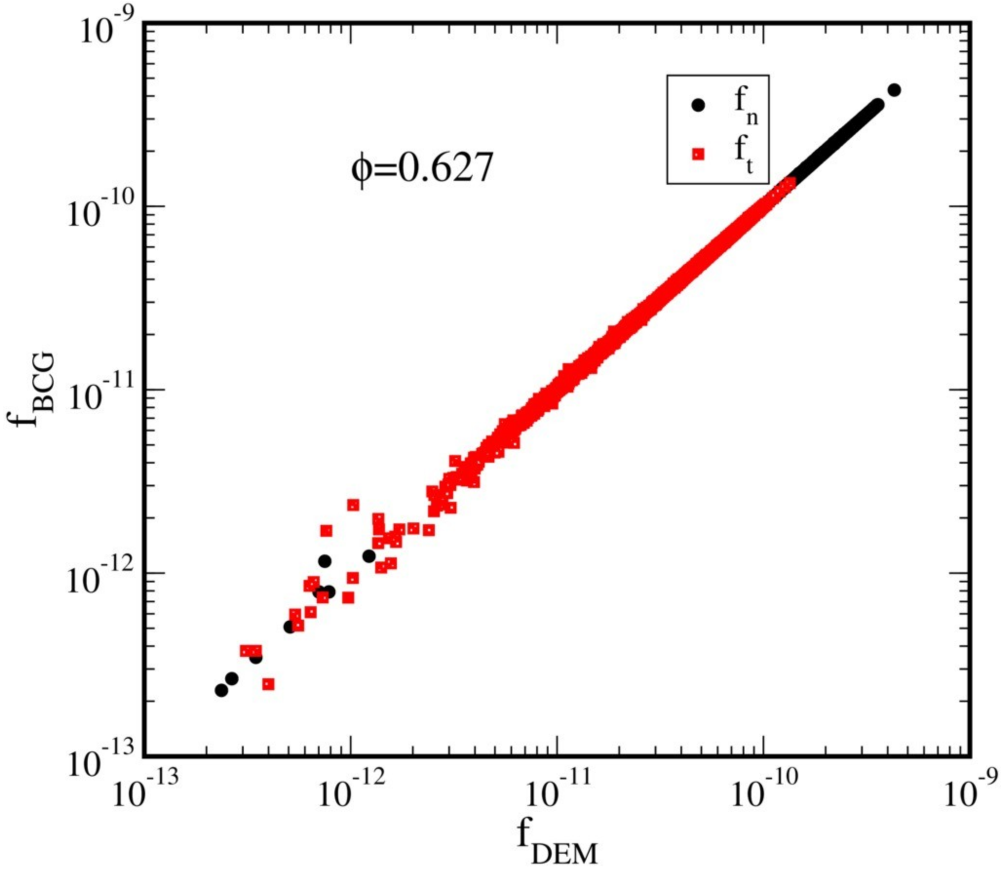
$$F=\begin{pmatrix} f^n_{12} \\ f^n_{13} \\ \vdots \\ f^\theta_{12} \\ f^\theta_{13} \\ \vdots \\ f^\phi_{12} \\ f^\phi_{13} \\ \vdots \end{pmatrix}$$

$$\begin{pmatrix}
R_1\hat{\phi}_{12}{}^{x} & R_1\hat{\phi}_{13}{}^{x} & \dots & -R_1\hat{\theta}_{12}{}^{x} & -R_1\hat{\theta}_{13}{}^{x} & \dots \\
R_2\hat{\phi}_{12}{}^{x} & 0 & \dots & -R_2\hat{\theta}_{12}{}^{x} & 0 & \dots \\
0 & R_3\hat{\phi}_{13}{}^{x} & \dots & 0 & -R_3\hat{\theta}_{13}{}^{x} & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
R_1\hat{\phi}_{12}{}^{y} & R_1\hat{\phi}_{13}{}^{y} & \dots & -R_1\hat{\theta}_{12}{}^{y} & -R_1\hat{\theta}_{13}{}^{y} & \dots \\
R_2\hat{\phi}_{12}{}^{y} & 0 & \dots & -R_2\hat{\theta}_{12}{}^{y} & 0 & \dots \\
0 & R_3\hat{\phi}_{13}{}^{y} & \dots & 0 & -R_3\hat{\theta}_{13}{}^{y} & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
R_1\hat{\phi}_{12}{}^{z} & R_1\hat{\phi}_{13}{}^{z} & \dots & -R_1\hat{\theta}_{12}{}^{z} & -R_1\hat{\theta}_{13}{}^{z} & \dots \\
R_2\hat{\phi}_{12}{}^{z} & 0 & \dots & -R_2\hat{\theta}_{12}{}^{z} & 0 & \dots \\
0 & R_3\hat{\phi}_{13}{}^{z} & \dots & 0 & -R_3\hat{\theta}_{13}{}^{z} & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots
\end{pmatrix}$$

$$\begin{bmatrix} R & 0 \\ 0 & T \end{bmatrix} |F\rangle = 0$$

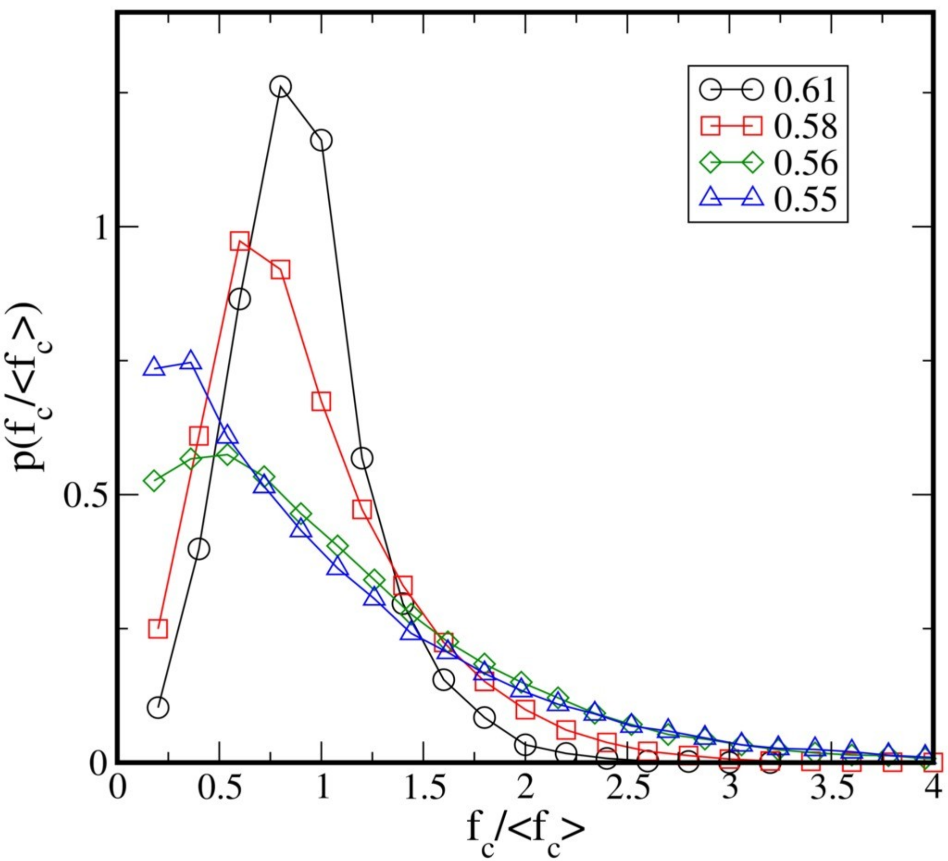
Estimating forces for a given geometry using solutions from DEM simulations

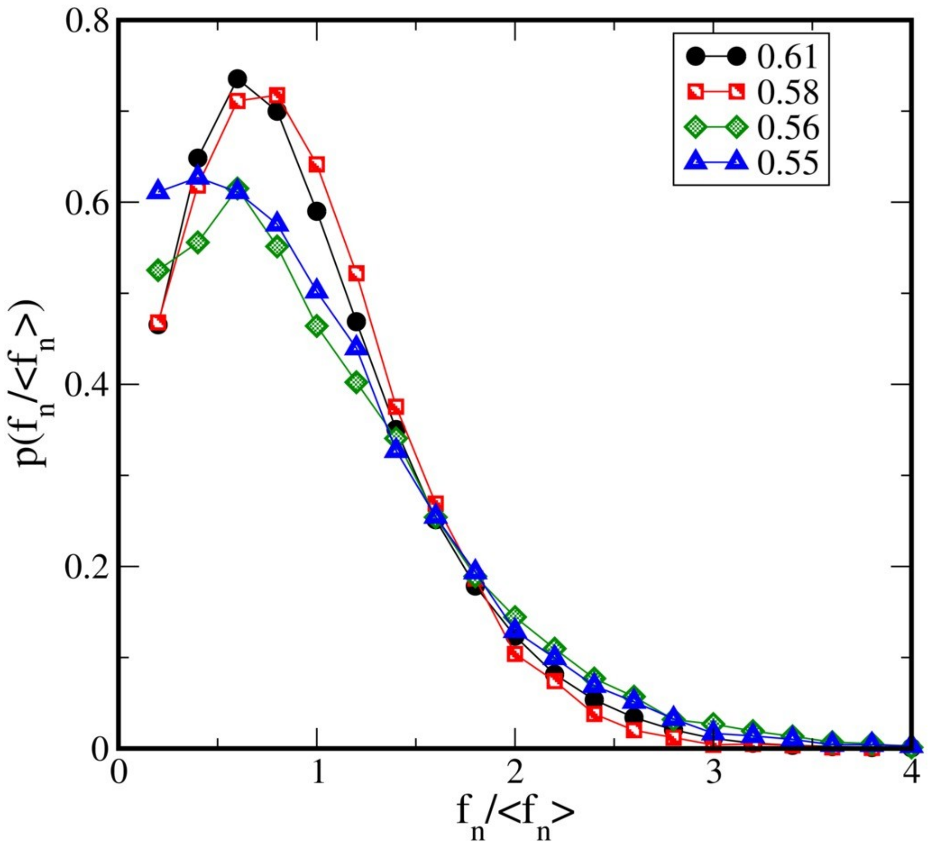
N=2000



Estimated forces match those obtained from frictional (DEM) simulations with the same initial SS configuration.

Force distributions





Forces satisfying force balance are obtained for steady state configurations using constrained minimization above Φ = 0.55. N=2000. Forces are initialized randomly.

Contact force distributions display peaks at finite values above Φ = 0.55 as observed above the jamming point, and obtained from sheared steady state configurations (with normal forces only).

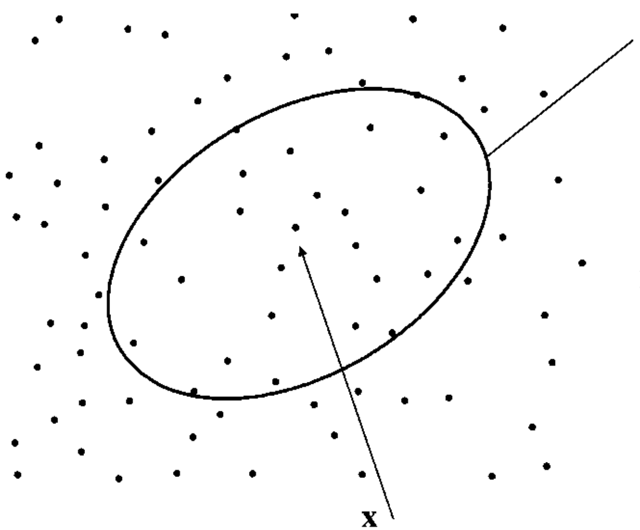
Hyperuniformity

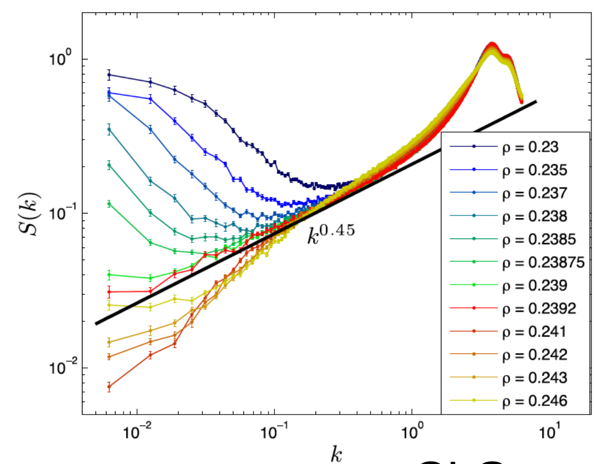
Number fluctuations in point patterns and sphere packings studied in the context of jamming. [Torquato, Stillinger (2003); Donev, Torquato & Stillinger (2005)]

Sub-extensive number fluctuations ~ vanishing zero wave length limit value of the structure factor, observed near the isotropic jamming point: S(k) ~ k

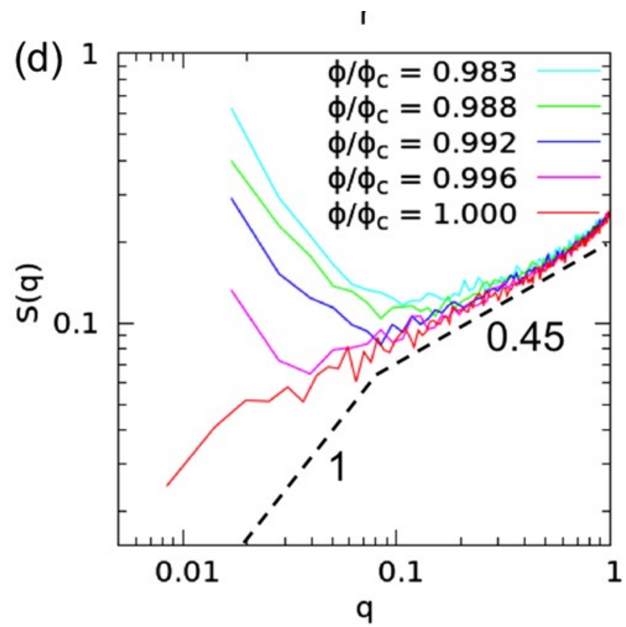
More recently: hyperuniform density fluctuations in periodically driven systems, but a crossover from S(k) ~ $k^{0.45}$ to S(k) ~ k, which isn't well explored yet.

Weijs et al, Hexner & Levine, Tjhung & Berthier (2015).



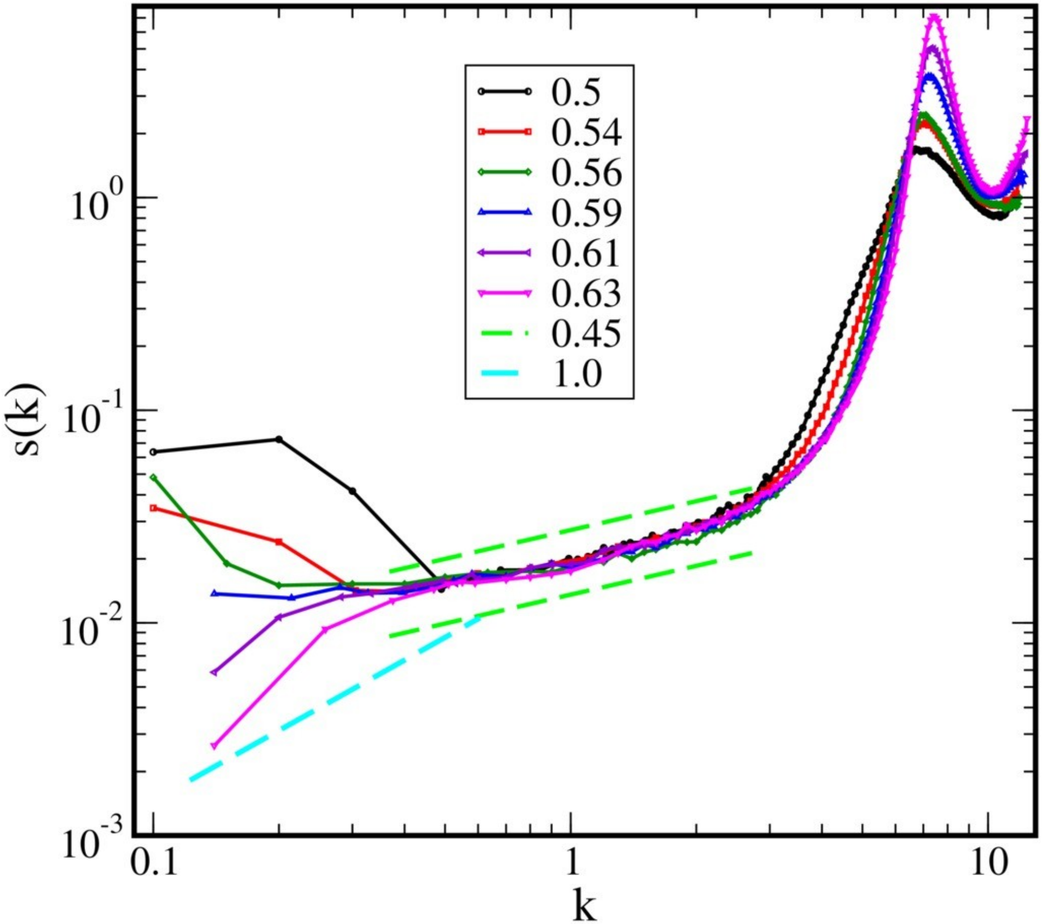


CLG



Hyperuniformity

In the steady state, with density as the parameter, we see a similar trend where at densities above Φ = 0.55 but below RCP Φ ~ 0.64, but need a better data for identifying the critical density, and to know the k → 0 limit.



N=10^5

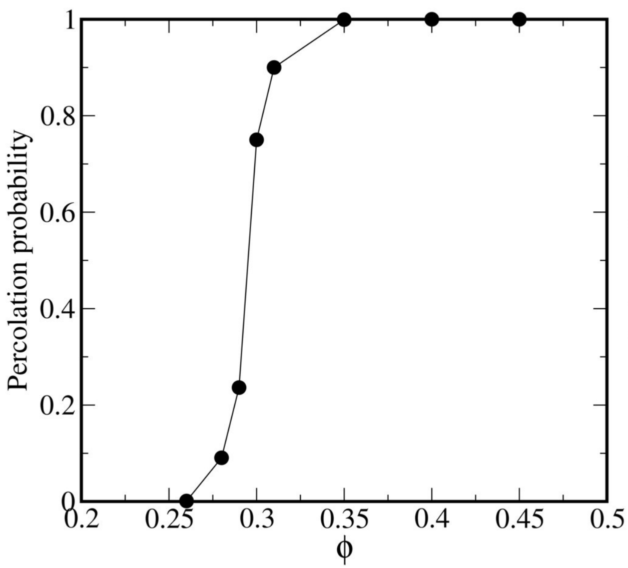
Percolation

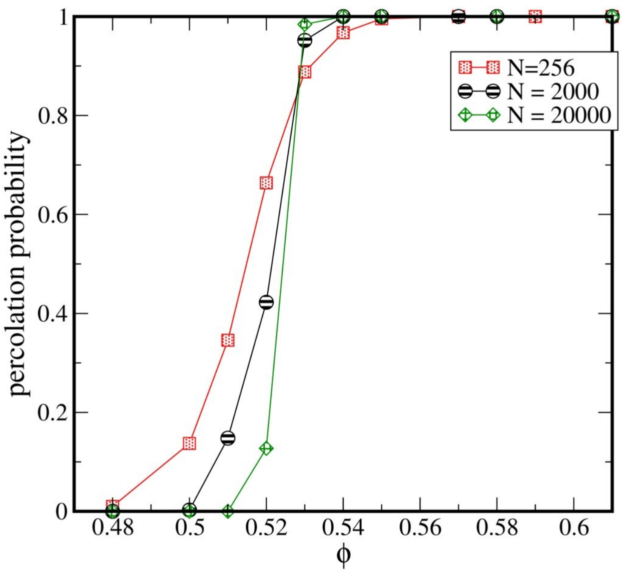
Interesting to understand shear jamming in terms of percolation of “rigidity”. But not very clear at present how that can be characterized.

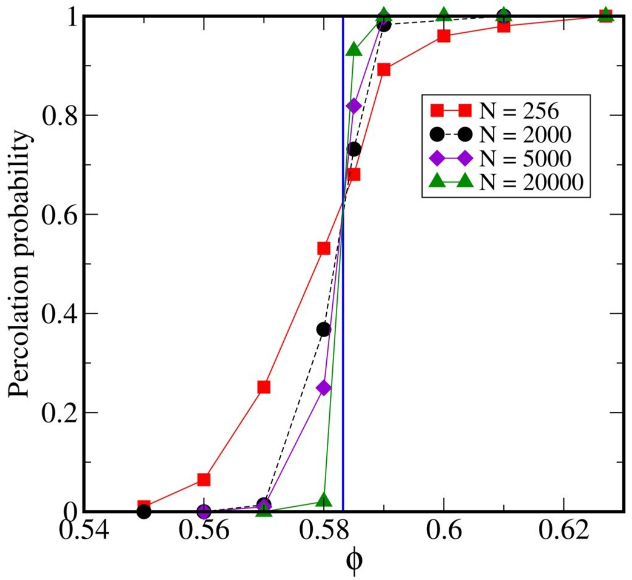
Contact percolation occurs at very low density, ~ 0.26

Percolation of locally jammed particles (Z>D) occurs at density 0.53.

Percolation of jammed particles (Z>=2D) occurs at density 0.58.

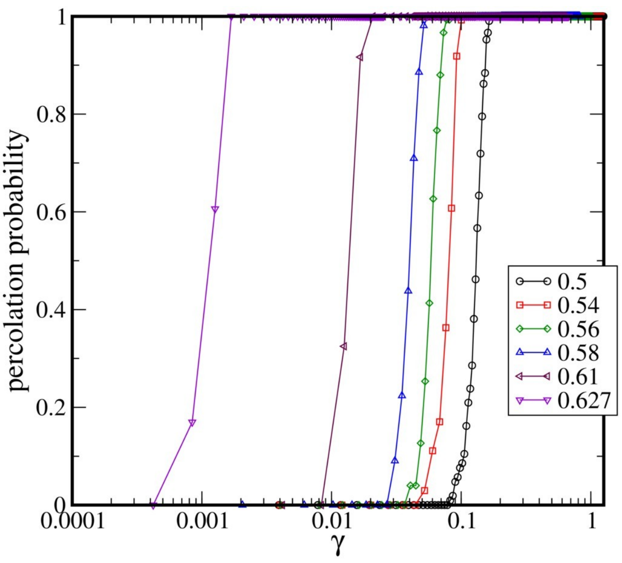




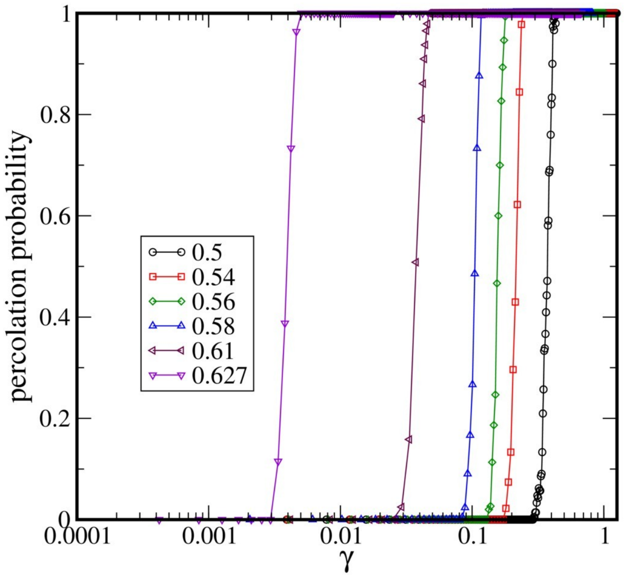


What is correct percolation problem to consider?

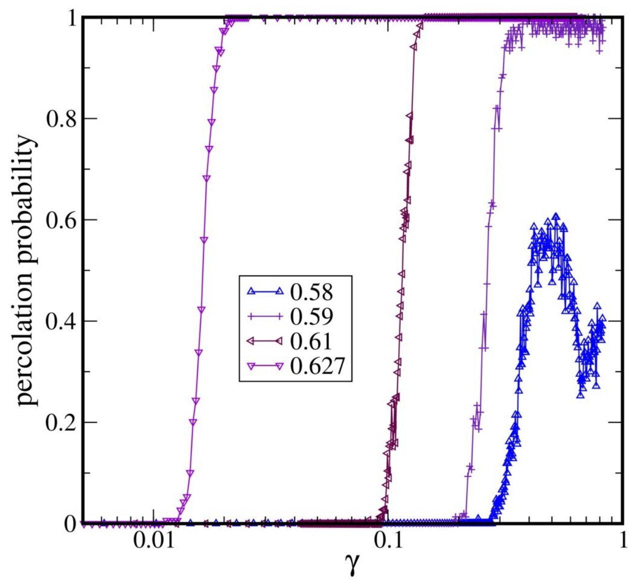
Percolation transition as a fuction of strain



Contact Percolation



Z >= D+1Percolation



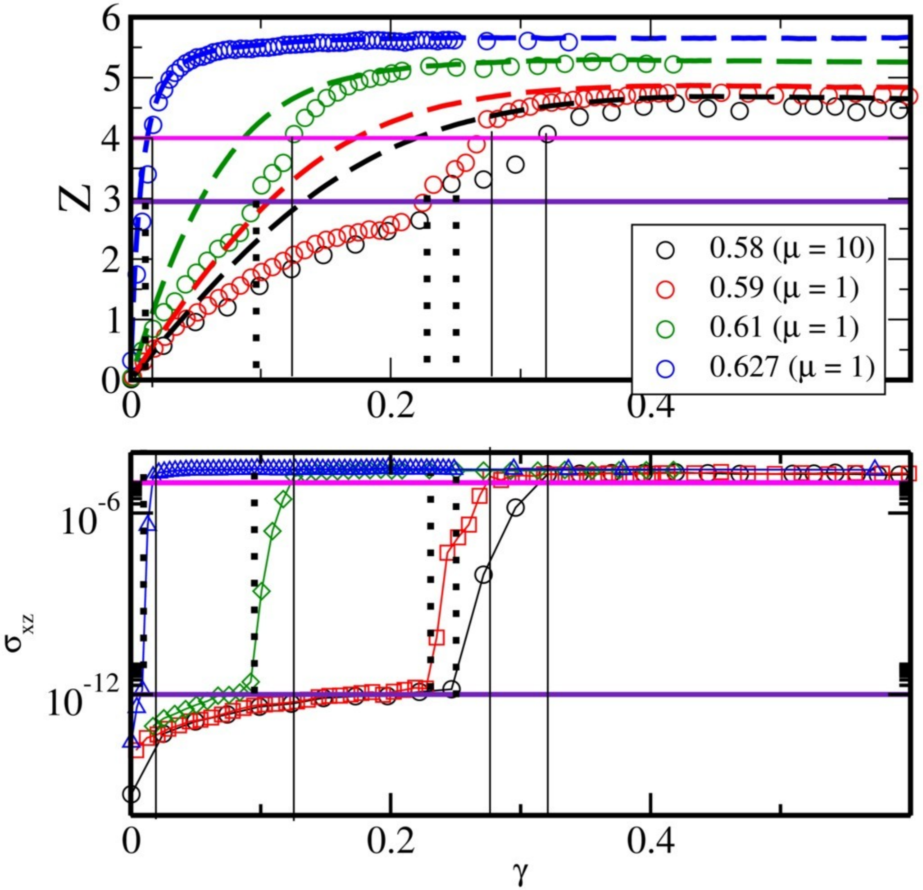
Z>= 2D Percolation

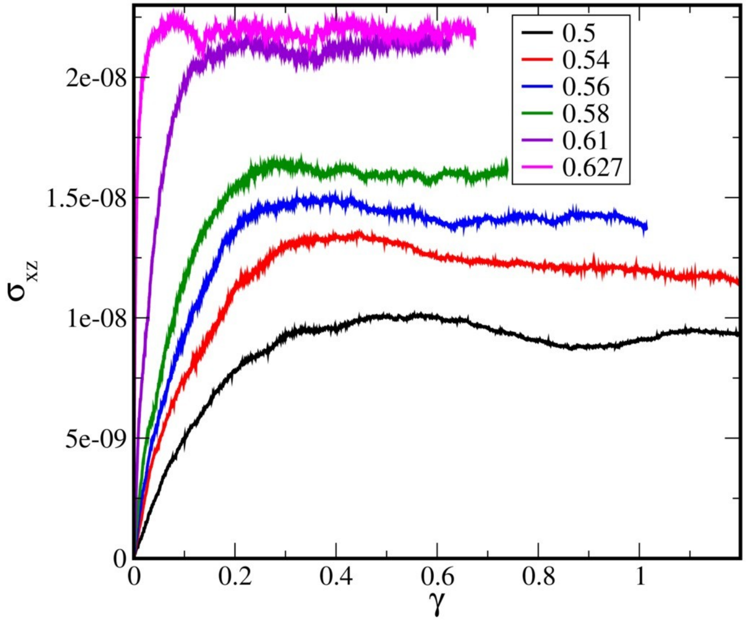
0.50

0.58

Evolution of Stress and Contact Number in the presence of Friction

Frictionless strained configurations are evolved at each strain by turning on friction.

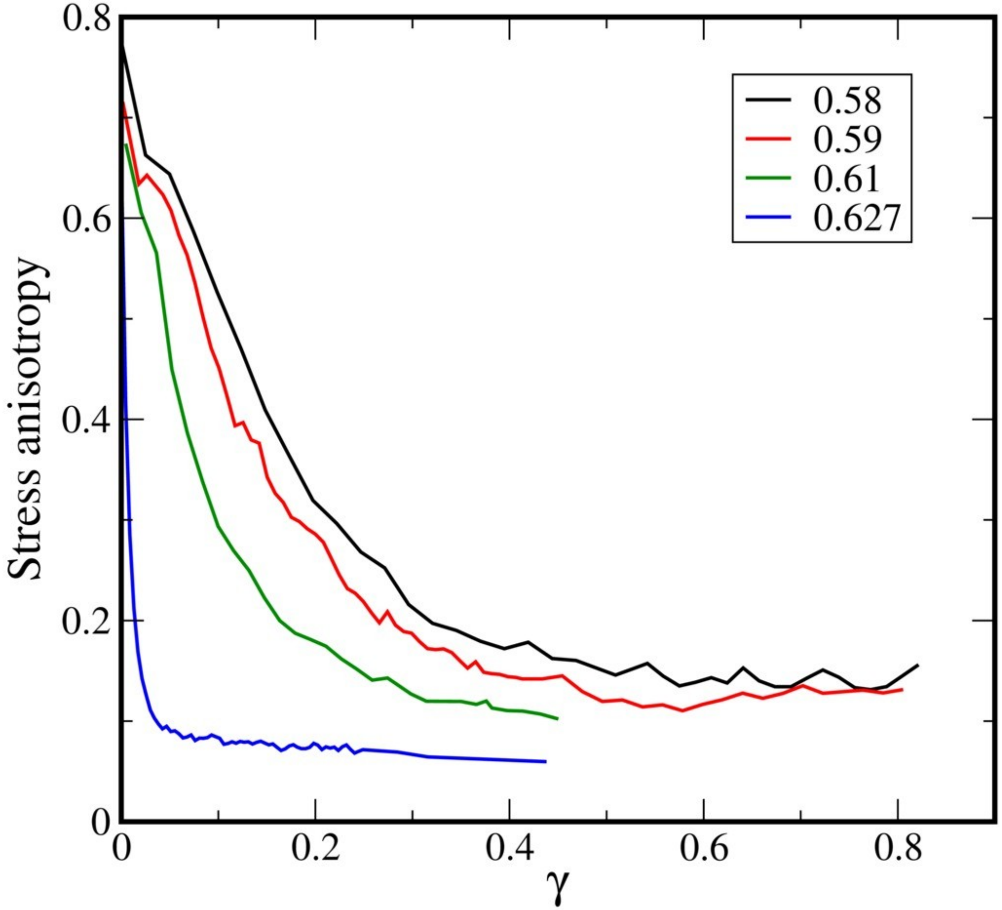




Contact number shows gradual change but there is discontinuous jump in stress. Z = D seems to trigger onset of jamming!!

Stress anisotropy & movies of evolution of Stress and Contact Number in the presence of Friction

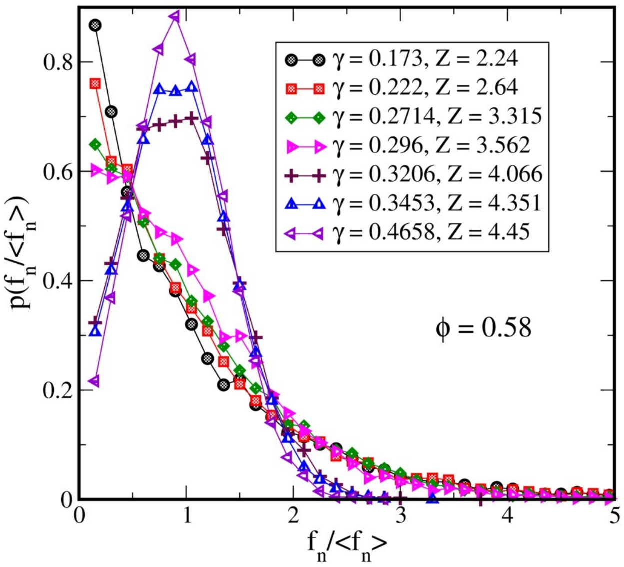
Stress tensor : $\hat{\sigma} = \frac{1}{V} \sum_{i \neq j} \mathbf{r}_{ij} \otimes \mathbf{f}_{ij}$



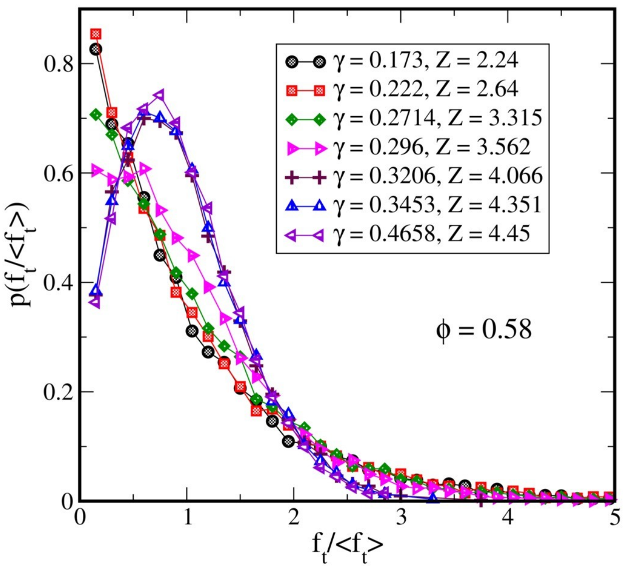
Stress anisotropy decreases with strain and reach a steady state.

Evolution of force distributions in the presence of Friction

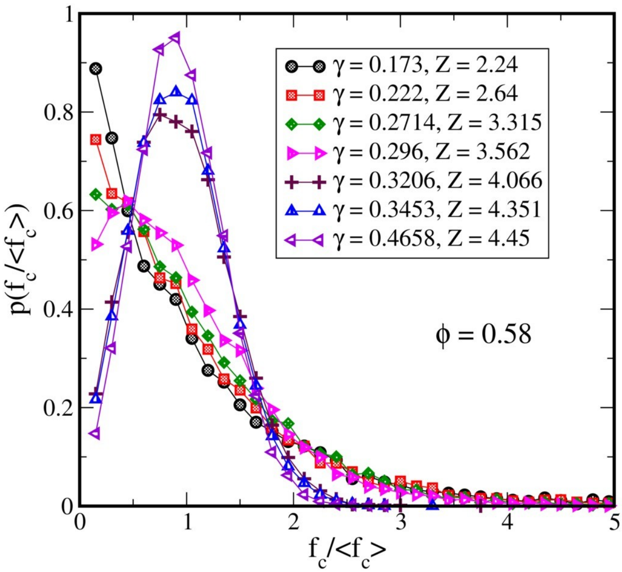
$\Phi = 0.58$



Normal forces



Tangential forces

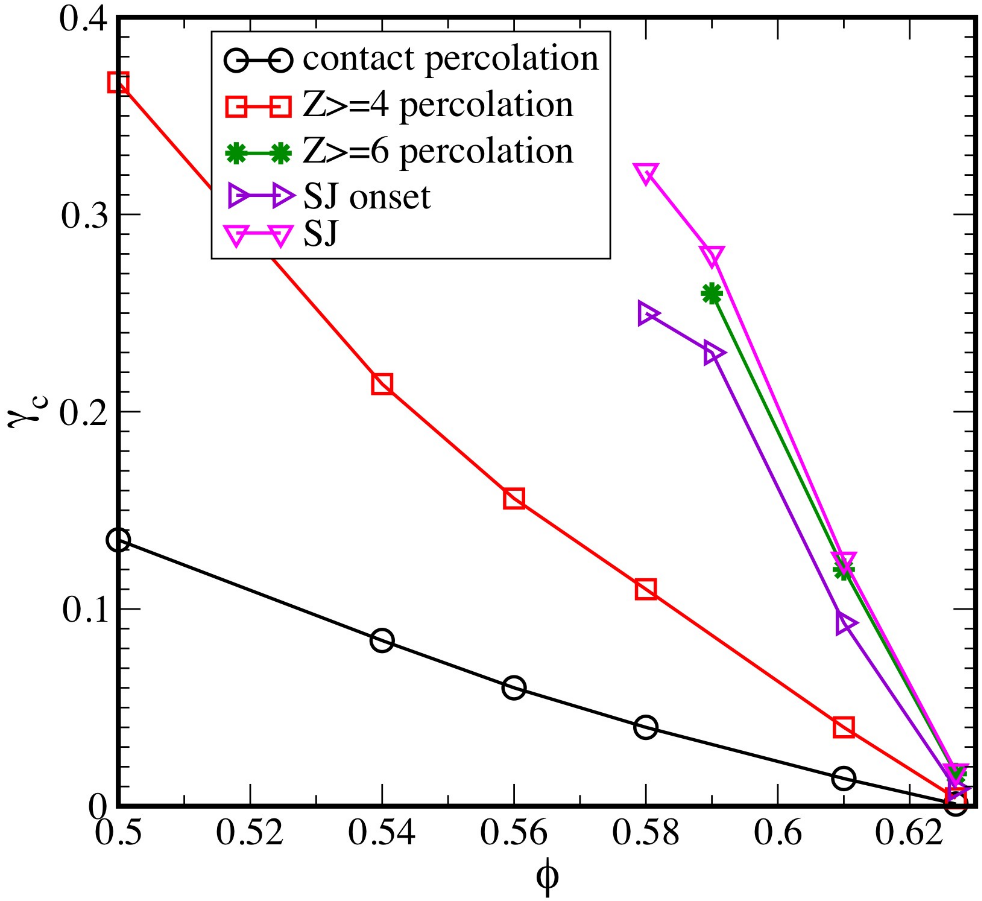


Normal & tangential forces

Force distributions begin to develop a peak at finite value of force near the onset of jamming.

At the strain value, where the coordination number Z=>4, the force distributions have a peak.

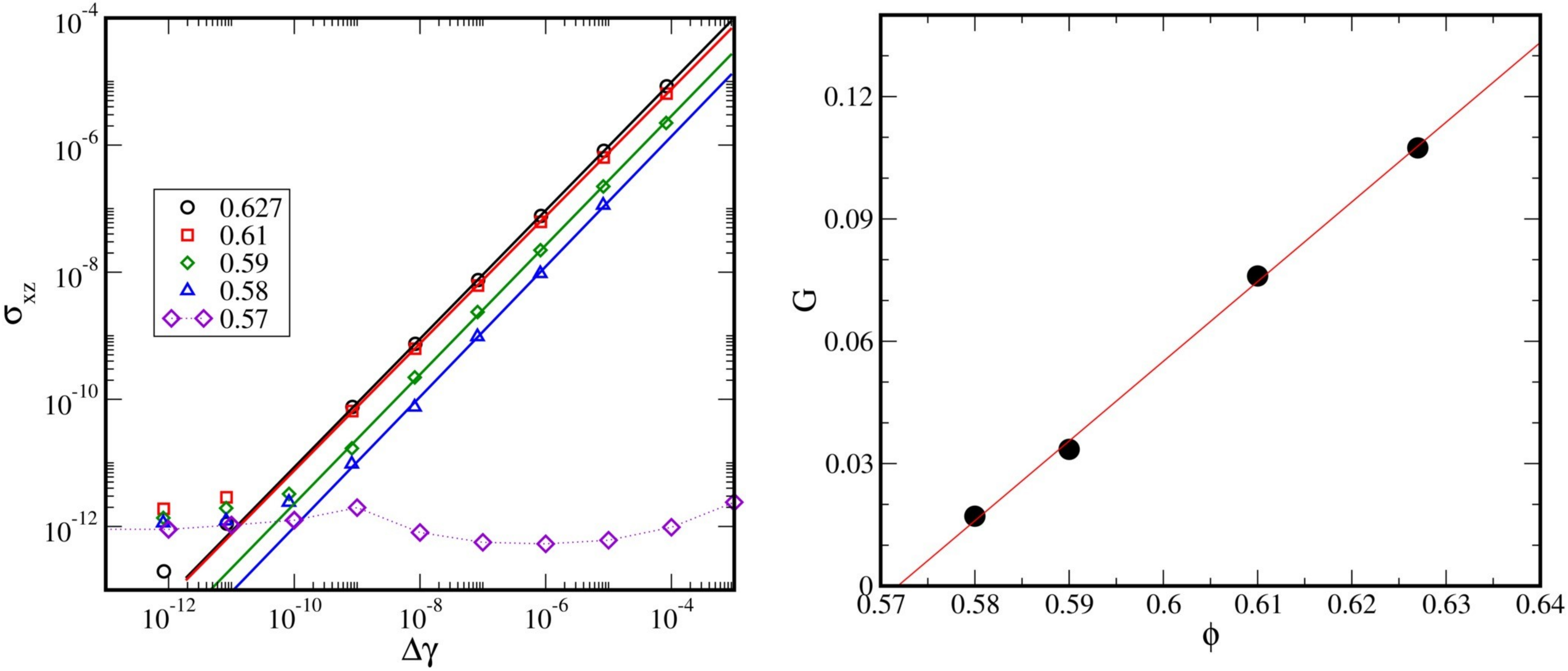
Jamming strain



Jamming occurs after the contact and the four coordinated percolations.

Z = D, D+1 percolations bracket the jamming transition!
Jamming transition ~ Z = 2D percolation!

Mechanical Characterization:
Shear modulus as a function of density



Steady state configurations show finite shear modulus above $\Phi = 0.57$.

Threshold density?

Summary

Shear deformation generates structures that exhibit geometric features characteristic of jammed structures, including hyperuniformity.

These structures can support load, when frictional forces are present in addition to normal forces, in a range of densities below the isotropic jamming point.

Force balance conditions can be solved based on geometric information alone, and results consistent with frictional jamming.

Percolation analysis and analysis of frictional jamming suggests that jamming occurs when spheres with contact number = 2D percolate.