The Jamming Transition

Everything you (possibly never) wanted to know about packing spheres

SIMONS FOUNDATION

STVDIVM VRBIS

Rafael Díaz Hernández Rojas

(Chimera Group)

Rome, May 17th, 2023

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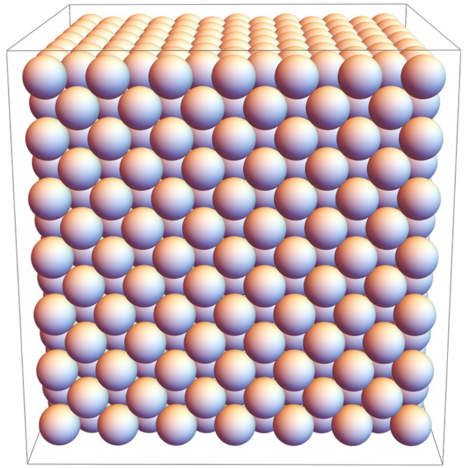
1) Regular Sphere Packings:
Geometric perspective



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2) Disordered packings:
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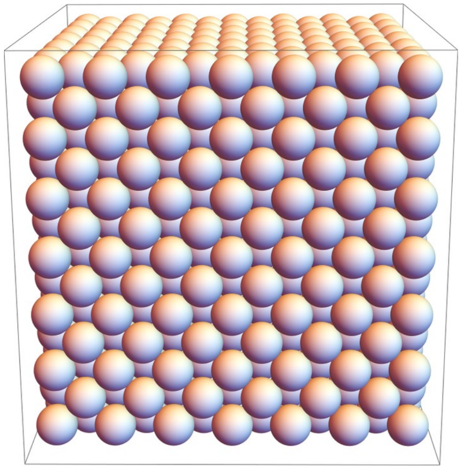

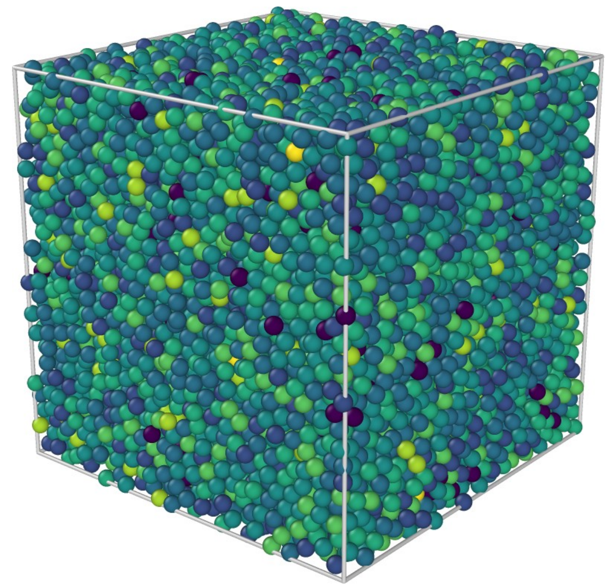

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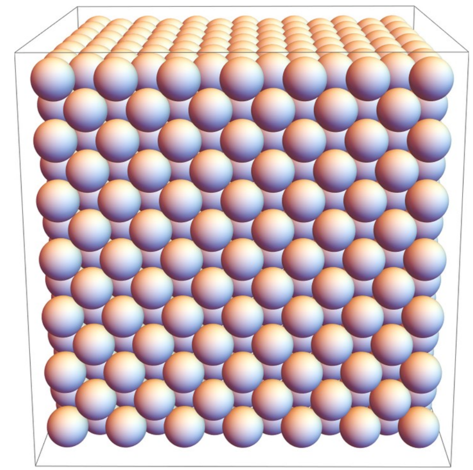

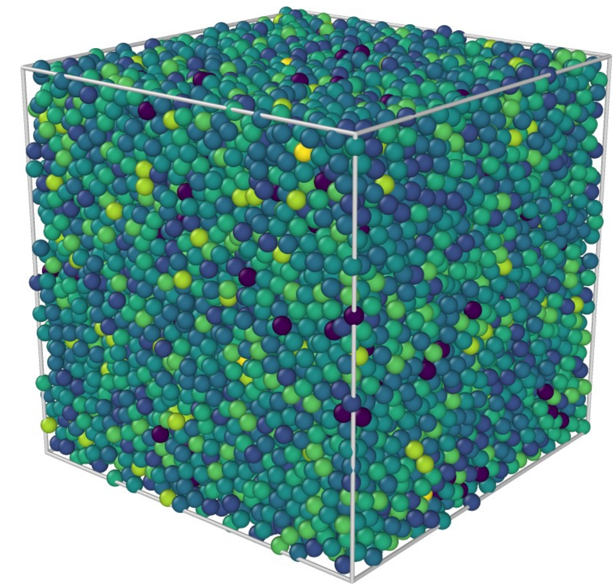

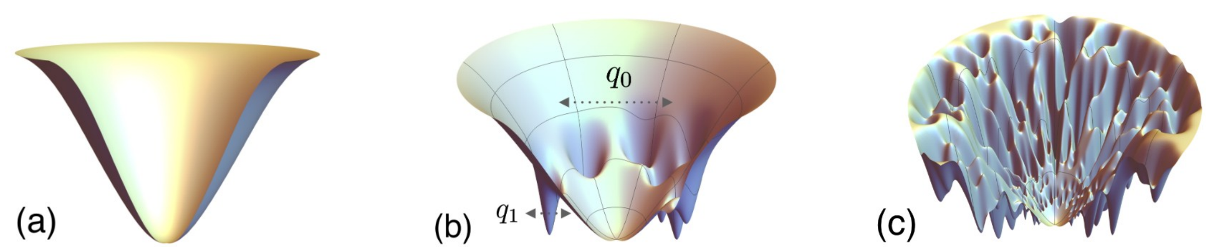

[Cugliandolo, *Ann. Rev. Cond. Matt*, **(to appear)**]

The sphere packing problem

How to place (infinitely) many equal spheres as efficiently as possible?

Find the configuration that maximizes the density (φ)

NO OVERLAPS BETWEEN SPHERES!!

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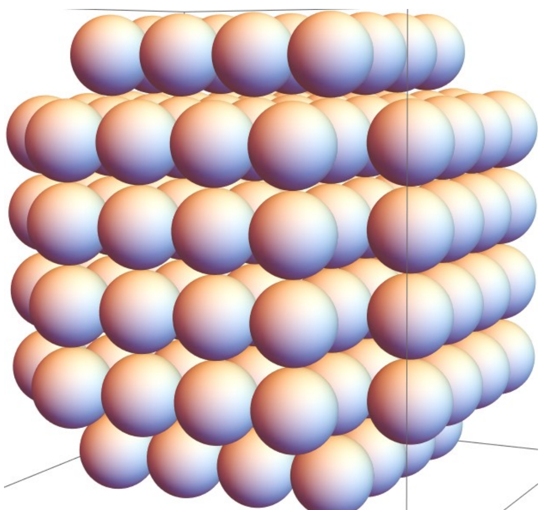
Simple cubic lattice



$$\varphi = \frac{\pi}{6} \approx 0.52$$

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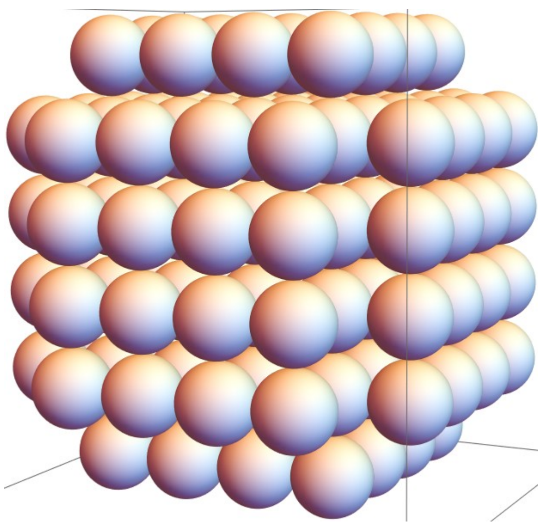

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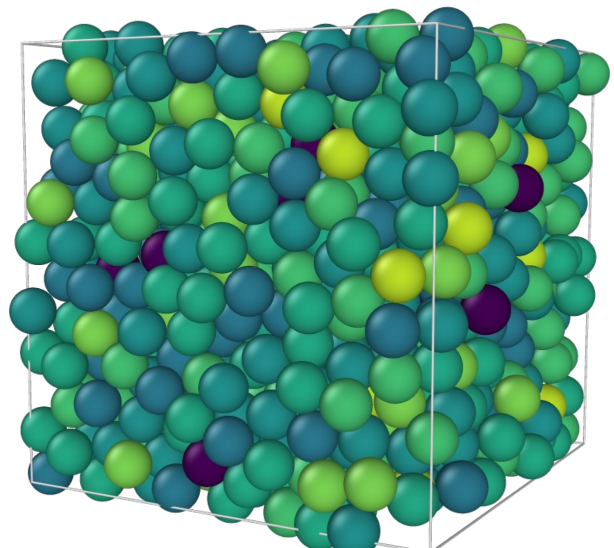
Random (mechanically stable)



$$\varphi \approx 0.635$$

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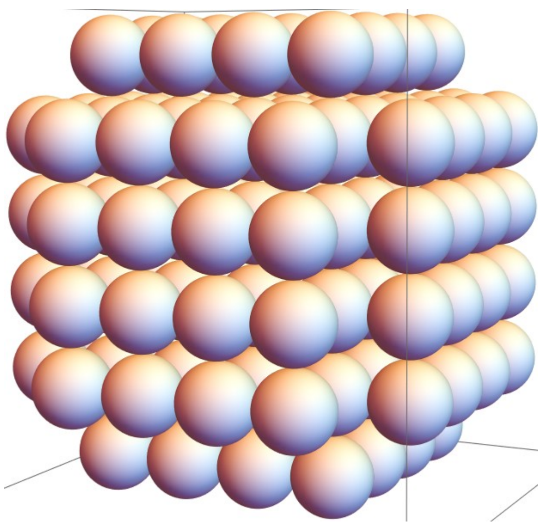

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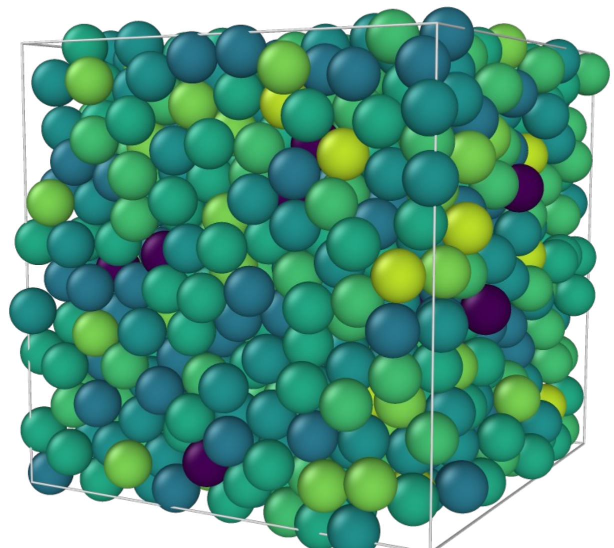

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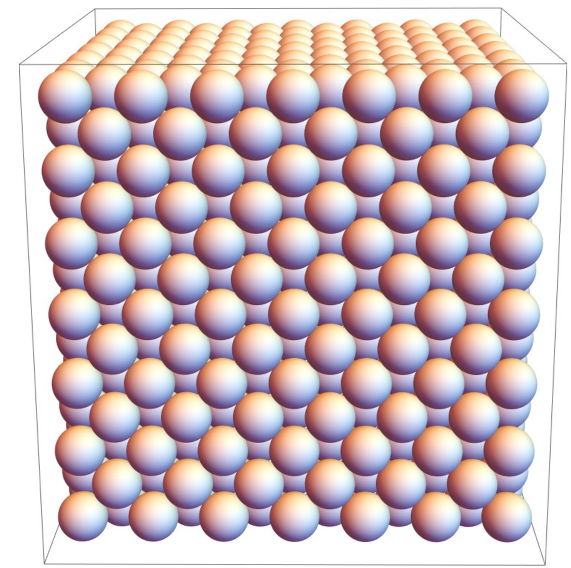
Face Centered Cubic lattice



$$\varphi^\star = \frac{\pi}{3\sqrt{2}} \approx 0.74$$

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[in d dimensions]

How to place (infinitely) many **hyper-**spheres as efficiently as possible?

The sphere packing problem

[in *d* dimensions]

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sphere: $\|\mathbf{x}\|^2 = \sum_{\alpha=1}^{d} x_\alpha^2 = r^2$

volume: $v_d(r) = \dfrac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} r^d$

no overlaps: $\|\mathbf{x}_i - \mathbf{x}_j\|^2 \geq 4r^2$

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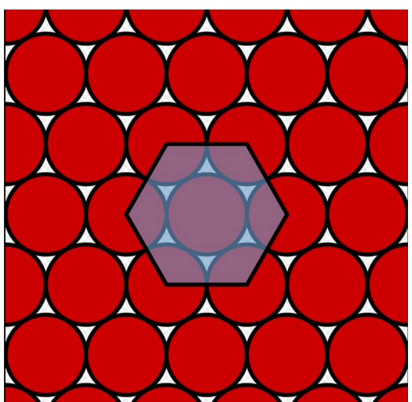

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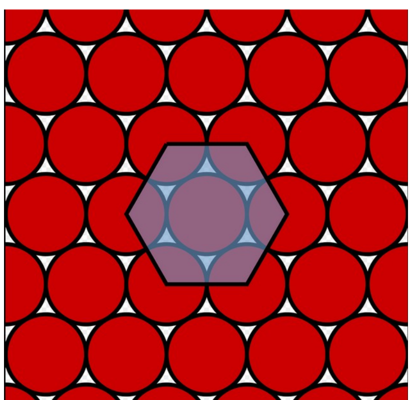

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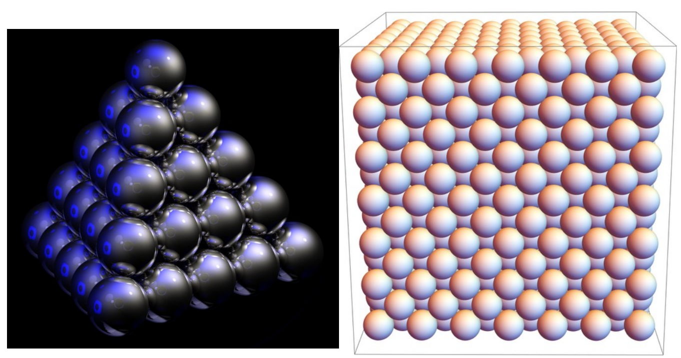
$d = 3$ (Kepler's Conjecture)



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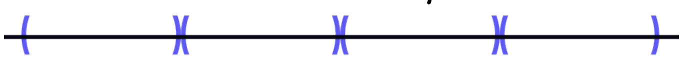
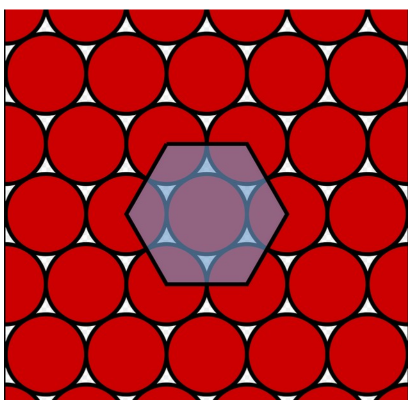


$d = 4, 5, 6, 7 \implies ???$

$d = 2$



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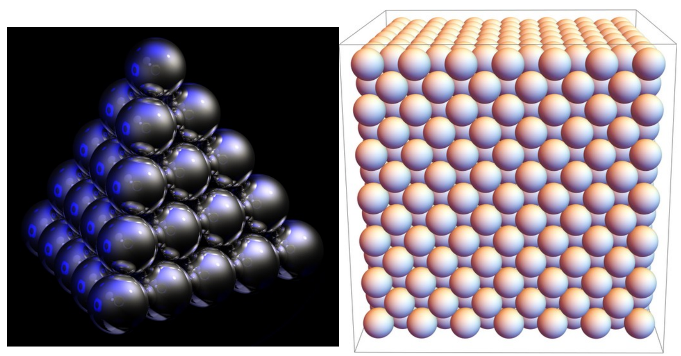

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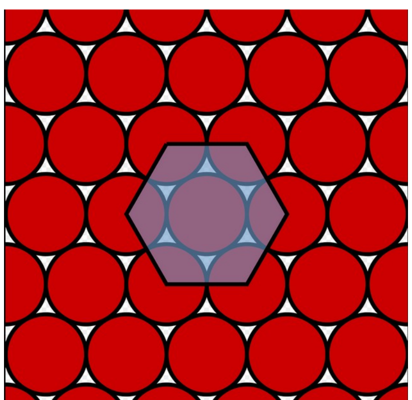

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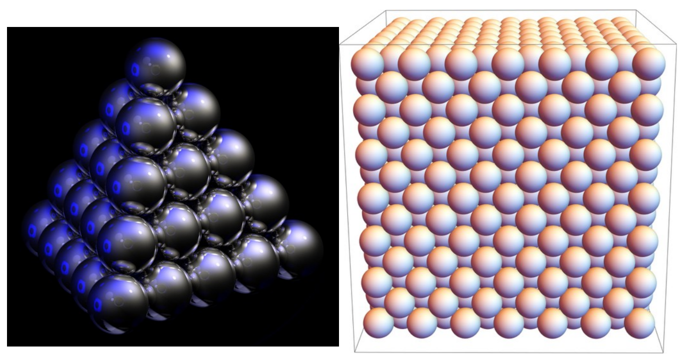

$\varphi^\star = \frac{\pi}{3\sqrt{2}} \approx 0.74$

$d = 8: \quad \varphi^\star = \frac{\pi^4}{384} \approx 0.25$

Maryna Viazovska
(Fields Medal winner 2022)

$d = 24: \quad \varphi^\star = \frac{\pi^{12}}{12!} \approx 0.0019$

Jamming and sphere packings in physics

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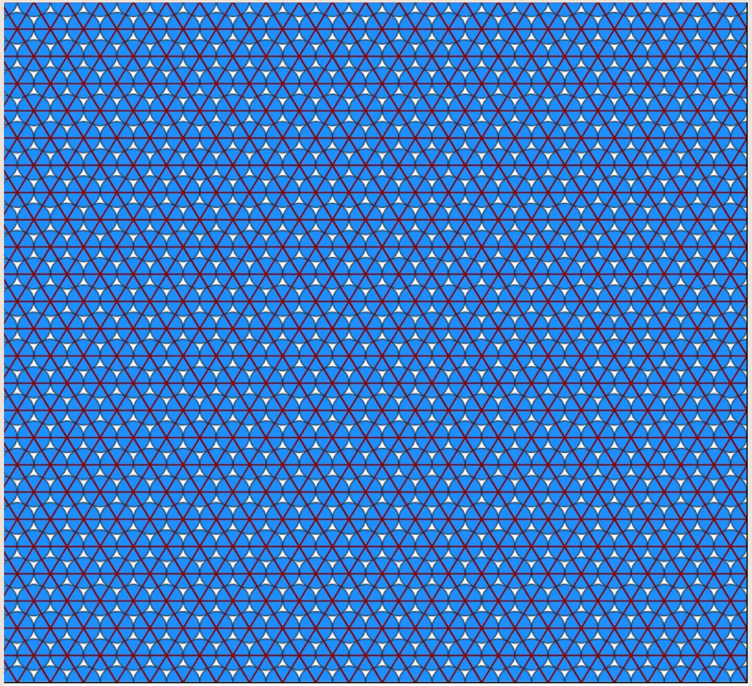
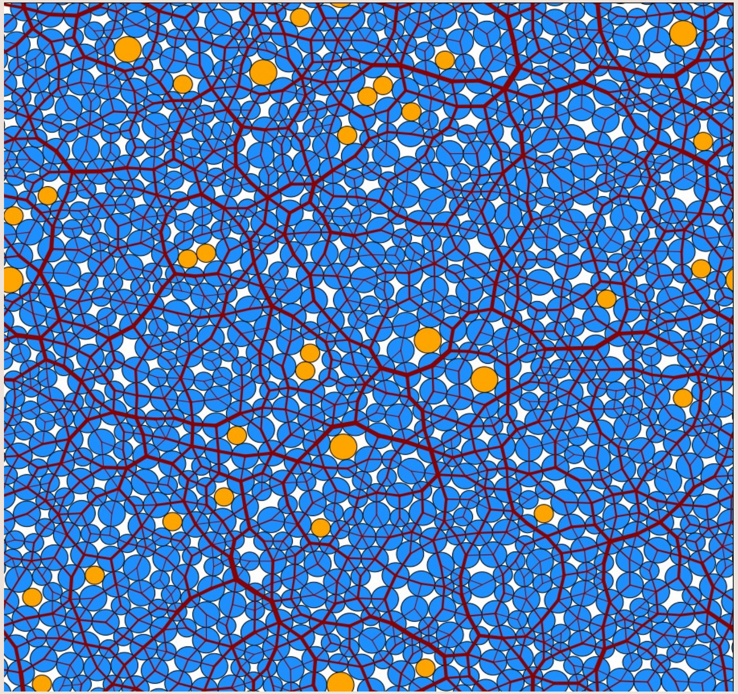


Enters disorder



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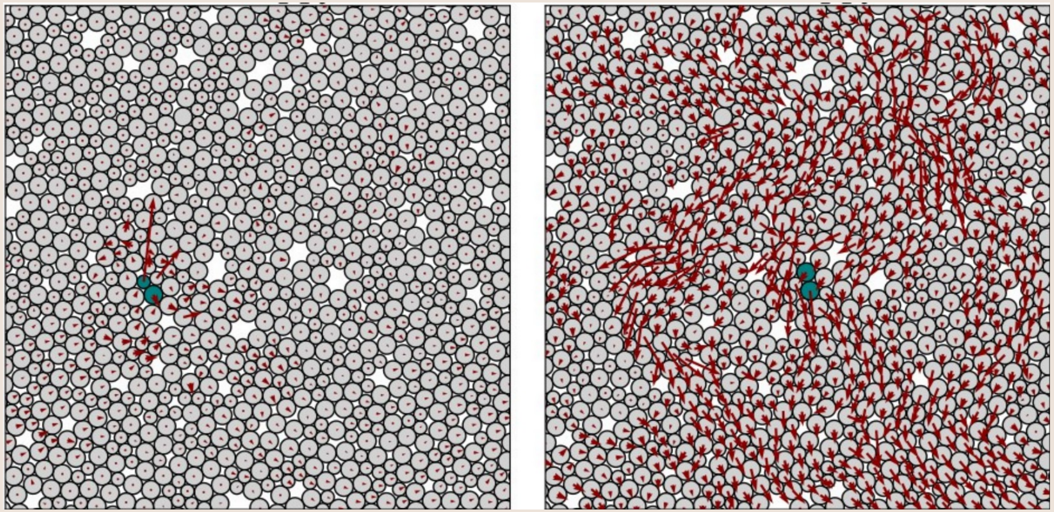

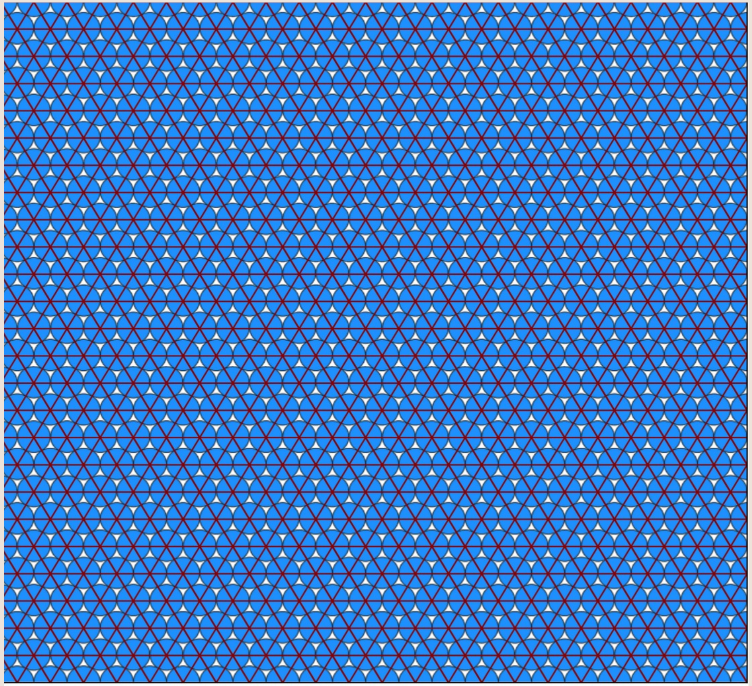

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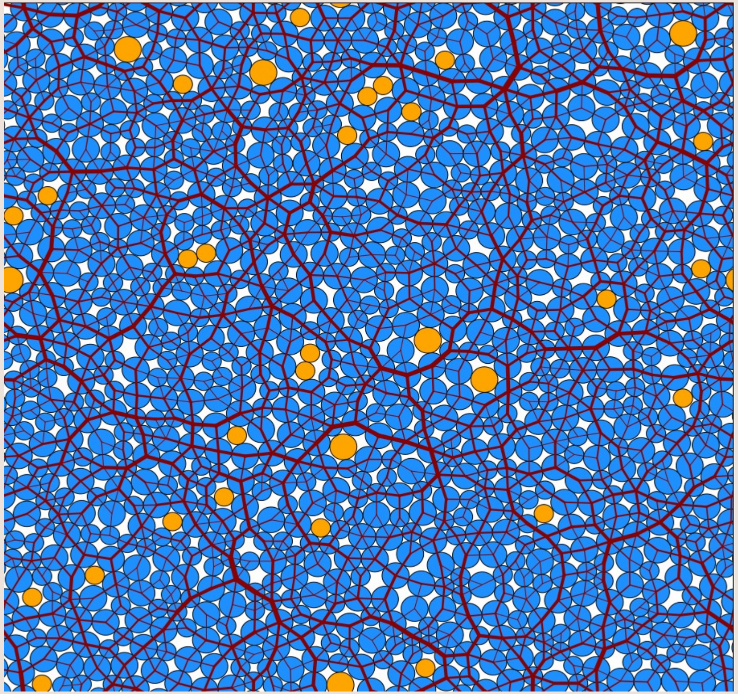

Jamming in Nature

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

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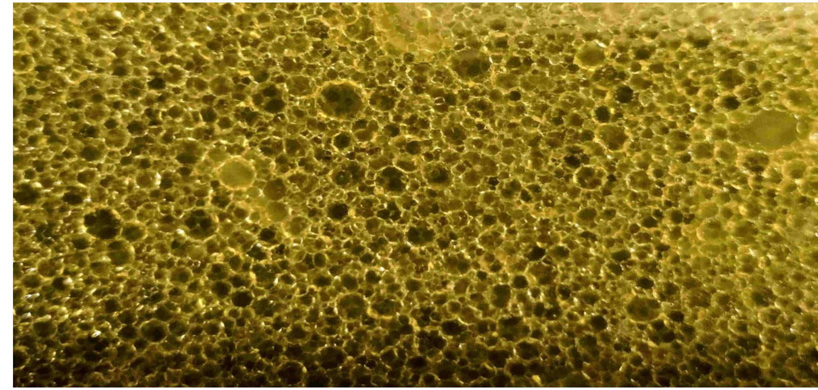

[Vinaigrette attempt; RDHR *unpublished recipe* (**2020**)]

(Glass from Tonalá. Jalisco, Mex.)

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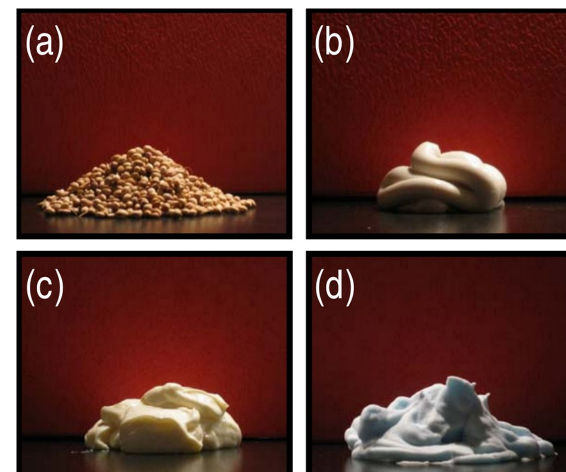

[van Hecke, J. Phys.: Cond. Matter (**2010**)]

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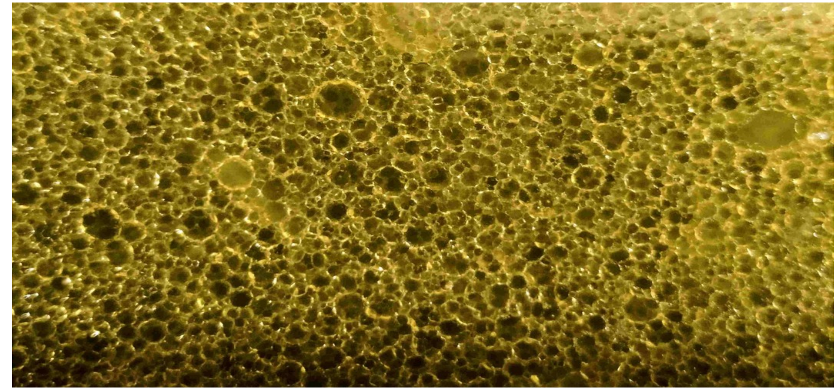

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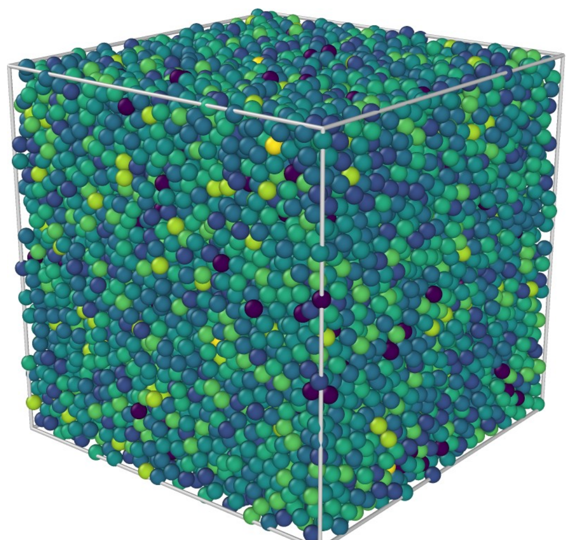

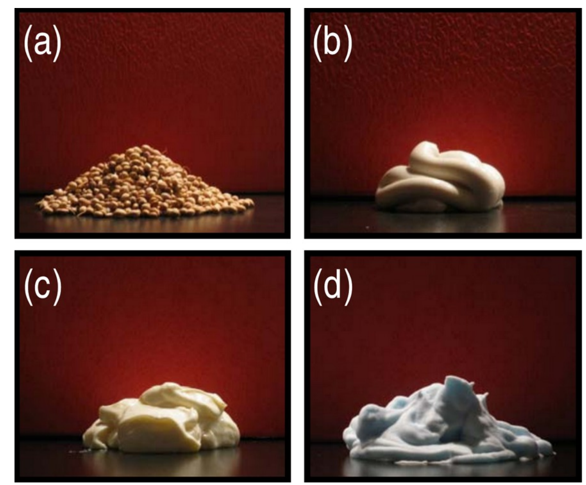

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Same components… many DIFFERENT macrostates (¿?)

$$\varphi_1 \quad \lesssim \quad \varphi_2 \quad \lesssim \quad \varphi_3$$

Same components... **many DIFFERENT macrostates** (¿?)

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"Give, and it will be given to you. A good measure, *pressed down, shaken together* and running over, will be poured into your lap. For with the measure you use, it will be measured to you."
Luke 6:38

Same components… **many DIFFERENT macrostates** (¿?) → Dependence on the (packing) <u>**protocol**</u>

$$\varphi_1 \lesssim \varphi_2 \lesssim \varphi_3$$

[no tapping]

[a bit of tapping]

[lots of tapping]

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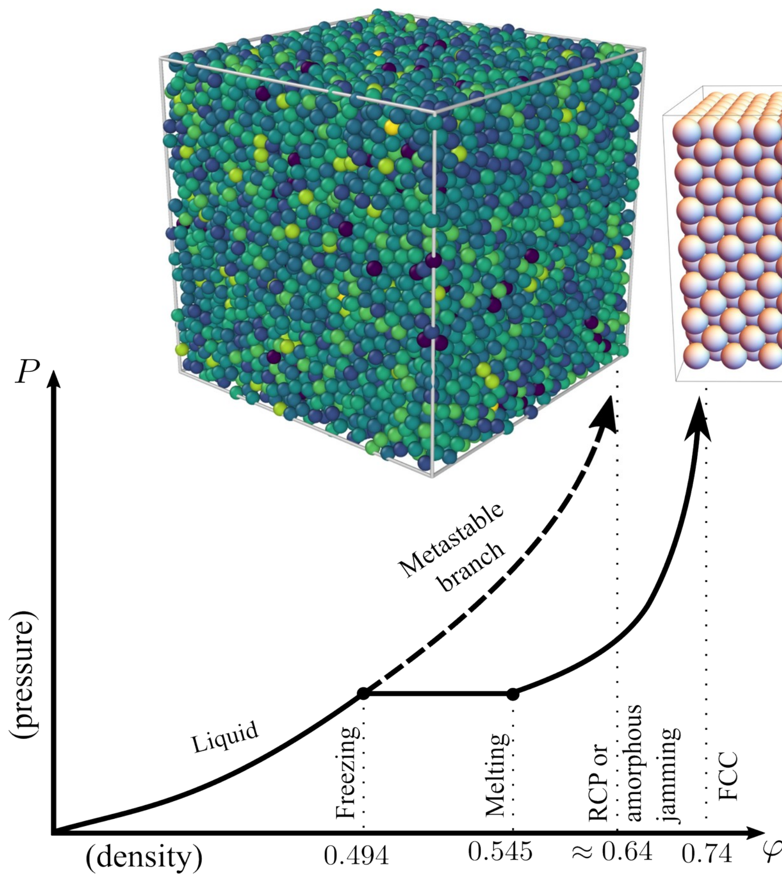
The jamming (rigidity) transition

Phase Diagram of **Hard-Spheres**



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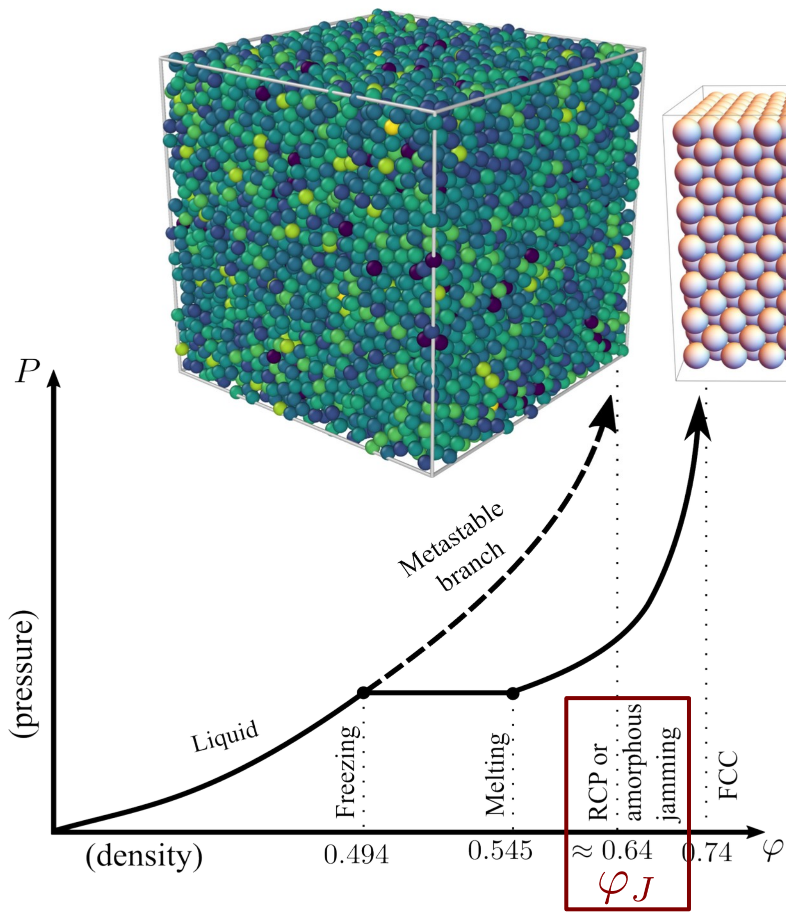

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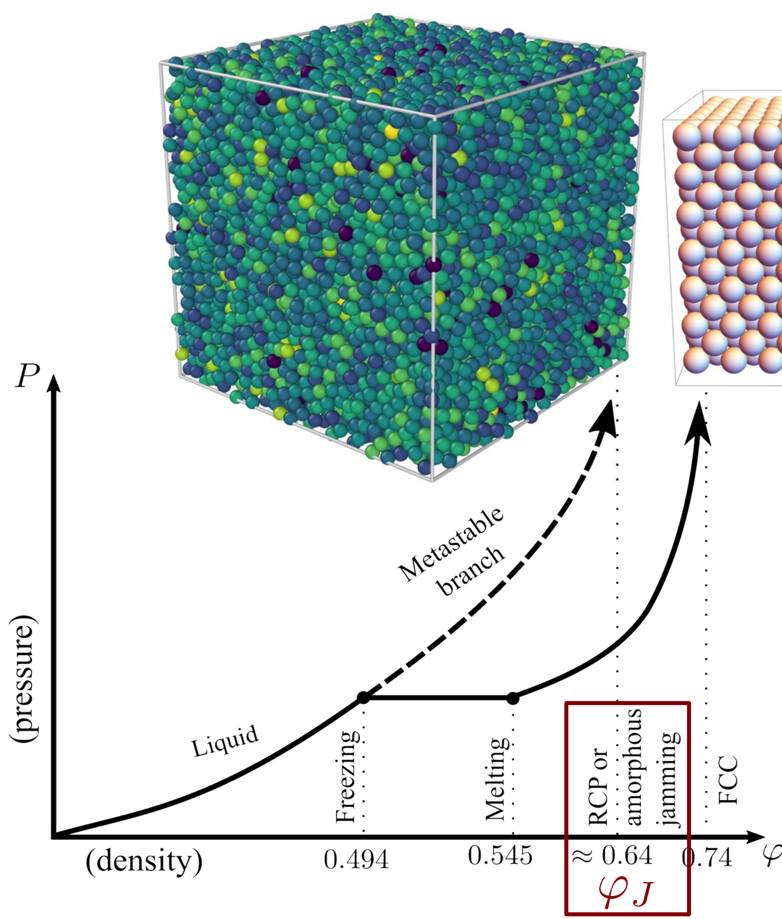

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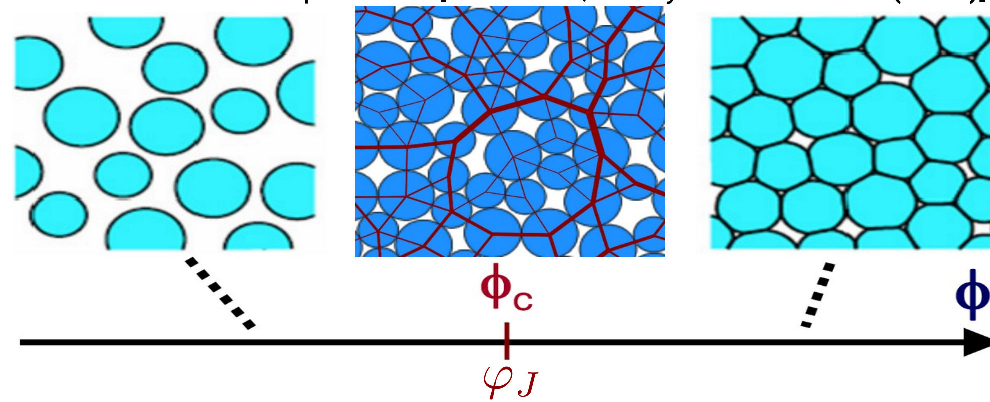

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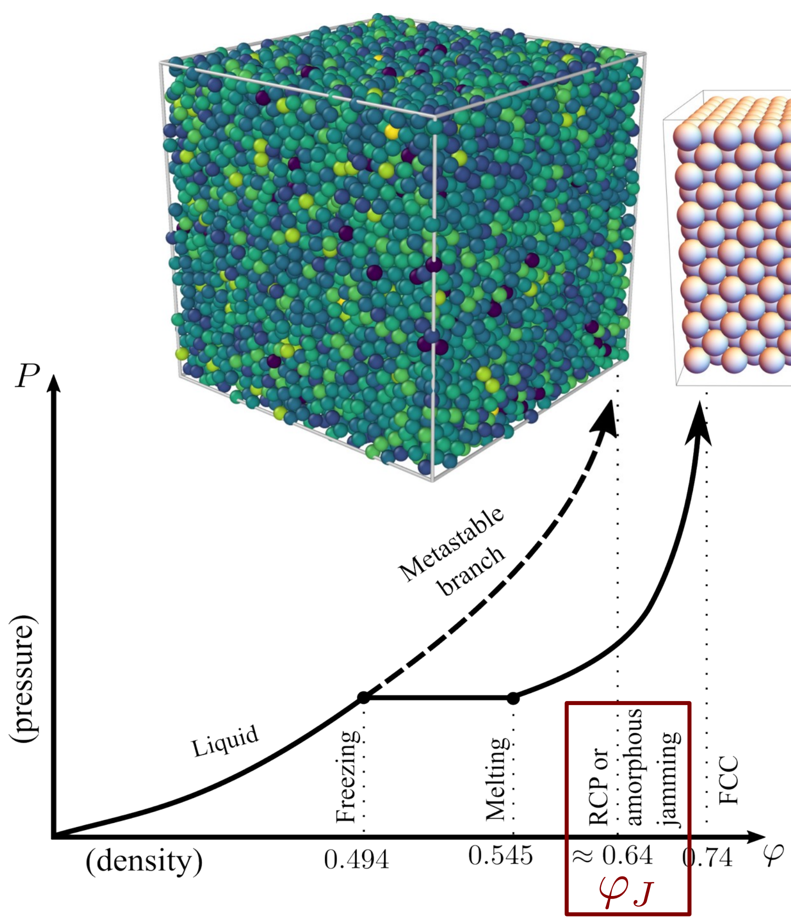

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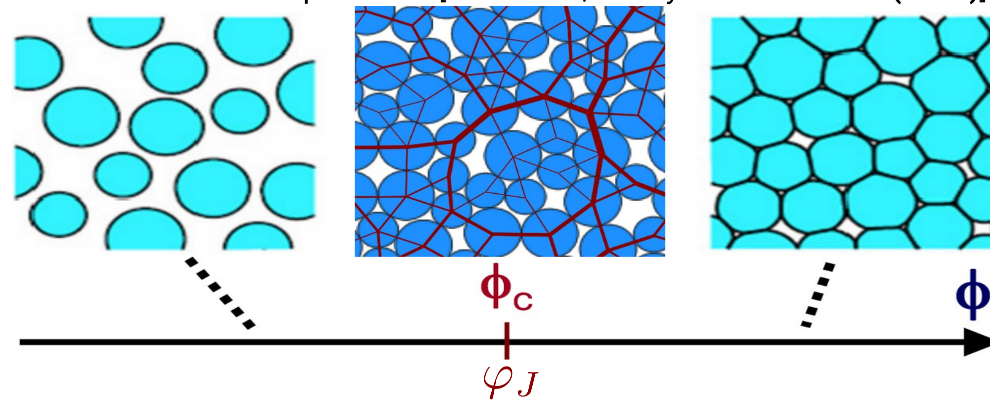

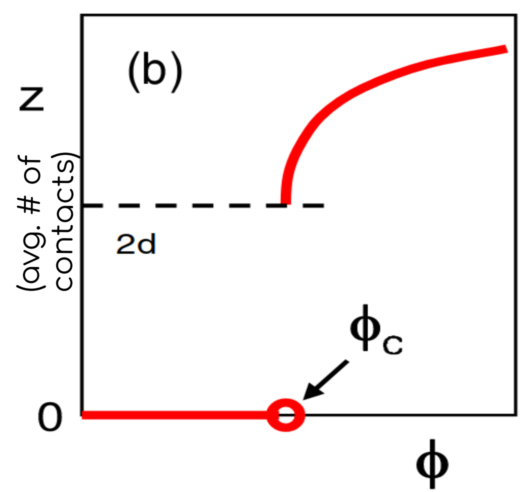

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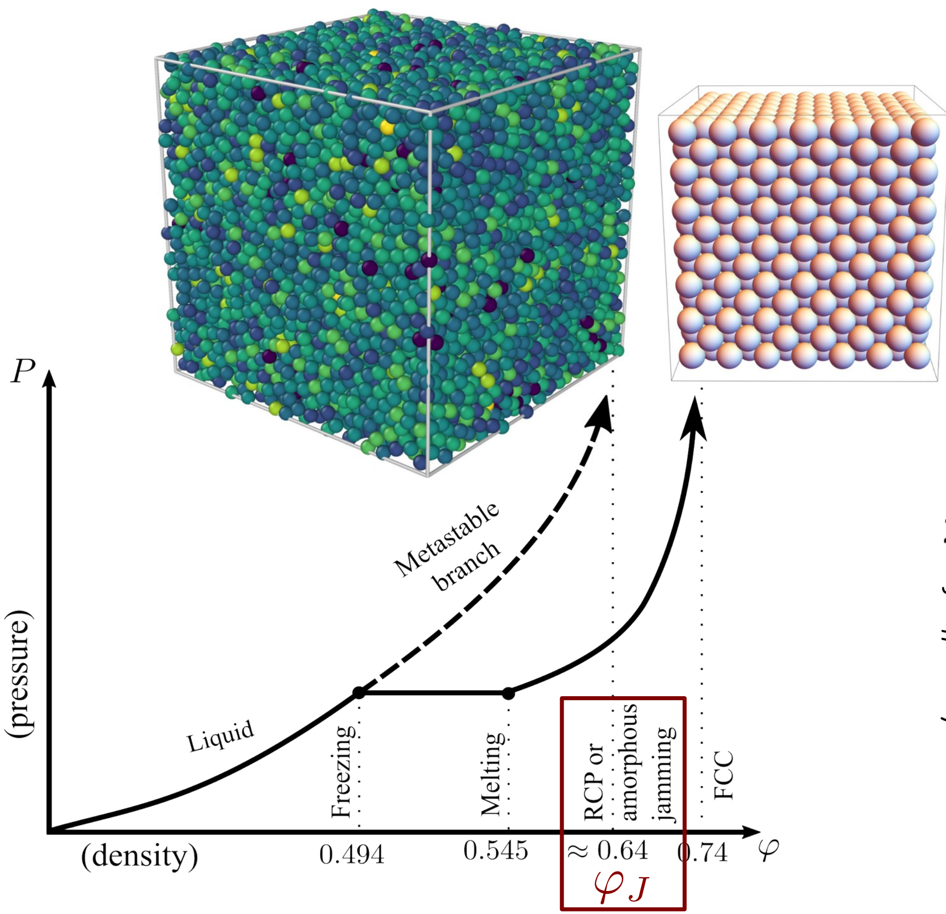

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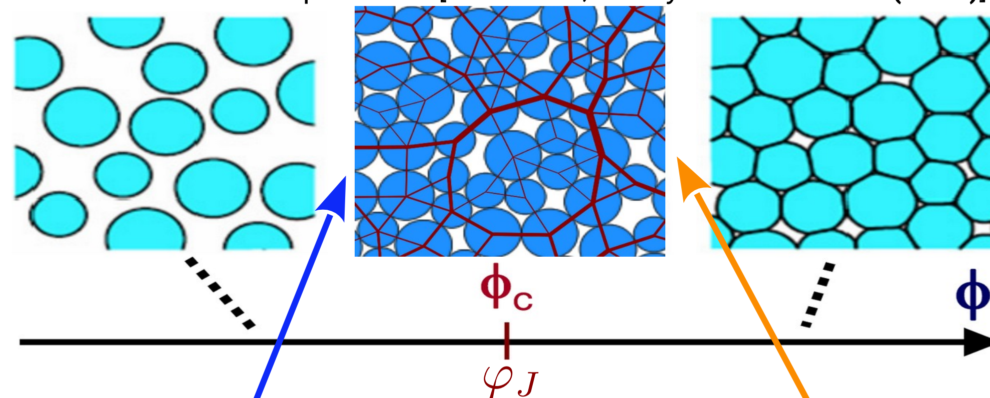

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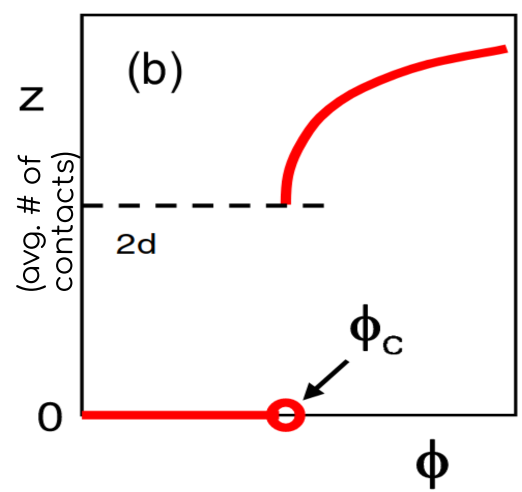
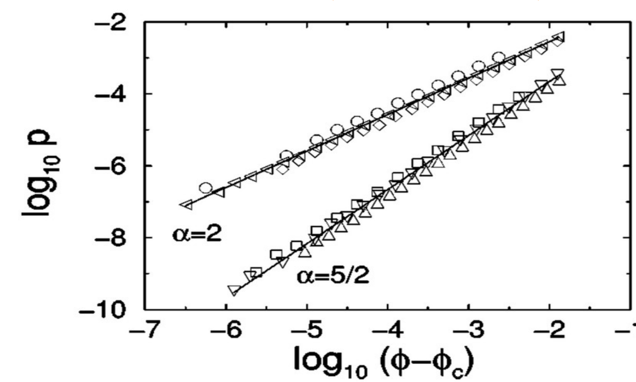
$$z - 2d \sim (\varphi - \varphi_J)^{1/2}$$



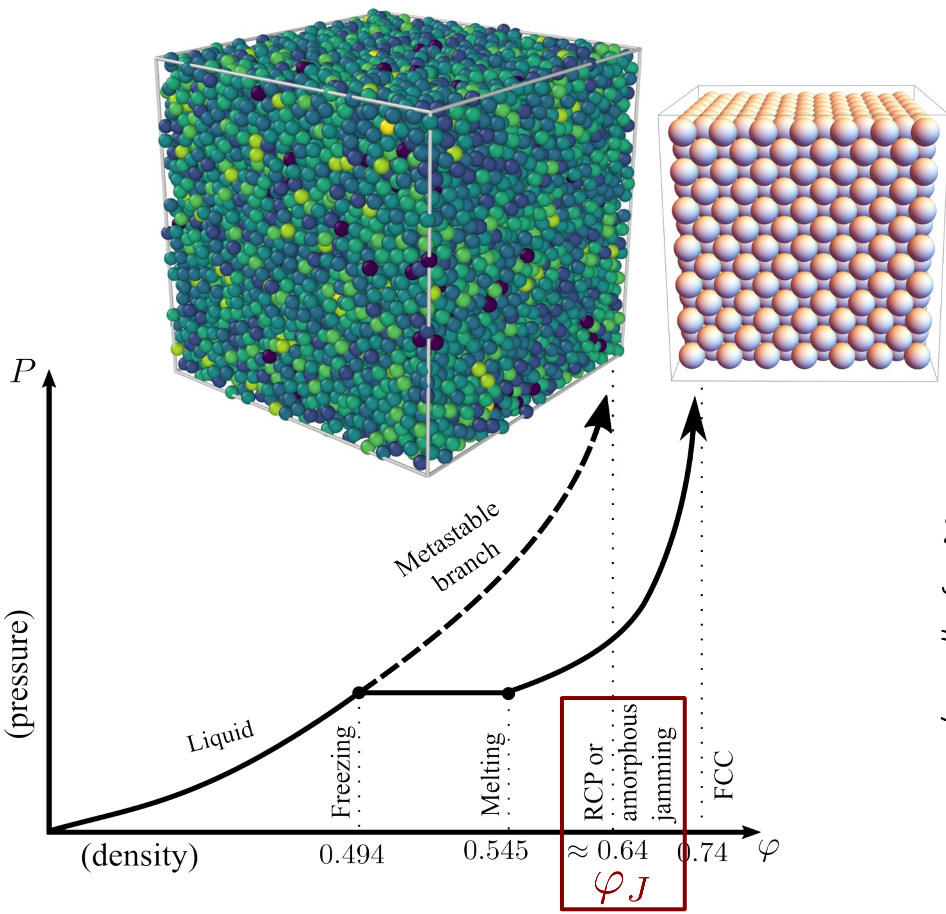


[O'Hern et al., *PRE* **(2003)**]

The jamming (rigidity) transition

In ALL dimensions !!! $(2 \leq d \leq 10)$

Phase Diagram of Hard-Spheres



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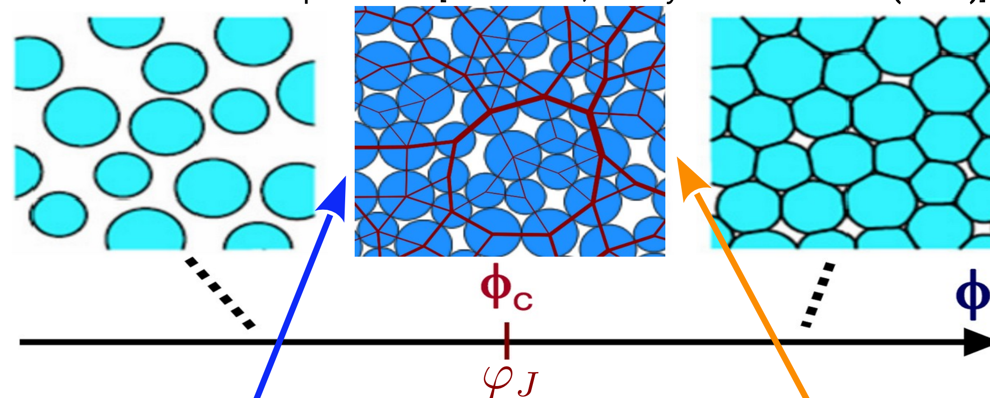

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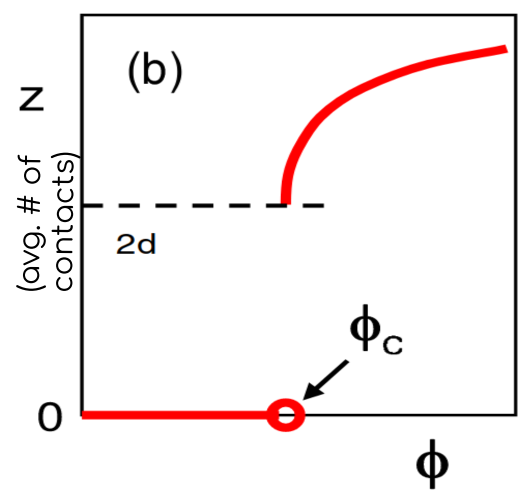

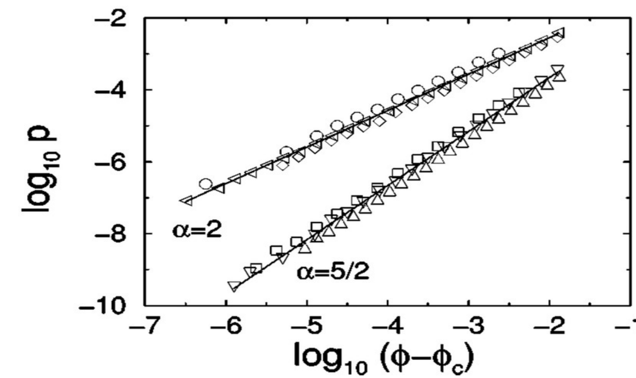

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How to understand (a bit of) Jamming using Statistical Physics?

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$d \to \infty$ ✓

(Exact) Mean-field theory developed by Charbonneau, Kurchan, Parisi, Urbani, Zamponi : ≈2010-today

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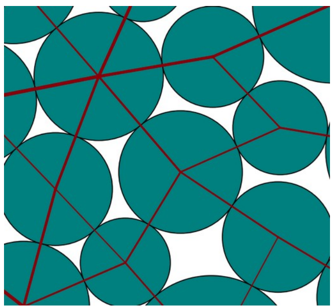
$d \to \infty \quad \checkmark$

(Exact) Mean-field theory developed by Charbonneau, Kurchan, Parisi, Urbani, Zamponi : ≈2010-today

$d = 2, 3 \quad \ldots ?$

No analytical theory available :'(
Good agreement between numerics and mean-field theory :D

Criticality of the MICROSTRUCTURE



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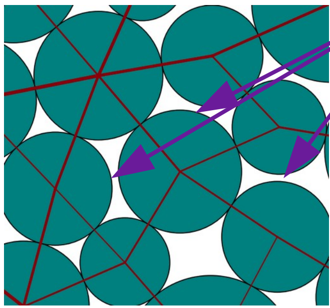

distance

Gaps $\left(h_{ij} = \frac{r_{ij}}{D_{ij}} - 1\right)$

Average diameter

$$g(h) \sim h^{-\gamma}; \;\; \gamma = 0.4127\ldots$$

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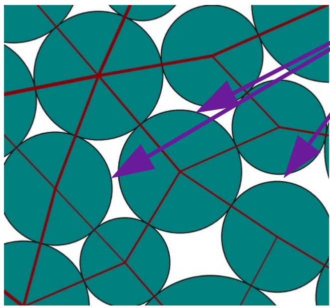

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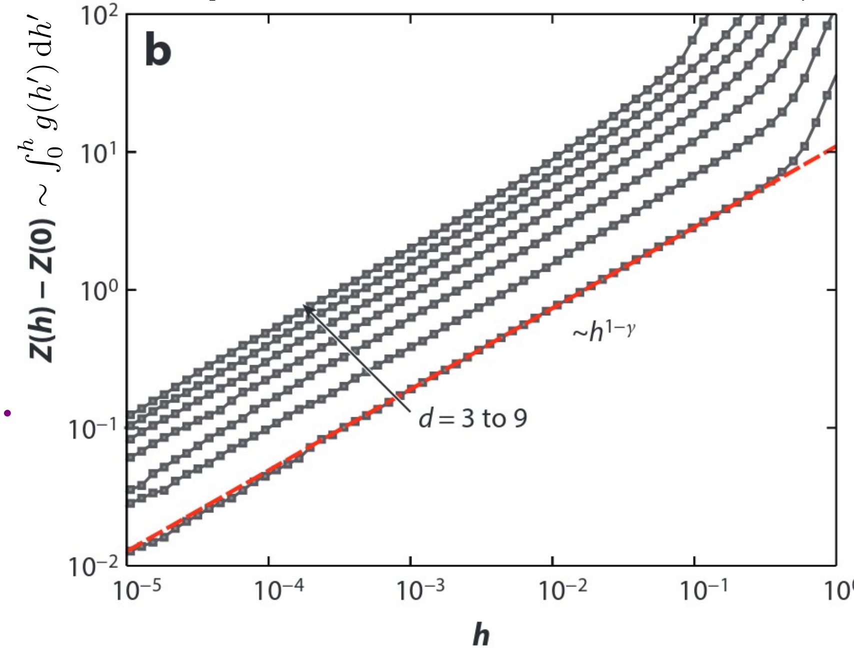
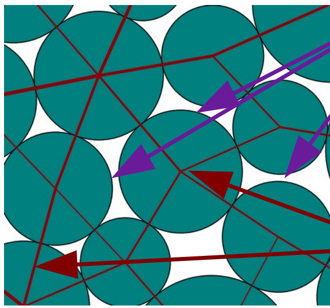
[Charbonneau, *et al*, Annu. Rev. Cond Matt. ***(2017)***]



Criticality of the MICROSTRUCTURE



Gaps $\left(h_{ij} = \frac{r_{ij}}{D_{ij}} - 1\right)$

distance

Average diameter

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Forces (magnitude)

$$p(f) \sim f^{\theta_e};\ \theta_e = 0.4231\ldots$$

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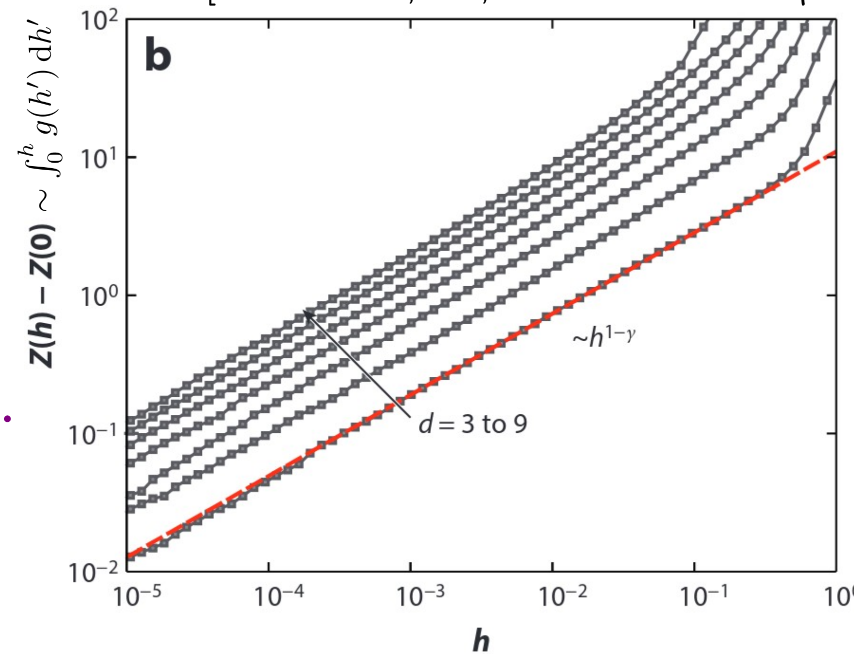

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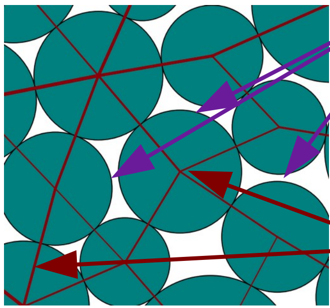

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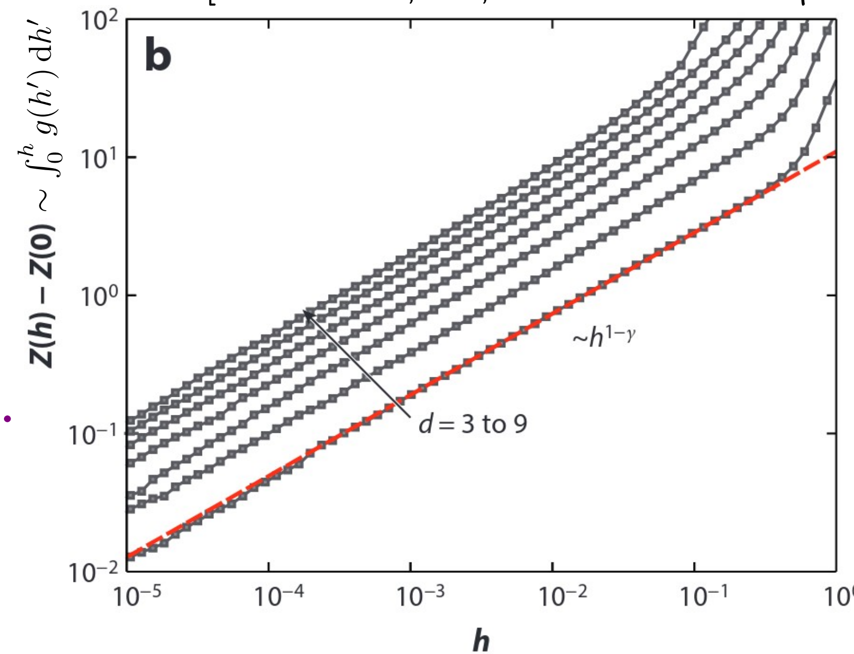
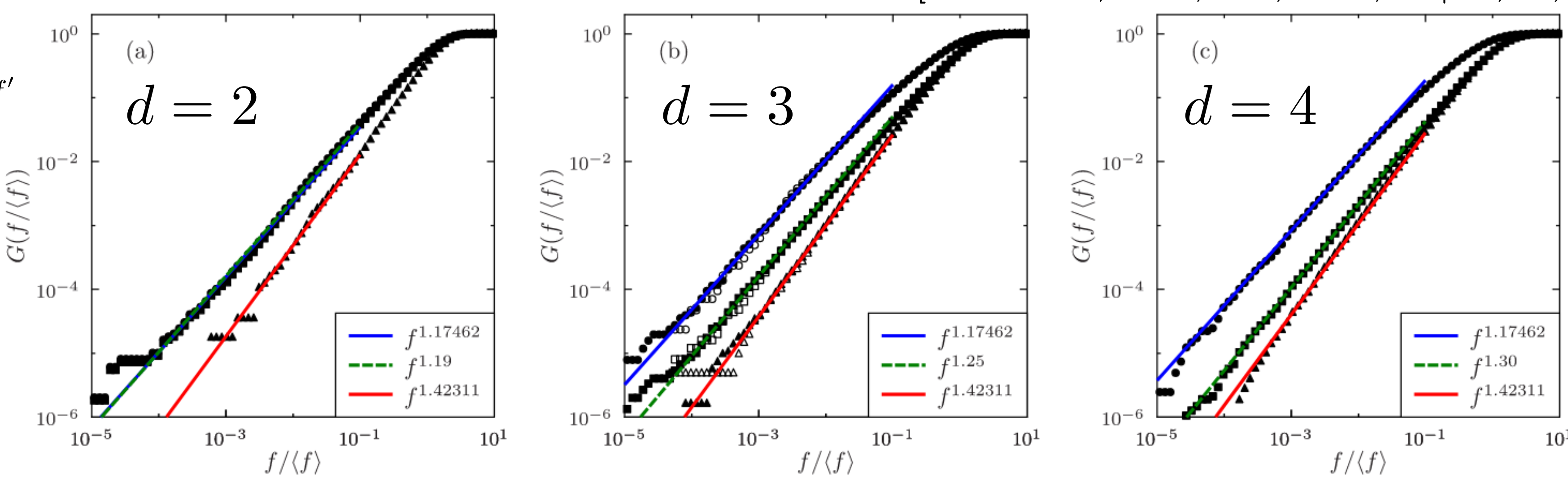


[Charbonneau, Corwin, Parisi, Urbani, Zamponi, *PRL*, ***(2015)***]

$\int_0^f p(f')\,\mathrm{d}f'$



Thermodynamics phases and free energy: Landscape picture

$$F(T) = U - TS = -T \log Z(T)$$

[thermodynamics def.] [Stat. Mech. definition]

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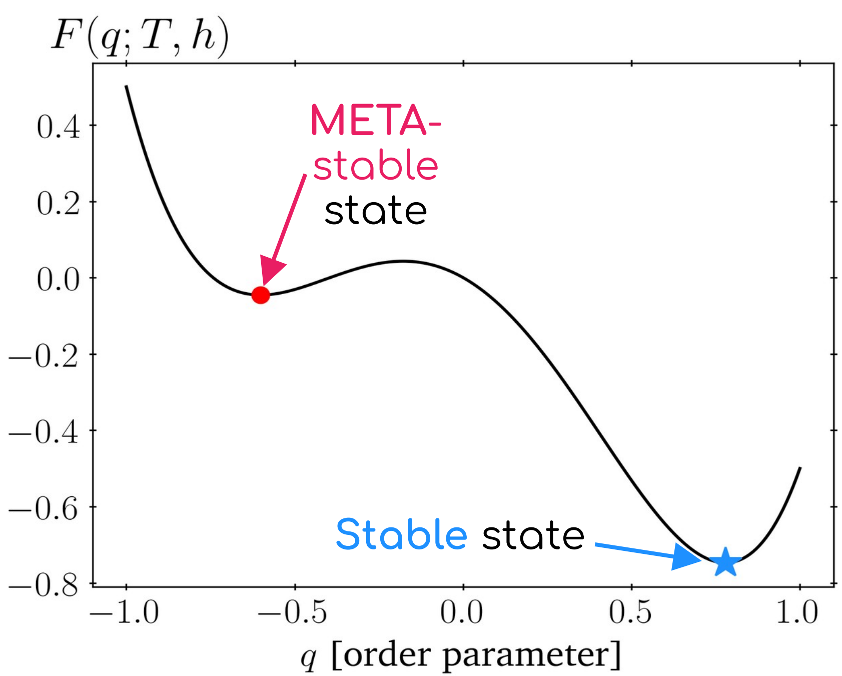

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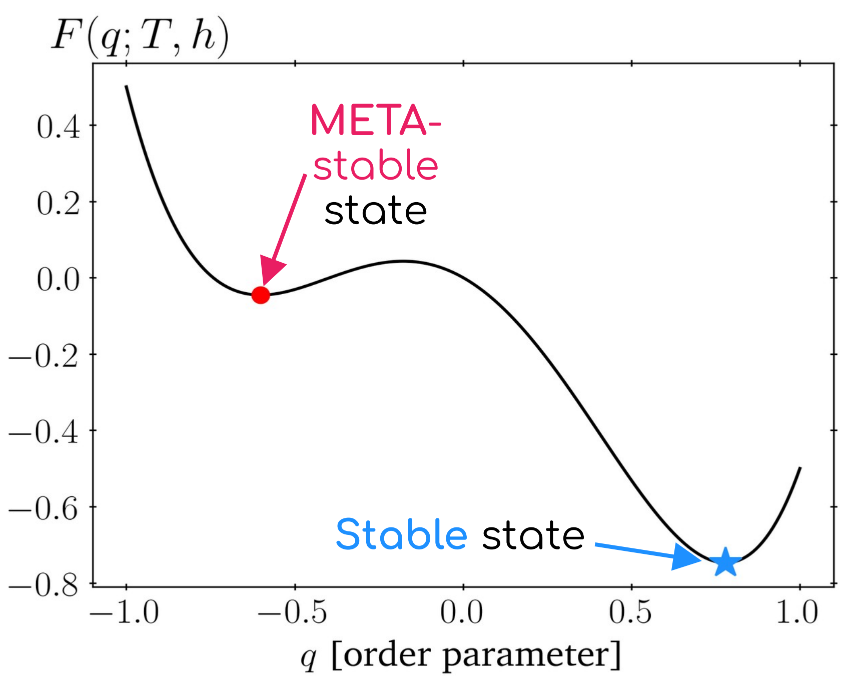

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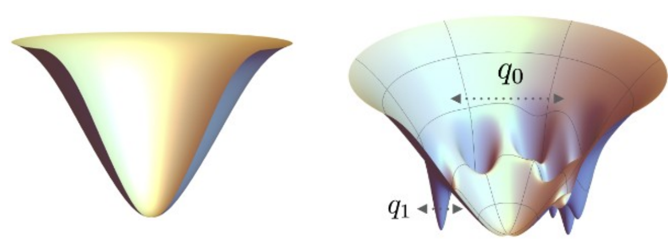

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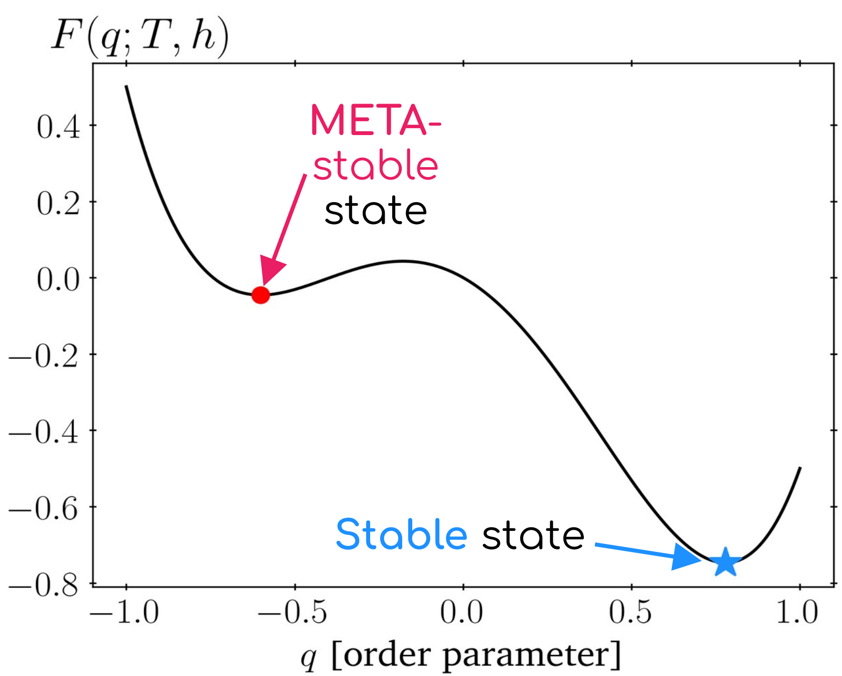
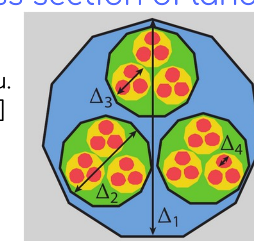


"cross section of landscape"

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



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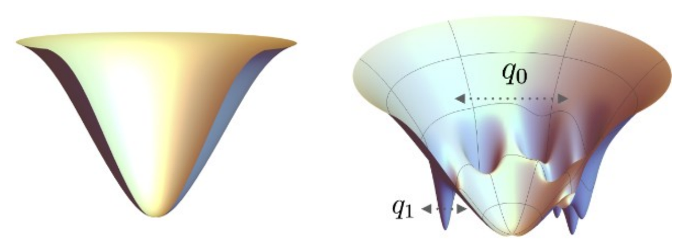

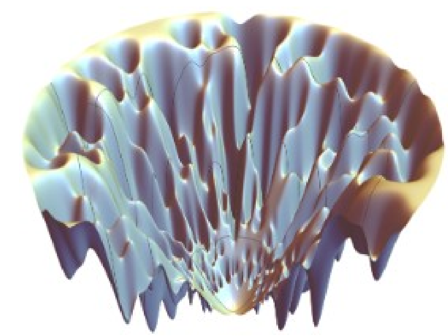

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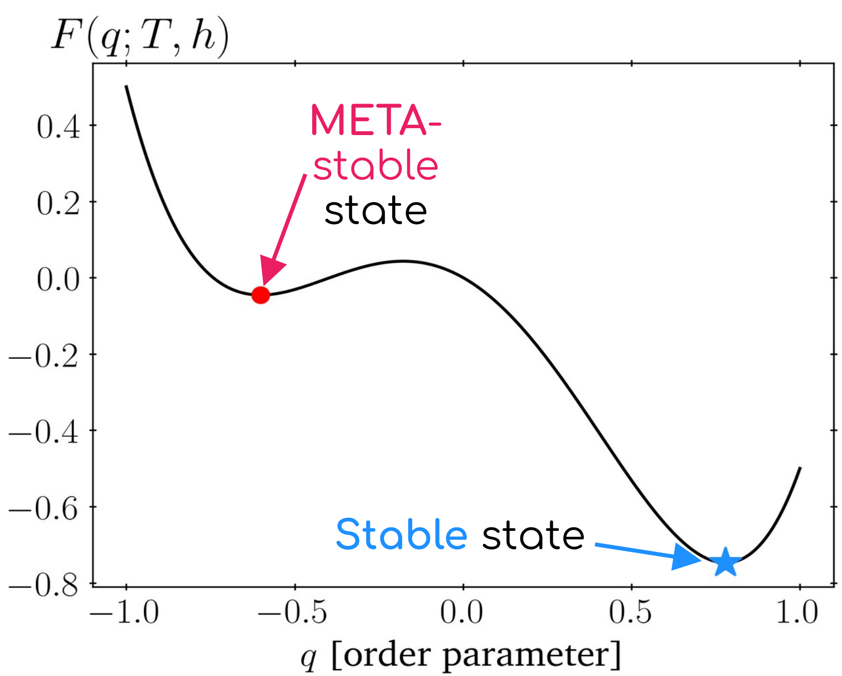

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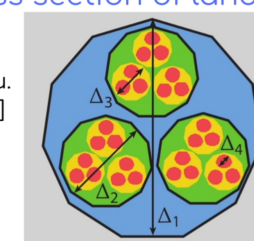

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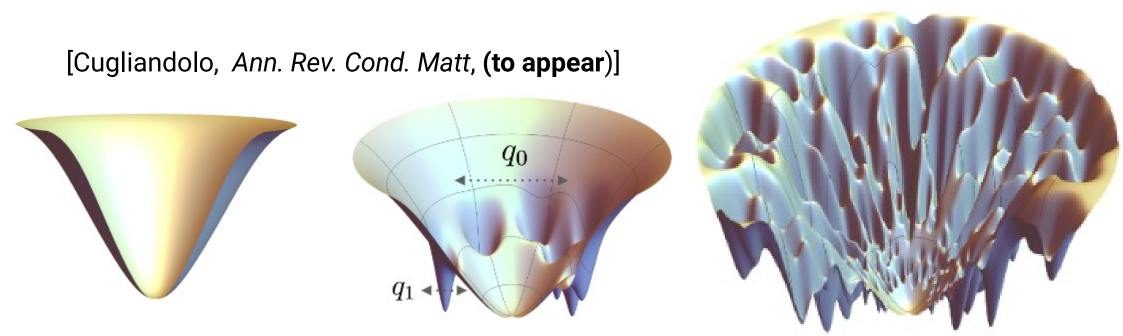

This is the picture in Hard Spheres φ

Jammed configuration:
minimum of a **very rough**
free energy landscape

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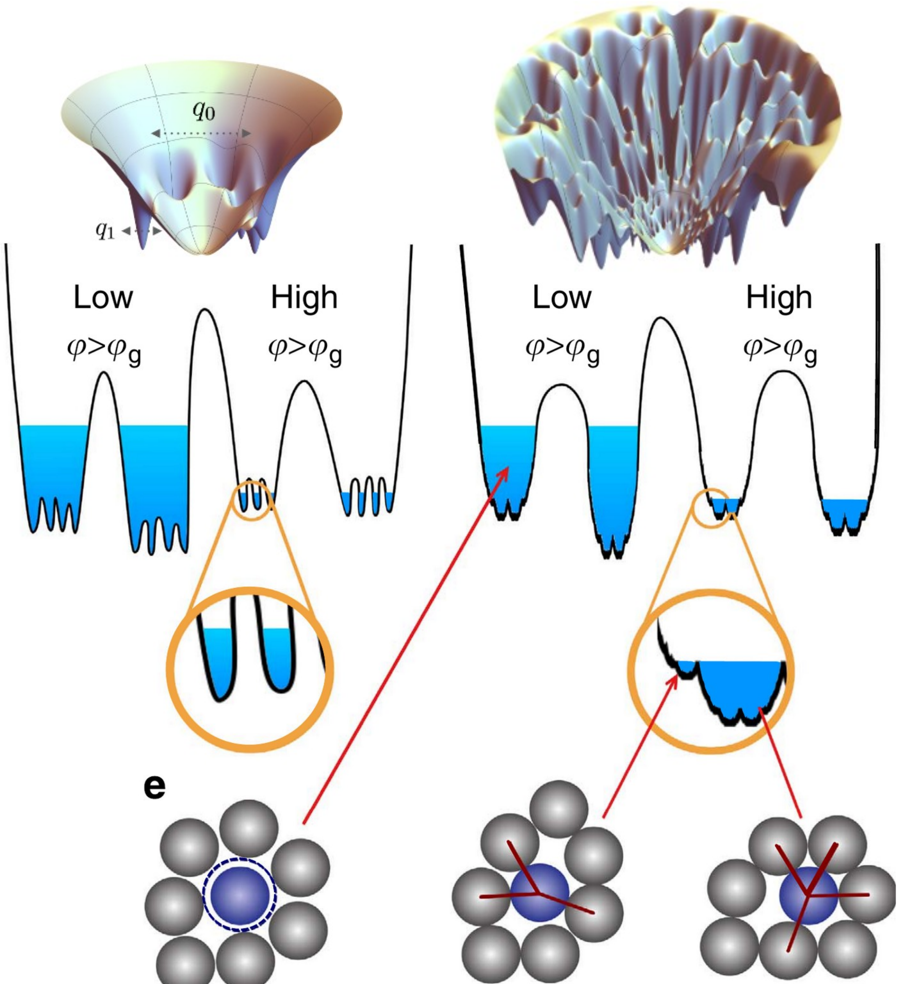

[Charbonneau, Kurchan, Parisi, Urbani, Zamponi, *Nat. Comms*, **(2014)**]

Jammed configuration:
minimum of a very rough
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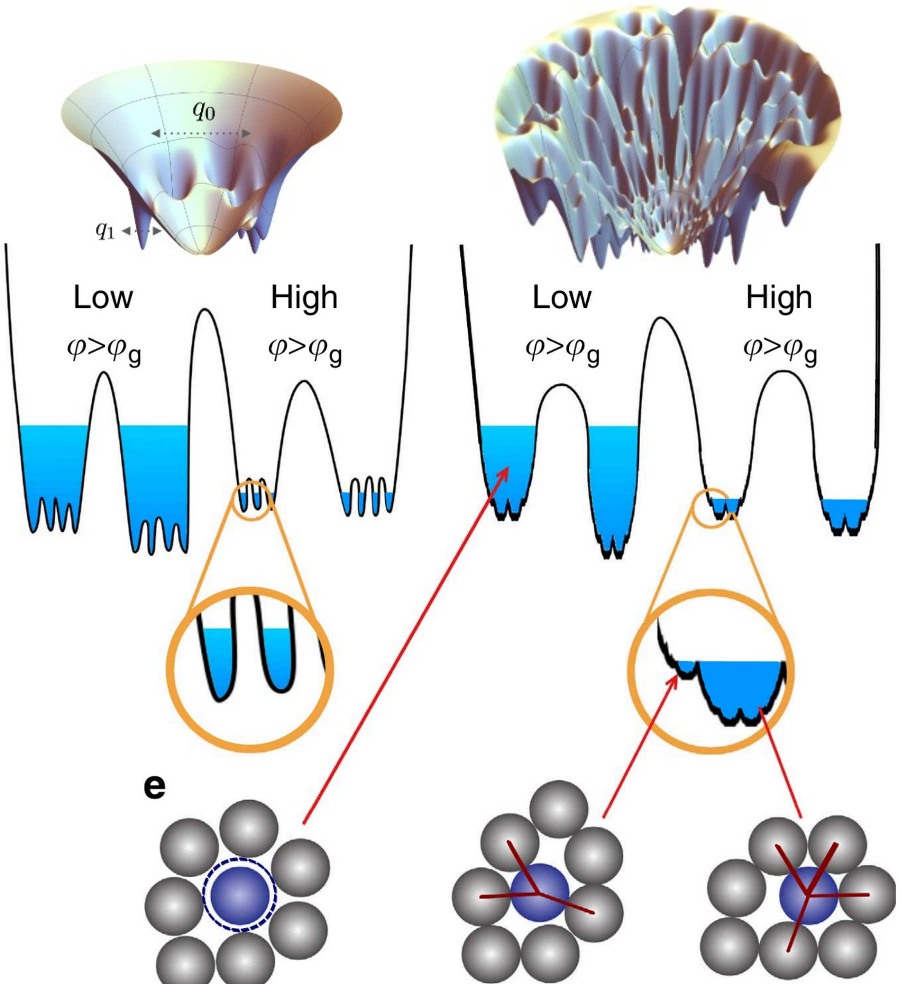
Each **minimum** (i.e. jammed packing) corresponds to a realization of a network of contacts $(\mathcal{N})$



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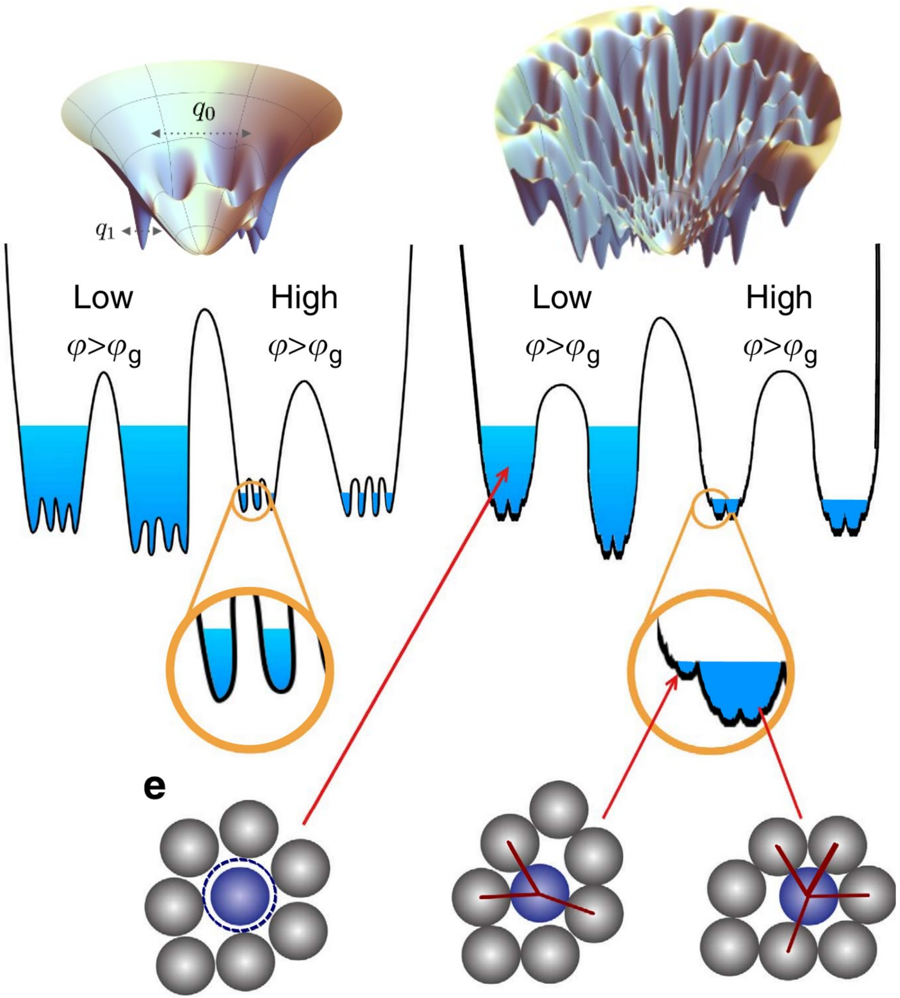
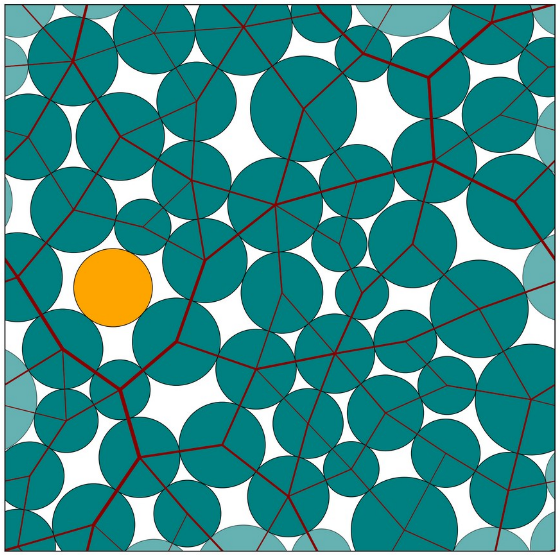


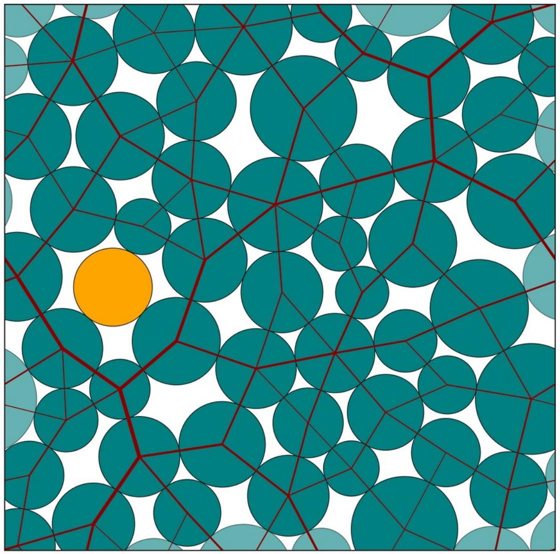
[Charbonneau, Kurchan, Parisi, Urbani, Zamponi, *Nat. Comms*, **(2014)**]

We can **test this model of the landscape** by measuring the similarity (a.k.a.*overlap*) between different packings!

"Order parameter" $q \sim \mathcal{N}_a \cap \mathcal{N}_b$



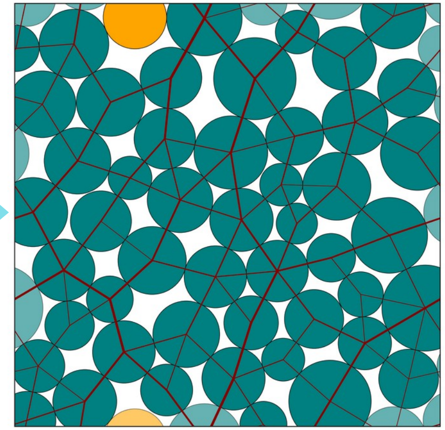
Reference packing



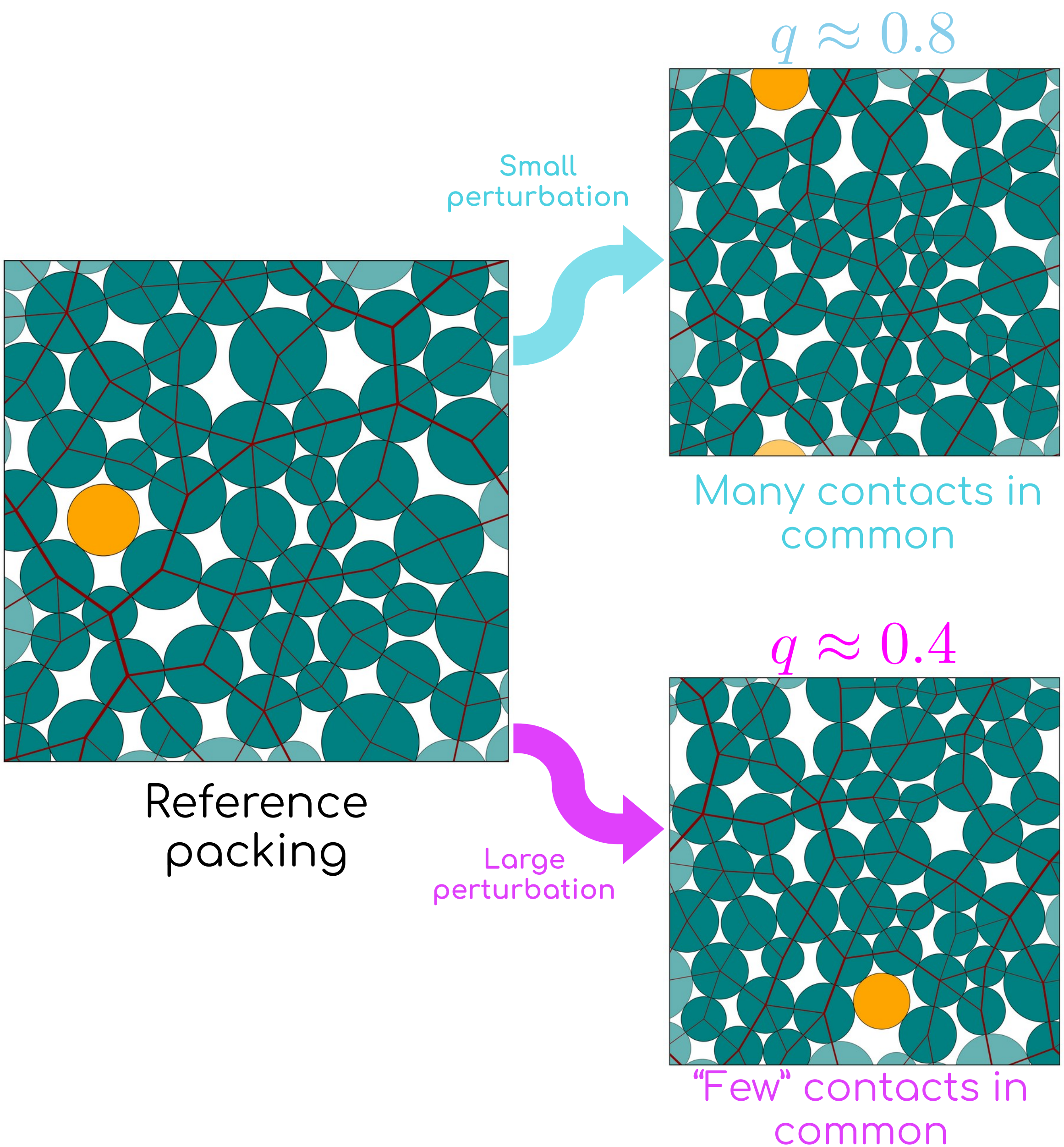
Reference packing

Small perturbation

$q \approx 0.8$



Many contacts in common


$q \approx 0.8$
Small perturbation
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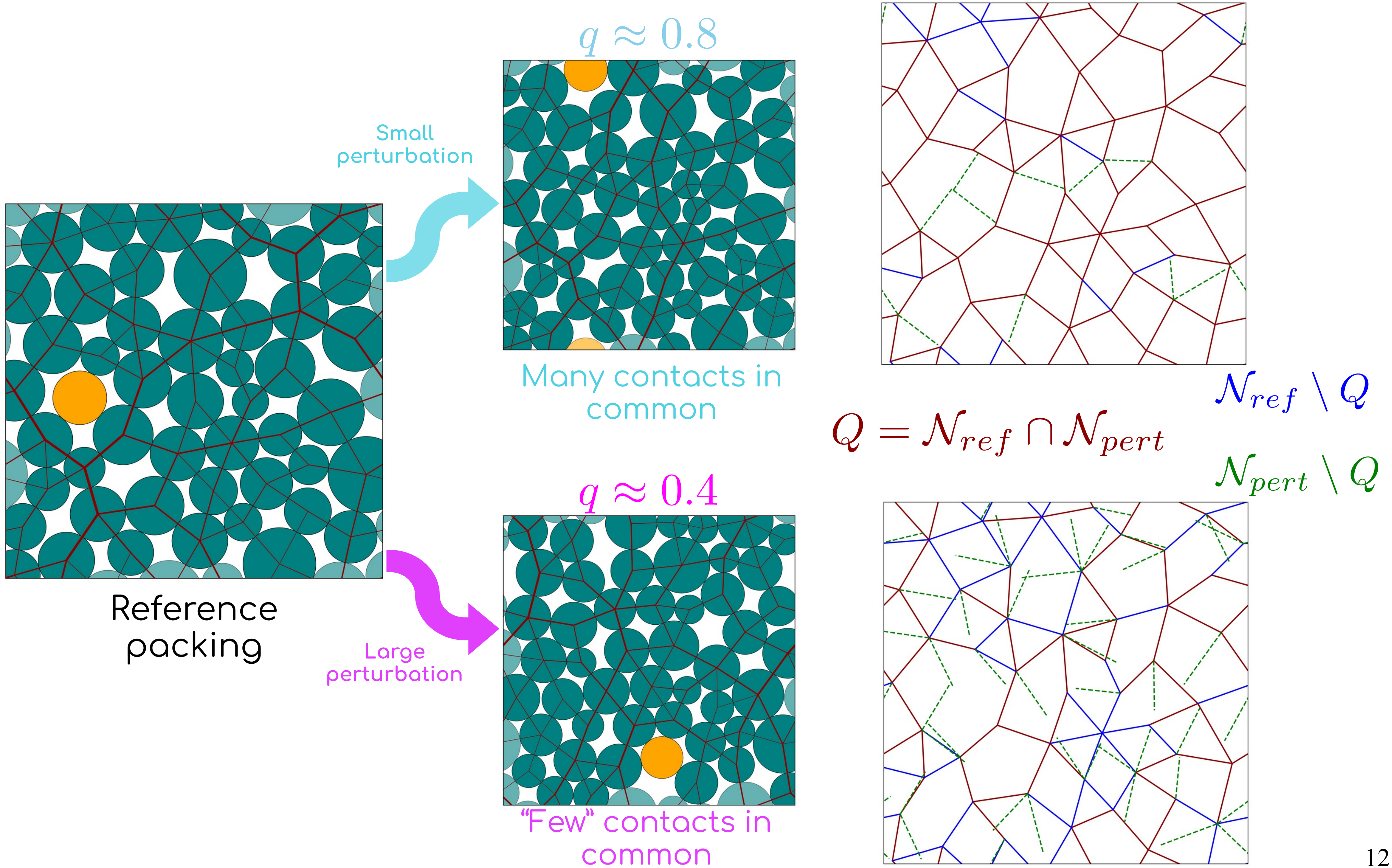
$q \approx 0.4$
Large perturbation
“Few” contacts in common



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Reference packing
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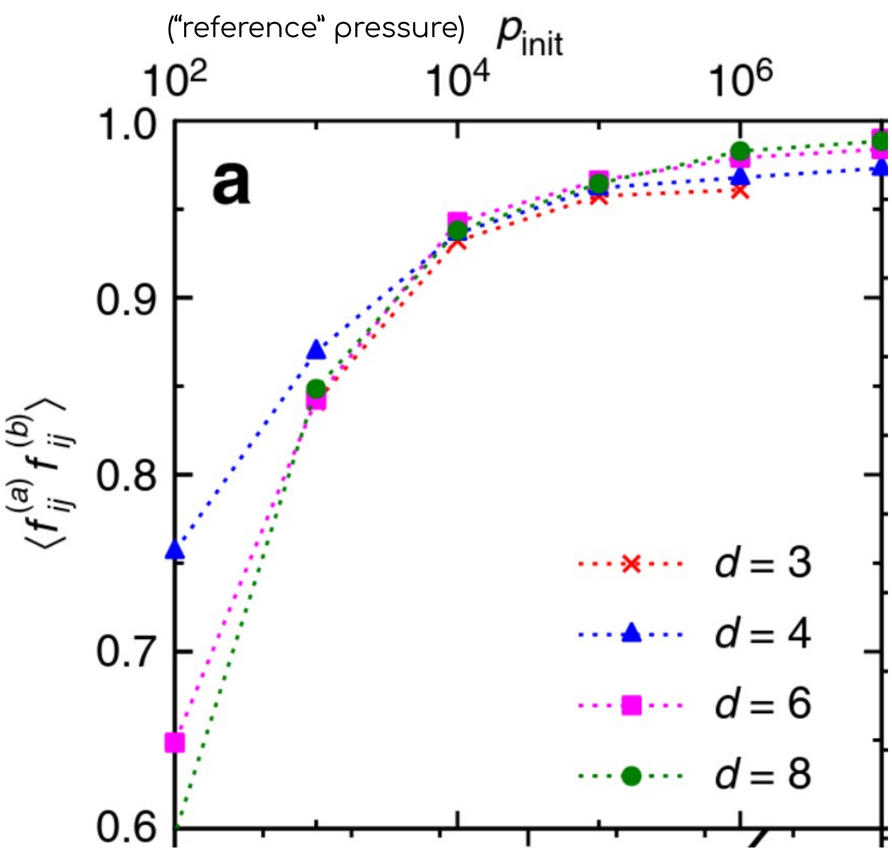
Large perturbation
"Few" contacts in common
$\mathcal{N}_{ref} \setminus Q$
$Q = \mathcal{N}_{ref} \cap \mathcal{N}_{pert}$
$\mathcal{N}_{pert} \setminus Q$



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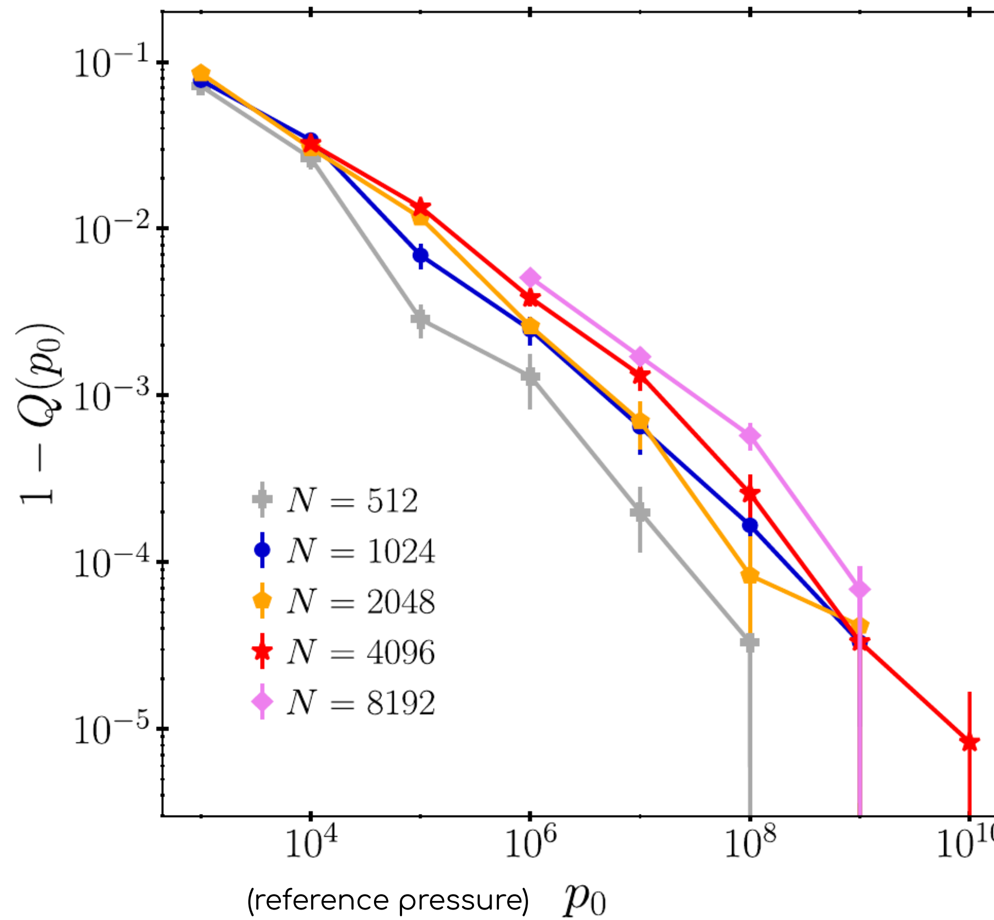
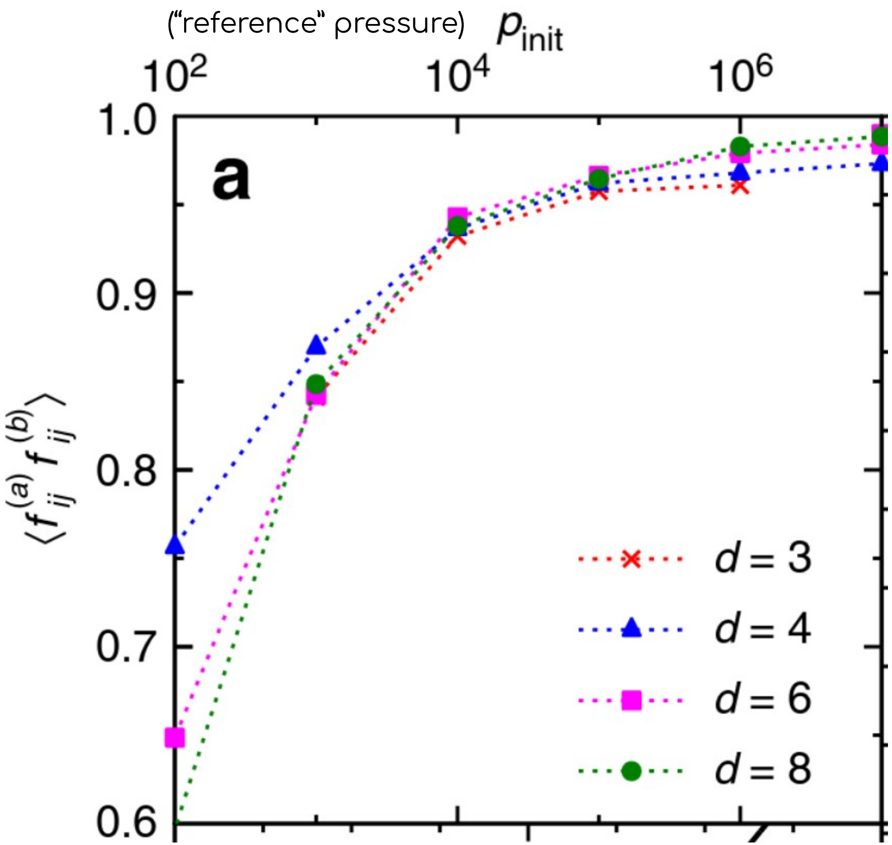


PROGRESSIVE increase in the similarity (overlap) between contacts networks

Free energy landscape has a **COMPLEX structure** (NOT made of simple, convex basins)



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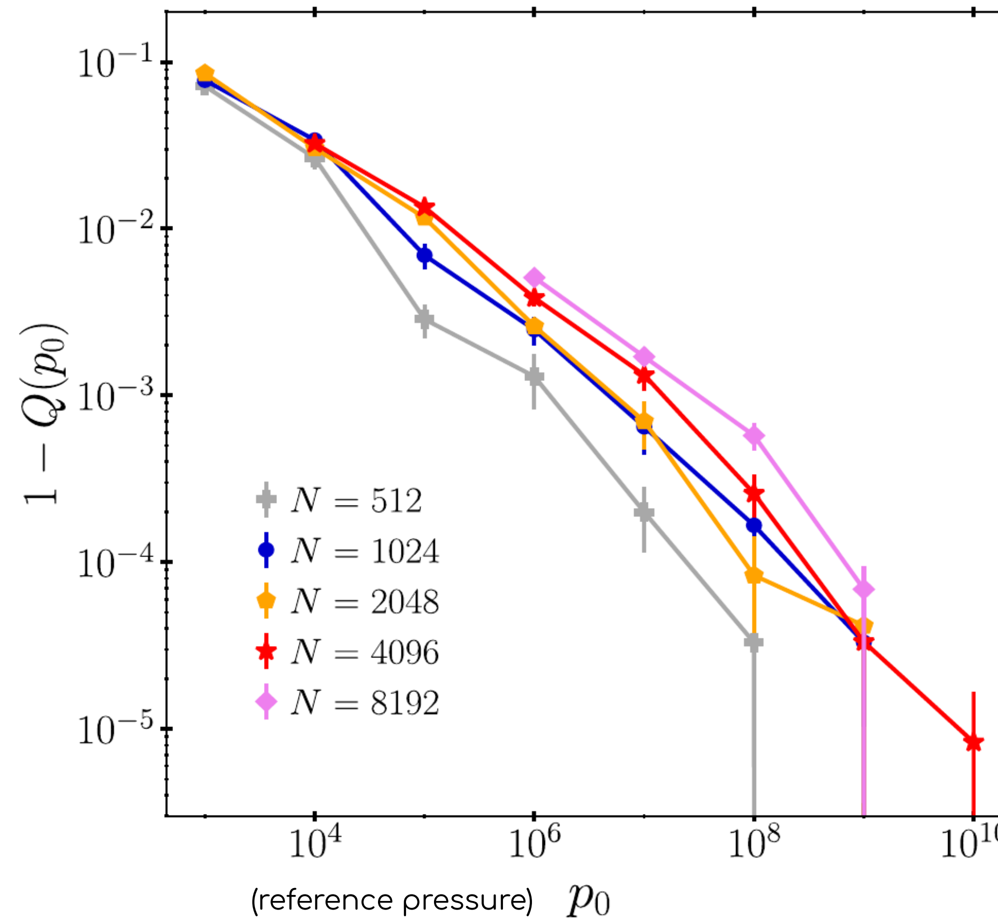
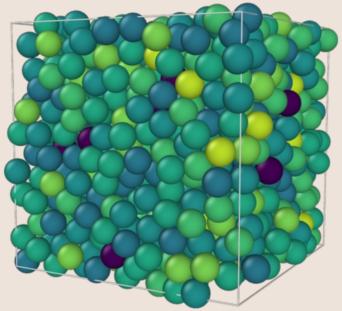
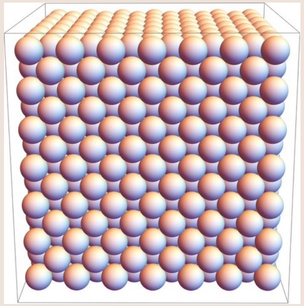


1) **(Disordered) Jamming** is different from the **geometric** sphere packing problem **[universality across dimensions]**



$\neq$



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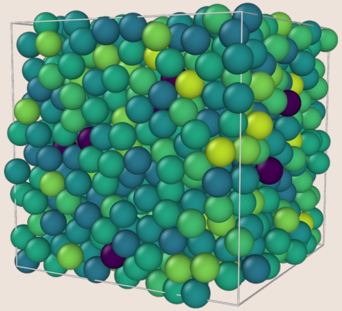

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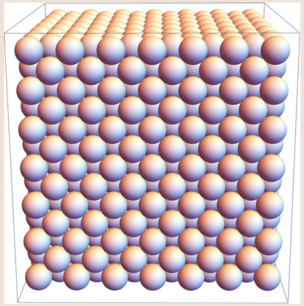
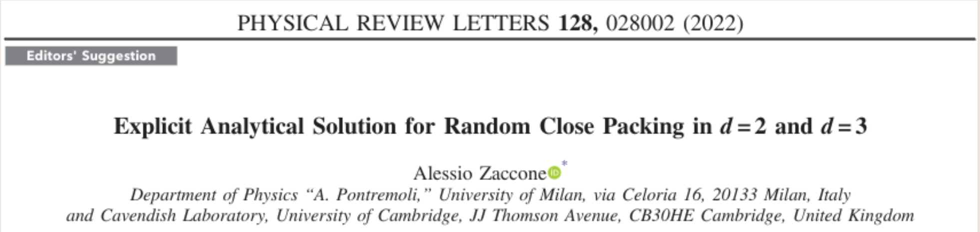


2) Jamming transition is **different** from usual phase transitions

a) It is an **<u>out equilibrium transition</u>**

b) We have NO idea how to compute (analytically) even basic quantities (φ_J)



PHYSICAL REVIEW LETTERS **128,** 028002 (2022)

Editors' Suggestion

Explicit Analytical Solution for Random Close Packing in $d=2$ and $d=3$

Alessio Zaccone*

Department of Physics "A. Pontremoli," University of Milan, via Celoria 16, 20133 Milan, Italy and Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, CB30HE Cambridge, United Kingdom

c) Do <u>NOT</u> believe in

[PERSONAL opinion]

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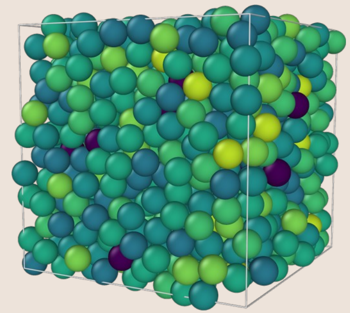

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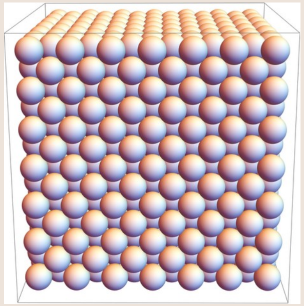

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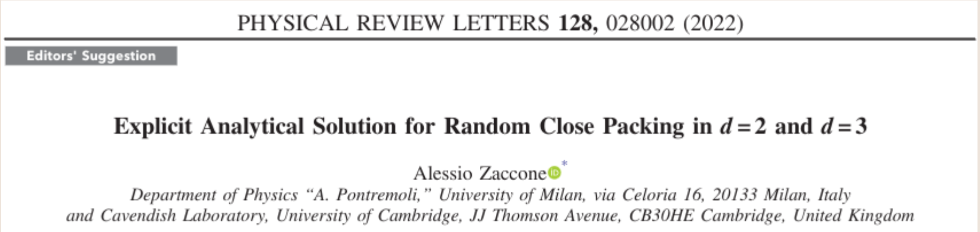

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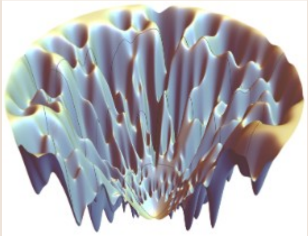

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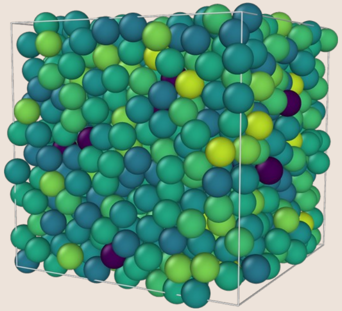

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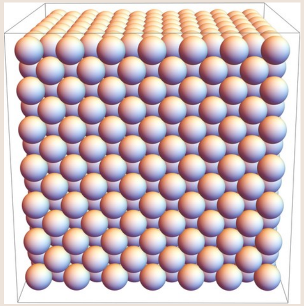

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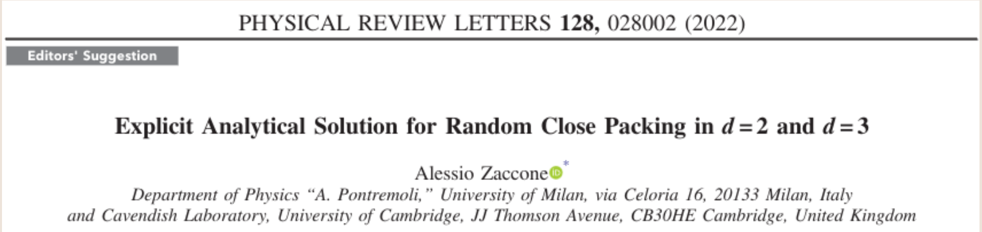
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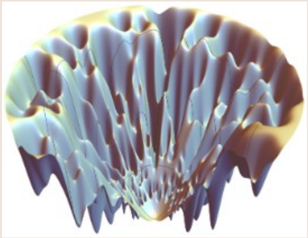

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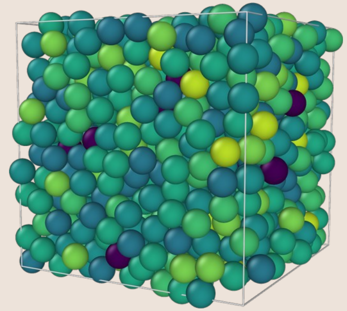

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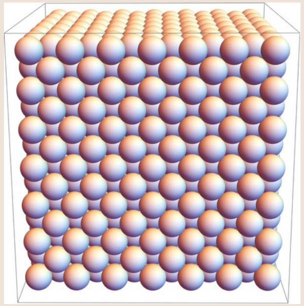

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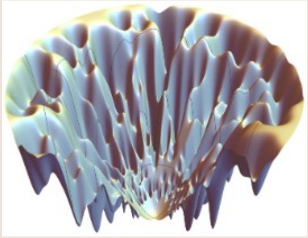


$$g(h) \sim h^{-\gamma};\ \gamma = 0.4127\ldots$$

$$p(f) \sim f^{\theta_e};\ \theta_e = 0.423\ldots$$

... why?!

4) Generating jammed packings is **numerically challenging!**

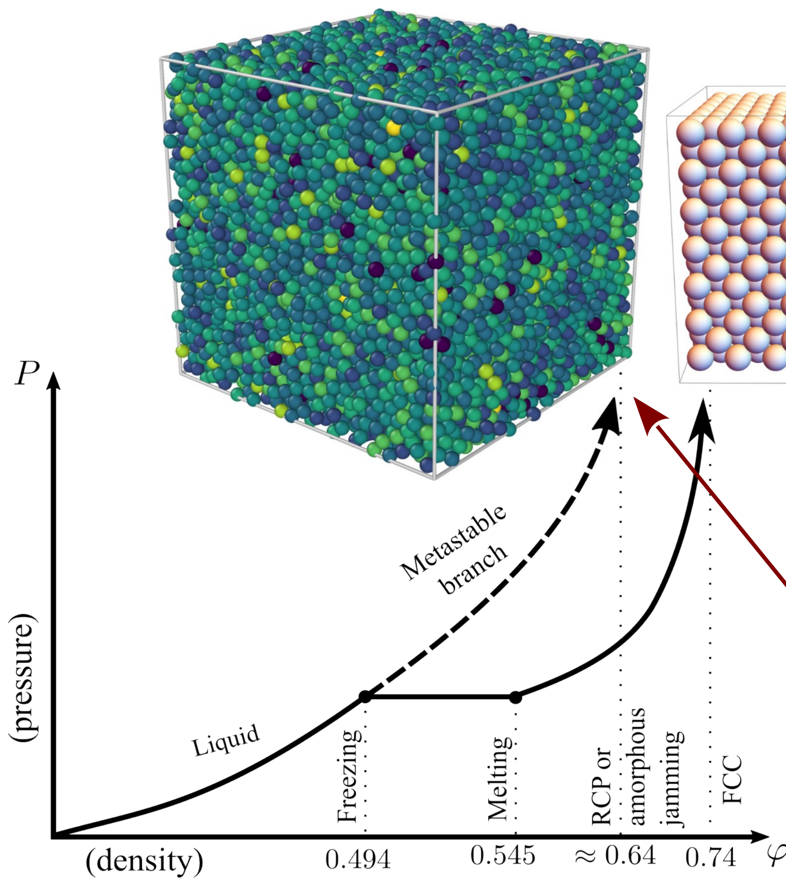
... can be discussed over a beer!

¡MUCHAS GRACIAS!

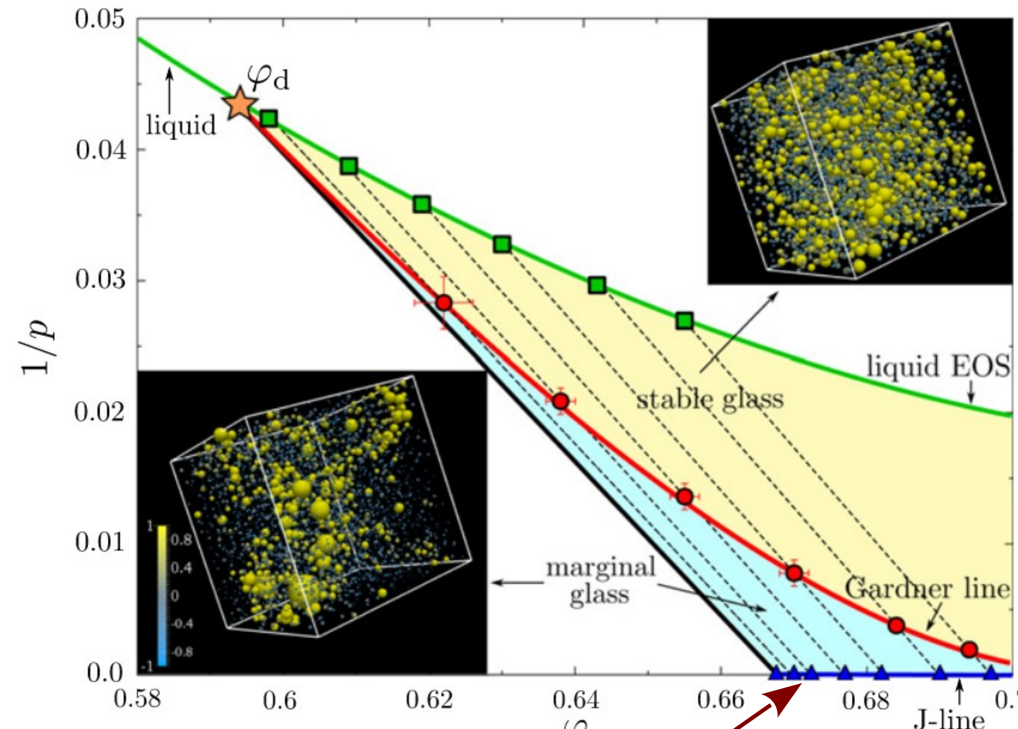
- Claudia Artiaco (now a postdoc @ Nordita)
- Prof. Federico Ricci Tersenghi
- Prof. Giorgio Parisi

Back-up slides

(A "crash course" on) Thermodynamics of Hard Spheres



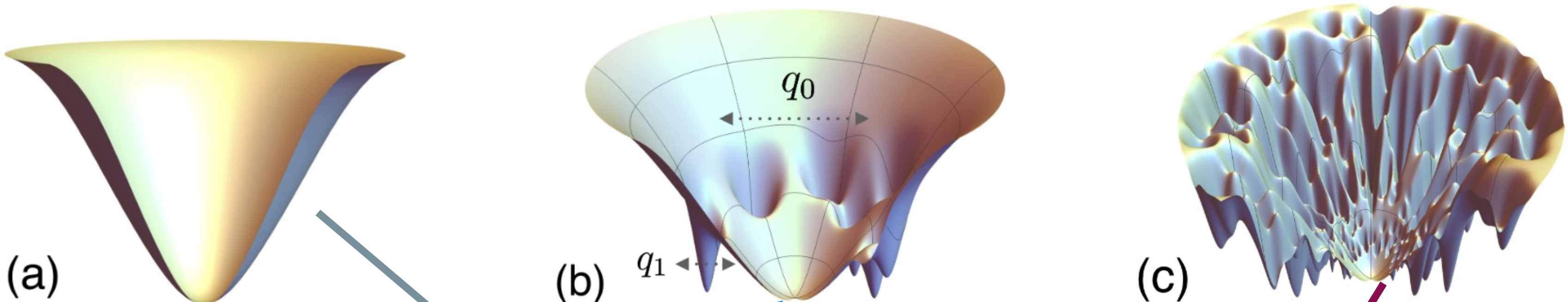
[Berthier, Charbonneau, Jin, Parisi, Seoane, Zamponi, *PNAS*, **(2016)**]

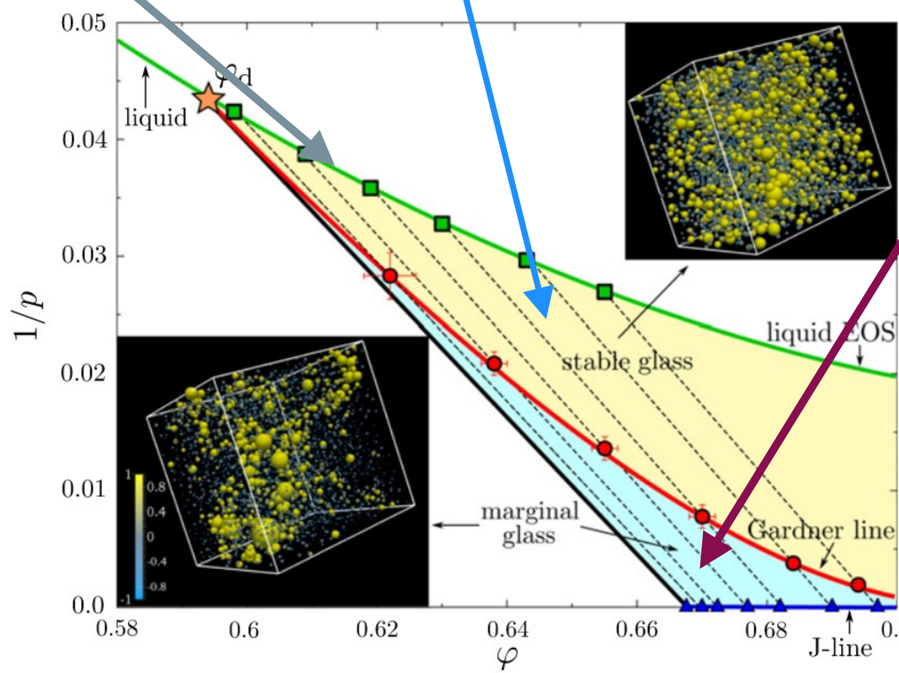


Jamming transition happens here
[universality class]

Free energy landscapes in disordered systems
[hard case]

[Cugliandolo, *Ann. Rev. Cond. Matt*, **(to appear)**]





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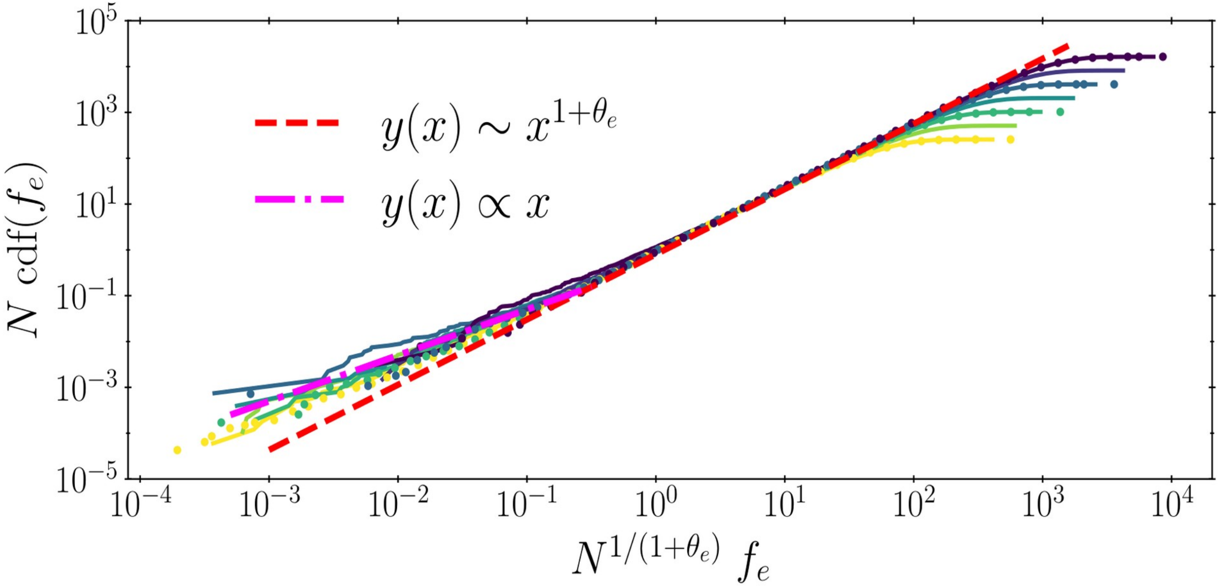
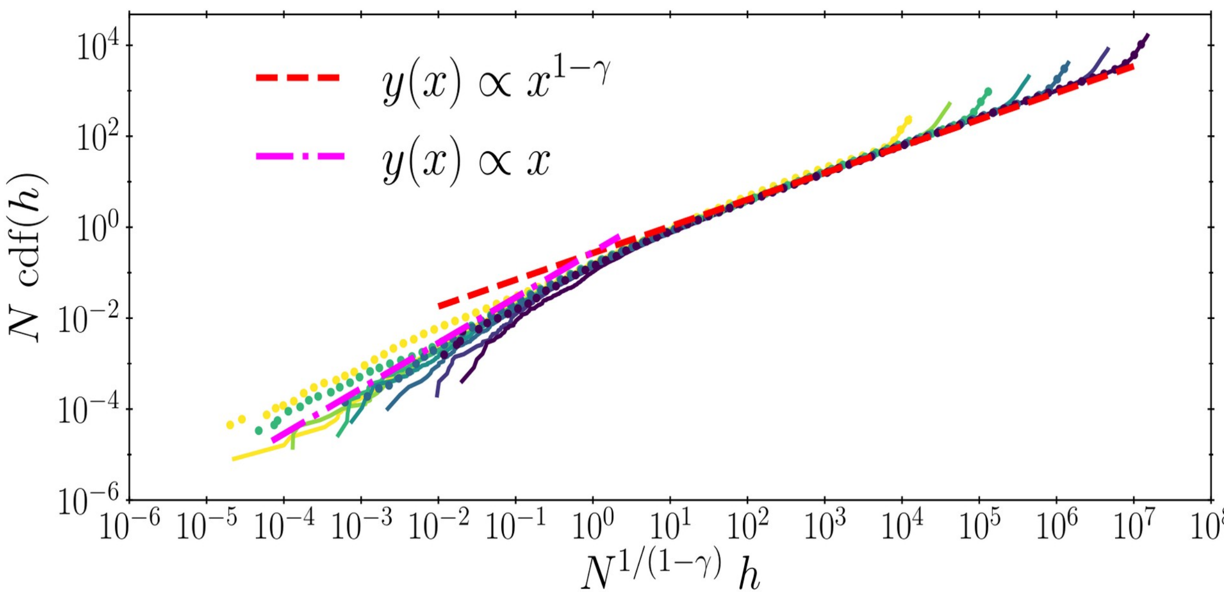
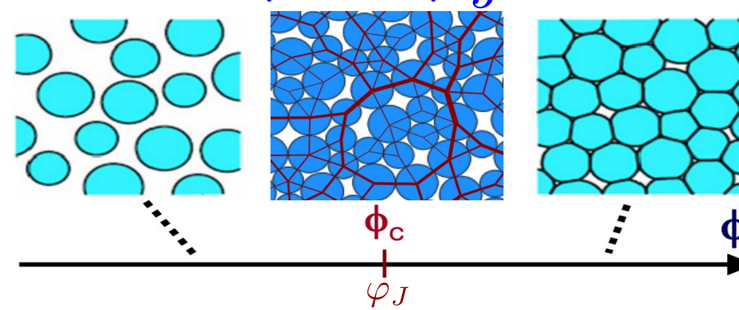




Same critical exponents <u>independently</u> of how the Jamming transition is reached!!

$$\varphi \to \varphi_J^{\pm}$$



[Charbonneau, Corwin, Denis, RDHR, Ikeda, Parisi, Ricci-Tersenghi, *PRE,* **(2021)**]

Hard-Spheres Jamming as an optimization problem

Inspired by [Donev *et al.* *J. Comp. Phys.* **(2004)**] & [Torquato and Jiao, *PRE* **(2010)**]

Given $\left(\begin{array}{l} \vec{\mathbf{r}} = \{\mathbf{r}_i\} \\ \vec{\sigma} = \{\sigma_i\} \\ \varphi < \varphi_J \end{array} \right)$ → Find the displacements (rearrangements) $\vec{\mathbf{s}} = \{\mathbf{s}_i\}$ → Density is *maximized* without overlaps!

$\mathbf{r}_i \to \mathbf{r}_i + \mathbf{s}_i$

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$$\max\ \Gamma$$

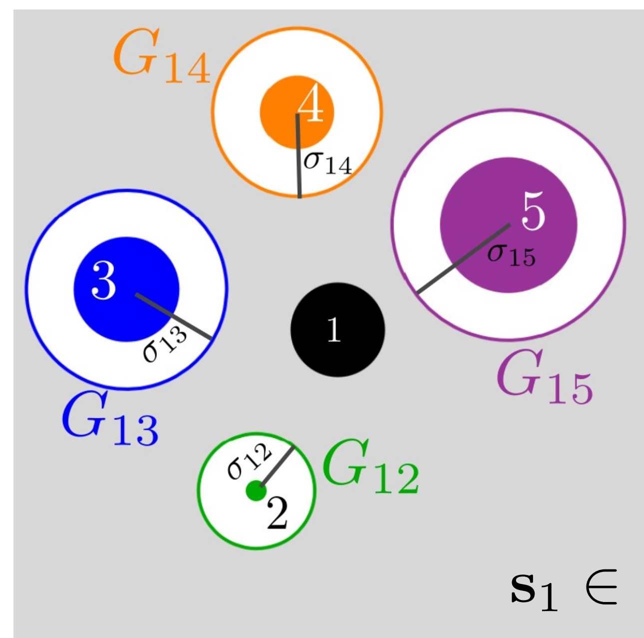
$$G_{ij}(\vec{\mathbf{s}}, \Gamma) : \left|\mathbf{r}_i + \mathbf{s}_i - (\mathbf{r}_j + \mathbf{s}_j)\right|^2 \geq \Gamma \sigma_{ij}^2$$

$$\forall 1 \leq i < j \leq N$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

$$\mathbf{r}_i \leftarrow \mathbf{r}_i + \mathbf{s}_i^{\star}$$

$$\sigma_i \leftarrow \sqrt{\Gamma^{\star}}\sigma_i$$



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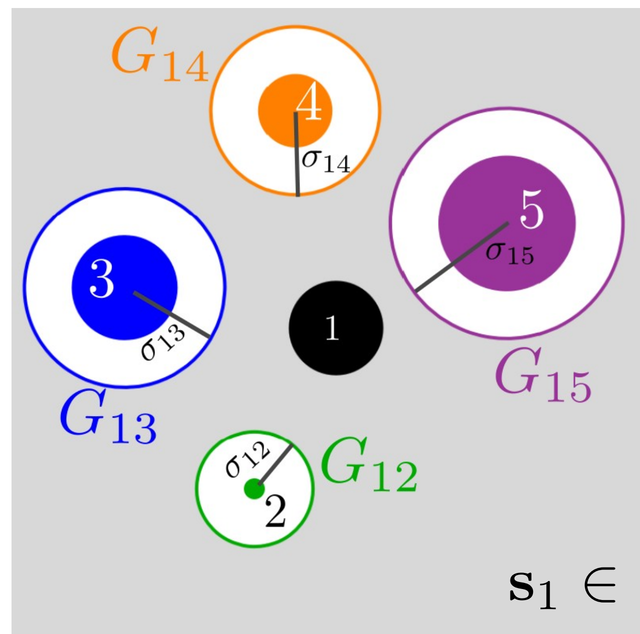


Constrained Optimization Problem

NON CONVEX

The Jamming LOP

If $\varphi \lesssim \varphi_J \implies |\mathbf{s}_{ij}| \ll |\mathbf{r}_{ij}|$

$\mathcal{O}\left(|\mathbf{s}_{ij}|^2\right)$ → Negligible

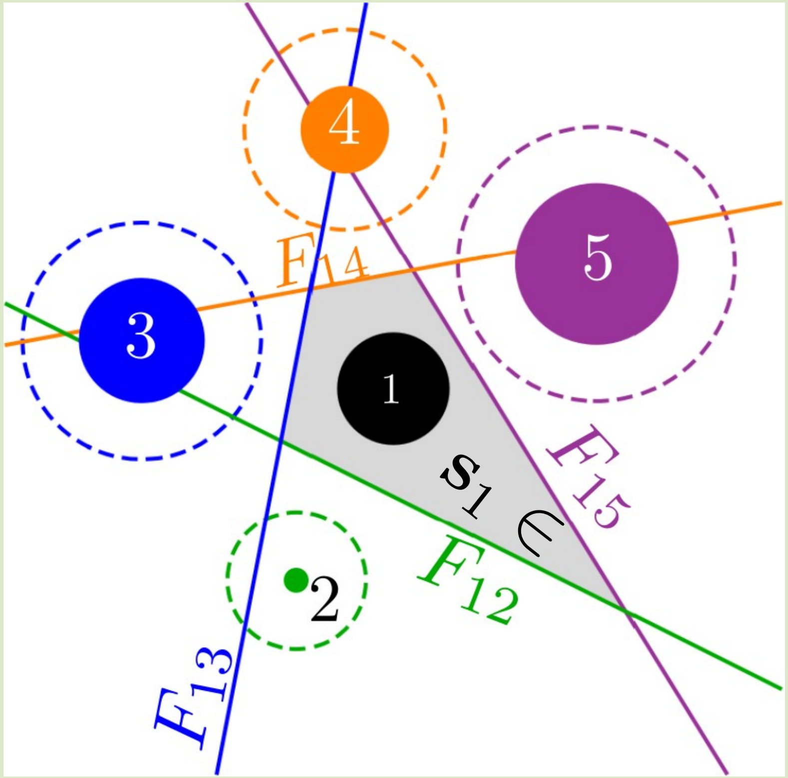
Linear Optimization Problem

LOP $\leftrightarrow$ easy

$$\max \ \Gamma$$

$$F_{ij}(\vec{\mathrm{s}}, \Gamma) : |\mathbf{r}_{ij}|^2 + 2\mathbf{r}_{ij} \cdot \mathbf{s}_{ij} \geq \Gamma \sigma_{ij}^2$$

$$\forall 1 \leq i < j \leq N$$

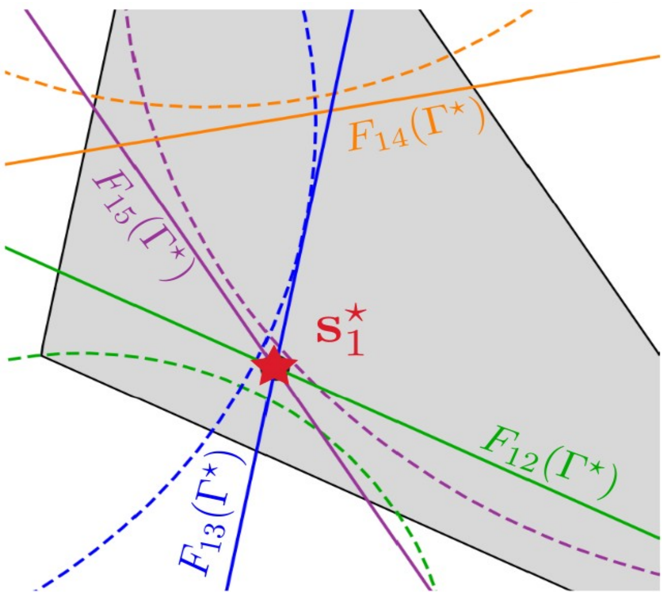


The Jamming LOP

First (*insufficient*) attempt

If $\varphi \lesssim \varphi_J \implies |\mathbf{s}_{ij}| \ll |\mathbf{r}_{ij}|$

$\mathcal{O}\left(|\mathbf{s}_{ij}|^2\right)$ → Negligible



Different optimizers of the <u>linear</u> and <u>exact</u> OPs!

Linear Optimization Problem

LOP ↔ easy

$$\max \ \Gamma$$

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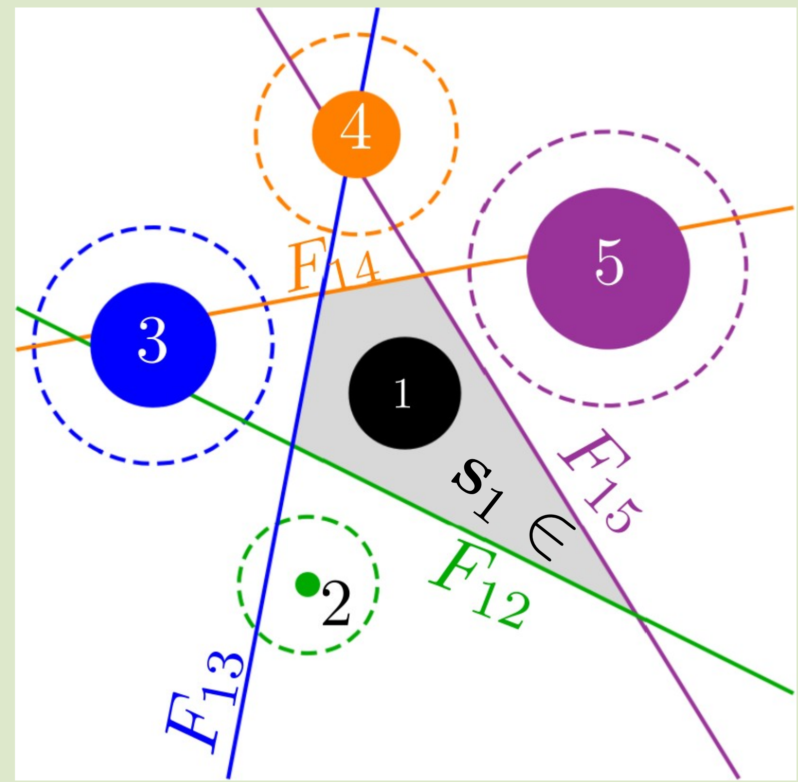

The CHAIN of Jamming LOPs

The new configuration:

$$\mathbf{r}_i \leftarrow \mathbf{r}_i + \mathbf{s}_i^\star \sigma_i \leftarrow \sqrt{\Gamma^\star}\sigma_i$$

1. Does not have any overlaps
2. Has a larger density

It can be used to generate a <u>NEW</u> instance of the jamming LOP

The CHAIN of Jamming LOPs

The new configuration:

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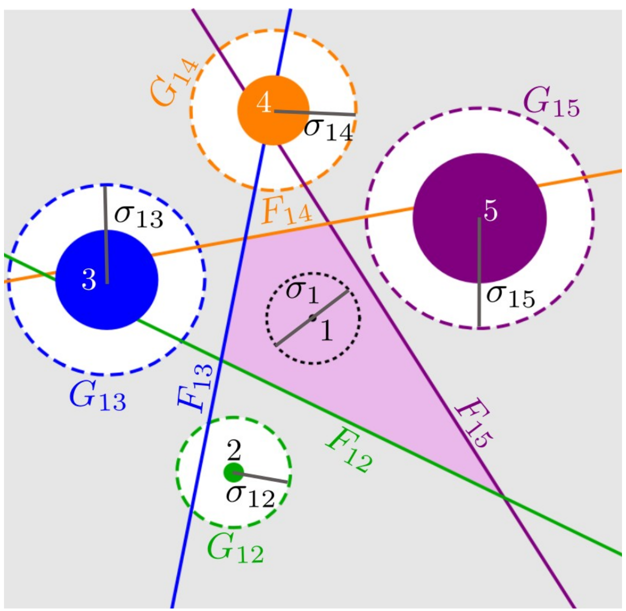
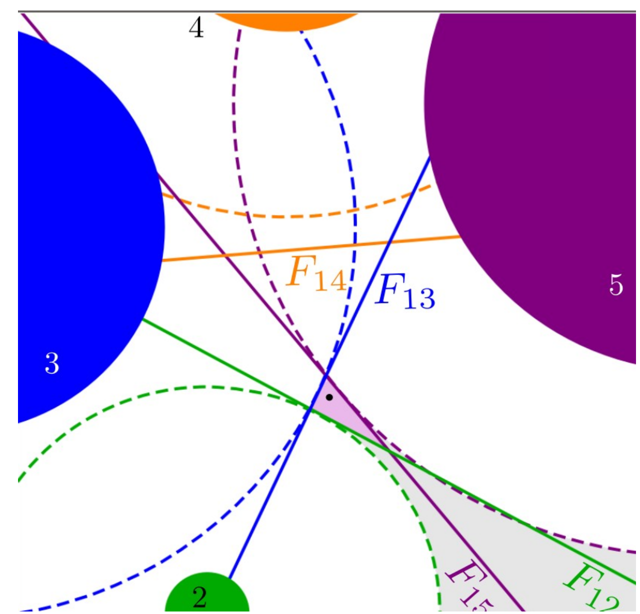
1. Does not have any overlaps
2. Has a larger density

It can be used to generate a NEW instance of the jamming LOP

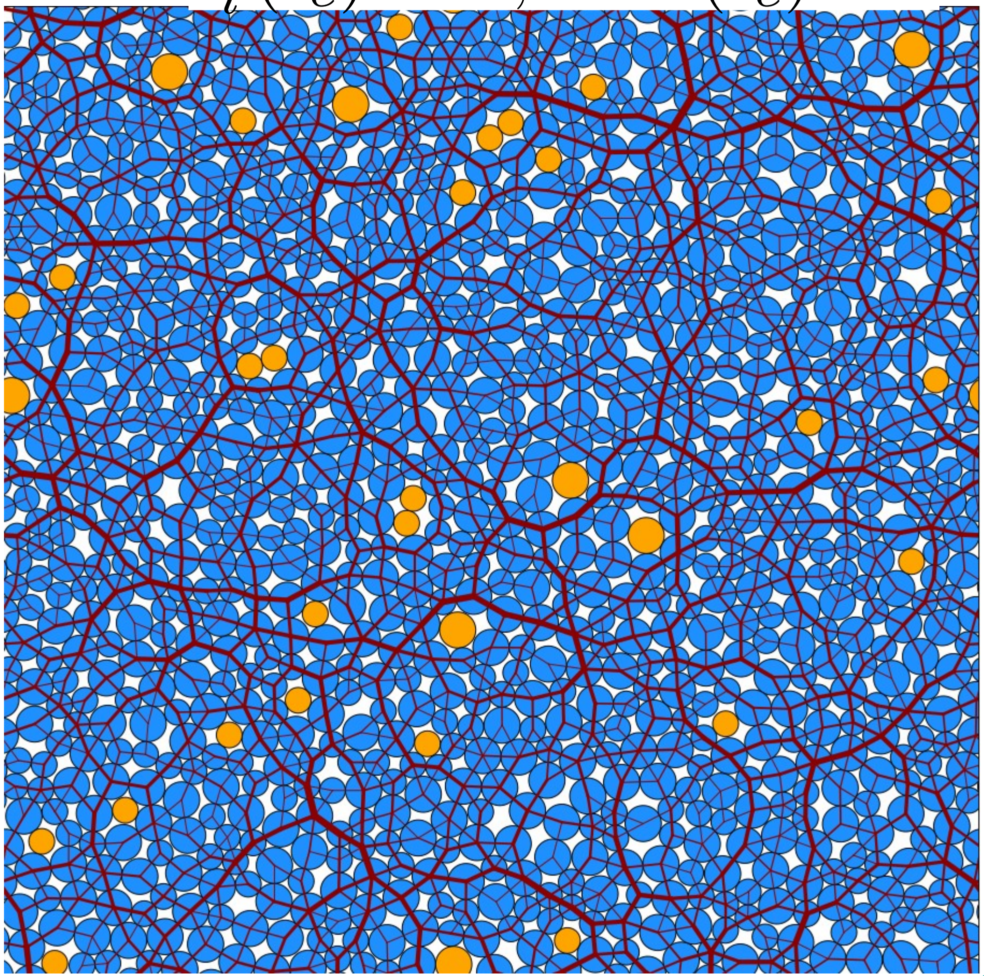
$$(\mathbf{r}_i(t+1), \sigma_i(t+1)) = \left(\mathbf{r}_i(t) + \mathbf{s}_i^\star(t), \sqrt{\Gamma^\star(t)}\sigma_i(t)\right)$$





Convergence

$$\mathbf{s}_i^\star(t_c) = \mathbf{0}, \quad \Gamma^\star(t_c) = 1$$



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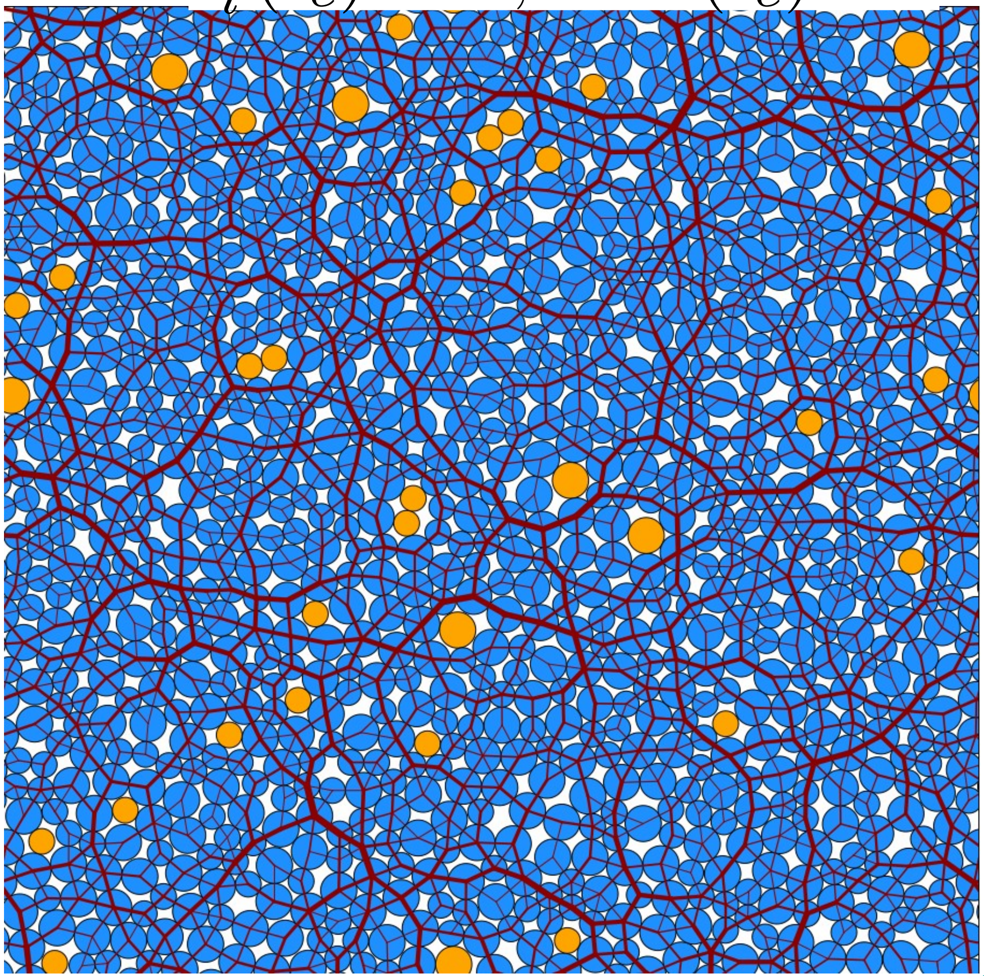

Forces ↔ Lagrange multipliers (>0)
(**active** dual variables)

$$F_{ij}(\vec{\mathbf{s}}, \Gamma) := \Gamma\sigma_{ij}^2 - 2\mathbf{r}_{ij}\cdot\mathbf{s}_{ij} - |\mathbf{r}_{ij}|^2 \le 0$$

$$F_{ij} \longrightarrow \lambda_{ij} \ge 0$$

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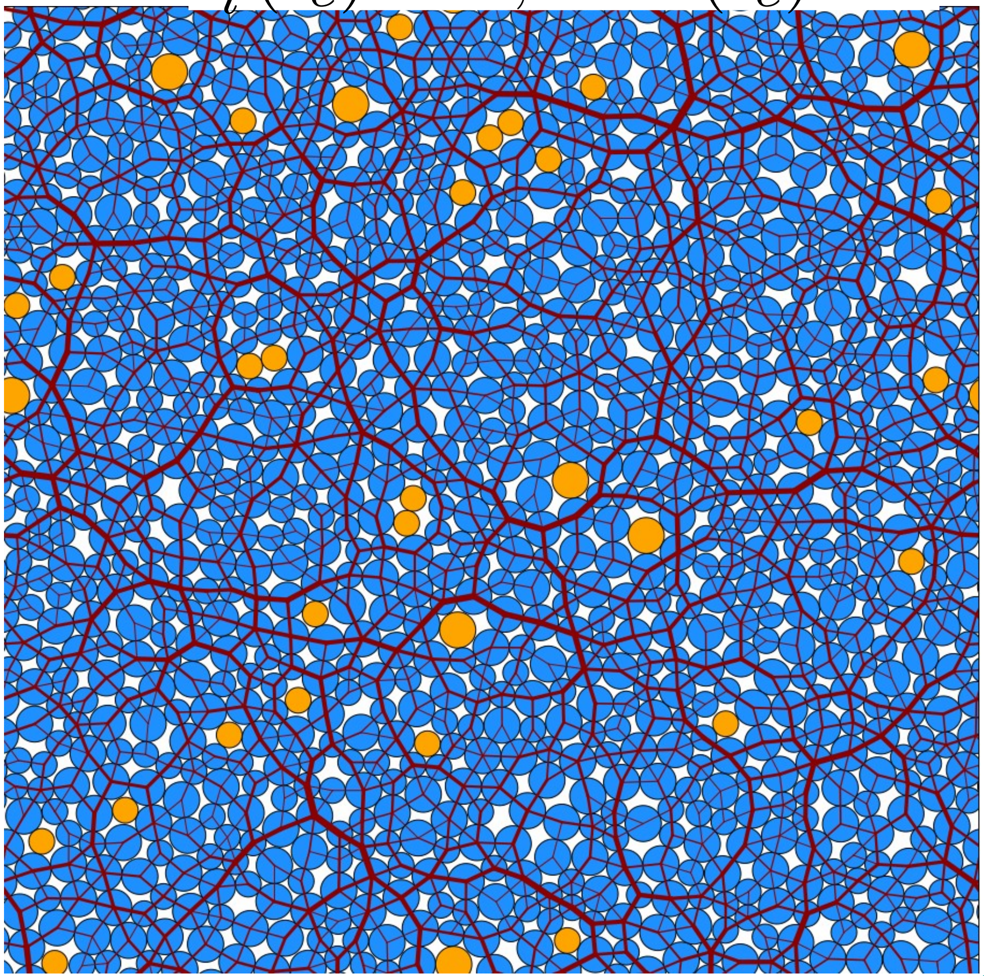

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$$F_{ij} \longrightarrow \lambda_{ij} \geq 0$$

For *any* Optimal Solution
(KKT conditions)

↓

Mechanical equilibrium

$$\sum_{j\in\partial i} \mathbf{f}_{ij} = 0$$

and isostaticity

$$N_c = d(N-1) + 1$$

CALiPPSO.jl

(Chain of Approximated Linear Programming for Packing Spherical Objects)

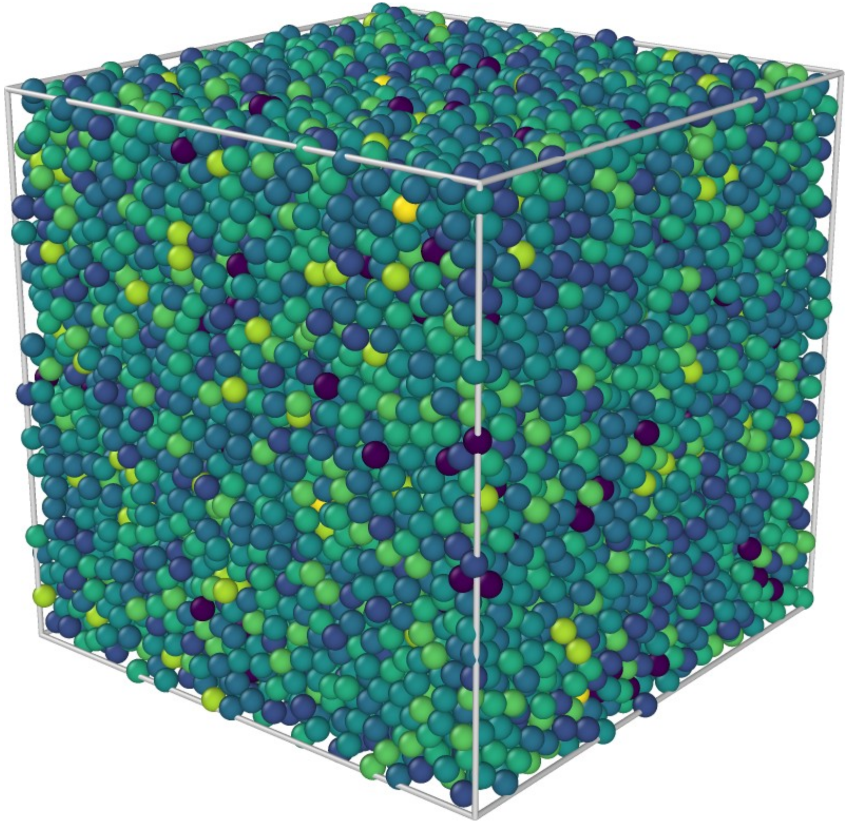
5 lines
To obtain **isostatic** jammed packings

In [1]:

```julia
using CALiPPSO

precompile_main_function()

const d, N, φ0, L = 3, 800, 0.3, 2.0
r0, Xs0 = generate_random_configuration(d, N, φ0, L)

packing, info, Γ_vs_t, Smax_vs_t, isostatic_vs_t = produce_jammed_configuration!(Xs0, r0; ℓ0=0.2*L, max_iters=500)
```

Optional (but recommended for speed)

```
        CALiPPSO converged!              Status of last LP optimization: OPTIMAL
Iterations to convergence = 456,       √Γ-1 = 2.220446049250313e-16,    Max displacement = 5.0e-15,     (ϕ, R) = [0.63326217, 0.11477086]
        Non_rattlers= 789       % of rattlers = 1.375   (Max, mean±std) constraints per particle per d: [15.0, 6.16, 3.91]
Isostaticity achieved: true      Non-rattlers = 789     % of rattlers = 1.375   N_contacts [in stable particles] = 2365.0        z in rattlers = 0
Maximum force equilibrium mismatch = 6.051041471403057e-15
Time to finish = 36.53 minutes;  Memory allocated (GB): 75.78
Checking for overlaps after convergence...
No overlaps found! :D


(3d Monodisperse packing         of N= 800 particles     of radius R= 0.11477086229012713
789 stable particles;    fraction of rattlers = 0.014
jammed: true      isostatic: true         and in mechanical equilibrium: true
```



Better initial condition:

$$\frac{\varphi_J - \varphi_0}{\varphi_J} \ll 1 \longleftrightarrow p \gg 1$$

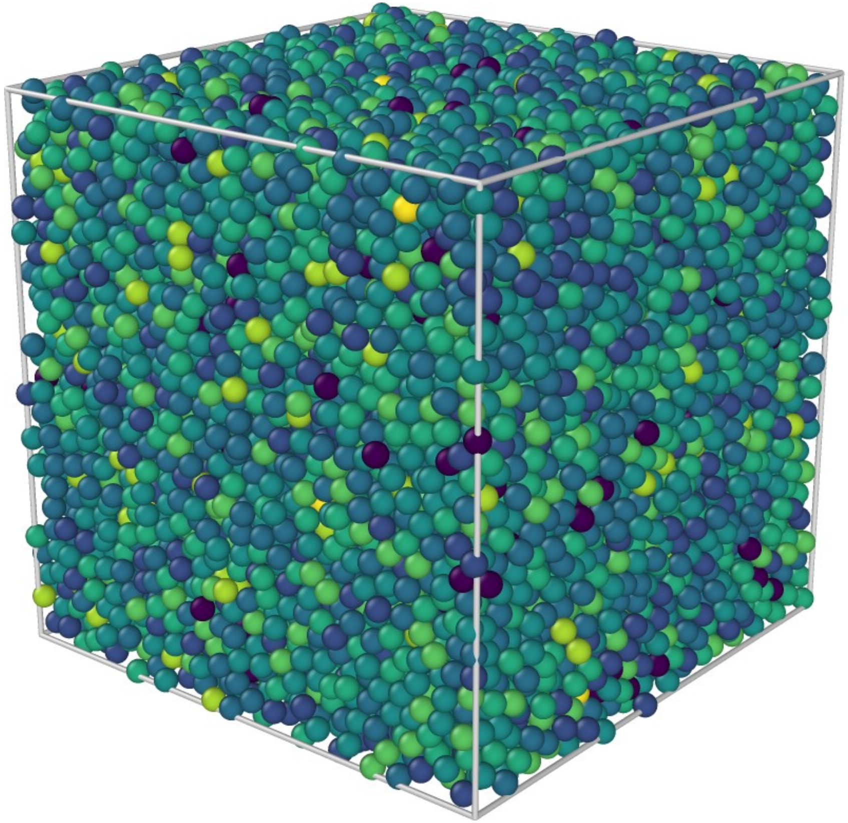
$N = 16,384$

$t_c \approx 30$ iterations

$\varphi_J = 0.644$

- Gaps and forces obtained independently
- Force balance ✓
- Isostaticity ✓

COMPLEXITY: $\tau \sim N^3$



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Study the landscape
[Artiaco, Baldan, Parisi, *PRE*, 2020]

and dynamics
[RDHR, Parisi, Ricci-Tersenghi, *Soft Mat.*, 2021]

of HS *near* jamming

Verify jamming *critical exponents* in HS=SS

$$p(f) \sim f^{\theta}, \quad \theta = 0.42311$$

$$g(h) \sim h^{-\gamma}, \quad \gamma = 0.41269$$

[Charbonneau, Corwin, Dennis, RDHR, Ikeda, Parisi, Ricci-Tersenghi *et al*, *PRE*, 2021]