Numerical study of the microscopic structure of jammed systems

from inferring their dynamics to finite size scaling

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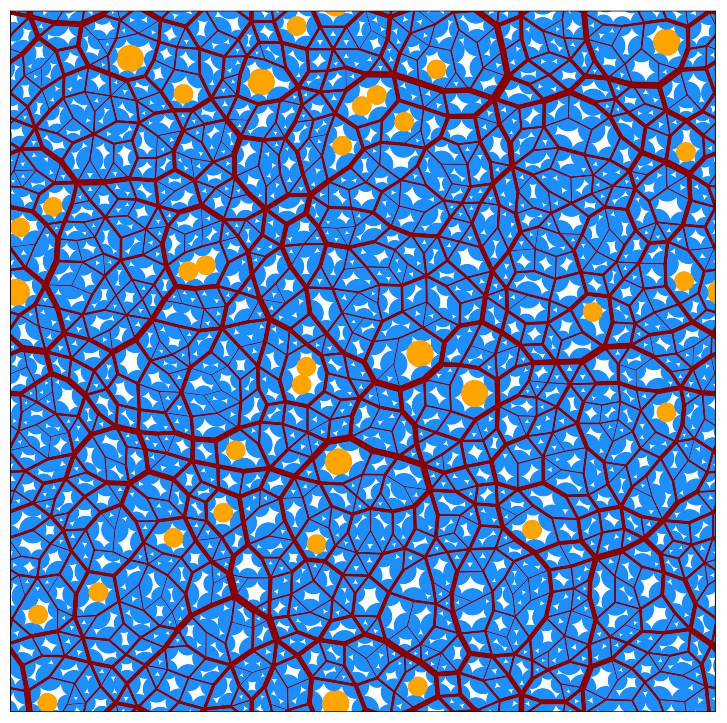
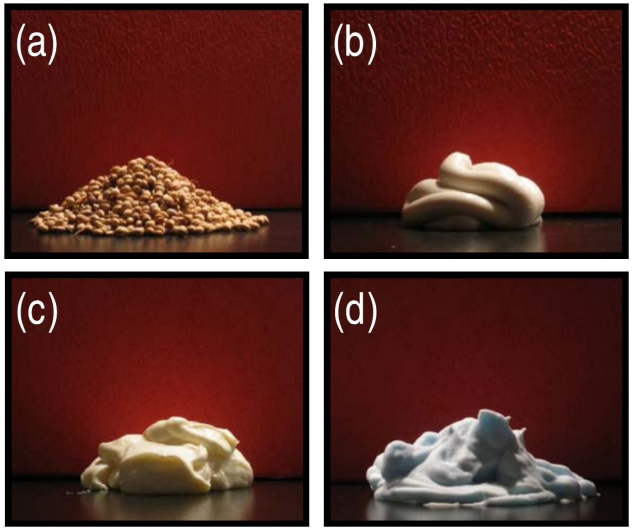
OUTLINE

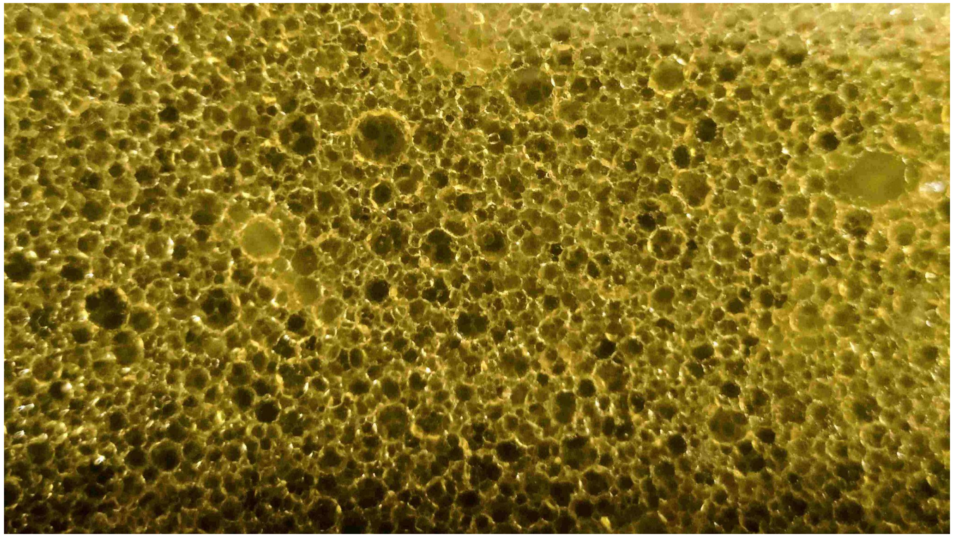


1. Introduction: Why should we care about jammed systems?
2. Producing jammed packings using ***Linear Programming***
3. Inferring the ***particle-wise dynamics*** *NEAR* the jamming point
4. **Finite size scaling** of microstructural criticality *@jamming*

What is Jamming?



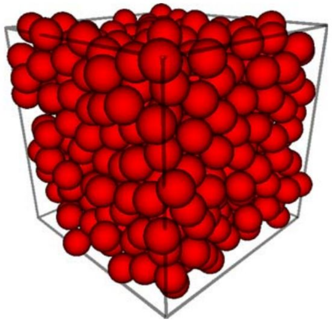
[van Hecke, *J. Phys.: Cond. Matter* **(2010)**]

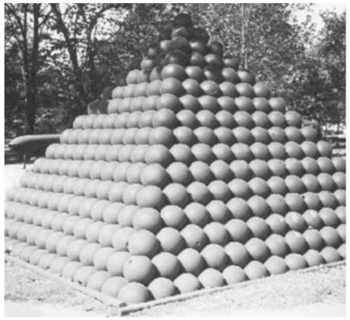


[Vinaigrette attempt; RDHR *unpublished recipe* **(2020)**]

In a ***jammed state*** all the degrees of freedom are completely frozen (*i.e.* blocked) due to geometric frustration.

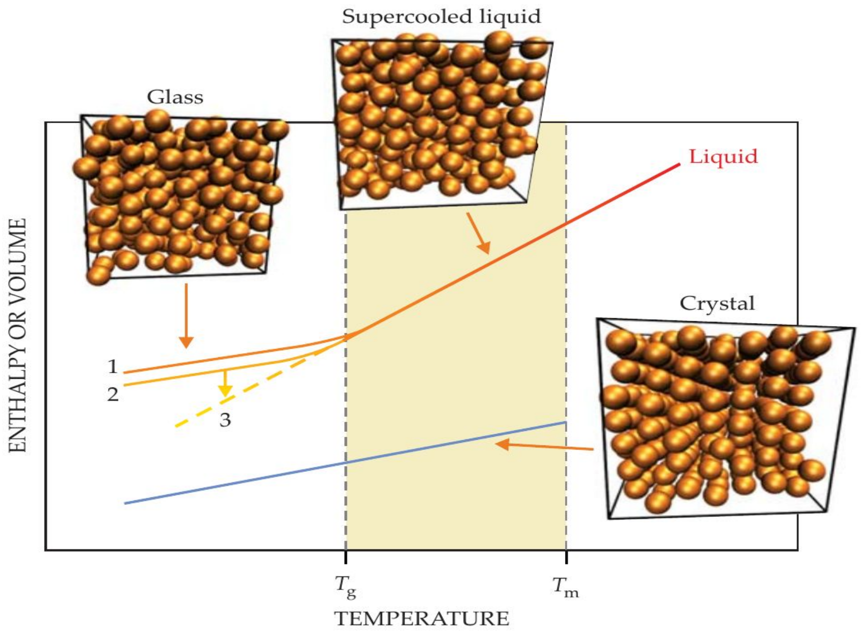
[Donev, *PhD Thesis* (Princeton) **(2006)**]



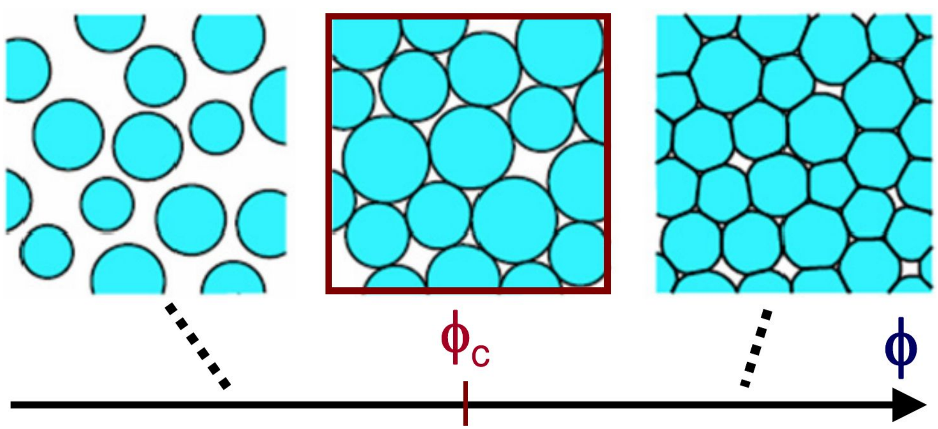


[Torquato and Stillinger, *Rev. Mod. Phys.*, 82, 3 **(2010)**]

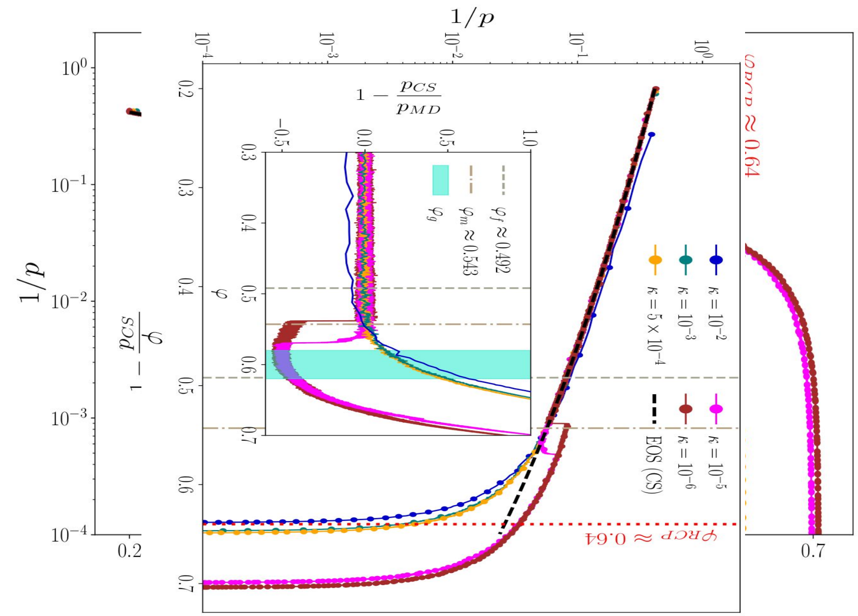
Glass and Jamming transitions

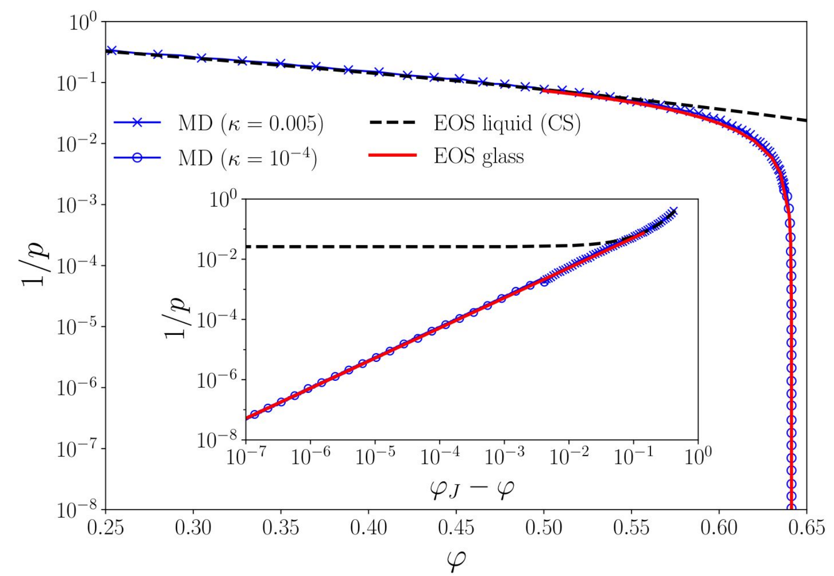


[Berthier and Ediger, *Physics Today 69* **(2015)**]



[van Hecke, *J. Phys.: Cond. Matter* **(2010)**]





Mean Field picture of glasses near jamming

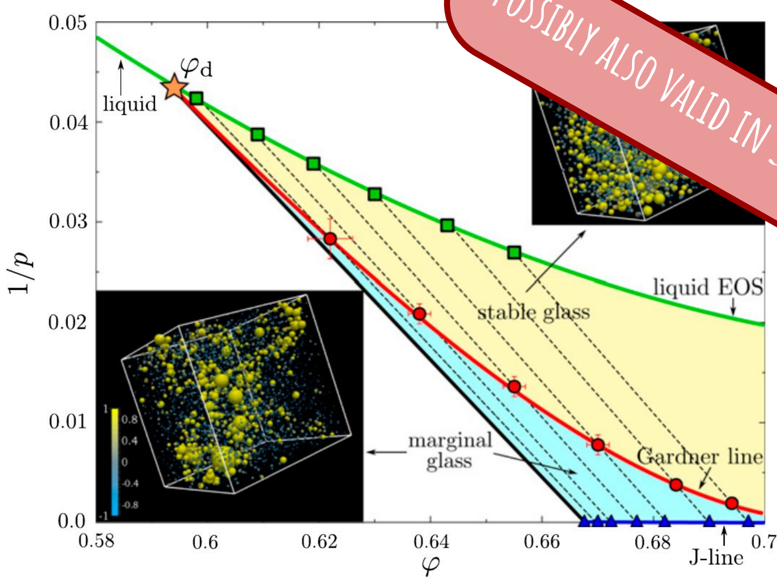
1. **Dynamical glass transition** at φ_d

2. An (equilibrated) glass state is identified by its values of p and φ

3. It can be *adiabatically compressed* (and decompressed) until a **Gardner transition** comes about, at φ_G

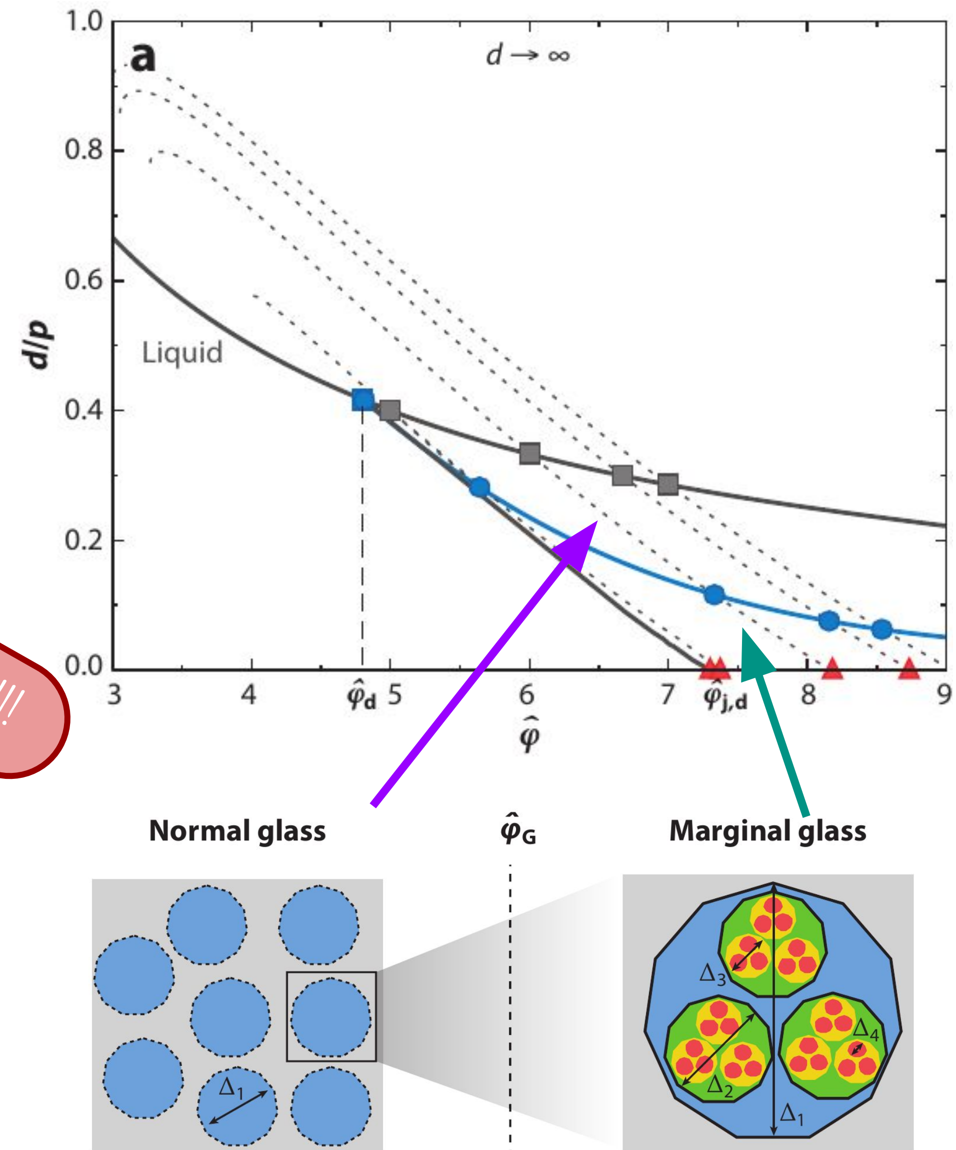
4. For $\varphi > \varphi_G$, the glass is in a **marginal phase**, that ends at jamming.

POSSIBLY ALSO VALID IN $3d$!!!

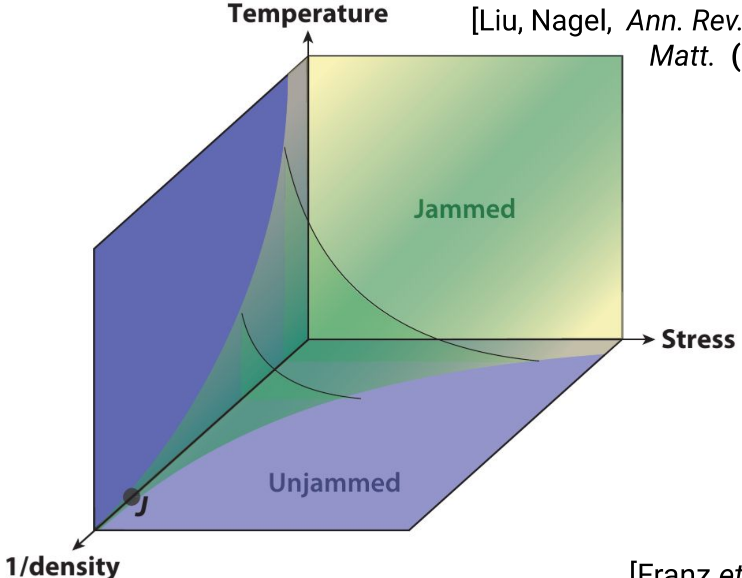


[Berthier *et al.*, *PNAS* **(2016)**]

[Charbonneau *et al.*, *Ann. Rev. Cond. Matt.* **(2017)**]



Jamming: same phenomena different systems

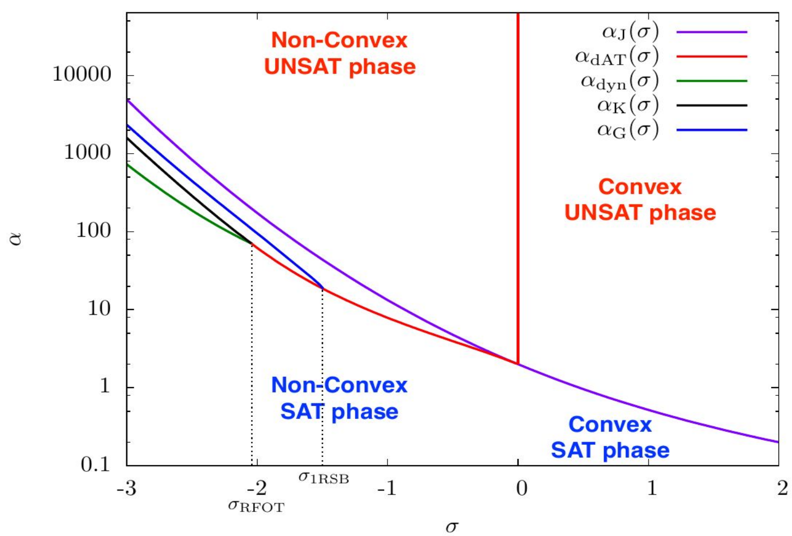


[Liu, Nagel, *Ann. Rev. Cond. Matt.* **(2010)**]

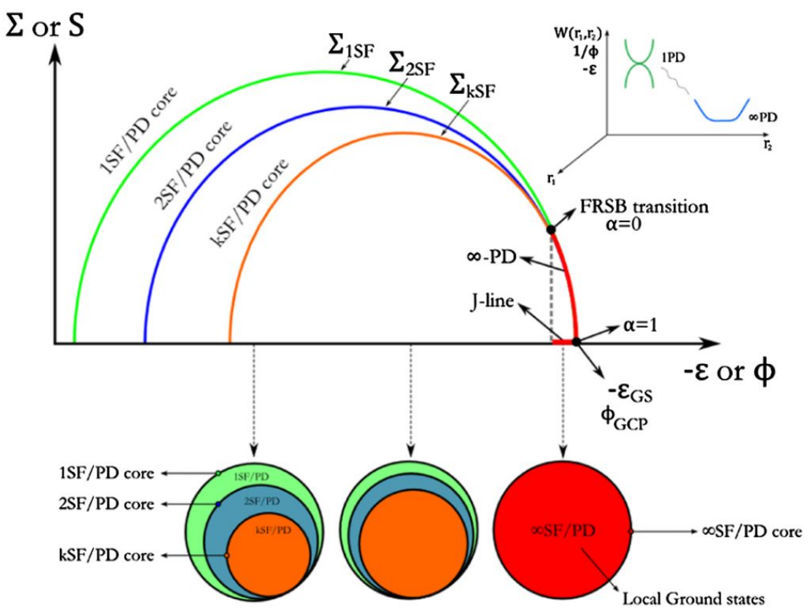
[Baule *et al.*, *Rev. Mod. Phys.* **(2018)**]

Athermal systems: foams, emulsions, grains

[Franz *et al.*, *SciPost* **(2017)**]



Constraint satisfaction problems:
Same universality class as spheres-based models



Edwards Stat Mech ⟷ FullRSB

Iterative Linear Programming Algorithm

Iterative LP Algorithm to reach jamming

Jamming as a *constrained optimization problem*: Rearrange particles in order to maximise the system density, **without any overlap between particles.**
Inspired by [Donev *et al. J. Comp. Phys.* **(2004)**] and [Torquato and Jiao, *PRE* **(2010)**]

$$\mathbf{r}_i \to \mathbf{r}_i + \mathbf{\Delta}_i \ , \quad \sigma_i \to \sqrt{\Gamma}\sigma$$

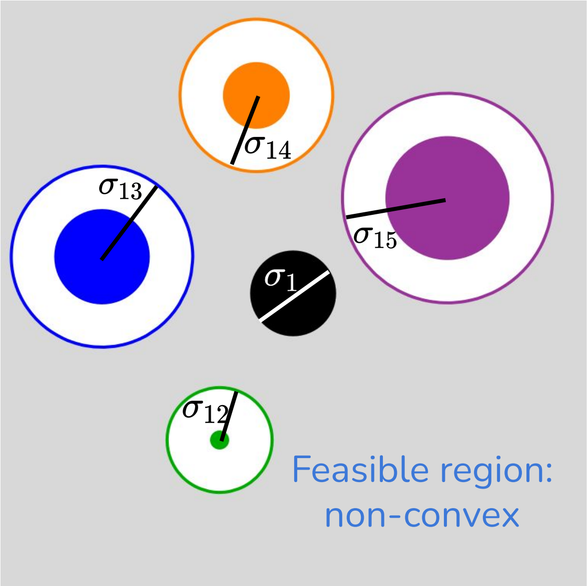
A version used for polydisperse spheres was introduced in [Artiaco, Baldan, Parisi *PRE,* **(2020)**]

EXACT FORMULATION:

$$\max \Gamma$$
$$\text{s.t.} \quad ||\mathbf{r}_i + \mathbf{\Delta}_i - (\mathbf{r}_j + \mathbf{\Delta}_j)||^2 \geq \Gamma \sigma_{ij}^2$$

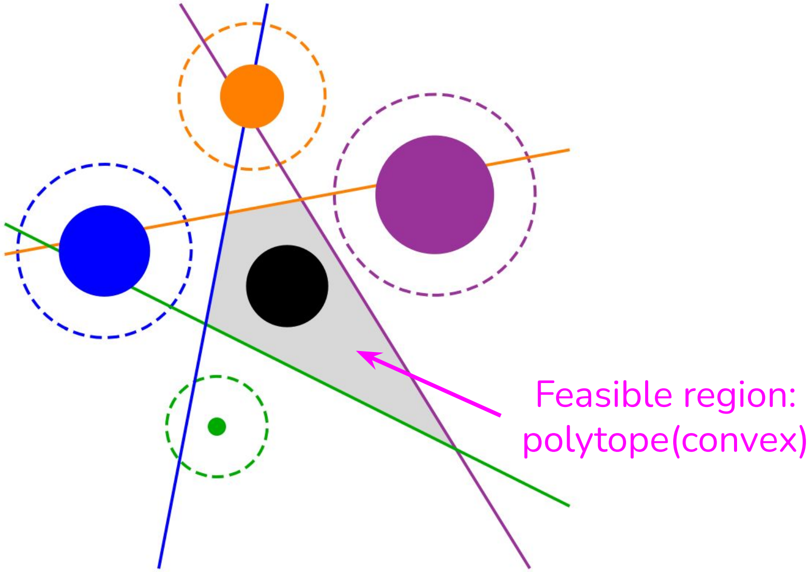
LINEAR APPROXIMATION:

$$\max \Gamma$$
$$\text{s.t.} \quad 2\,(\mathbf{\Delta}_i - \mathbf{\Delta}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j) \geq \Gamma \sigma_{ij}^2 - ||\mathbf{r}_i - \mathbf{r}_j||^2$$



Non-convex problem

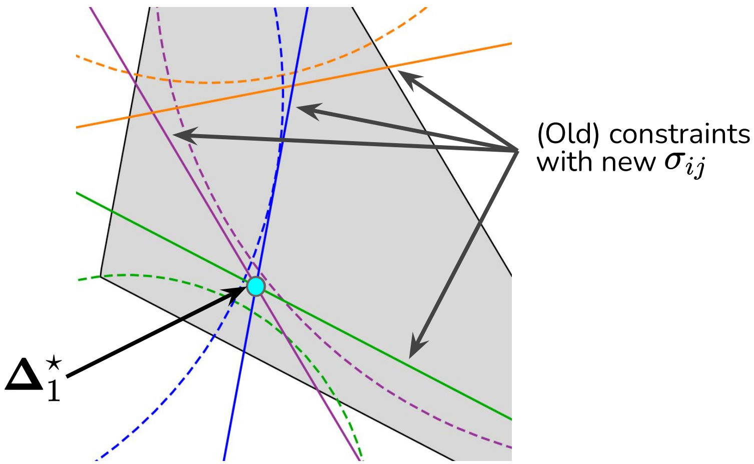
(Very hard!!)



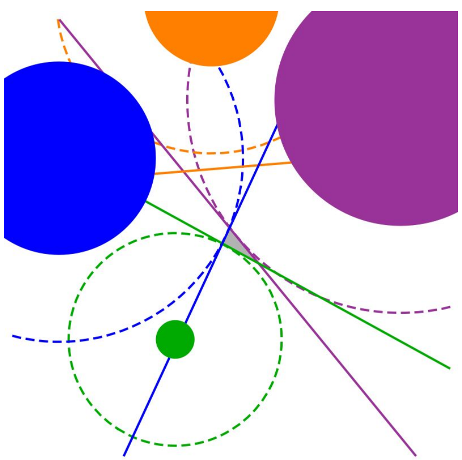
- Not huge error if close to jamming
- Easy (Linear Programming)
- Several iterations to reach jamming

Iterative LP Algorithm to reach jamming

Optimal solution: **saturates** linear constraints

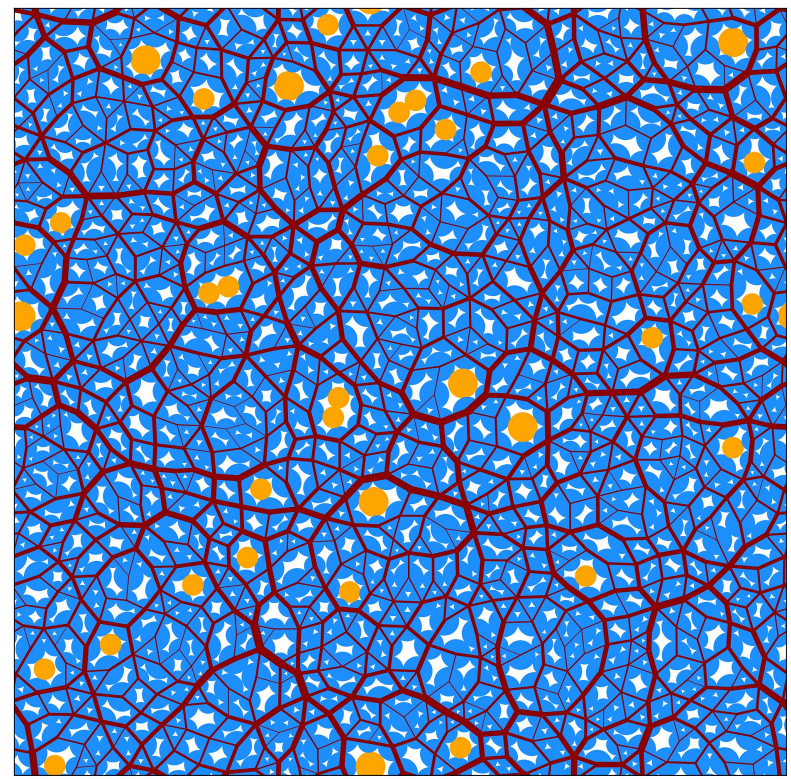


$$\max \Gamma$$
$$\text{s.t.} \quad 2\,(\boldsymbol{\Delta}_i - \boldsymbol{\Delta}_j)\cdot(\mathbf{r}_i - \mathbf{r}_j) \geq \Gamma \sigma_{ij}^2 - ||\mathbf{r}_i - \mathbf{r}_j||^2$$



Generate new instance of LP with

- Updated sizes
- Updated positions
- **Repeat!**



- *Forces* ⇔ ***active** dual variables*
- *Rattlers* ⇔ *particles with $< d+1$ contacts*

Until... $\Gamma^\star = 1\,, \quad \boldsymbol{\Delta}_i^\star = 0$

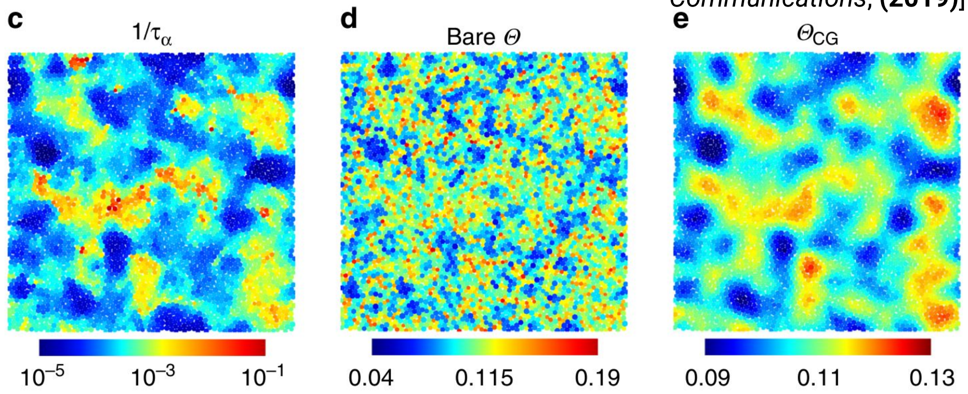
Dynamics near the jamming point

Díaz Hernández Rojas, Ricci-Tersenghi, Parisi
"Inferring the particle-wise dynamics of amorphous solids from the local structure at the jamming point",
Soft Matter 17, 1056–1083 ***(2020)***

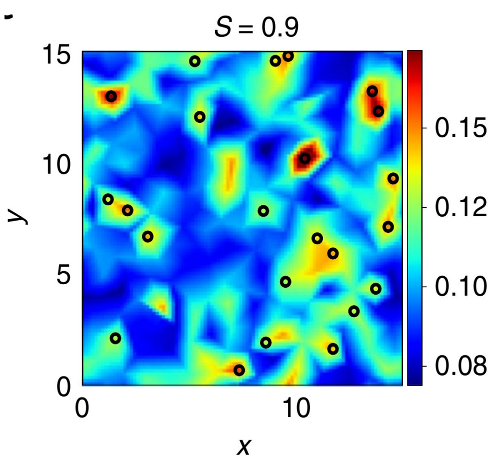
Correlation of structure and dynamics

Find a <u>connection</u> **between dynamical features** (*e.g.* relaxation time) and **local structure** (*i.e. inherent structures)*

[Tong and Tanaka, *Nat. Communications*, **(2019)**]



Require coarse graining! (*a posteriori*)



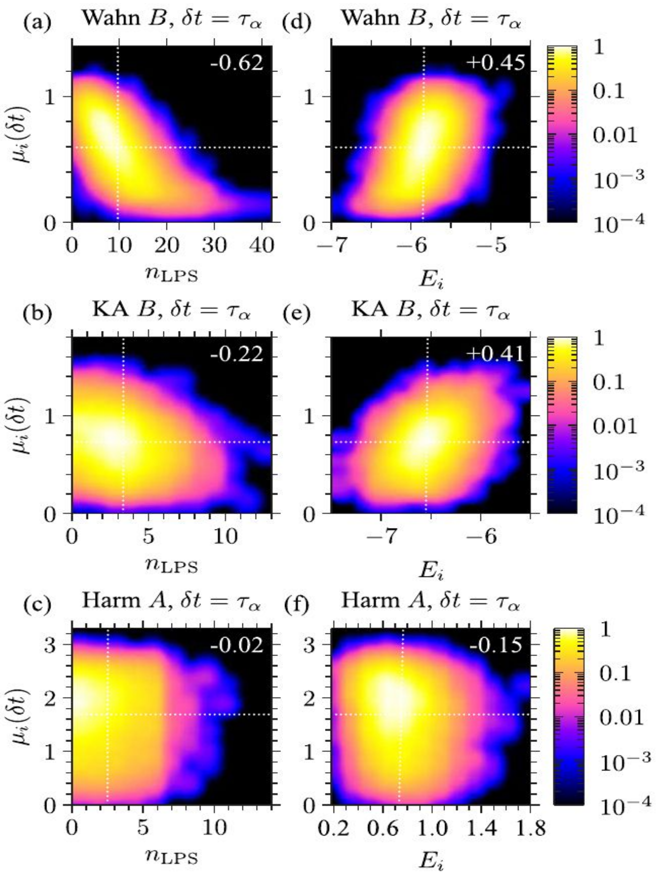
[Bapst *et al.*, *Nat. Phys.*, **(2020)**]

Machine and deep learning methods

High quality predictions of most mobile particles (black) from local structure.

Hard to obtain a physical picture (**interpretability problem**)

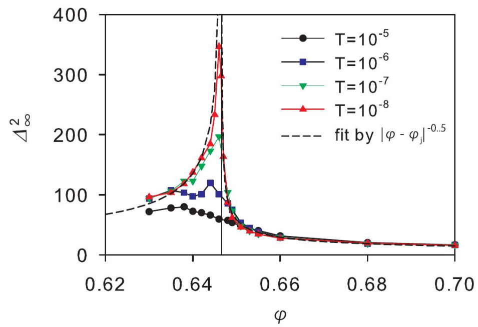
[Hocky et al, *PRL* 113, **(2014)**]

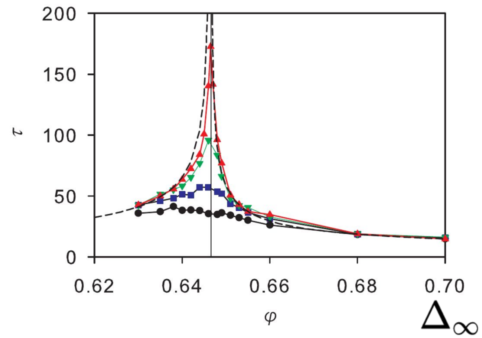


<u>**Iso-configurational ensemble**</u> (ICE):
Generate many trajectories with the same initial conditions.

- Study statistical properties of mobility
- Strong system dependence if using the wrong structural variable

... and near jamming?



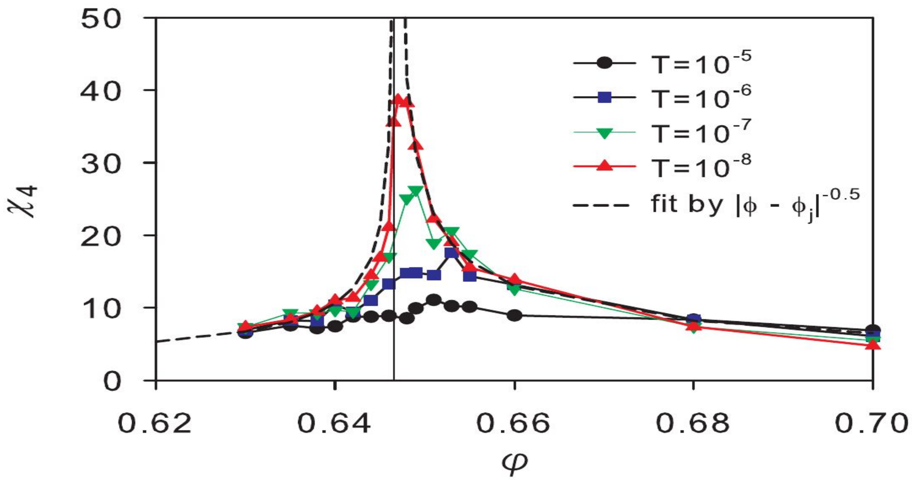


Dynamic criticality NEAR jamming

- Identified from normal modes estimation
- Mainly valid at long times
- Results derived for a **generic potential**
- Critical behaviour: $\varphi \to \varphi_J^{\pm}$
- No **single-particle** analysis

$$U(r_{ij}) \sim |r_{ij}/\sigma_{ij} - 1|^{\alpha}$$

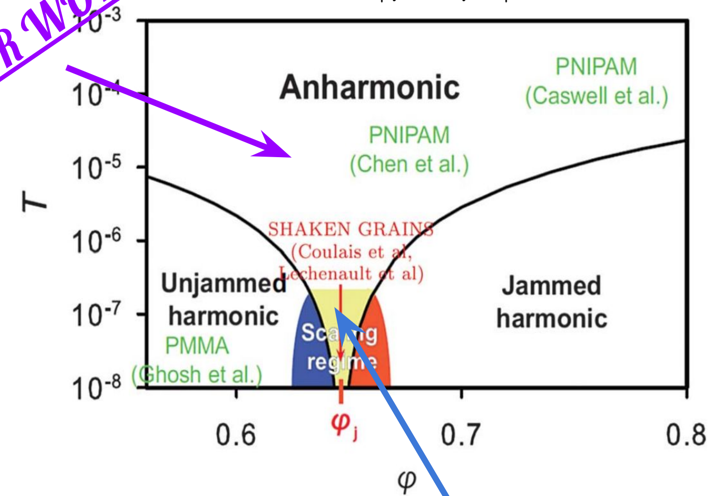
$$\Delta_{\infty} \sim \tau \sim \chi_4 \sim \xi_4^2 \sim |\varphi - \varphi_J|^{-1/\alpha}$$



[Ikeda, Berthier, Biroli, *J.Chem. Phys*, **(2013)**]

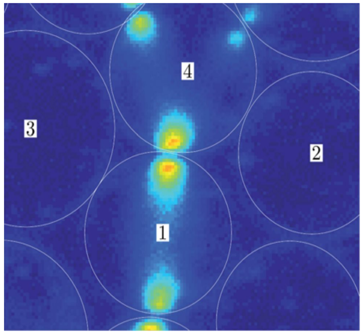
OUR WORK

$$T > T^* \sim |\varphi - \varphi_J|^{\alpha}$$



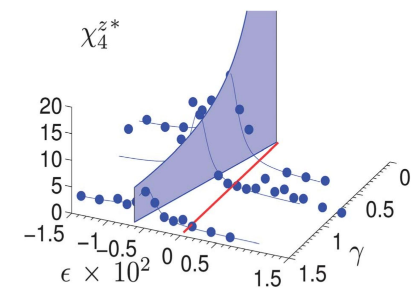
Very close to jamming.

They belong to the **anharmonic regime**



EXPERIMENTS!!!

Shaken rigid particles and viscoelastic disks



[Coulais, Behringerb, Dauchot, *Soft Matter*, **(2014)**]

Our approach:

I. Begin with an isostatic jammed configuration $(N{=}1024)$
(**generated via *iLP***)

II. Move away from the jamming point by a *small amount* to generate trajectories

$\{\delta\mathbf{r}_i(t)\}_{i=1}^{N}$

$\{|\delta\mathbf{r}_i(t)|^2\}_{i=1}^{N}$

MOLECULAR DYNAMICS
with **hard spheres**

$$0.98 \leq \varphi/\varphi_J \leq 0.999$$

5,000 independent trajectories

MONTE CARLO simulations
at small *T*

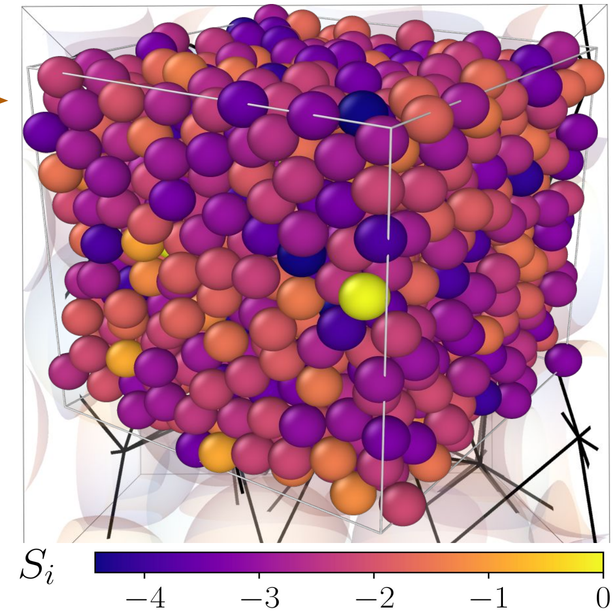
$$U(r_{ij}) = |r_{ij} - D_J|^{\alpha}\,\Theta(D_J - r_{ij})$$

$$\alpha = \{3/2,\ 2,\ 5/2\}$$

1,000 independent trajectories

Always with the **same initial condition** $\mathbf{r}_i(0) = \mathbf{r}_i^{(J)}$

I.e. We'll sample from the ICE



$$\mathbf{n}_{ij} = \frac{\mathbf{r}_i^{(J)} - \mathbf{r}_j^{(J)}}{|\mathbf{r}_i^{(J)} - \mathbf{r}_j^{(J)}|}$$

$$\mathbf{C}_i = \sum_{j\in\partial i} \mathbf{n}_{ij}$$

$$S_i = \sum_{j<k\in\partial i} \mathbf{n}_{ij}\cdot\mathbf{n}_{ik}$$

III. Study statistics of displacements

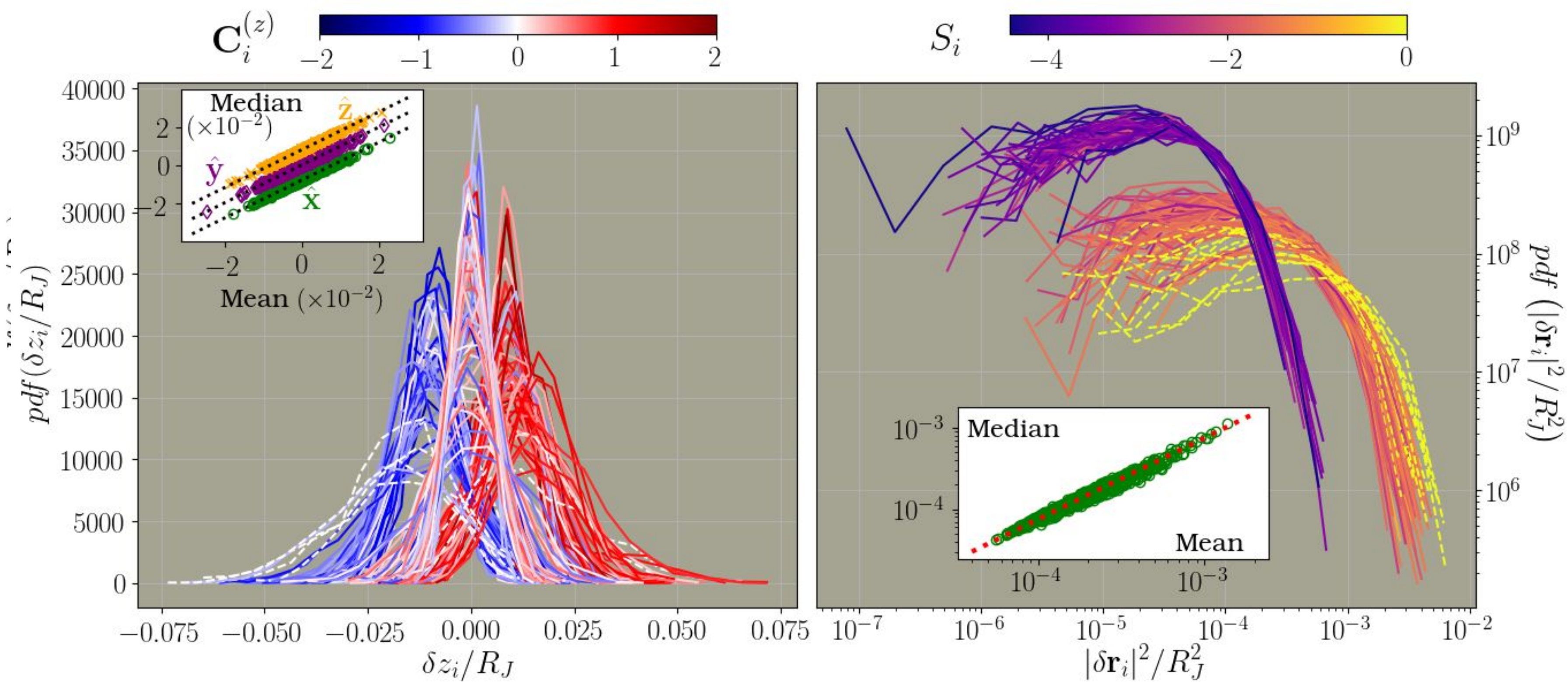
[per particle]

a) Find preferential directions

b) How much do particles move

Statistical correlations ?

How do particles move?



Preferential directions of motion

$$\langle \delta \mathbf{r}_i \rangle \neq 0$$

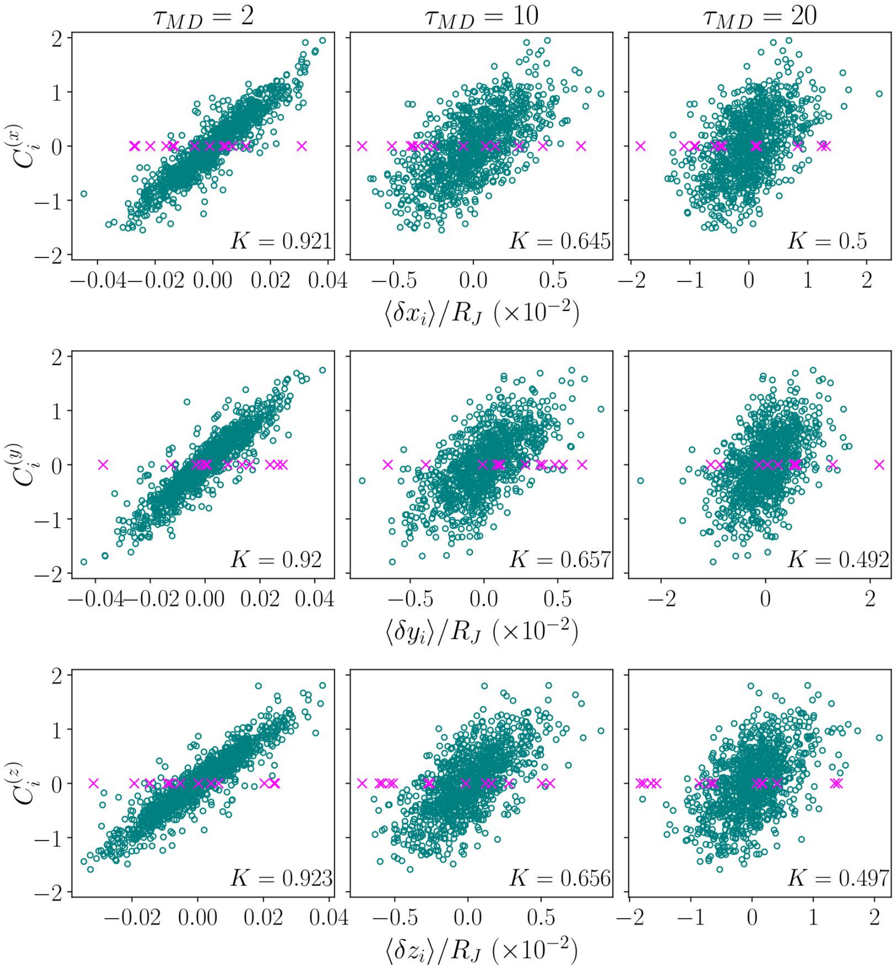
- Broad range of mobilities
- Non-negligible sample to sample fluctuations

We will use the first moments instead of the full distribution

Correlation in hard sphere systems (Mol. Dyns.)

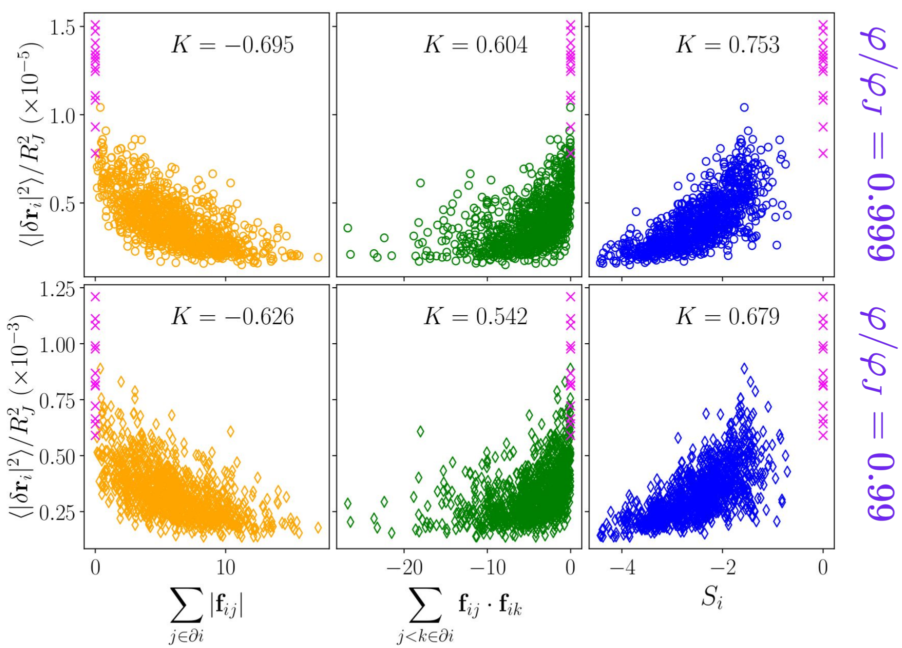
$(\beta = 10)$

$\varphi = 0.995\varphi_J$



Test different (scalar) structural variables

$(\tau_{MD} = 10)$



$$S_i \sim \langle |\delta \mathbf{r}_i|^2 \rangle$$

$$\mathbf{C}_i \sim \langle \delta \mathbf{r}_i(t) \rangle$$

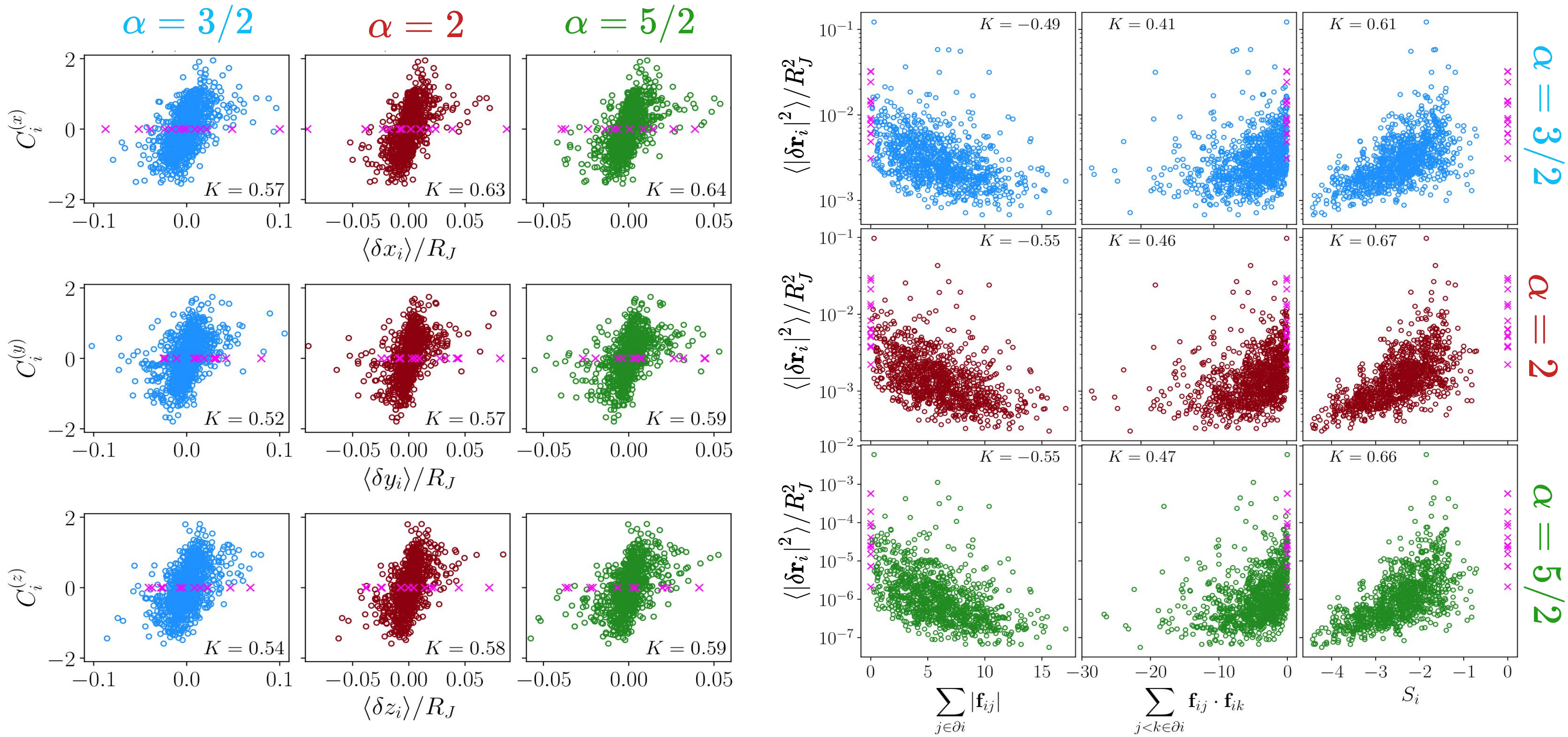
K = Spearman correlation

× → Rattlers

τ → Collisions/particle

Correlation in soft sphere systems (Monte Carlo)

$(\varphi = \varphi_J)$



Very simply and robust method:

- Applicable to *different dynamical protocols* and *potentials*
- "**Universal**" decorrelation rate
- We can predict mobilities and preferential directions, by ranking according to S_i (short times)

K = Spearman correlation
× → Rattlers
(τ =250 MC steps)

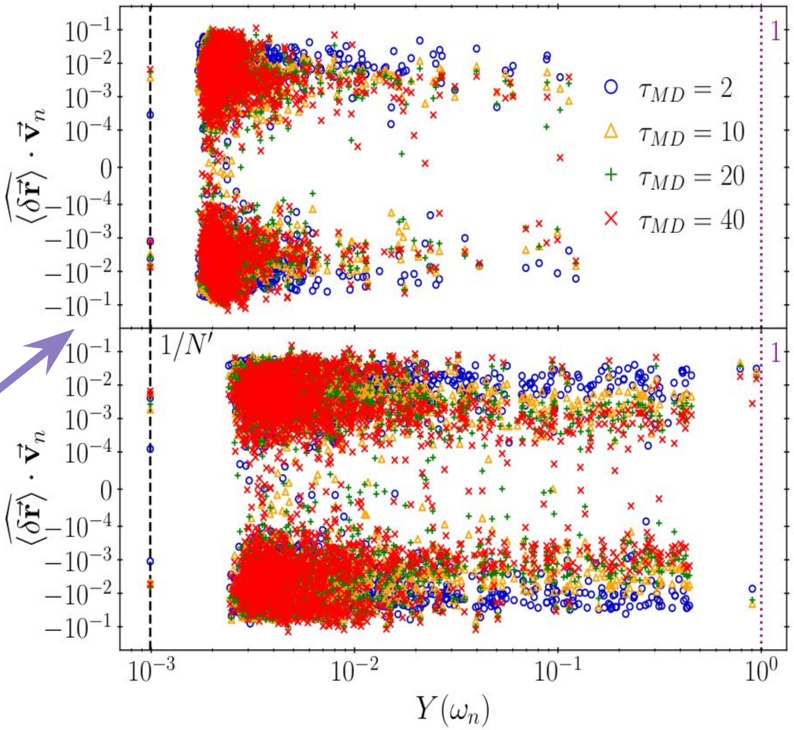
In summary

1. Nearest neighbours (contacts) can be used to infer statistical properties of short time dynamics.
   a. We obtained a particle-wise description of:
      i. Preferential directions: $\langle \delta \mathbf{r}_i \rangle \sim \mathbf{C}_i$
      ii. Mobility: $\langle |\delta \mathbf{r}_i|^2 \rangle \sim S_i$
   b. Information about the forces is redundant and **worsens** the quality of the inference.

2. Particles not only vibrate around an energy minimum configuration. ⇒ Normal mode description fails!
   a. Displacements do not occur along eigenmodes.
   b. No criterion for selecting the relevant modes.

3. System independent decorrelation: likely related to how the configuration initially explores a meta-basin.

$$\mathcal{H}\mathbf{v}_n = \omega_n^2 \mathbf{v}_n$$



ToDo's

- Perform inference on full distribution of displacements and mobilities (not only their first moment).
- Analyse correlations of structural variables: if particles are **dynamically** correlated, they must also be **structurally**
- Improve duration of inference by, *e.g.* including more neighbours and coarse graining.

Finite size scaling of critical distributions of forces and gaps

In collaboration with:

- Patrick Charbonneau
- Eric Corwin
- Cameron Dennis
- Harukuni Ikeda

"Finite size effects in the microscopic critical properties of jammed configurations: a comprehensive study of the effects of different types of disorder",
arXiv:2011.10899 ***(PRE accepted)***

Scaling collapse to validate critical exponents

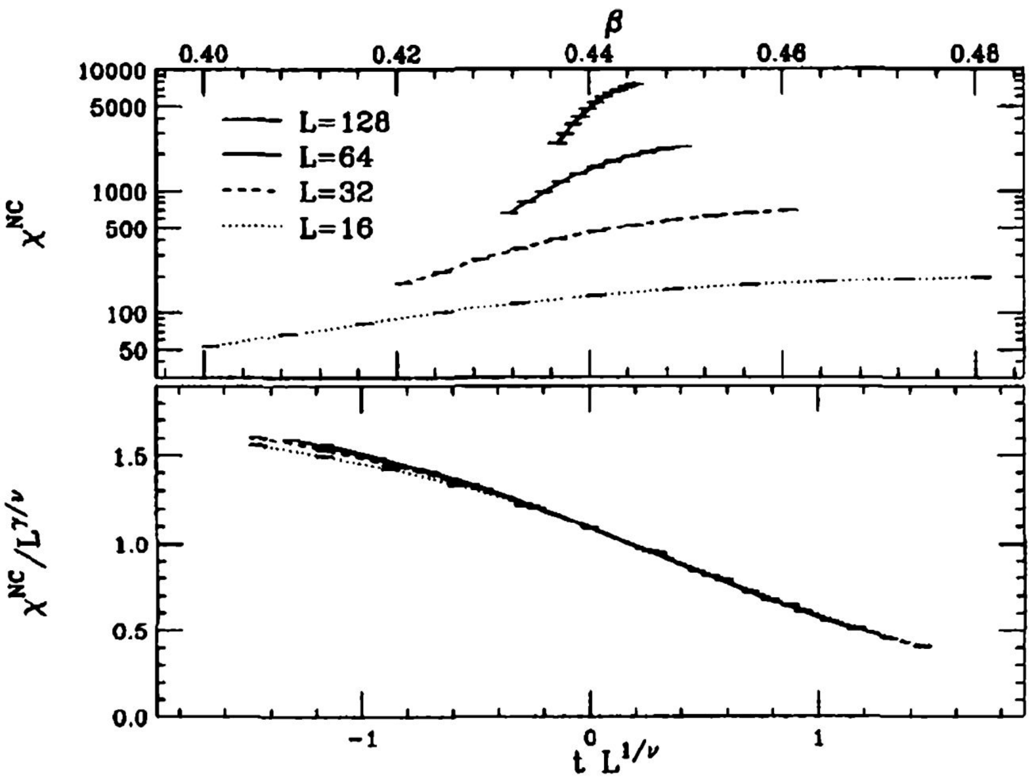
$$\chi = V[\langle m^2 \rangle - \langle m \rangle^2] \sim |t|^{-\gamma}$$

$$t = \frac{T - T_c}{T_c} \qquad \xi \sim |t|^{-\nu}$$

Divergence at the critical point!!

Only in the **thermodynamic limit**, $L \to \infty$

[Amit, Martín-Mayor, *Field Theory, RG, and Critical Phenomena* **(2005)**]



In finite systems:

$\xi \leq L \qquad \chi \sim \xi^{\gamma/\nu}$

$$\chi \sim |t|^{-\gamma} F(L\,|t|^{-\nu}) \sim L^{\gamma/\nu} \widetilde{F}(L^{1/\nu}|t|)$$

Validating *Jamming criticality* as $\varphi \to \varphi_J^+$

What happens exactly at $\varphi = \varphi_J$?

$v(h) = \frac{1}{\alpha}|h|^{\alpha}\Theta(-h)$

$h = \frac{r_{ij}}{\sigma_{ij}} - 1$

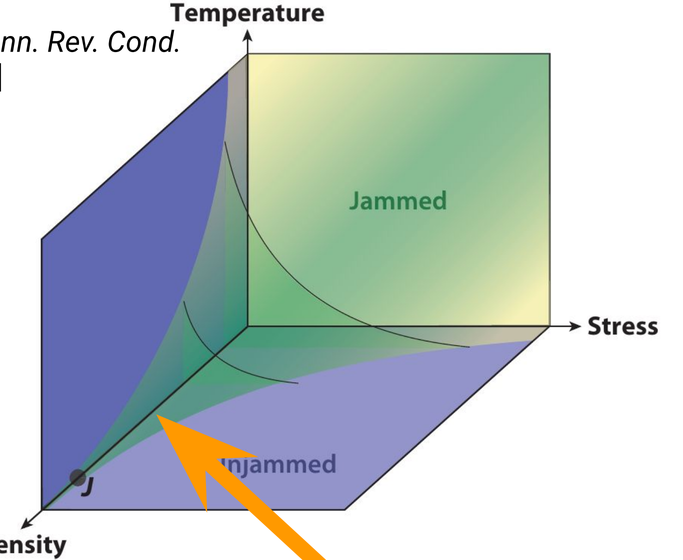
E

$p \sim$

B -

Z -

[Liu, Nagel, *Ann. Rev. Cond. Matt.* **(2010)**]



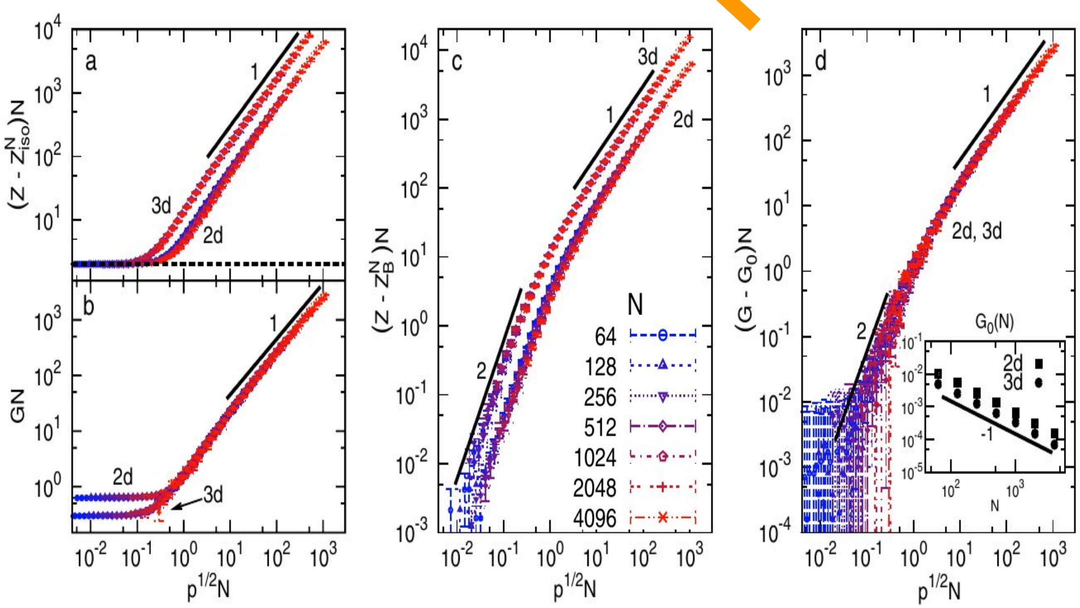
Criticality at the jamming transition:

1. There is **NO** (usual) **correlation length**
2. Size scaling is caused by the condition of **Single State of Self Stress**:

$$N_c = \frac{Z}{2} = N_{iso} + 1$$
$$N_{iso} = N_{dof} = d(N-1)$$

3. Scaling relations can be thus obtained:

$$Z - Z_N^{iso} \sim \frac{1}{N} F(p^{1/2} N)$$

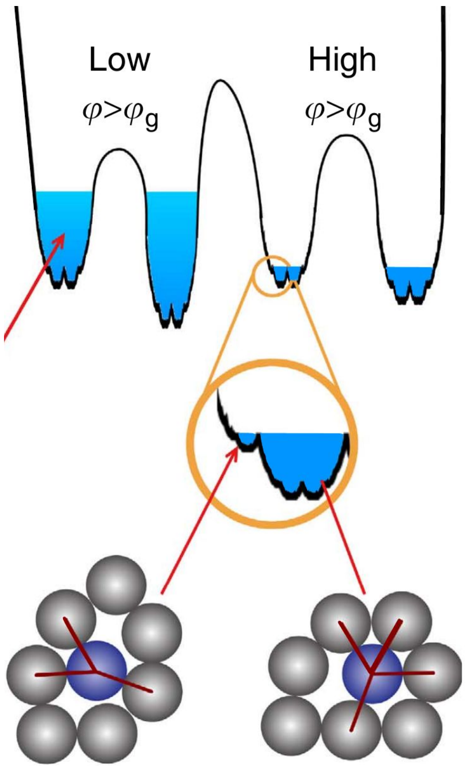


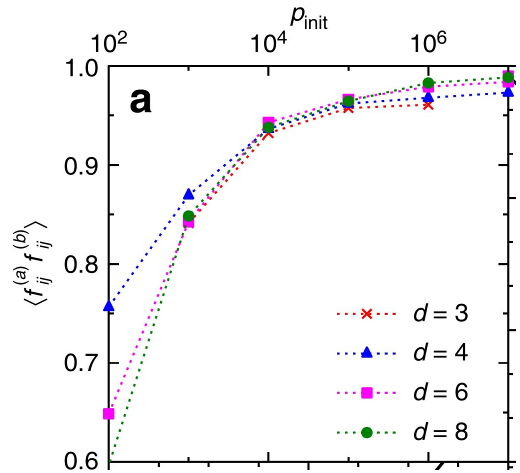
[Goodrich, Liu, Nagel, *PRL* **(2012)**]

Hierarchical free energy landscape

[Charbonneau, Kurchan, Parisi, Urbani, Zamponi, *Nat. Communications*, **(2014)**]

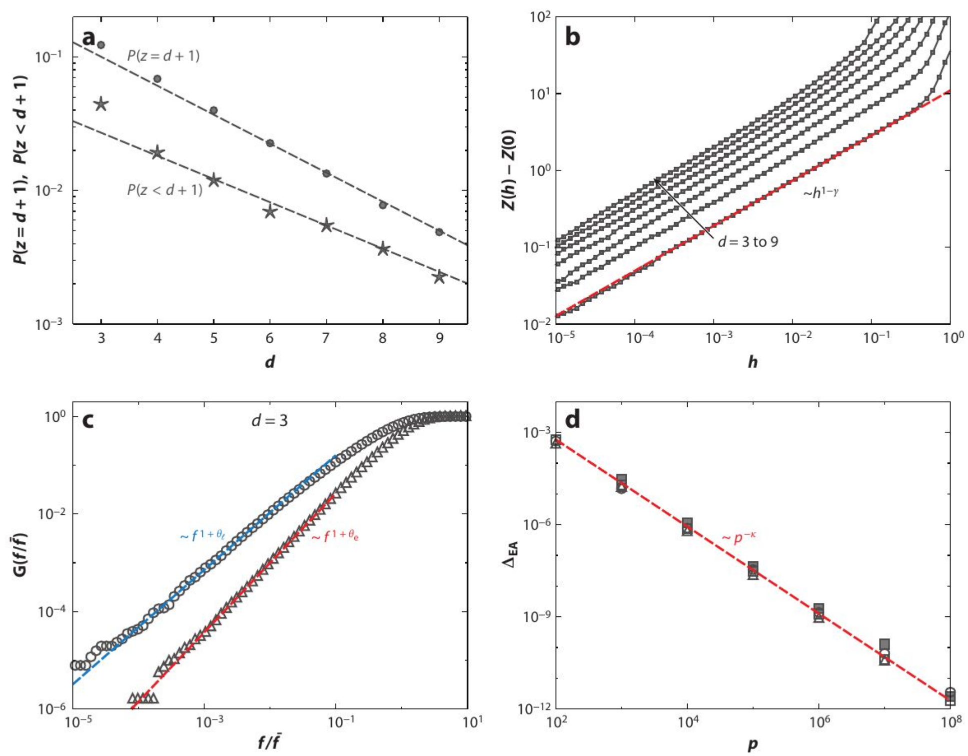
*Forces are determined **gradually** when going down a meta-basin*





Test similarity of network of contacts between different jammed states

$$f_{ij}^{(a)} f_{ij}^{(b)} = \begin{cases} 1 & (i,j) \text{ in contact in both configurations} \\ 0 & \text{otherwise} \end{cases}$$



$$h_{ij} = \frac{r_{ij}}{\sigma_{ij}} - 1$$

$$p(h) \sim h^{-\gamma}$$

$$\gamma = 0.41269\ldots$$

$$\Delta_{EA} \sim p^{-\kappa}$$

$$\kappa = 1.4157\ldots$$

$$p(f_e) \sim f_e^{\theta_e}$$

$$\theta_e = 0.42311\ldots$$

[Charbonneau *et al.*, *Ann. Rev. Cond. Matt.* **(2017)**]

Why studying Finite Size Effects at jamming?

1. **Exact** MF predictions for the contact forces and interparticle gaps $(h_{ij} = \frac{r_{ij}}{\sigma_J} - 1)$

$$\begin{cases} p(f) \sim f^{\theta_e}, & \theta_e = 0.42311\dots \\ g(h) \sim h^{-\gamma}, & \gamma = 0.41269\dots \end{cases}$$

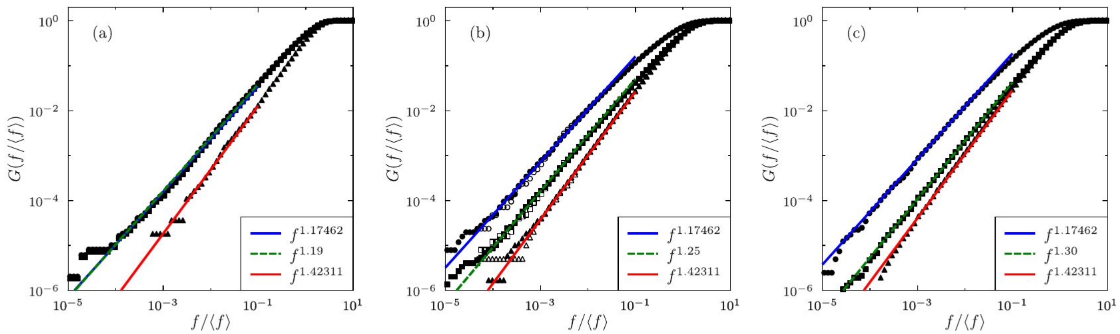
... but uses $d \to \infty$ assumption

2. But maybe also valid in d=2,3,...

Not systematic study so far.

In *finite d* another contribution: **localized forces ⟺ bucklers**

$$p(f_\ell) \sim f_\ell^{\theta_\ell}, \quad \theta_\ell \approx 0.17$$



[Charbonneau, Corwin, Parisi, Zamponi, *PRL*, **(2015)**]

3. Stability bounds **(SATURATED)**

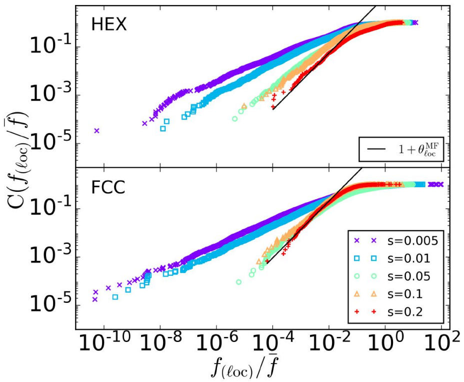
$$\gamma \geq \frac{1}{2+\theta_e} \qquad \gamma \geq \frac{1-\theta_\ell}{2}$$

An accurate estimation is very important.

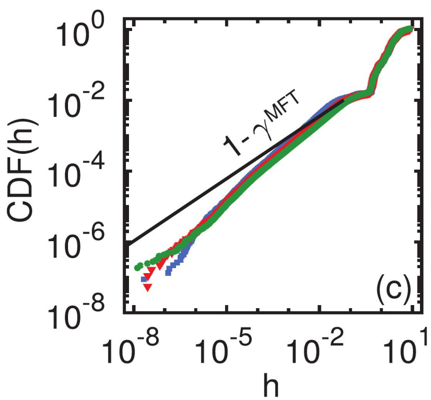
FSS is a <u>very precise technique</u> for estimating critical exponents.

Already tested in perceptron; see [Kallus, *PRE*, **(2016)**]

4. Other models (crystals) have ***different*** scalings



[Tsekenis, arXiv: *2006.07373*, **(2020)**]



[Charbonneau *et al.*, *PRE*, **(2019)**]

Our models and methods

Rigid particles
Jamming via
MD+iLP

Mari-Kurchan model in *d=3*
(MF-like, useful reference)

Monodisperse spheres

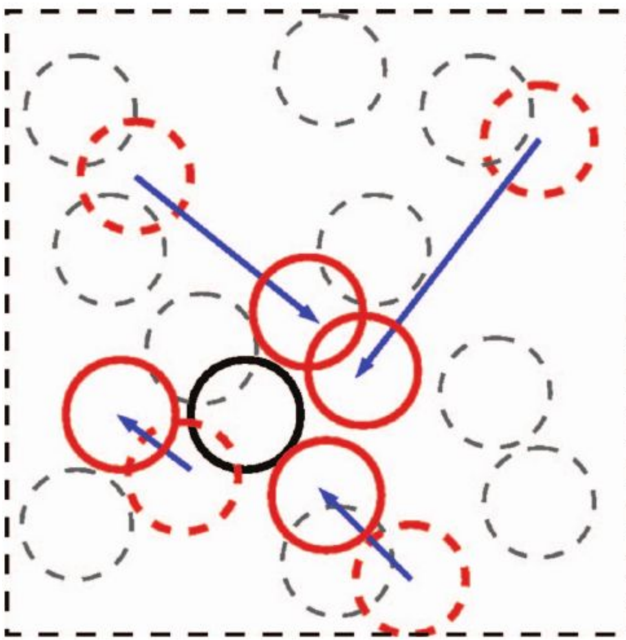
Polydisperse disks
(upper critical dimension)

Near crystals
(3d, minimally polydisperse)

Soft particles
Jamming via
FIRE

$\varphi \to \varphi_J^-$

$\varphi \to \varphi_J^+$



[Mari, Kurchan, *J. Chem. Phys.* **(2011)**]

$$D(\mathbf{r}_i, \mathbf{r}_j) = |\mathbf{r}_i - \mathbf{r}_j + \mathbf{A}_{ij}|$$

samples

aps in each

if $\rho(x) \sim x^\alpha \implies \int_0^{x_{\min}} \rho(x)\,\mathrm{d}x \sim x_{\min}^{1+\alpha} \sim \frac{1}{N}$

$$\rho(x) \sim N^{\frac{-\alpha}{1+\alpha}}\ \tilde{\rho}\left(xN^{\frac{1}{1+\alpha}}\right)$$

$$D(\mathbf{r}_i, \mathbf{r}_j) \simeq \sigma_{ij}$$

he same N

$$D(\mathbf{r}_i, \mathbf{r}_k) \simeq \sigma_{ik}$$

$$\int_0^x \rho(x')\,\mathrm{d}x'$$

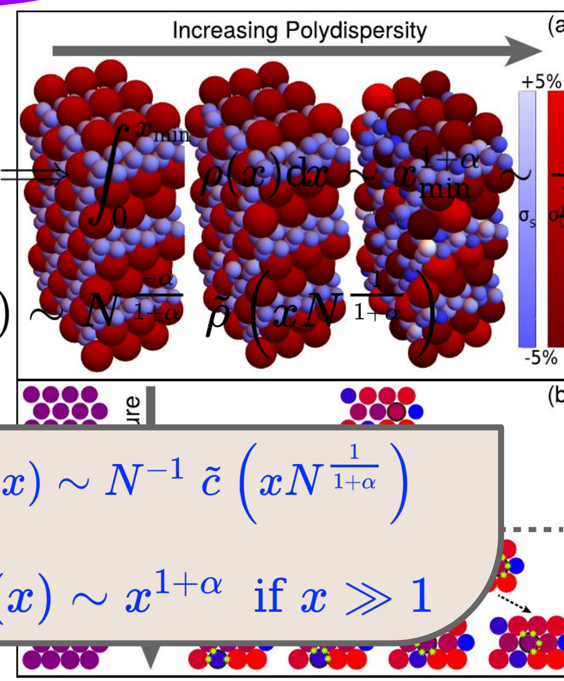
$\mathbf{A}_{ij} \sim \mathrm{Unif}(V)$

nt N using

ts and

$$D(\mathbf{r}_j, \mathbf{r}_k) \gg \sigma_{jk}$$

lapse



$$c(x) \sim N^{-1}\ \tilde{c}\left(xN^{\frac{1}{1+\alpha}}\right)$$

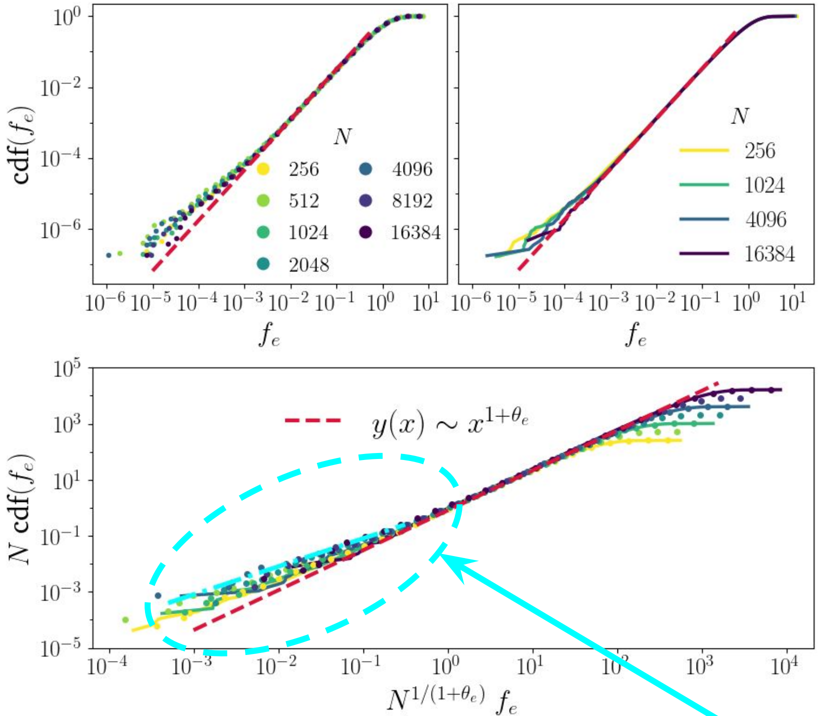
$$\tilde{c}(x) \sim x^{1+\alpha} \quad \text{if } x \gg 1$$

[Charbonneau at *et al*, *PRE* **(2019)**]

Results with monodisperse spheres

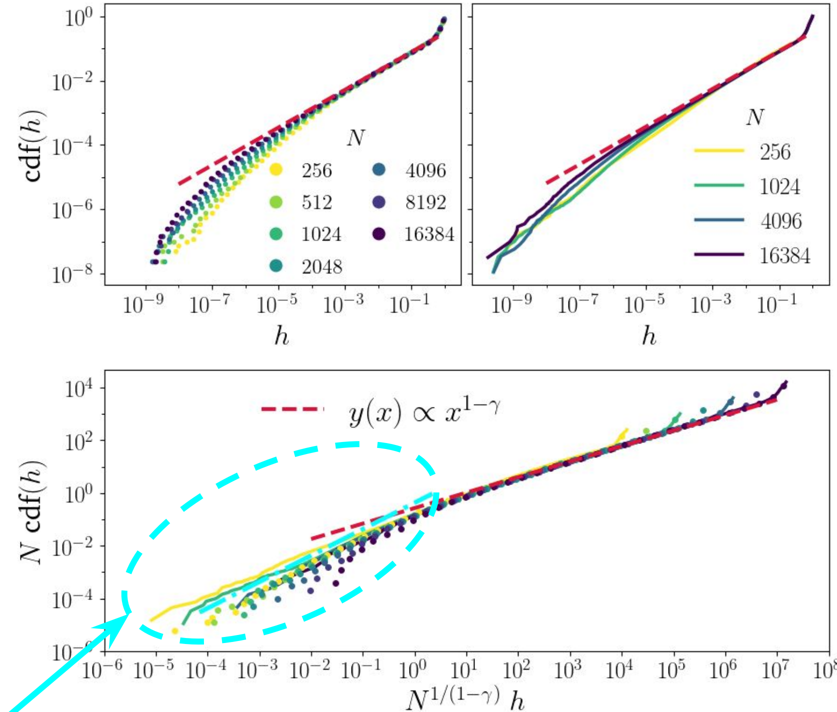
FORCES (extended): negligible size effects.

Hard spheres | Soft spheres



GAPS: clear signatures of finite N corrections

Hard spheres | Soft spheres



$\theta_e =$ MF prediction

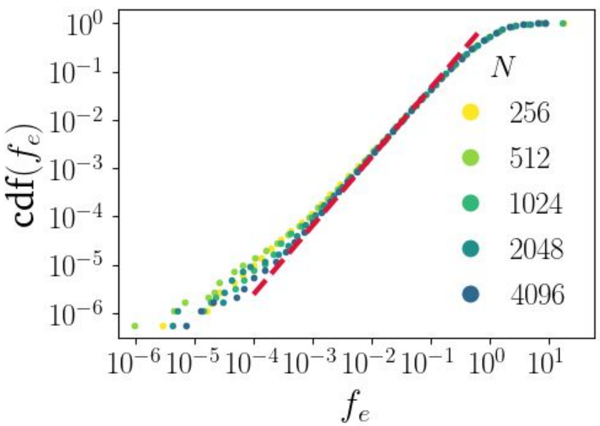
Linear regime!!

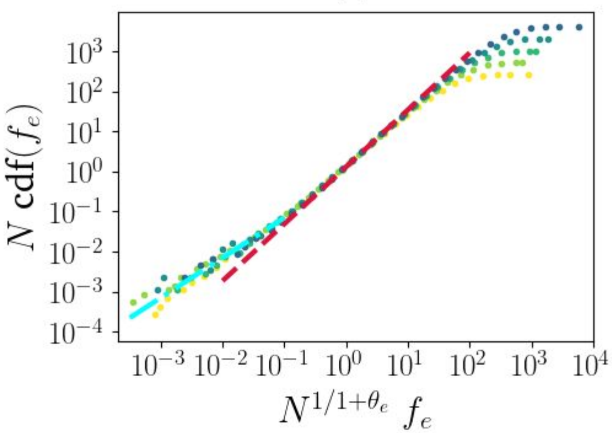
$\gamma =$ MF prediction

Perfect matching of both limits: $\varphi \to \varphi_J^{\pm}$

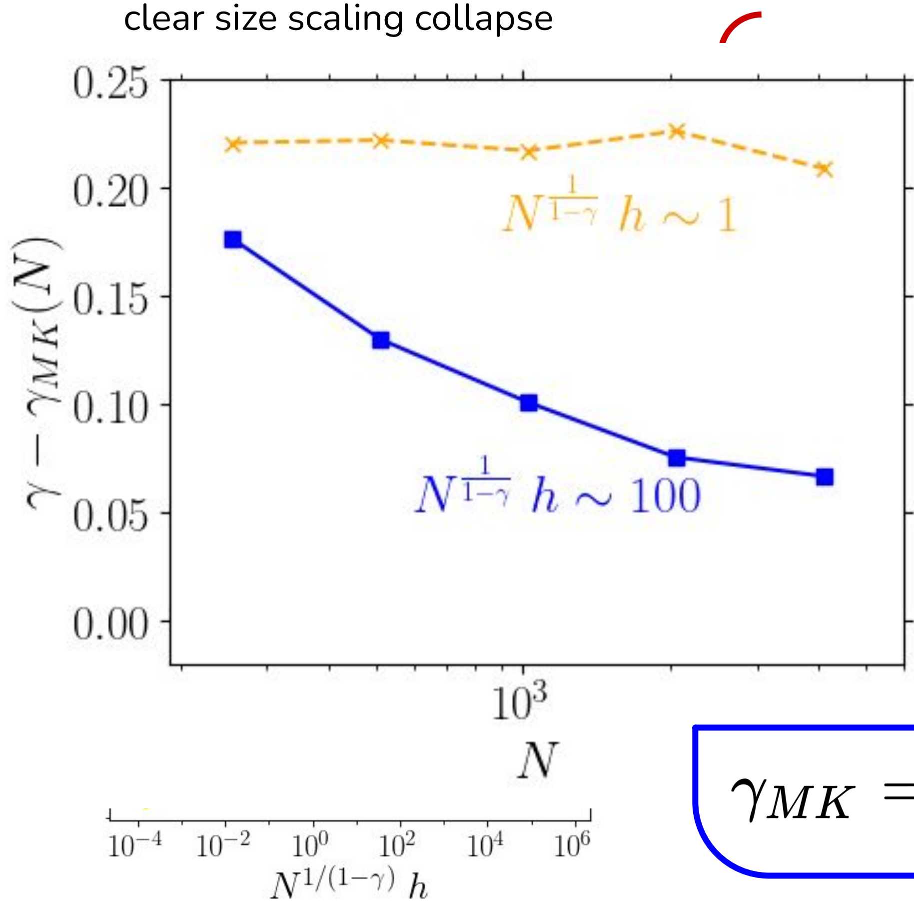
Scaling in MK model

FORCES (extended):
Small but noticeable size effects





GAPS:
clear size scaling collapse



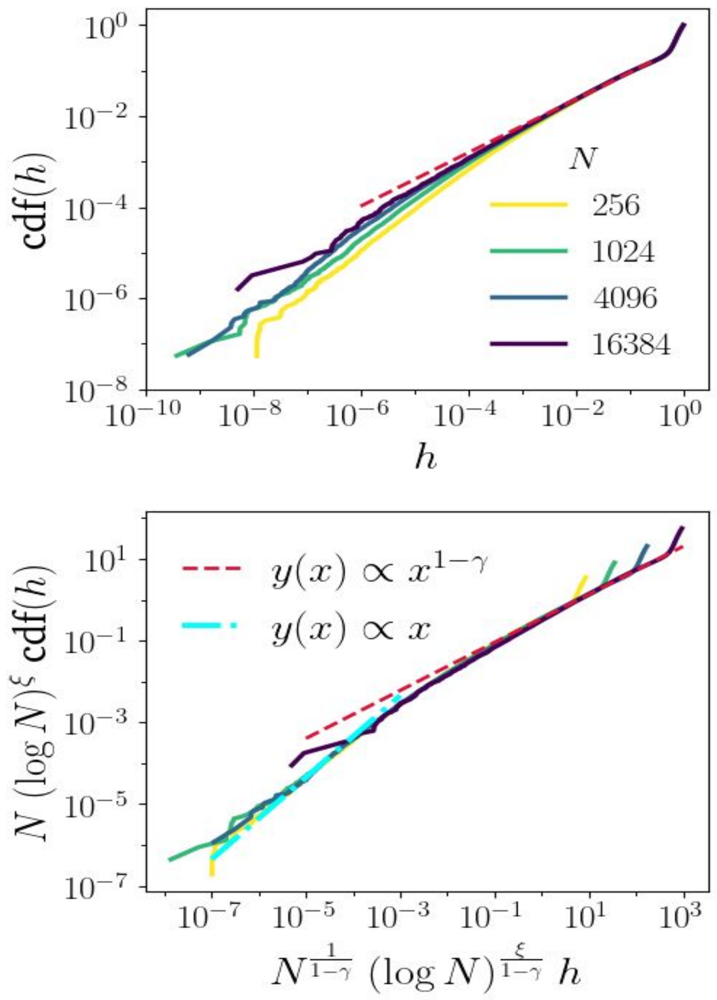
$$\gamma_{MK} = \gamma$$

Pronounced finite N effects due to:

1. **Fully connected** MF model
   ⇒ *very large systems needed to observe thermodynamic limit behaviour*
2. Very high connectivity (1% of spheres have $z > 12$) and large particles ($\varphi_J \geq 3.1$)
   ⇒ **Reduced effective size**

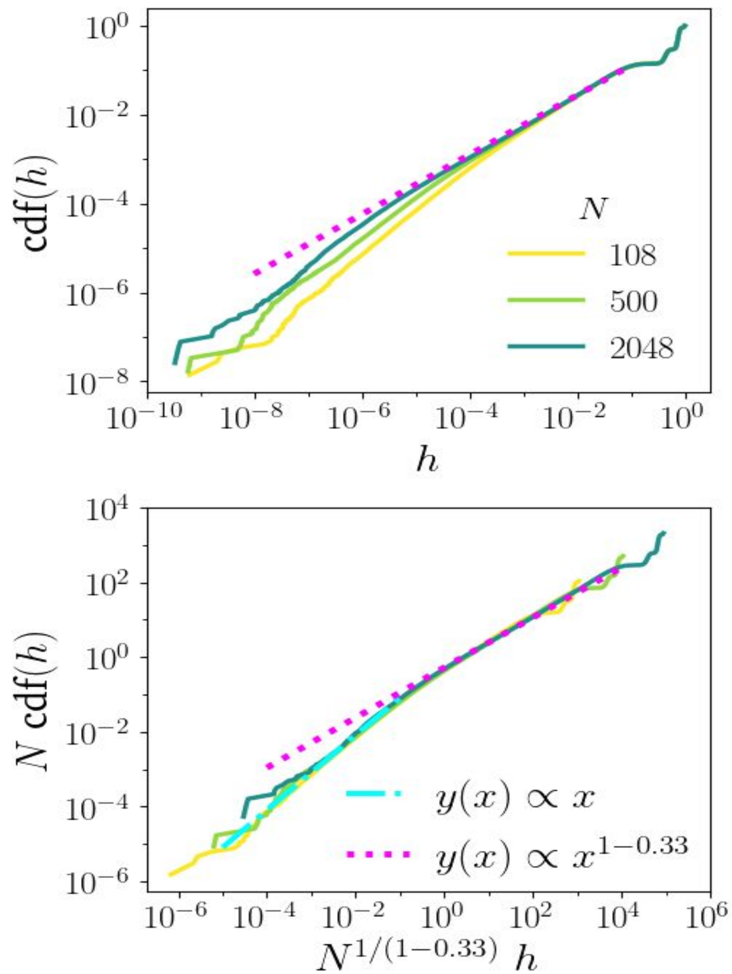
Gaps scaling in other models

Polydisperse disks (radii ~ log-normal dist.)



Upper crit. dim. ⇒ **Logarithmic corrections**

Minimally polydisperse FCC crystal



$\gamma_{FCC} \neq \gamma$

(Violates stability bounds!!)

What did we learn?

1. **Verified the exponents** predicted by *Mean Field theory*

$$p(f_e) = \begin{cases} N^{\frac{-\theta_e}{1+\theta_e}} p_0(fN^{\frac{1}{1+\theta_e}}), & \text{if } fN^{\frac{1}{1+\theta_e}} \ll 1 \\ f^{\theta_e}, & \text{if } fN^{\frac{1}{1+\theta_e}} > 1 \end{cases} \xrightarrow{p_0(x) \sim 1} \tilde{c}(x) \sim \begin{cases} x, & x \ll 1 \\ x^{1+\alpha}, & x \gg 1 \end{cases}$$

2. *d=2* is **the upper critical dimension** (corroborated by logarithmic corrections to scaling)

3. Scaling collapse **much clearer in gaps** distribution (+ forces in MK)

¿¿¿

$$\xi_h \geq N^{1/d}, \quad \xi_f \ll N^{1/d} \implies \xi_h \gg \xi_f$$

???

4. **Crystalline ordering** seems to break universality (*localized forces and gaps*).

5. Linear regime is notoriously robust (present in **all the models**). It can be observed clearly in gaps distribution and possibly also in the (extended) forces distribution.

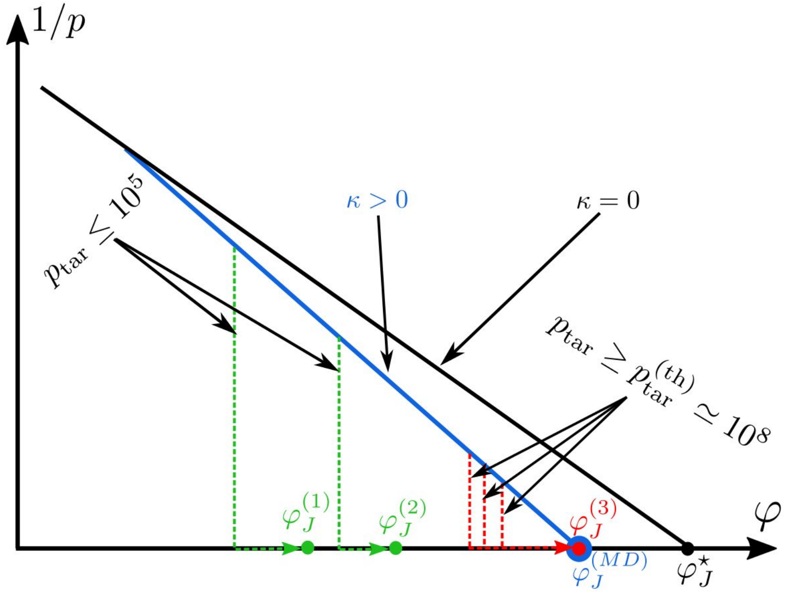
Possibly due to **1S-SS** condition (global property)

6. It is likely that *stability bounds need to be generalized* to deal with *other types of disorder* (**near crystals, MK**)

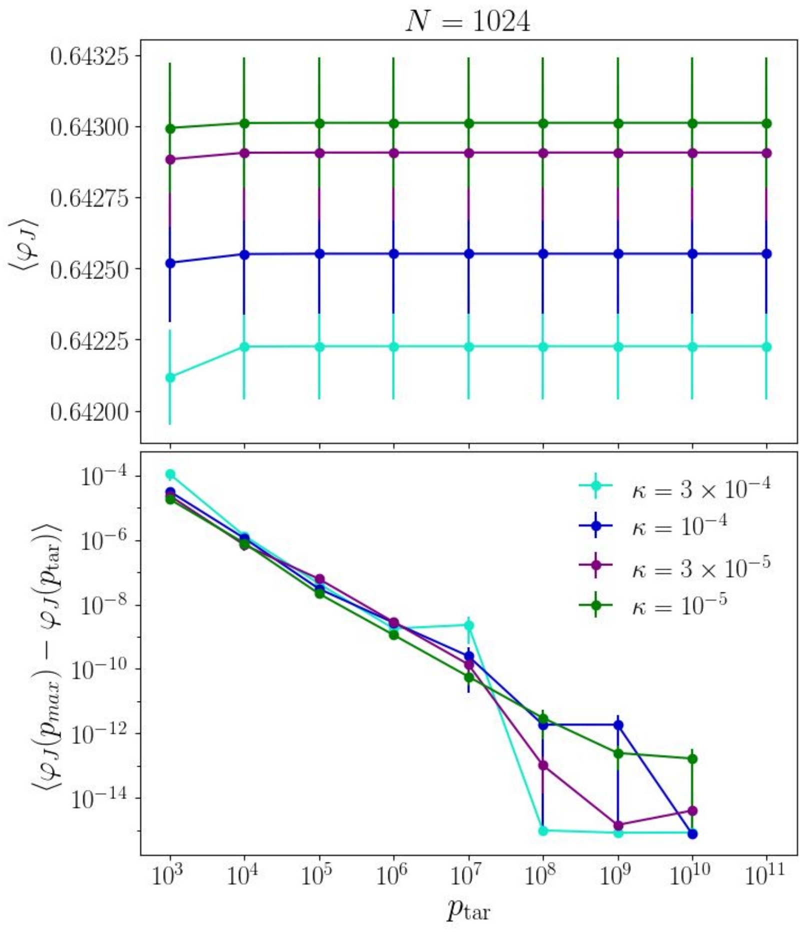
MUCHAS GRACIAS!!!

iLP can be accelerated with Molecular Dynamics

To approach jamming ($p \to \infty$) we used MD with a Lubachevsky-Stillinger compression: $\dot{\sigma}(t) = \kappa$



1. Fast compression up to p=*500* (avoid crystal)
2. Slow compression to a given target p
3. Use high p configuration as <u>*initial condition*</u> of iLP.



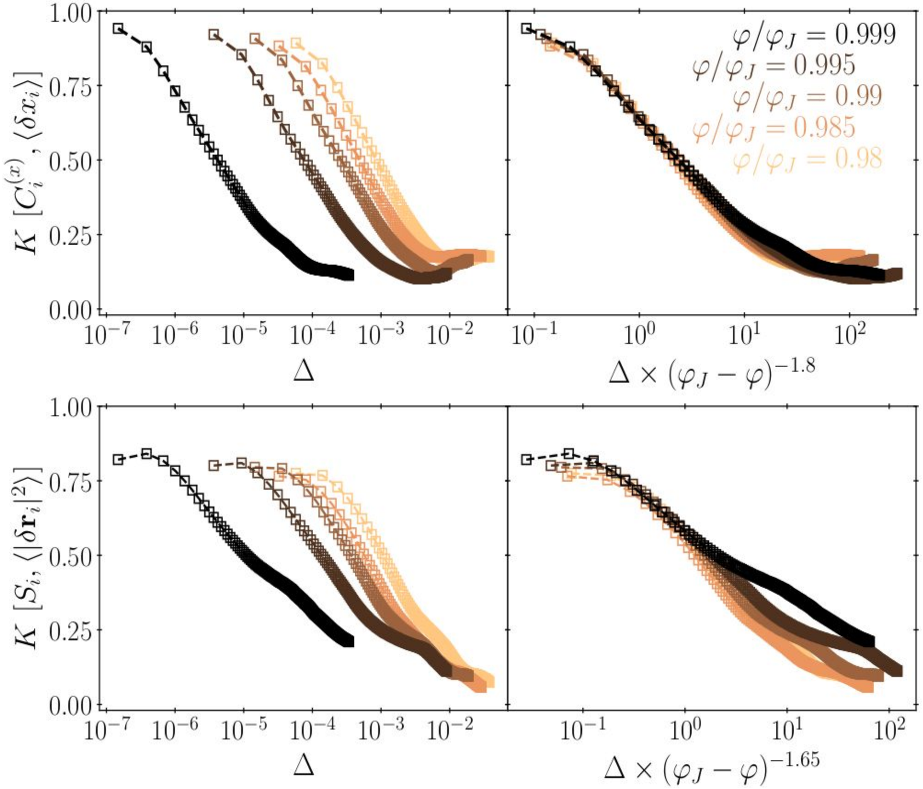
MD compression:

1. Very fast (asynchronous event-driven)
2. Many configurations can be produced simultaneously

iLP algorithm:

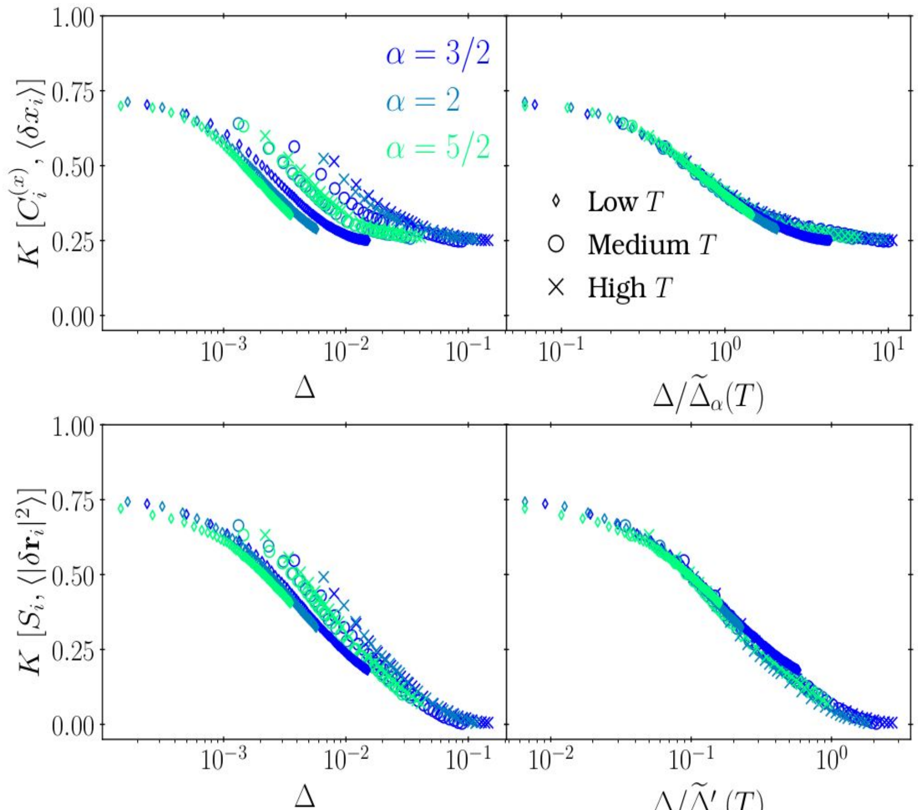
1. Benefits from interior-point (concurrent) solvers
2. Limited by system's size (about ~N^3)

“Universal” decorrelation rate



$$\Delta_\alpha \sim T^{\gamma_\alpha}$$

$\gamma_{3/2} = 0.84$ $\gamma_2 = 0.64$ $\gamma_{5/2} = 0.51$



The *loss of correlation* seems to be a <u>general function</u> of:

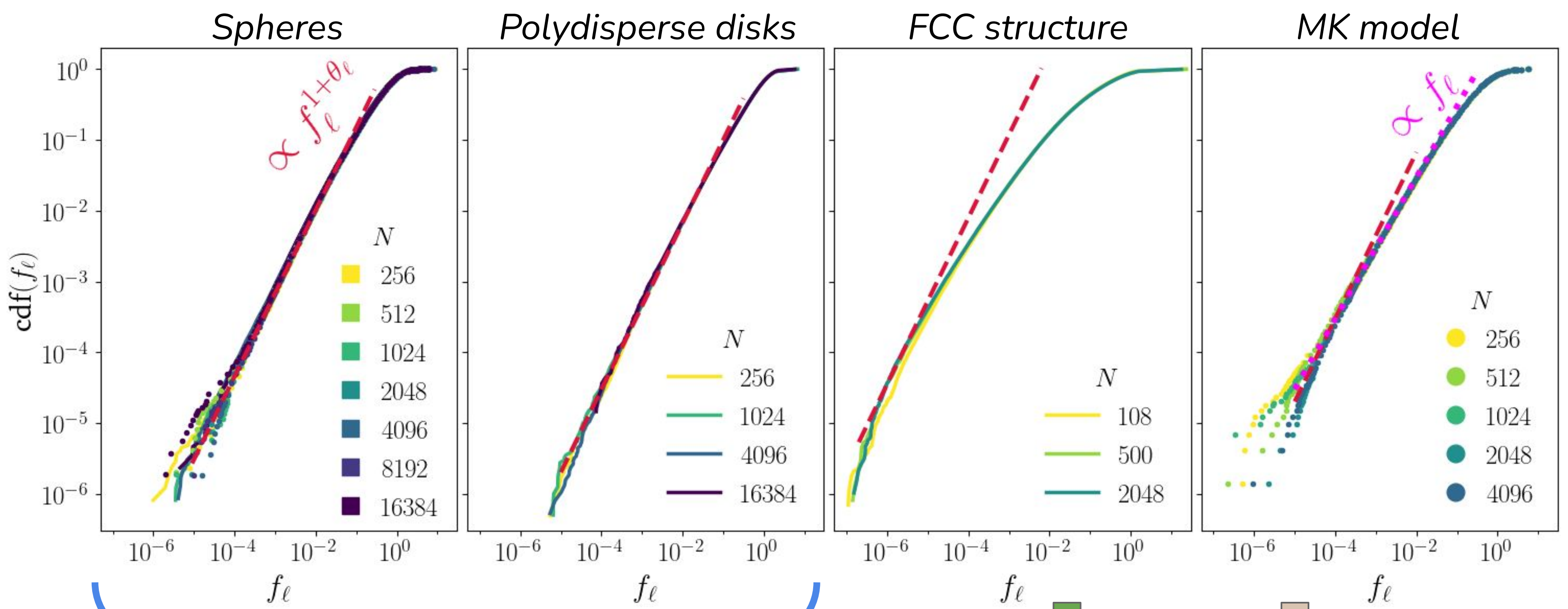
- **Evolution of the configuration** (measured by Δ)
- **Distance from jamming point** $(\varphi_J - \varphi)$ T

$$\widetilde{\Delta}_\alpha \sim T^{\delta_\alpha}$$

$\delta_{3/2} = 0.45$ $\delta_2 = 0.40$ $\delta_{5/2} = 0.35$

Localized forces

No presence of finite size corrections ...expected



$\theta_\ell = 0.17$

No power law!

$\theta_{\ell,MK} = 0$

(Unstable!)