Jamming and the Anticrystal

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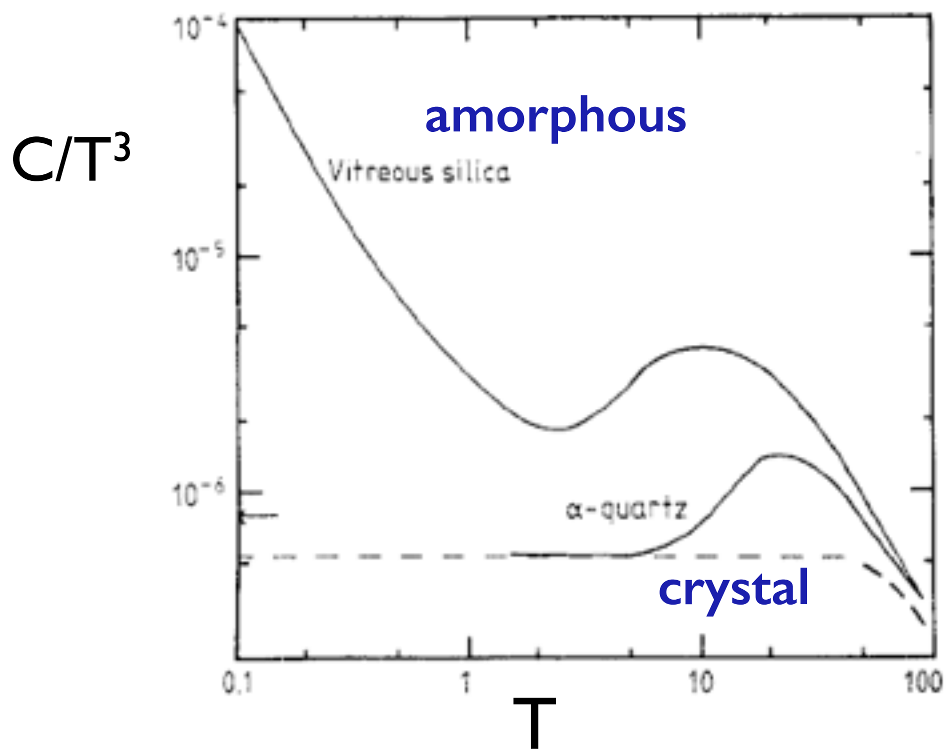
Glasses and the Glass Transition

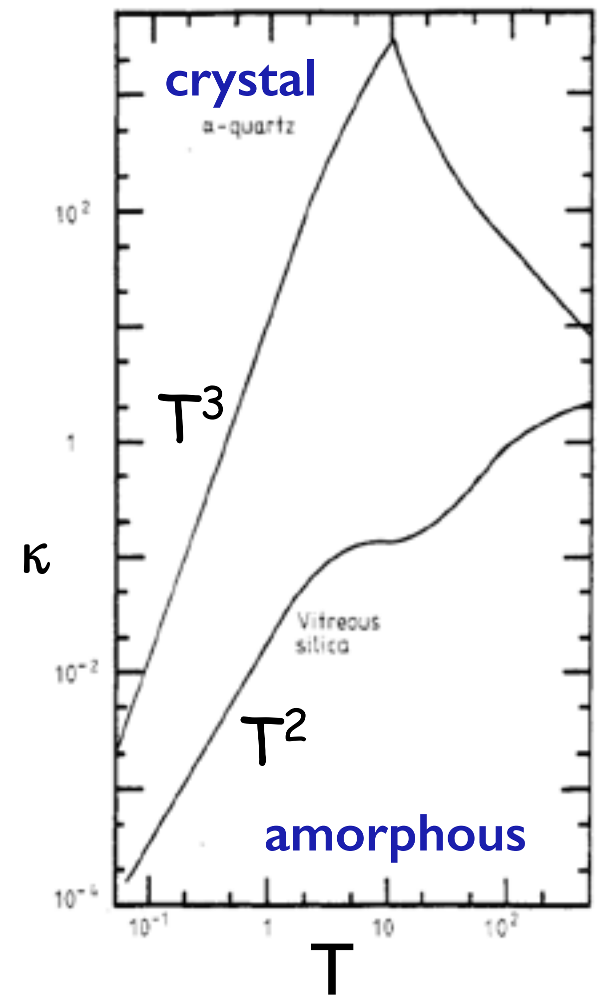
Earliest glassmaking 3000BC

Glass vessels from around 1500BC

- When liquid is cooled through glass transition
  - Particles remain disordered
  - Stress relaxation time increases continuously
  - Can get 10 orders of magnitude increase in 20 K range
- When system can no longer equilibrate on a reasonable time scale, it is called a glass
- All liquids undergo glass transitions if cooled quickly enough

Glasses Share Common Features





- Behavior of glasses is
  - very different from that of crystals
  - similar in all glasses, no matter how they are made
  - low T behavior ascribed to quantum two-level systems

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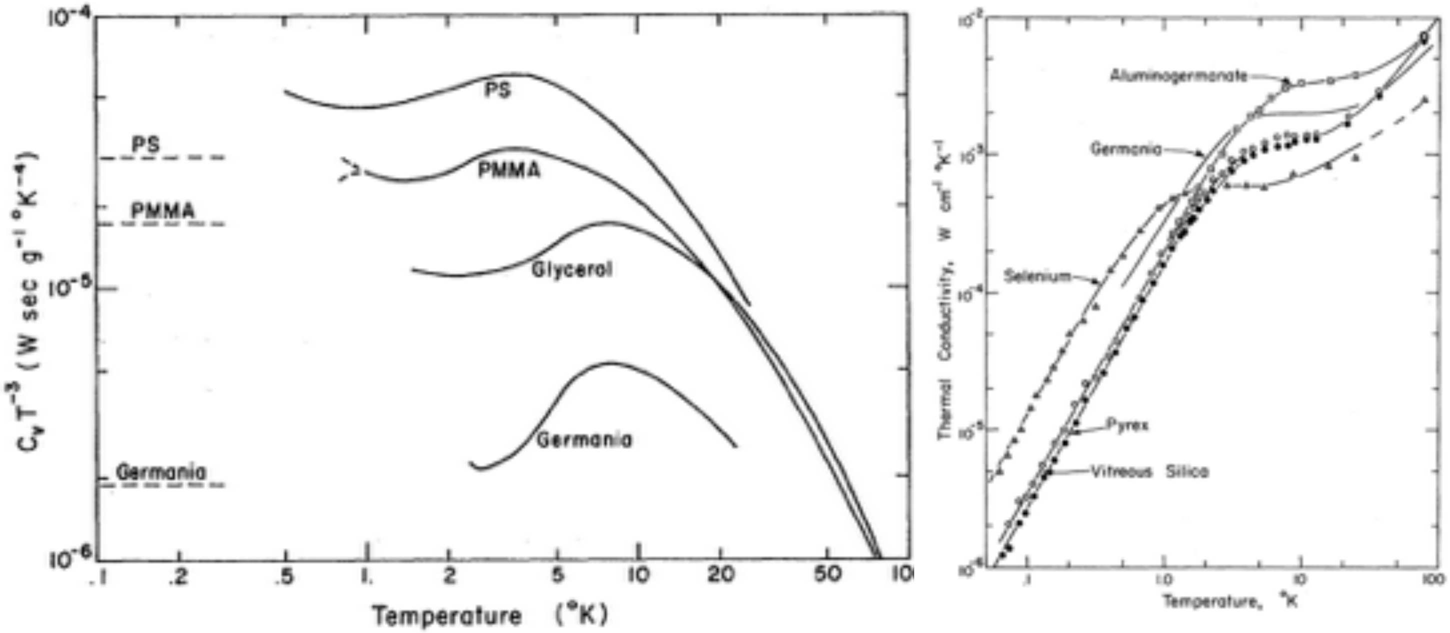

Zeller & Pohl, PRB 4, 2029 (1971).

- Behavior of glasses is
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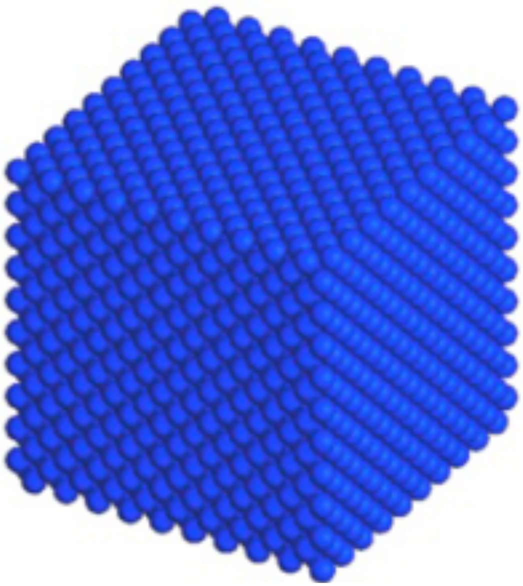
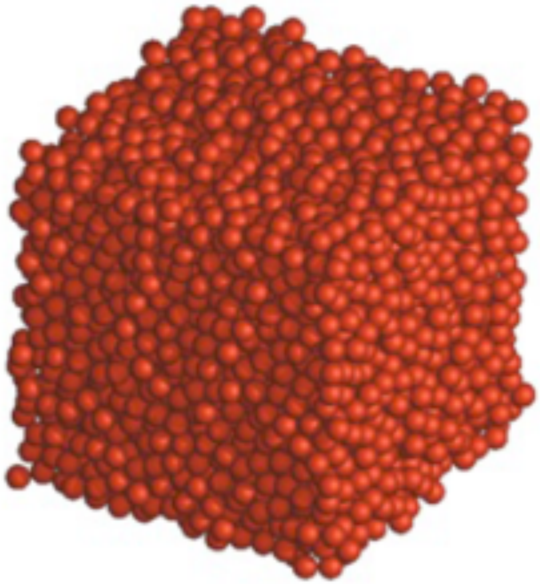
Is There an OPPOSITE POLE to the Crystal?

- Perfect crystal is epitome of order at T=0
- What is the epitome of disorder —the anticrystal—at T=0?



- Why is this a useful question?
  - Important for understanding glasses
    - cannot get there by perturbing a crystal (ie adding defects)
    - Need new way of thinking about solids



  - To understand glass transition, it might help to understand what liquid is making transition to

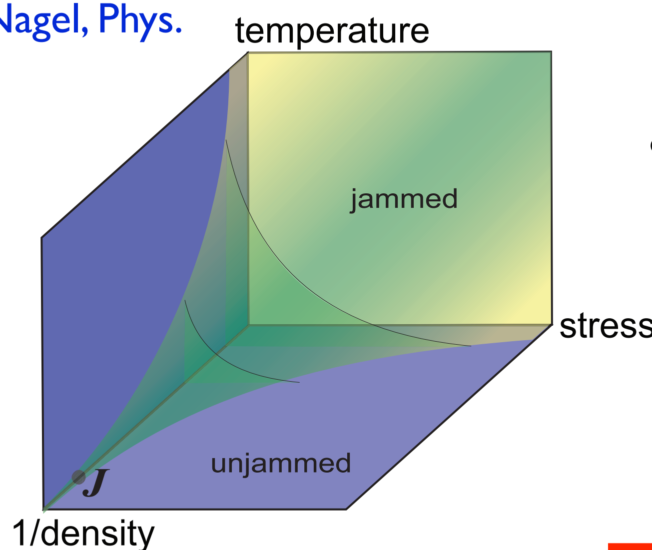
Jamming Transition for "Ideal Spheres"

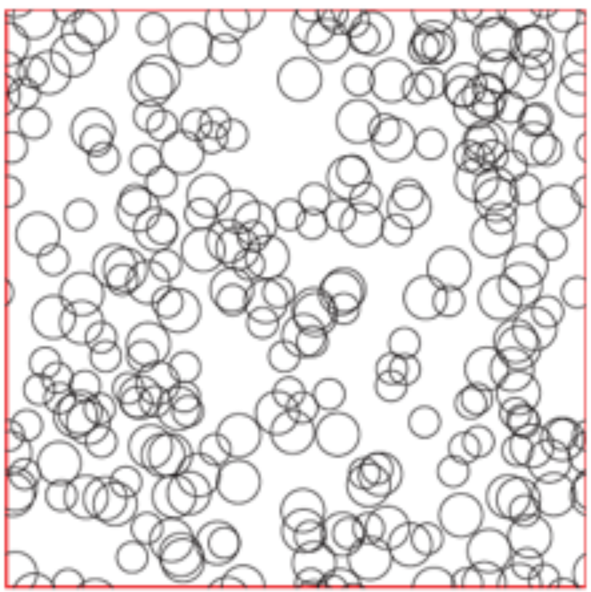
C. S. O'Hern, S. A. Langer, A. J. Liu and S. R. Nagel, Phys. Rev. Lett. **88**, 075507 (2002).

C. S. O'Hern, L. E. Silbert, A. J. Liu, S. R. Nagel, Phys. Rev. E **68**, 011306 (2003).

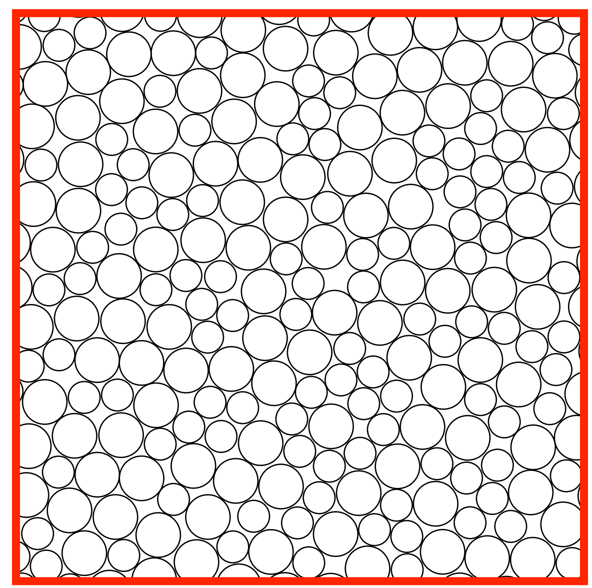
Ideal spheres exhibit standard glass transition phenomenology

$$V(r) = \begin{cases} \dfrac{\varepsilon}{\alpha}\left(1-\dfrac{r}{\sigma}\right)^{\alpha} & r \le \sigma \\ 0 & r > \sigma \end{cases}$$



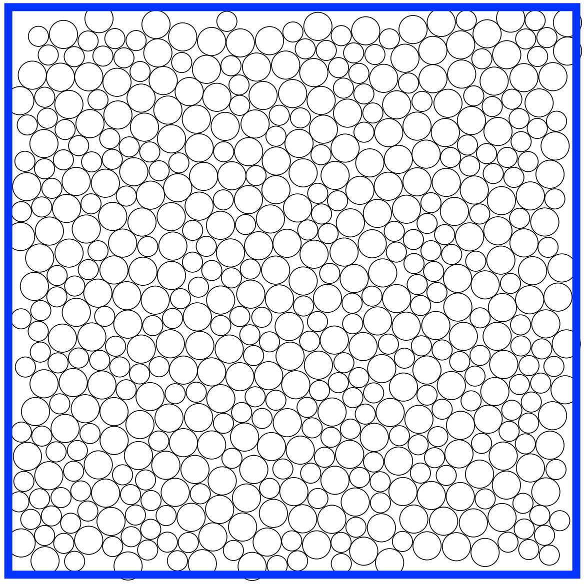


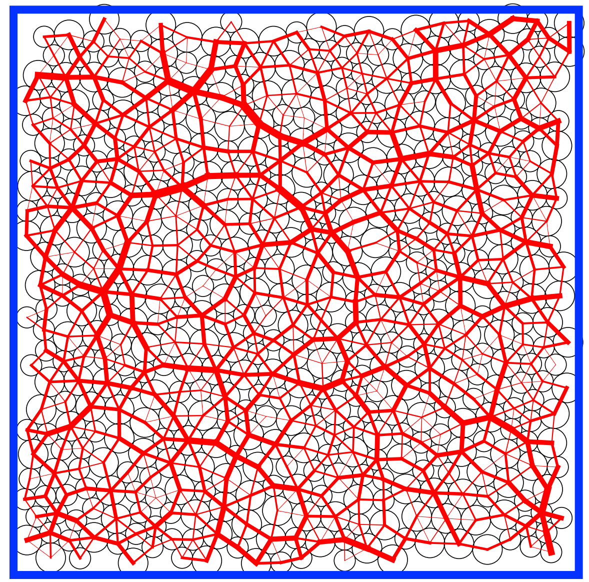
Quench to local energy minimum (T=0)



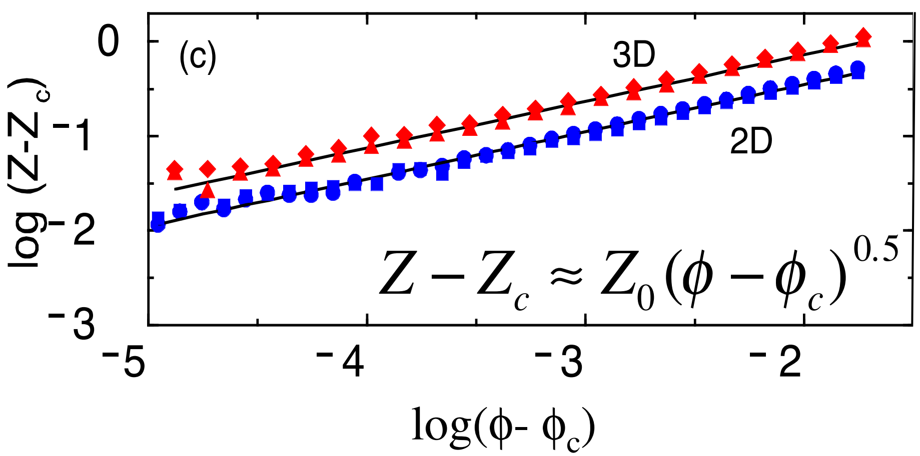
Onset of Overlap has Discontinuous Character

Just below φ_c, no particles overlap





Just above φ_c there are Z_c overlapping neighbors per particle



$Z_c = 3.99 \pm 0.01$ 2D

$Z_c = 5.97 \pm 0.03$ 3D

Verified experimentally:
G. Katgert and M. van Hecke, EPL **92**, 34002 (2010).

Durian, PRL **75**, 4780 (1995).
O'Hern, Langer, Liu, Nagel, PRL **88**, 075507 (2002).

Isostaticity

- What is the minimum number of interparticle contacts needed for mechanical equilibrium?
- No friction, N repulsive spheres, d dimensions
- Match
  - number of constraints=NZ/2
  - number of degrees of freedom =Nd
- Stable if $Z \geq 2d$
- So at overlap, sphere packing has minimum number of contacts needed for mechanical stability. Is it stable?

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James Clerk Maxwell

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YES

- Onset of overlap is onset of rigidity. This is the jamming transition.

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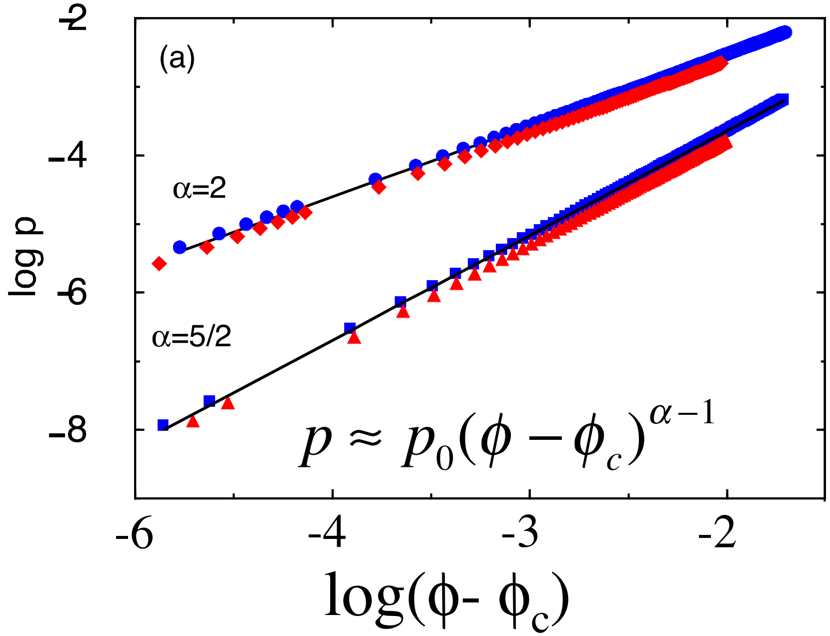

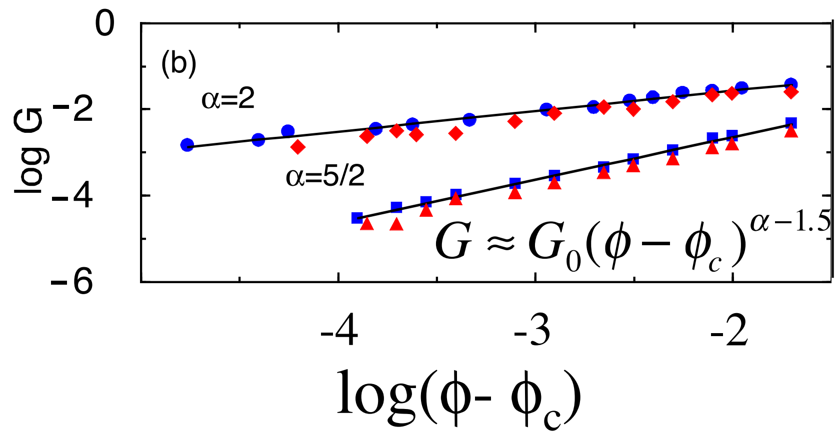

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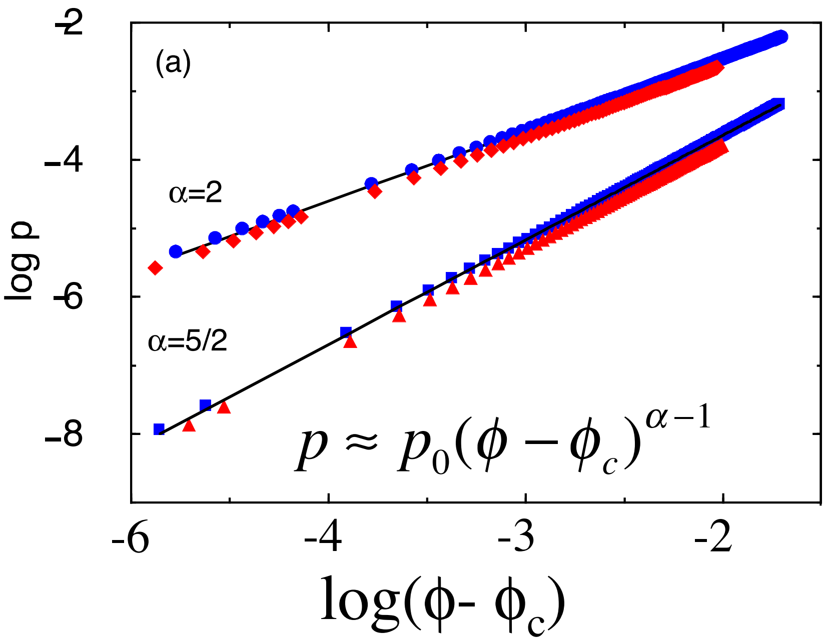
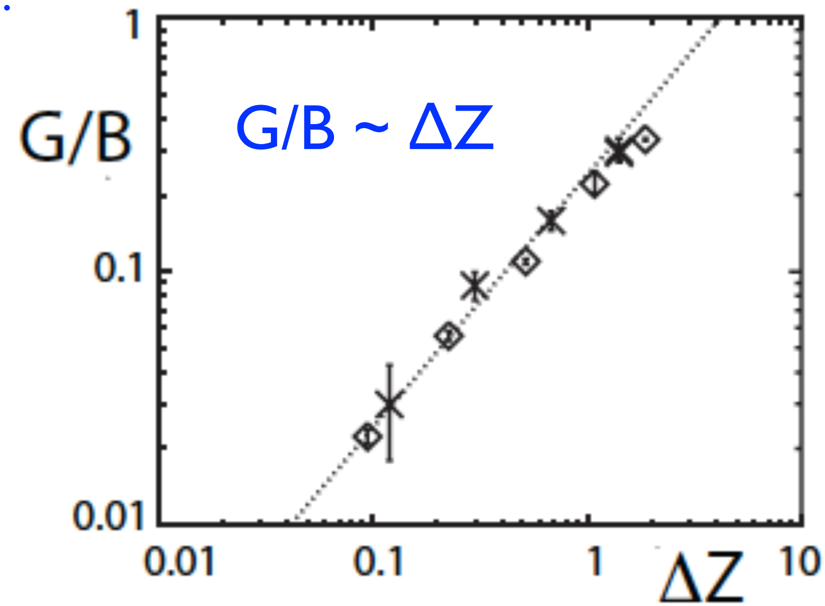
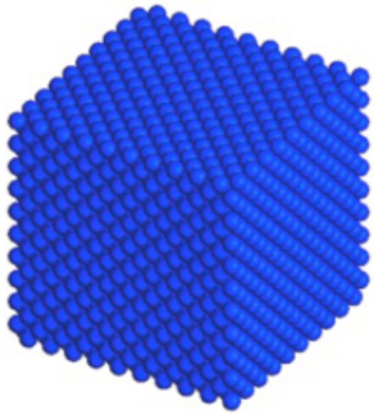
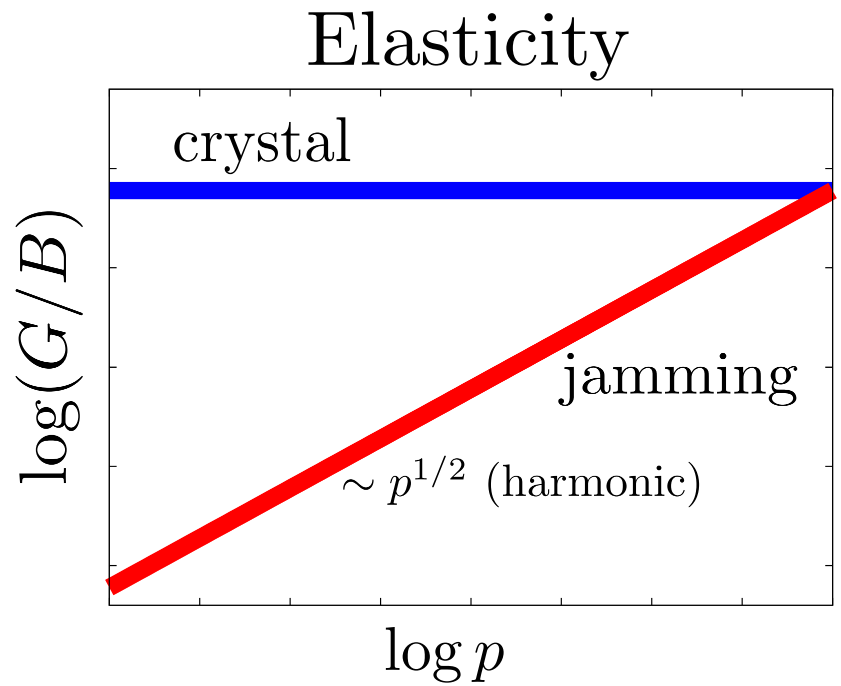


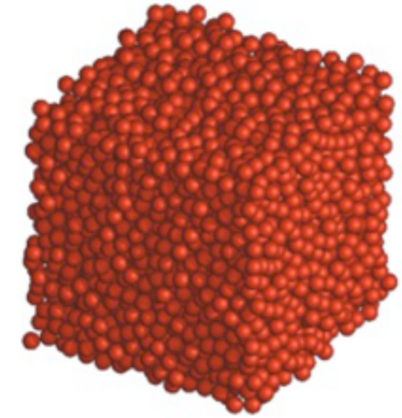
Ellenbroek, Somfai, van Hecke, van Saarloos, PRL 97, 257801 (2006).



Compare to crystal







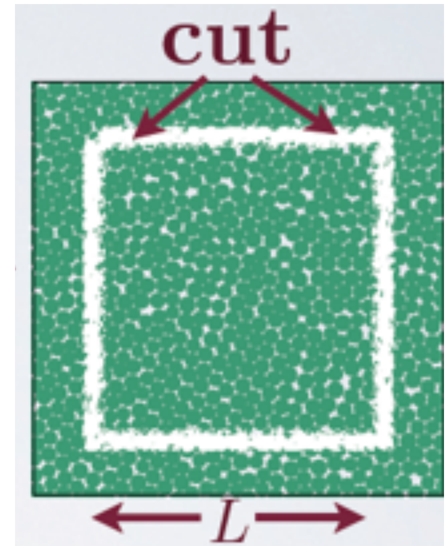
- G/B→0 at jamming transition (like liquid)
- jammed solid marginally stable to pressure (Wyart)

- jammed state is anticrystal; opposite pole to perfect crystal
- anticrystal defined in terms of rigidity, not structure

Marginal Stability Leads to Diverging Length Scale

M. Wyart, S.R. Nagel, T.A. Witten, EPL **72**, 486 (05)

- For system at ϕ_c, Z=2d
- Removal of one bond makes entire system unstable by adding a soft mode
- This implies diverging length as ϕ-> $\phi_c^{\ +}$



For $\phi > \phi_c$, cut bonds at boundary of size L

Count number of soft modes within cluster

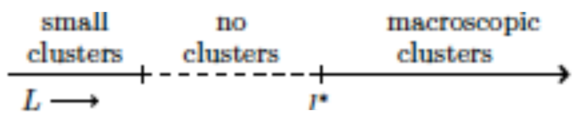
$$N_s \approx L^{d-1} - (Z - Z_c)L^d$$

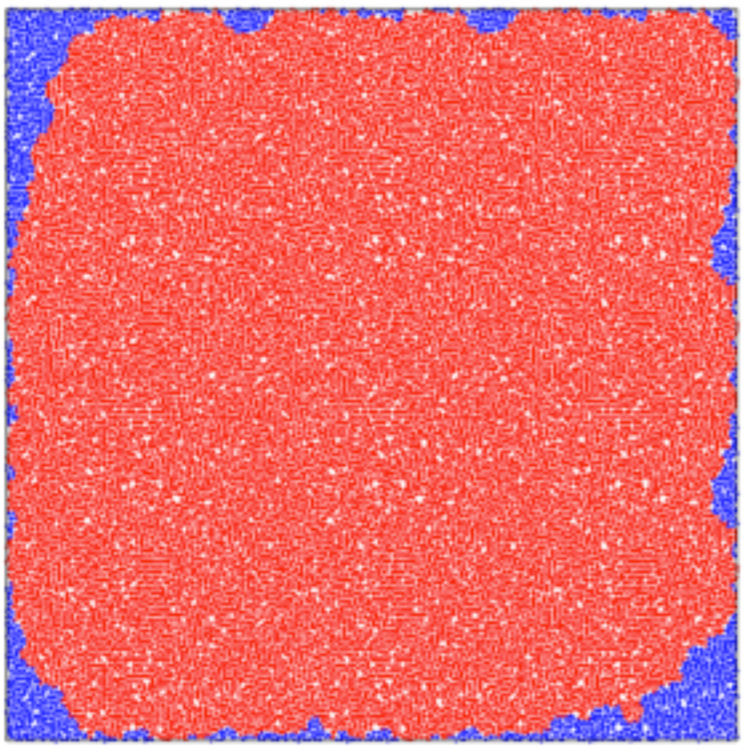
Define length scale at which soft modes just appear

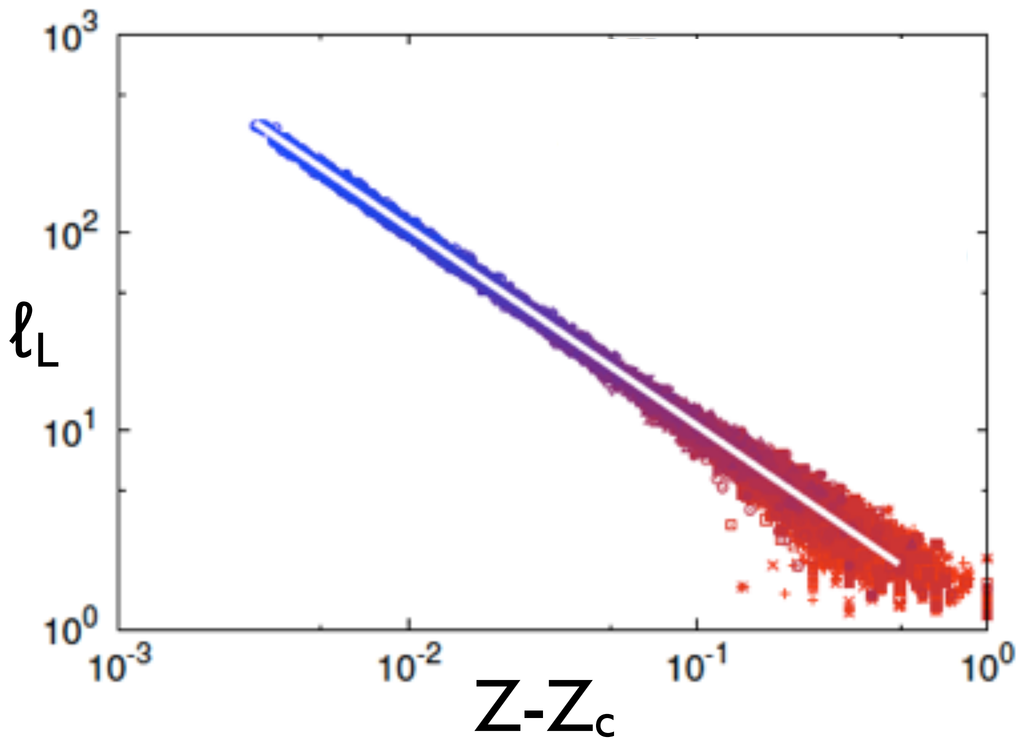
$$\ell_L \sim \frac{1}{Z - Z_c} \equiv \frac{1}{\Delta z} \sim (\phi - \phi_c)^{-0.5}$$

More precisely

Define ℓ^* as size of smallest macroscopic rigid cluster for system with a free boundary of any shape or size







Goodrich, Ellenbroek, Liu Soft Matter (2013)

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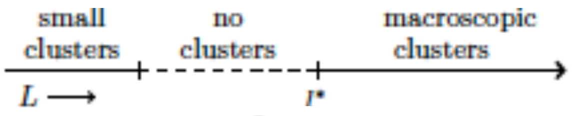

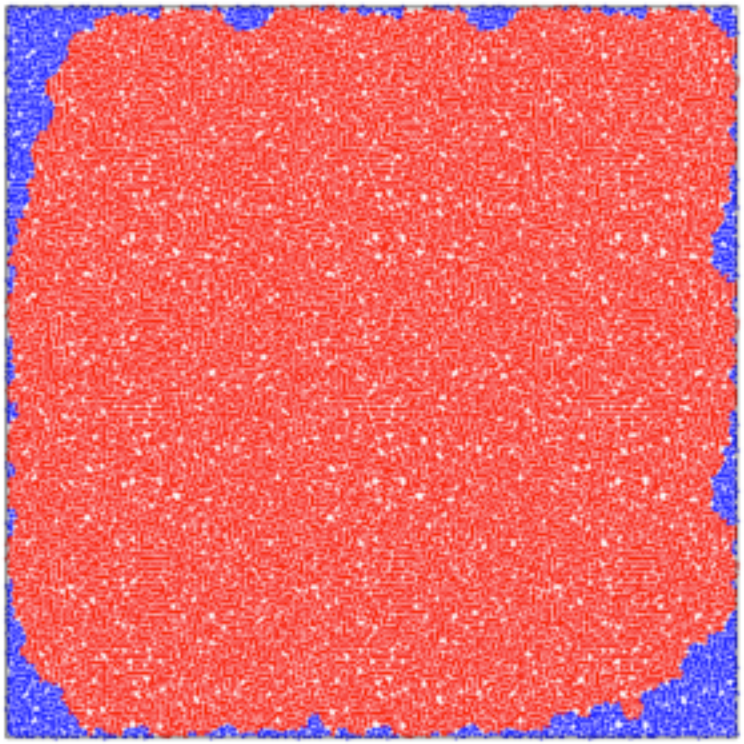

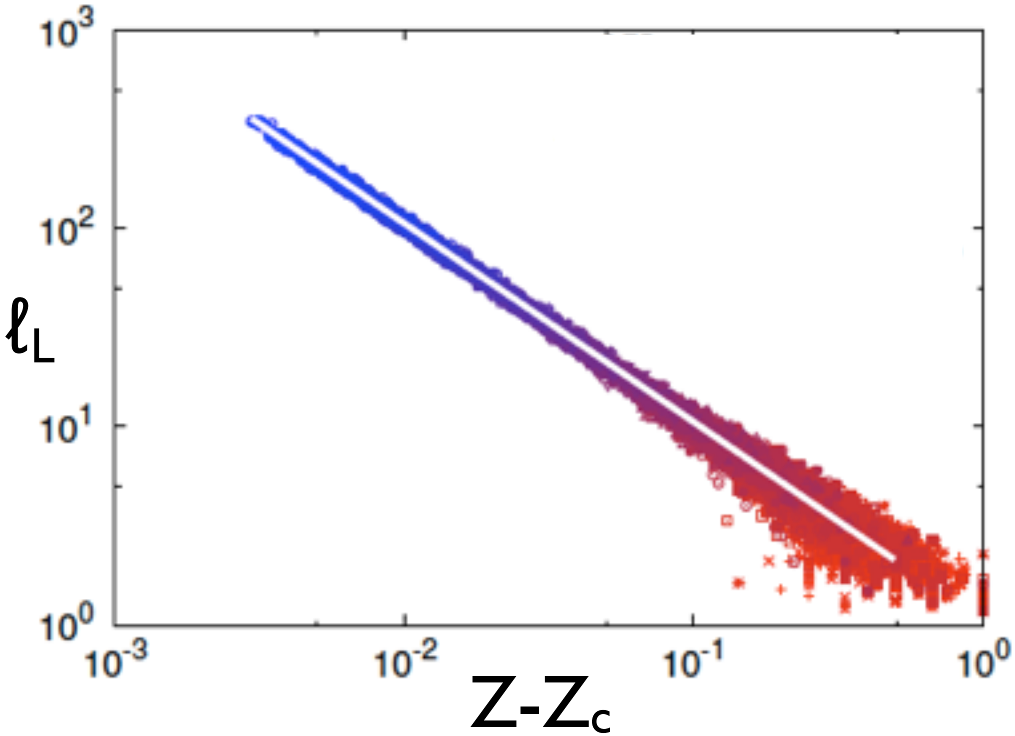

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Vibrations in Disordered Sphere Packings

- Crystals are all alike at low T or low ω
  - density of vibrational states $D(\omega) \sim \omega^{d-1}$ in d dimensions
  - heat capacity $C(T) \sim T^d$
- Why?

Low-frequency excitations are sound modes. Long wavelengths average over disorder so all crystalline solids behave this way

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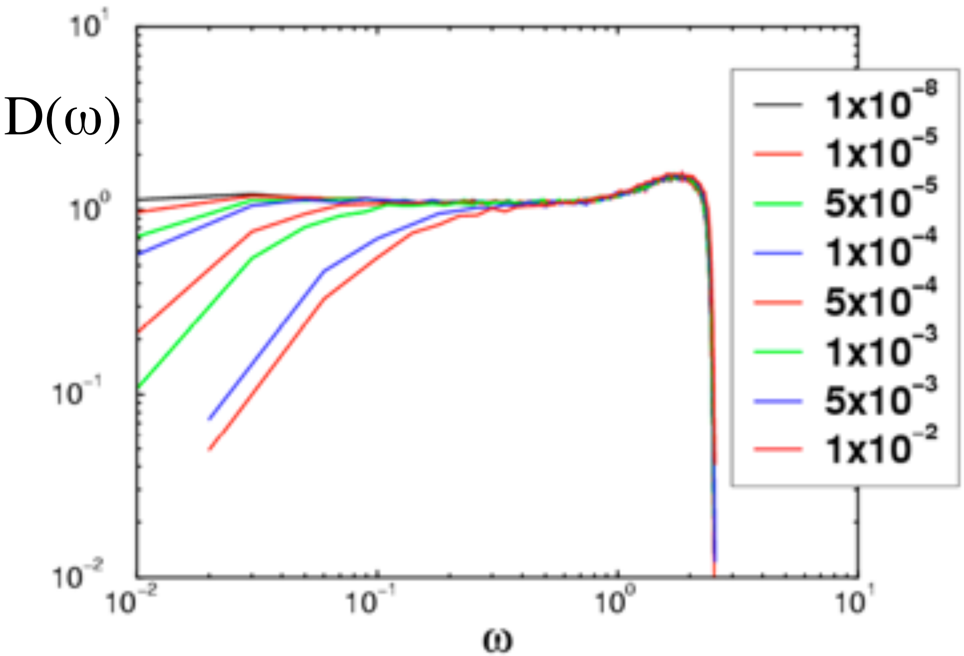
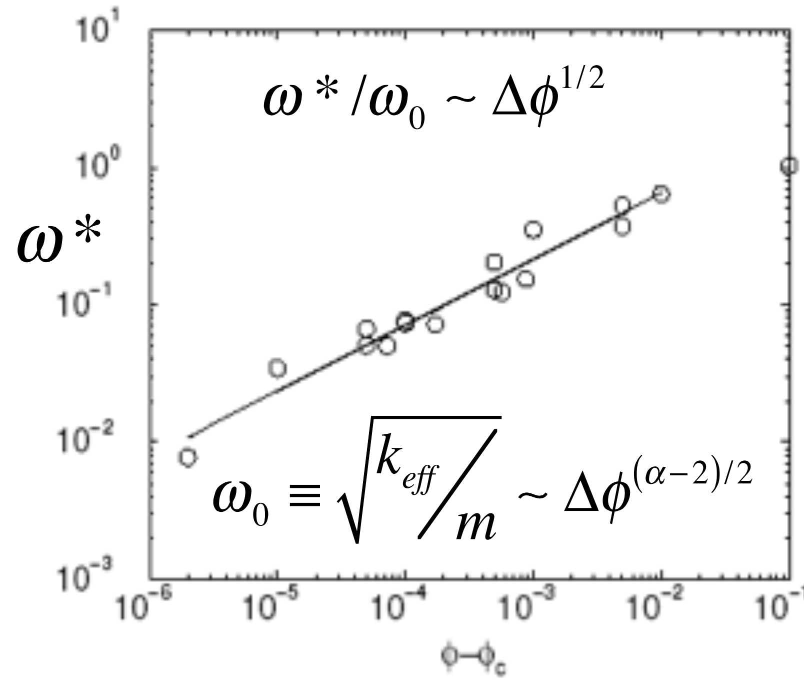
BUT near at Point J, there is a diverging length scale ℓ_L

So what happens?

Vibrations in Sphere Packings

L. E. Silbert, A. J. Liu, S. R. Nagel, PRL **95**, 098301 ('05)





- New class of excitations originates from soft modes at Point J M. Wyart, S.R. Nagel, T.A. Witten, EPL **72**, 486 (05)

- Generic consequence of diverging length scale: $\ell_L \simeq c_L/\omega^*$
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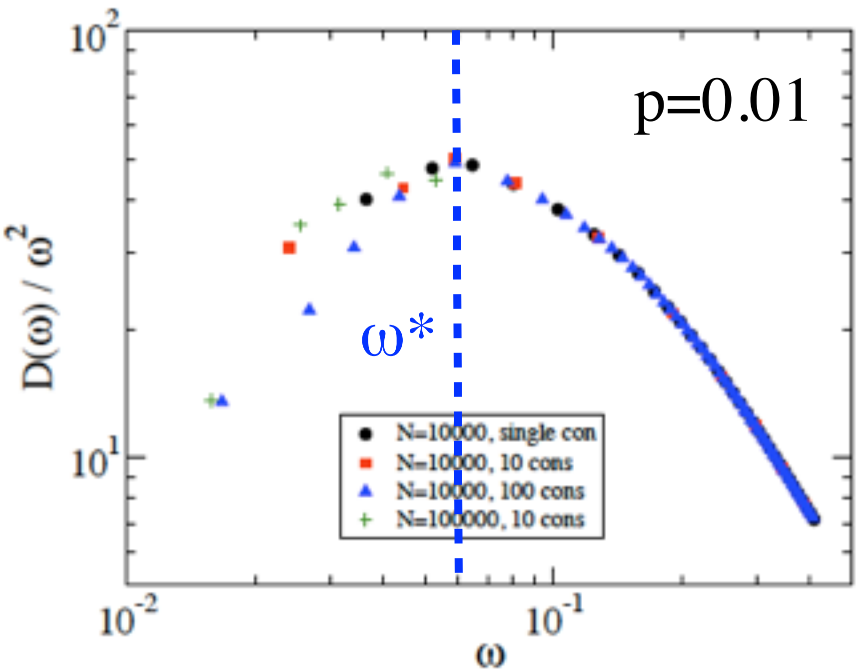

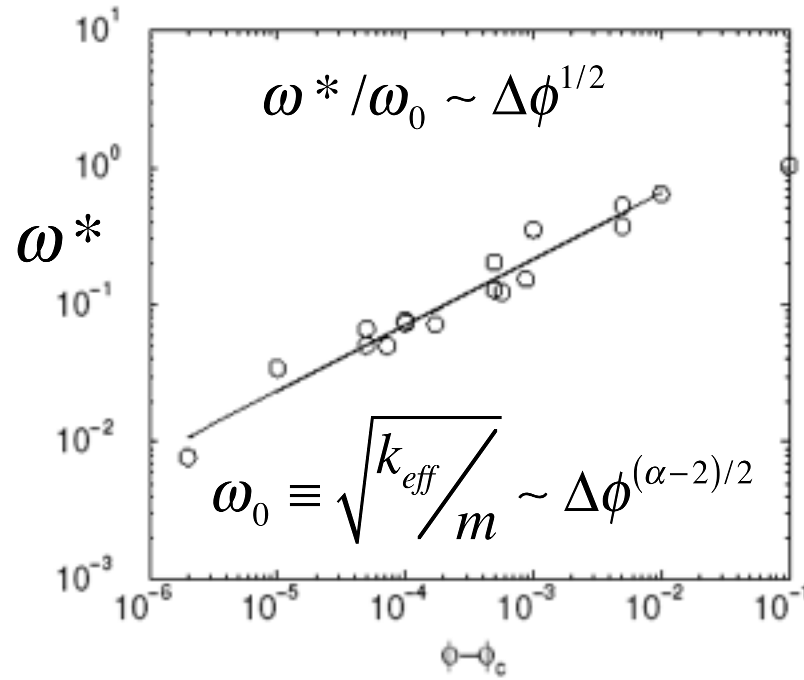

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Critical Scaling near Jamming Transition

- Mixed first-order/second-order transition (RFOT)
- Number of overlapping neighbors per particle

$$Z = \begin{cases} 0 & \phi < \phi_c \\ Z_c + z_0 \Delta\phi^{\beta \cong 1/2} & \phi \geq \phi_c \end{cases} \qquad V(r) = \begin{cases} \dfrac{\varepsilon}{\alpha}\left(1 - \dfrac{r}{\sigma}\right)^{\alpha} & r \leq \sigma \\ 0 & r > \sigma \end{cases}$$

- Static shear modulus/bulk modulus

$$G / B \sim \Delta\phi^{\gamma \cong 1/2}$$

- Two diverging length scales

$$\ell_L \sim \Delta\phi^{-\nu^* \cong -1/2} \qquad \ell_T \sim \Delta\phi^{-\nu^\dagger \cong -1/4}$$

- Vanishing frequency scale

$$\omega^* / \omega_0 \sim \Delta\phi^{\varsigma \cong 1/2}$$

A. J. Liu and S. R. Nagel, Ann. Rev. Cond. Mat. Phys. (2010)

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$$Z = \begin{cases} 0 & \phi < \phi_c \\ Z_c + z_0 \Delta\phi^{\beta \cong 1/2} & \phi \geq \phi_c \end{cases}$$

Exponents are

- independent of potential
- independent of dimension

Mean field

- Static shear modulus/bulk modulus

$$G / B \sim \Delta\phi^{\gamma \cong 1/2}$$

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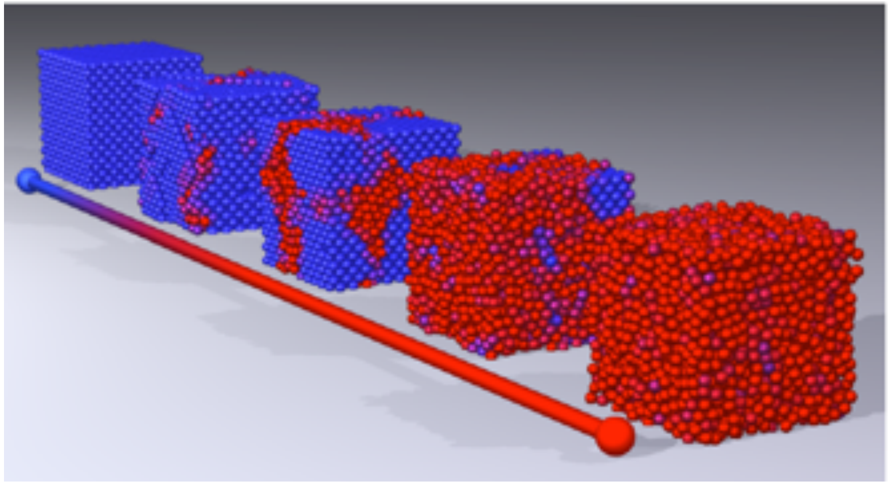
Tuning from perfect order to perfect disorder



Goodrich, Liu, Nagel, Nature Phys (2014)

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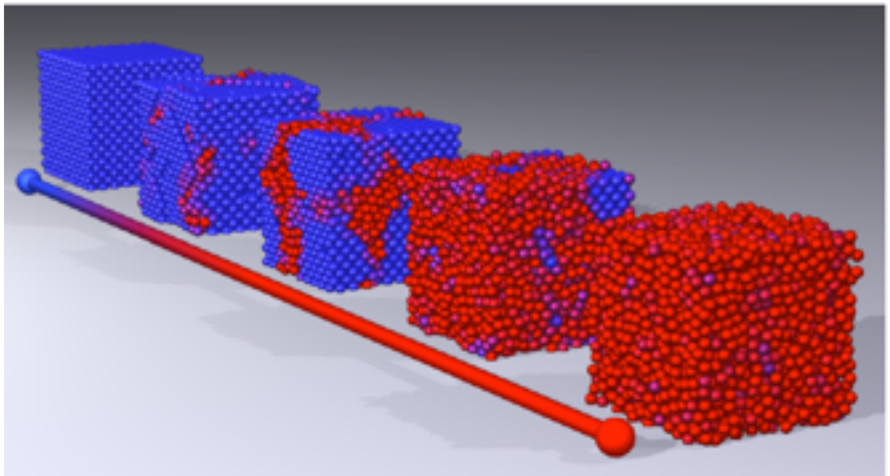
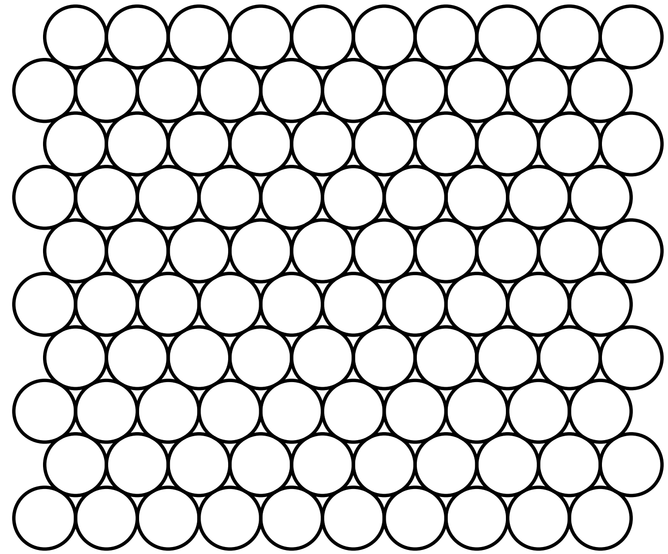


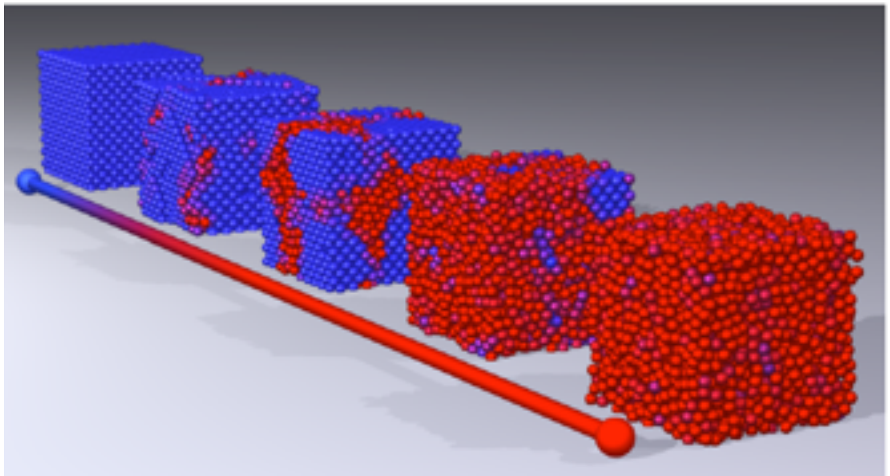


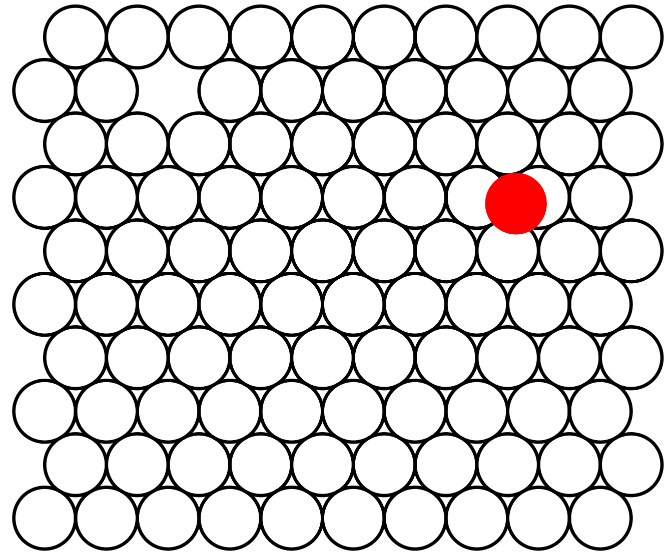
$2d$ illustration

1. start with a perfect FCC crystal

Goodrich, Liu, Nagel, Nature Phys (2014)

Tuning from perfect order to perfect disorder





$2d$ illustration

1. start with a perfect FCC crystal
2. introduce 1 vacancy-interstitial pair

Goodrich, Liu, Nagel, Nature Phys (2014)

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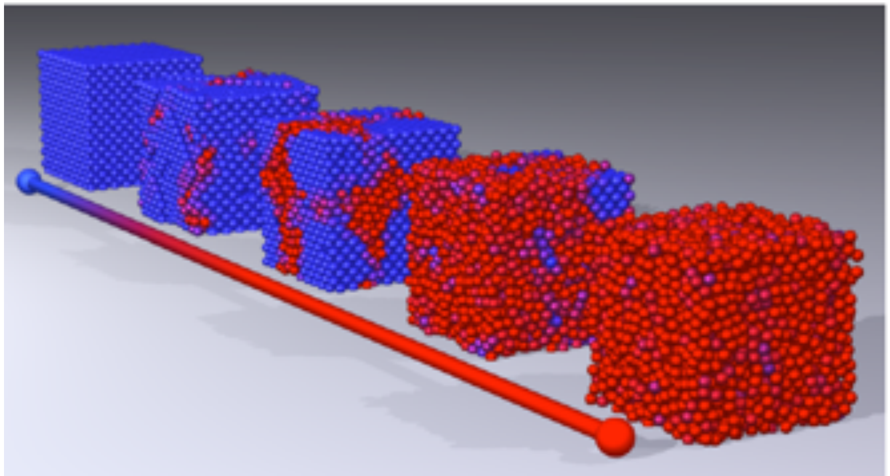

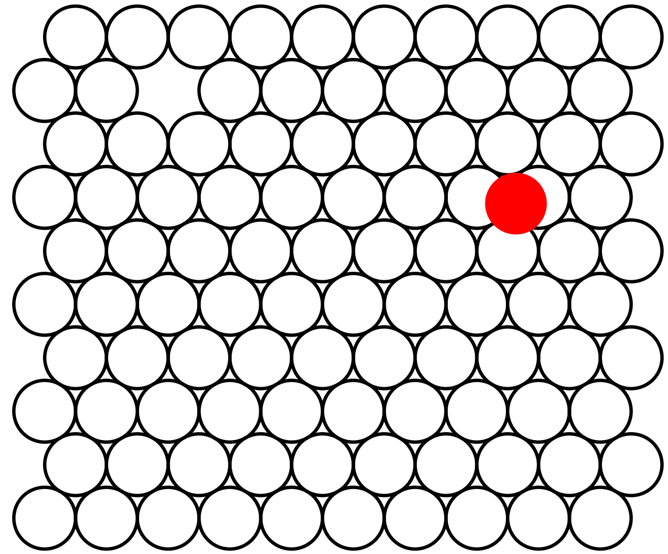

$2d$ illustration

1. start with a perfect FCC crystal
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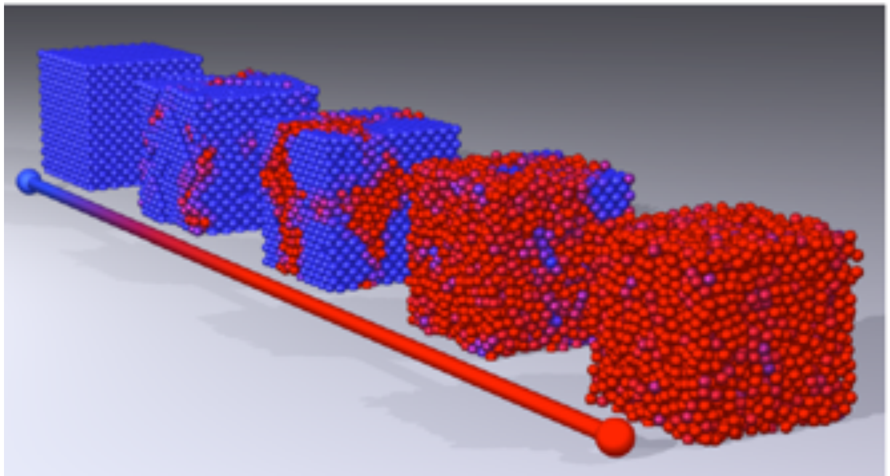
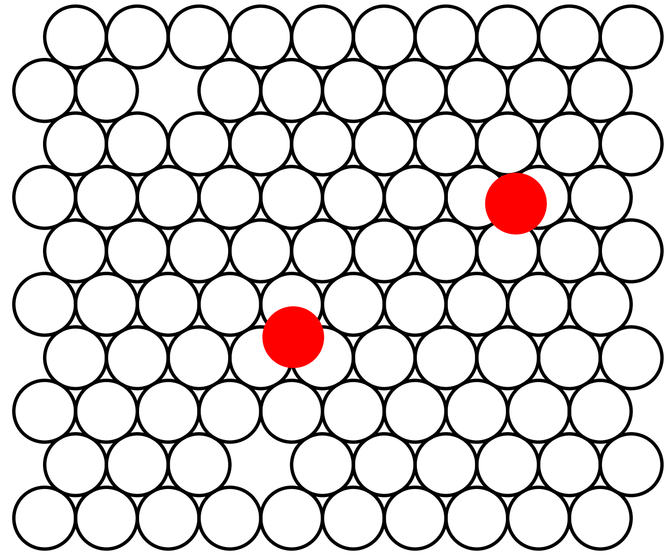
3. minimize the energy

Goodrich, Liu, Nagel, Nature Phys (2014)

Tuning from perfect order to perfect disorder



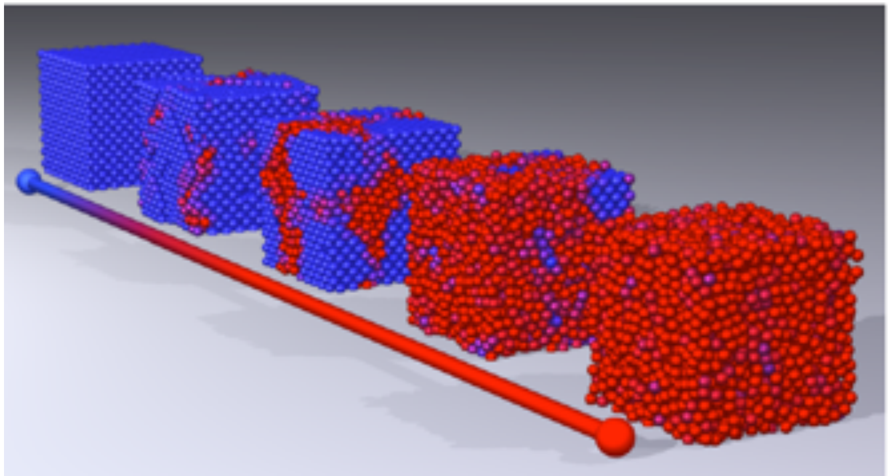


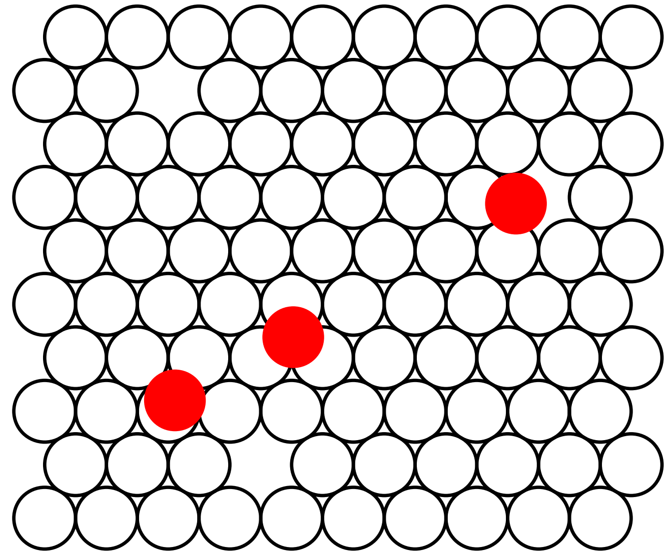
$2d$ illustration

1. start with a perfect FCC crystal
2. introduce 2 vacancy-interstitial pairs
3. minimize the energy

Goodrich, Liu, Nagel, Nature Phys (2014)

Tuning from perfect order to perfect disorder



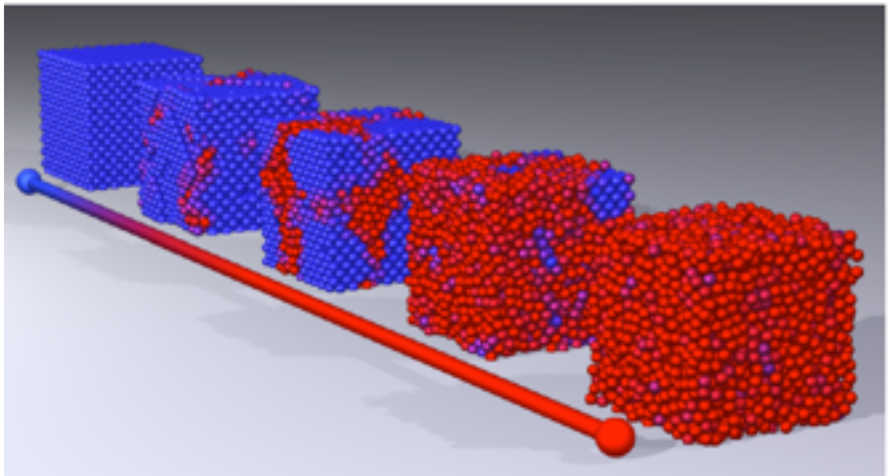


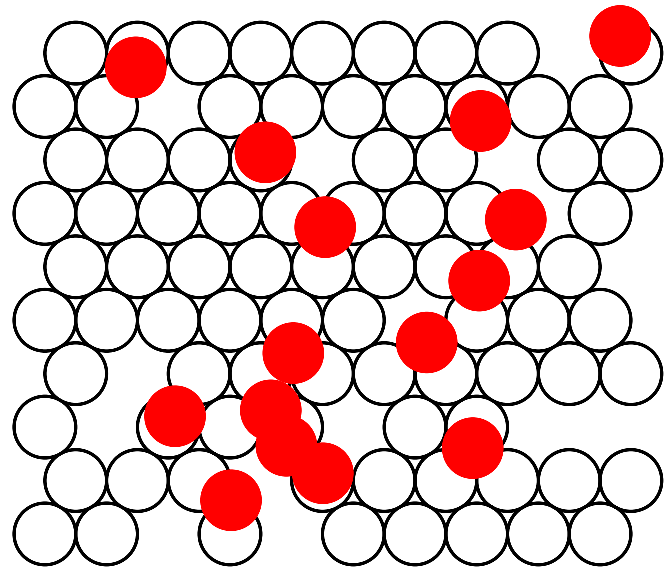
$2d$ illustration

1. start with a perfect FCC crystal
2. introduce 3 vacancy-interstitial pairs
3. minimize the energy

Goodrich, Liu, Nagel, Nature Phys (2014)

Tuning from perfect order to perfect disorder





$2d$ illustration

1. start with a perfect FCC crystal
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Goodrich, Liu, Nagel, Nature Phys (2014)

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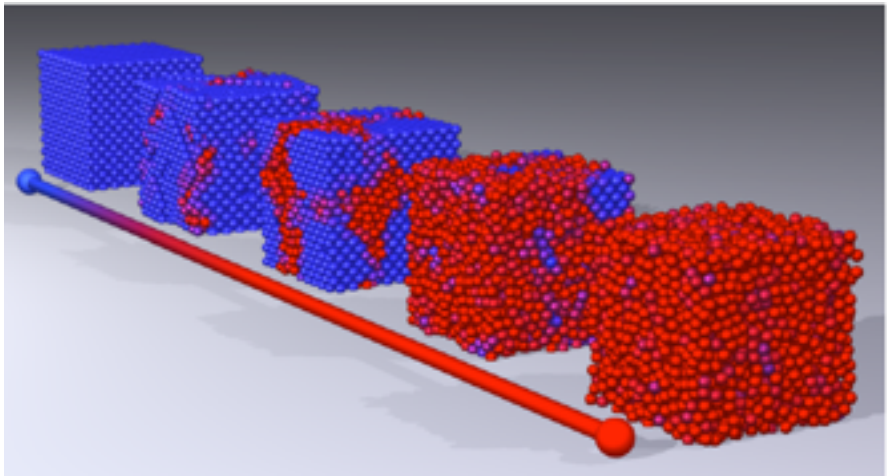
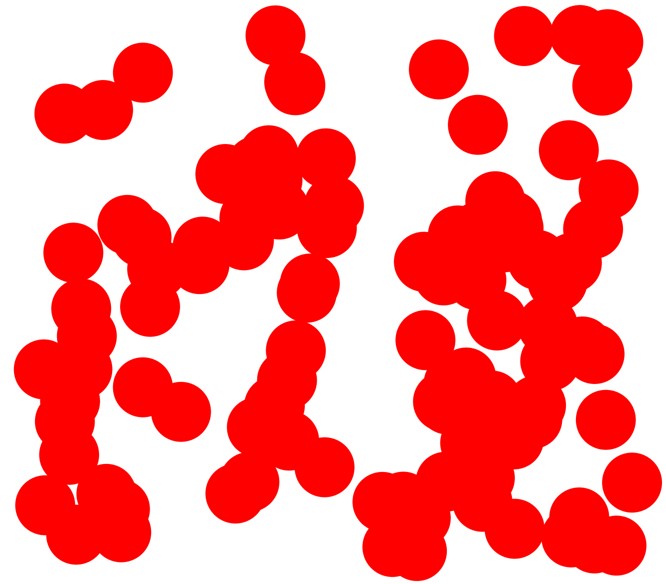


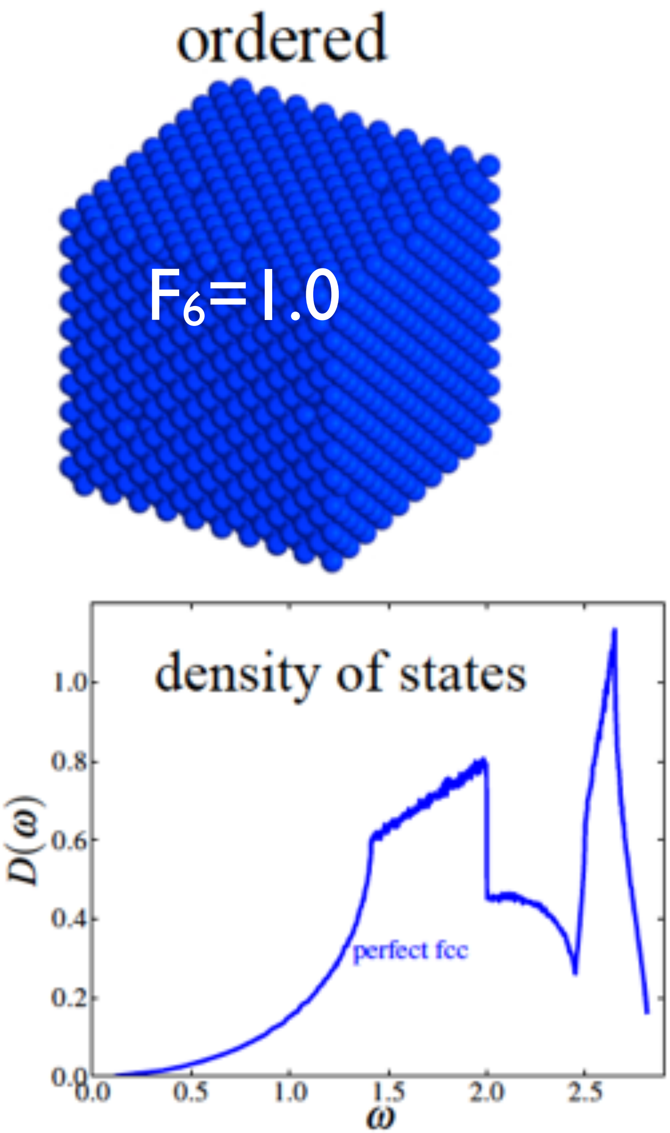


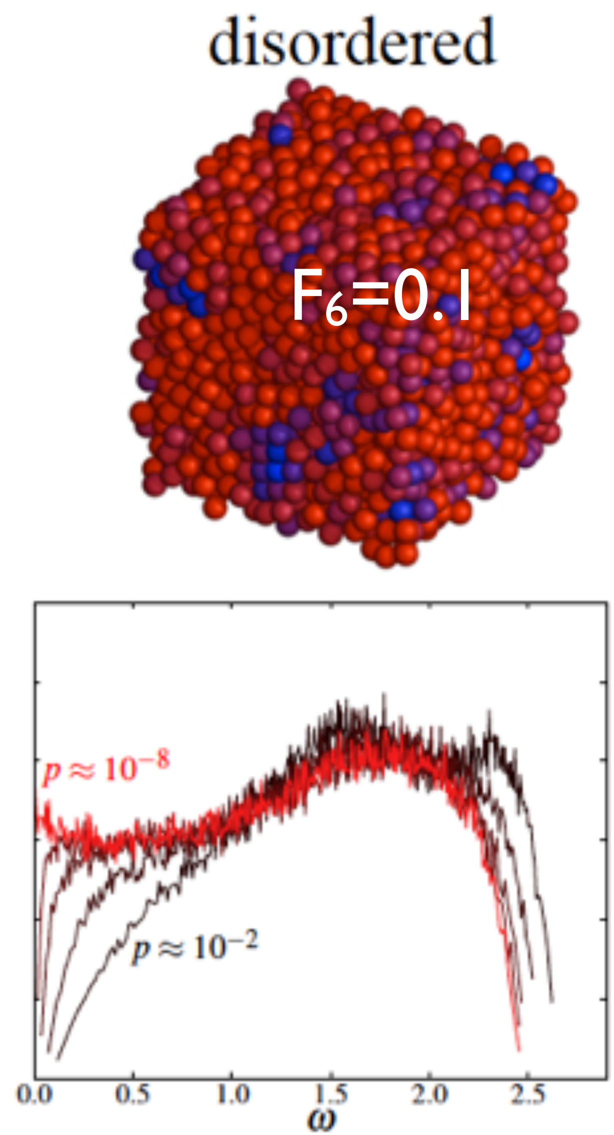
$2d$ illustration

1. start with a perfect FCC crystal
2. introduce $\texttt{N}$ vacancy-interstitial pairs
3. minimize the energy

Goodrich, Liu, Nagel, Nature Phys (2014)

From Order to Disorder: When does Disorder Win?





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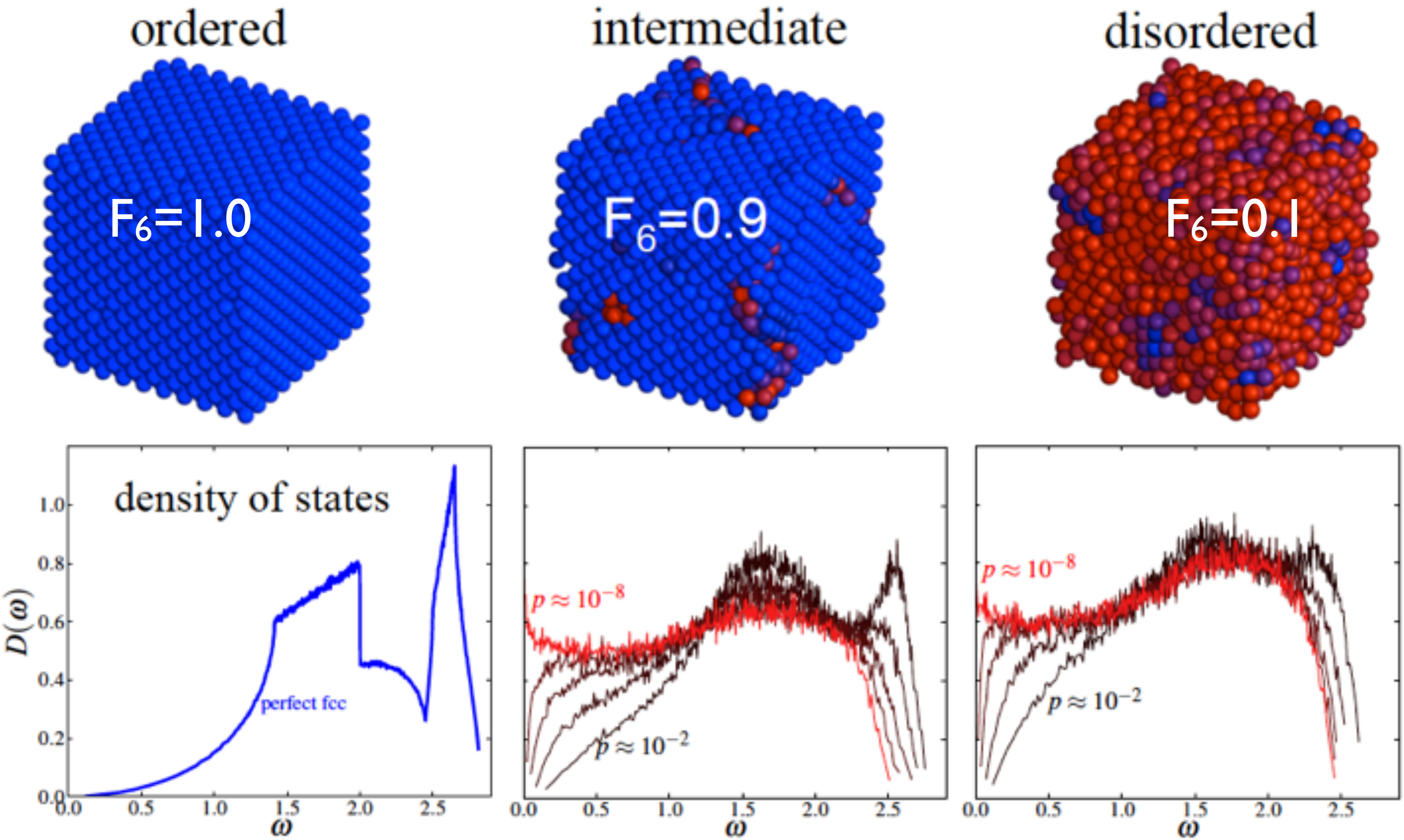

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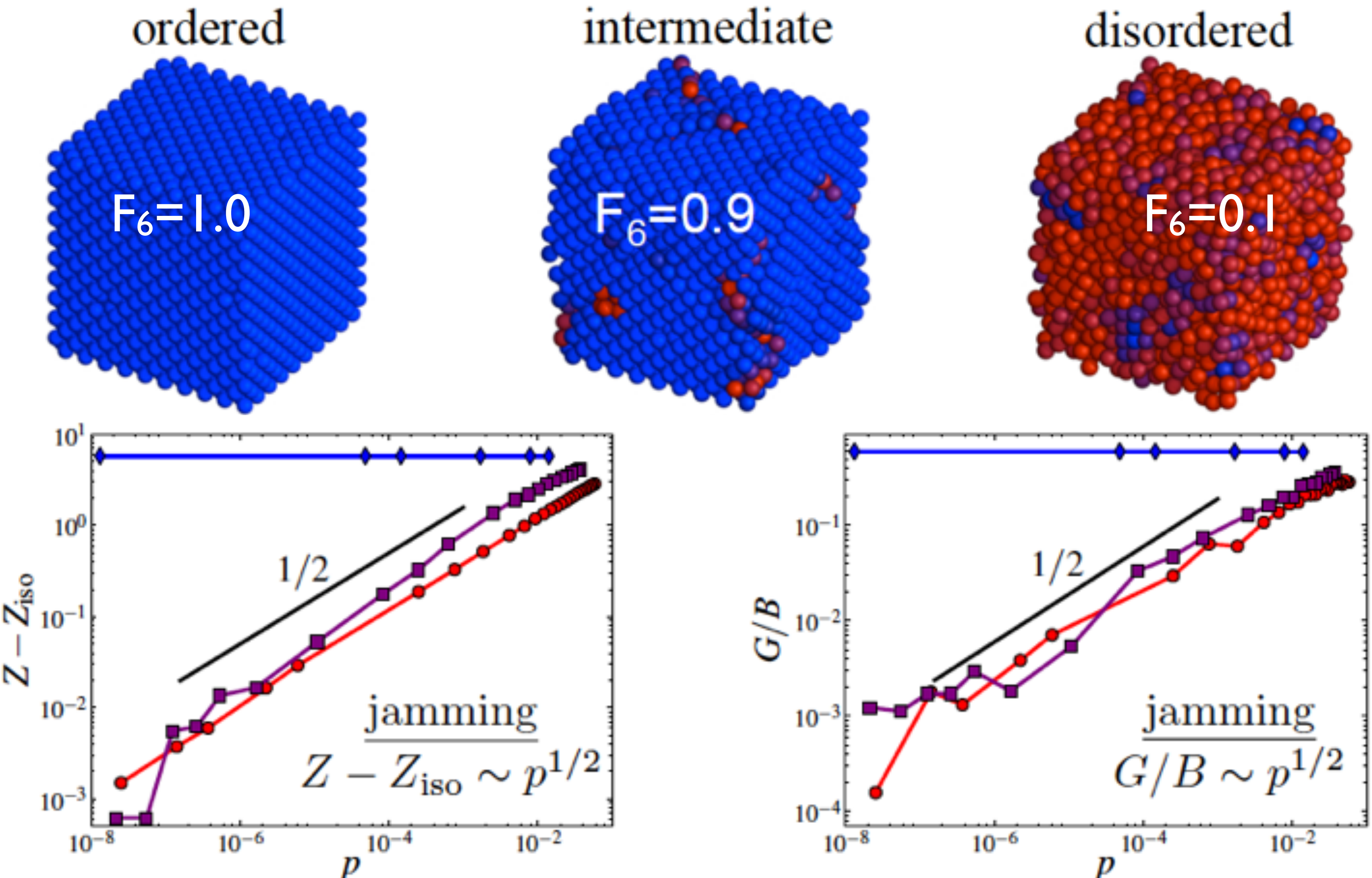

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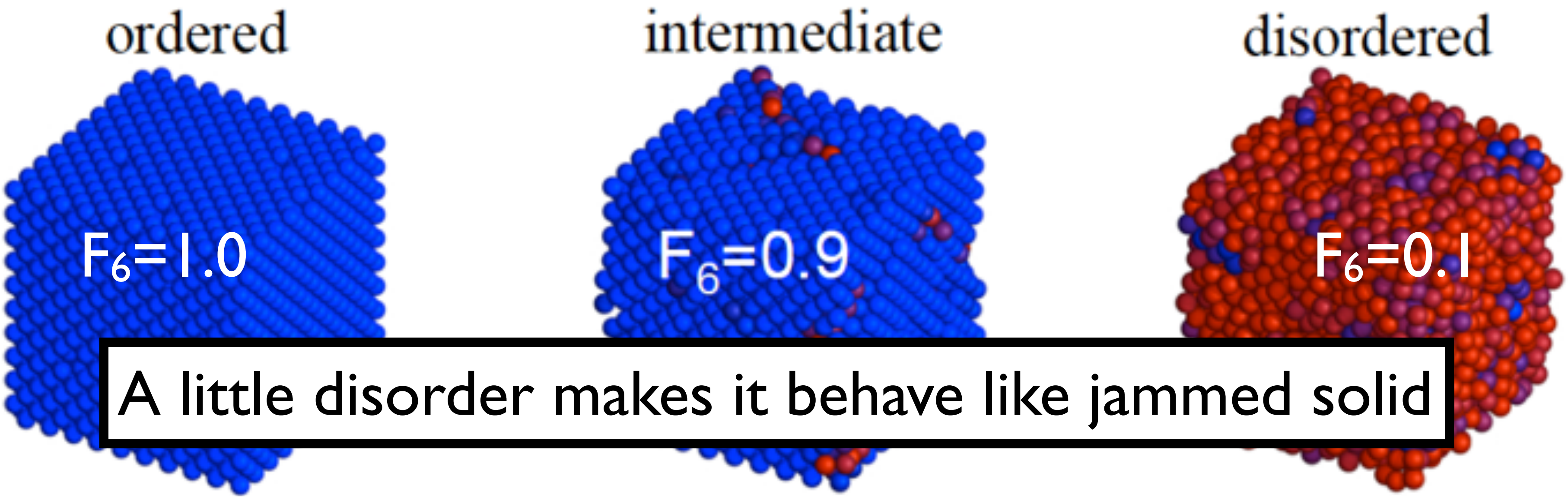
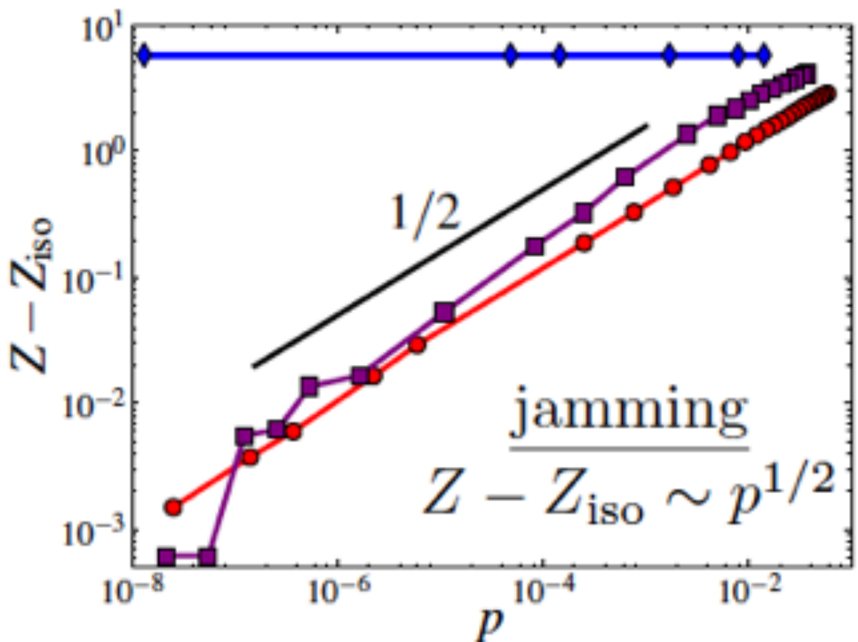
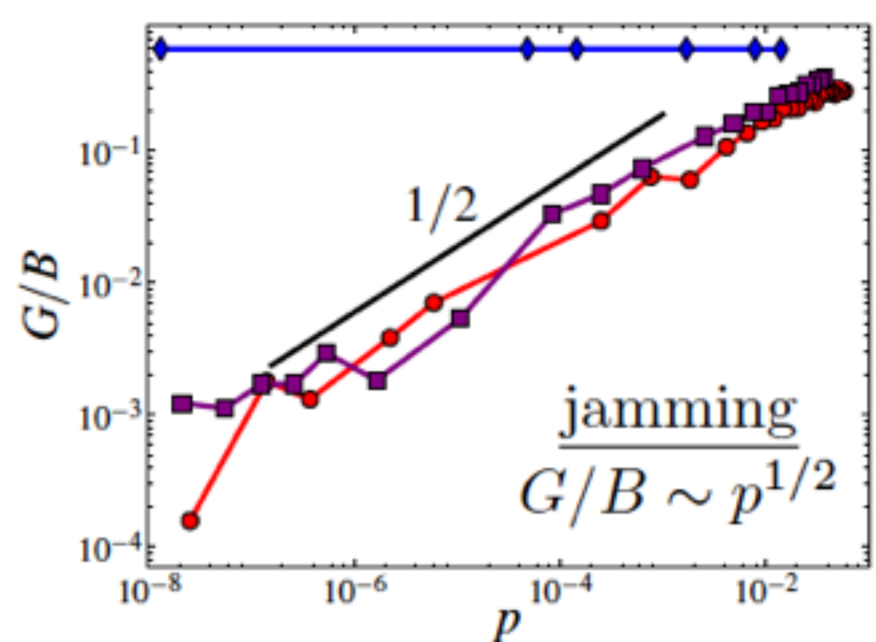


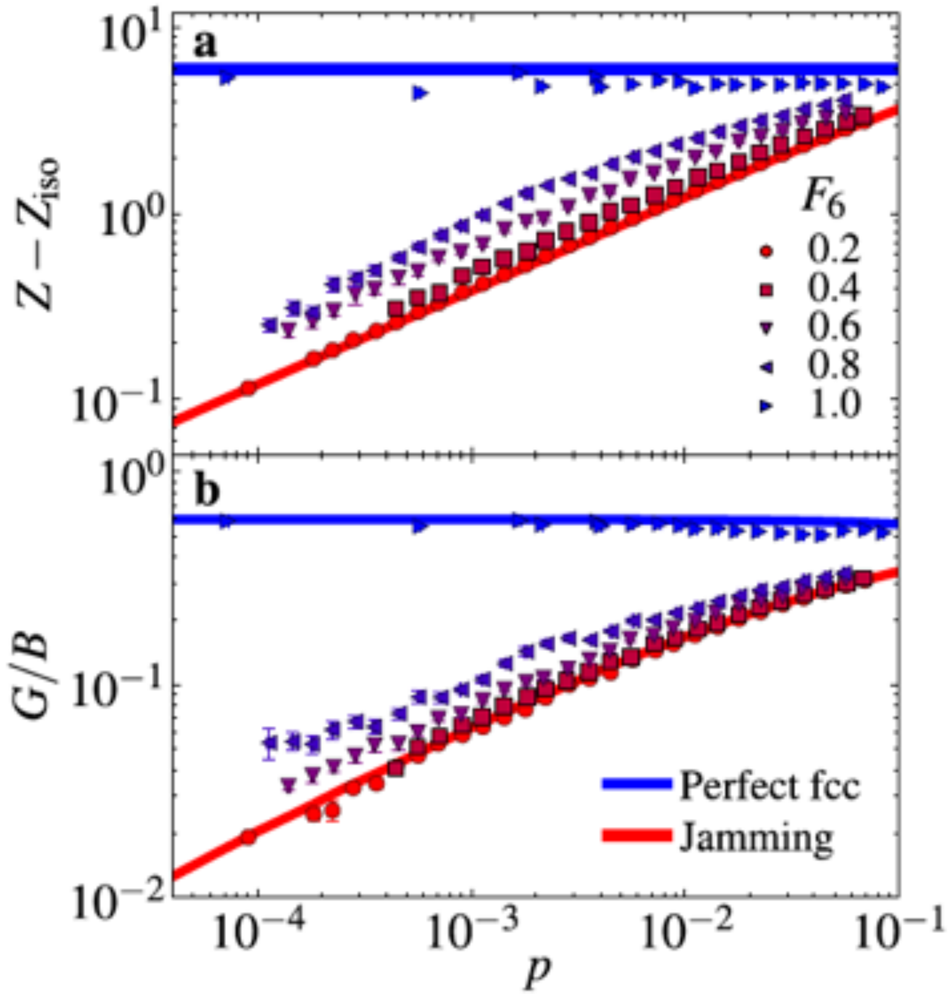
A little disorder makes it behave like jammed solid





Look at thousands of packings

Elasticity



Even very ordered systems behave mechanically like jammed solids

What Have We Left Out? ALMOST EVERYTHING

- long-ranged interactions

  N. Xu, et al. PRL 98 175502 (2007).

- attractions

  N. Xu, et al. PRL 98 175502 (2007).

- 3-body interactions (e.g. bond-bending)

  J. C. Phillips, J. Non-Cryst. Solids (1979), **43**, 37 (1981); M. F. Thorpe, J. Non-Cryst. Solids(1983); P. Boolchand, et al., Phil. Mag. (2005).

- temperature

  Z. Zhang, et al. Nature (2009); L. Berthier and T. A. Witten, EPL (2009); K. Chen, et al. PRL (2010); A. Ikeda, et al. J Chem Phys (2013), T. Still, et al. PRE (2014).

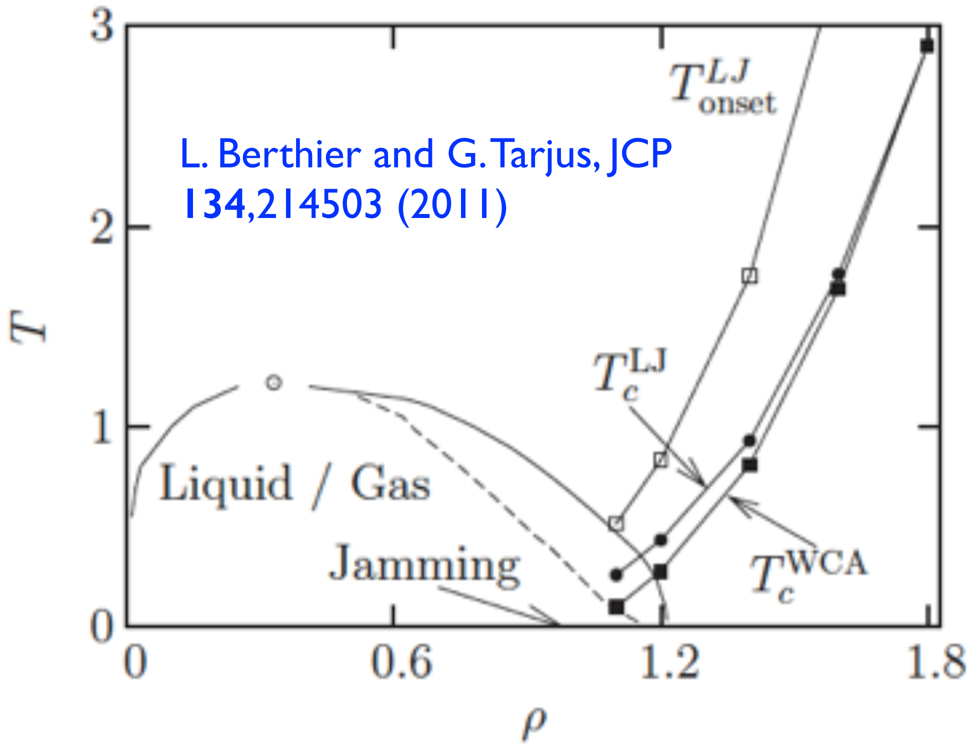
- non-spherical particle shape

  Z. Zeravcic, N. Xu, A. J. Liu, S. R. Nagel, W. van Saarloos, EPL (2009), Mailman, et al. PRL (2009).

- friction

  K. Shundyak, et al. PRE (2007); E. Somfai, et al. PRE (2007); S. Henkes, et al. EPL (2010), D. Bi, et al. Nature (2011); T. Still et al. PRE (2014).

Long-ranged interactions & attractions



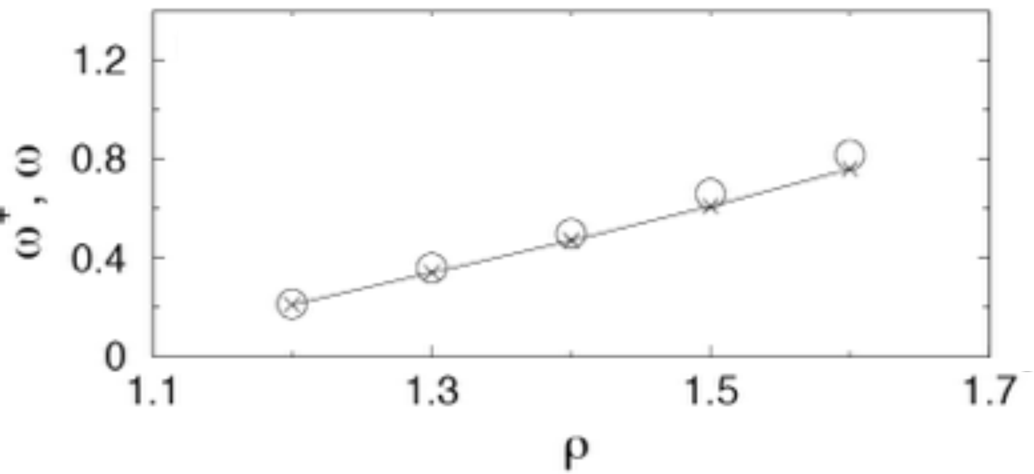
Attractions serve to hold system at high enough density that repulsions come into play (WCA)

- Point J lies inside liquid-vapor coexistence curve so it doesn’t exist
- But in liquid state theory, physics is controlled by finite-ranged repulsions

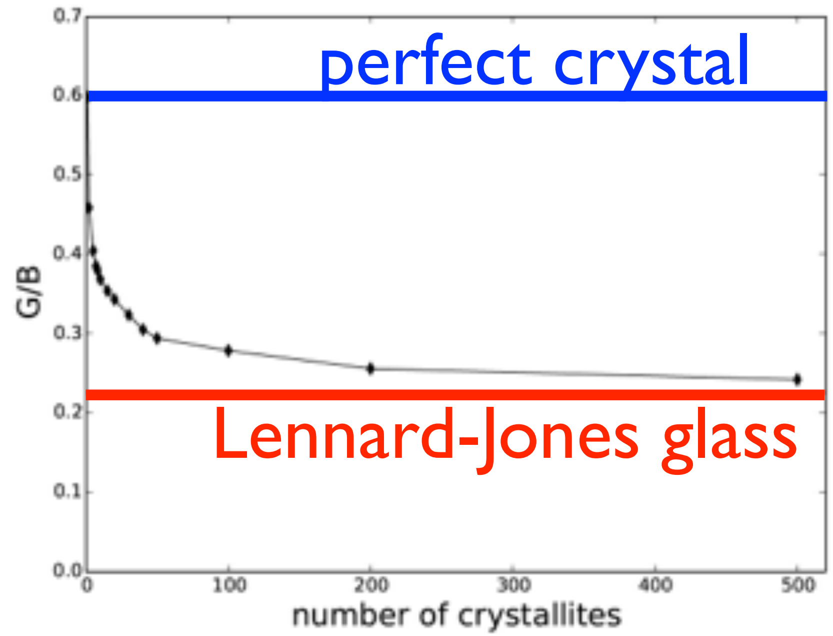
Lennard-Jones Interactions

- Can treat long-ranged interactions as correction in variational theory to predict shift in boson peak frequency (and G/B)

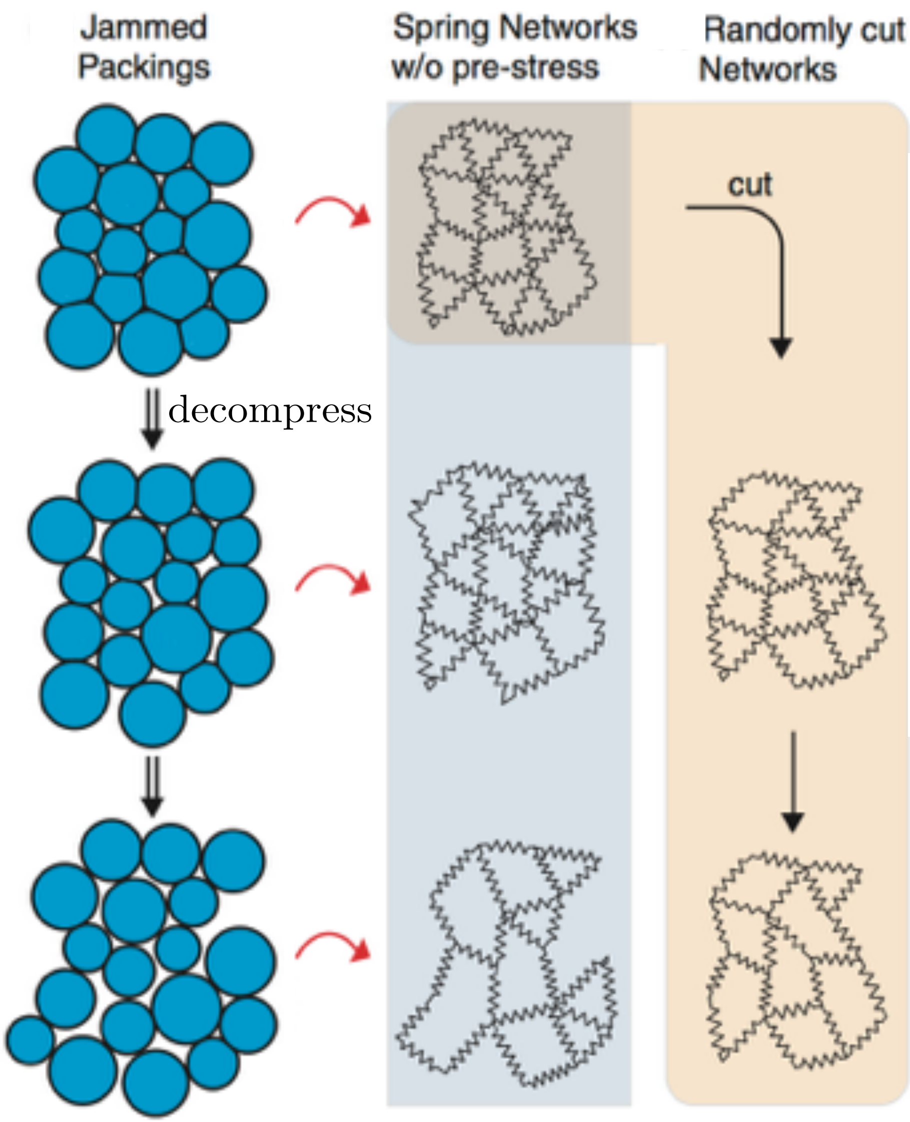
N. Xu, M. Wyart, A. J. Liu, S. R. Nagel, PRL (2007).

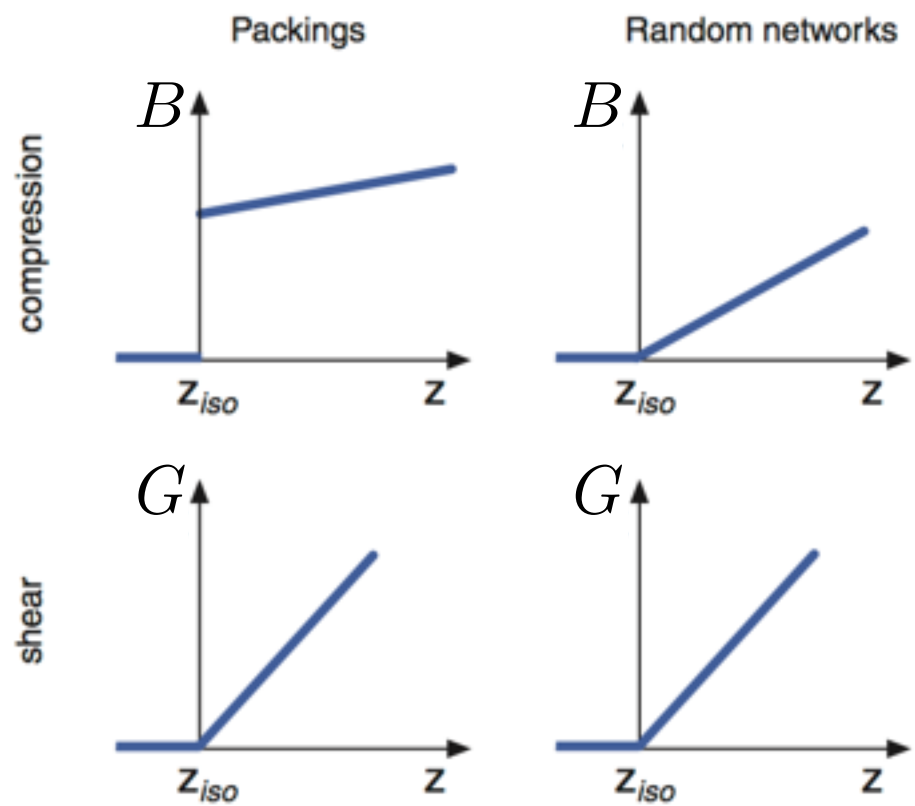


- Lennard-Jones polycrystal
- For >6 crystallites, G/B closer to disordered limit than to perfect crystal



Understanding the Scaling of G/B





$G/B \sim \Delta Z$

same as jamming

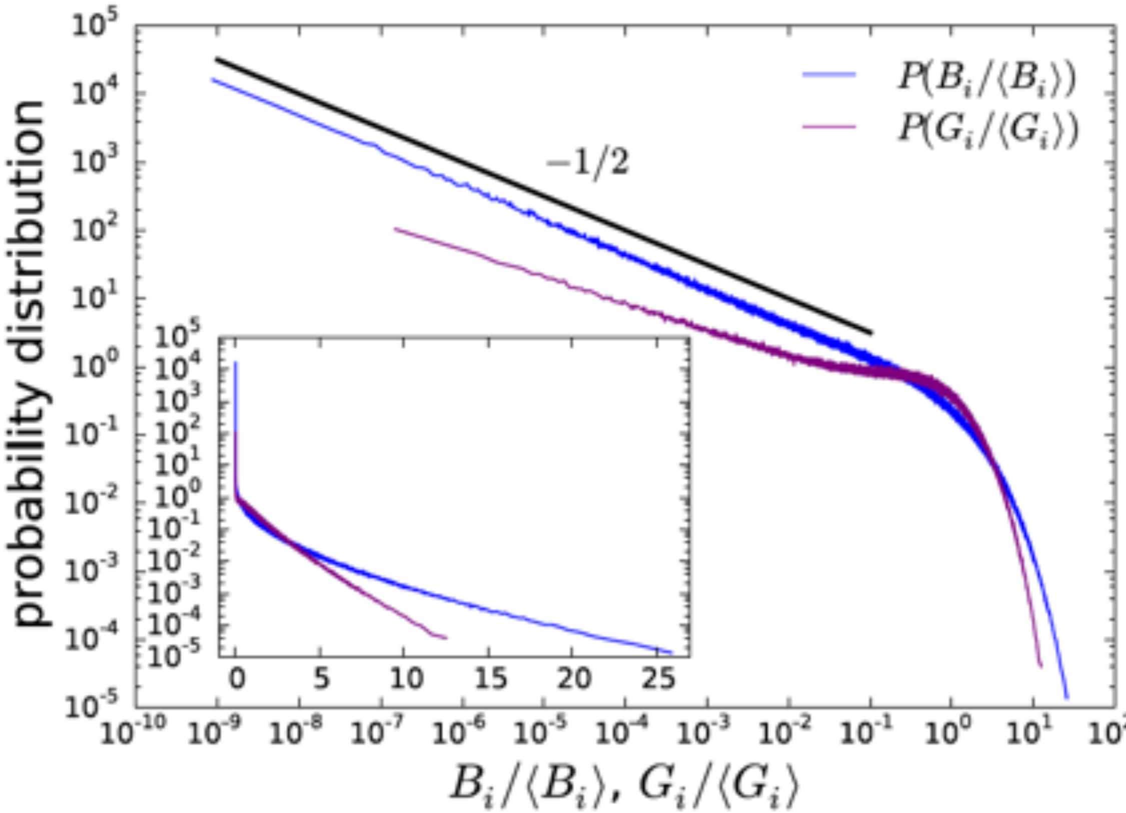
$G/B \sim 1$

rigidity percolation

Ellenbroek, et al. EPL (2009).

Bond Contributions to G, B

- Calculate contribution of each spring to G, B



3D
ΔZ=0.127

- Distribution is continuous down to B_i, G_i=0 & fairly broad
- Perfect fcc: sum of a few delta functions

Tuning by pruning

<u>prune bonds with smallest B_i</u>

$G \sim$

$B \sim$

<u>random</u>

$G \sim \Delta Z$

$B \sim \Delta Z$

<u>prune bonds with largest B_i</u>

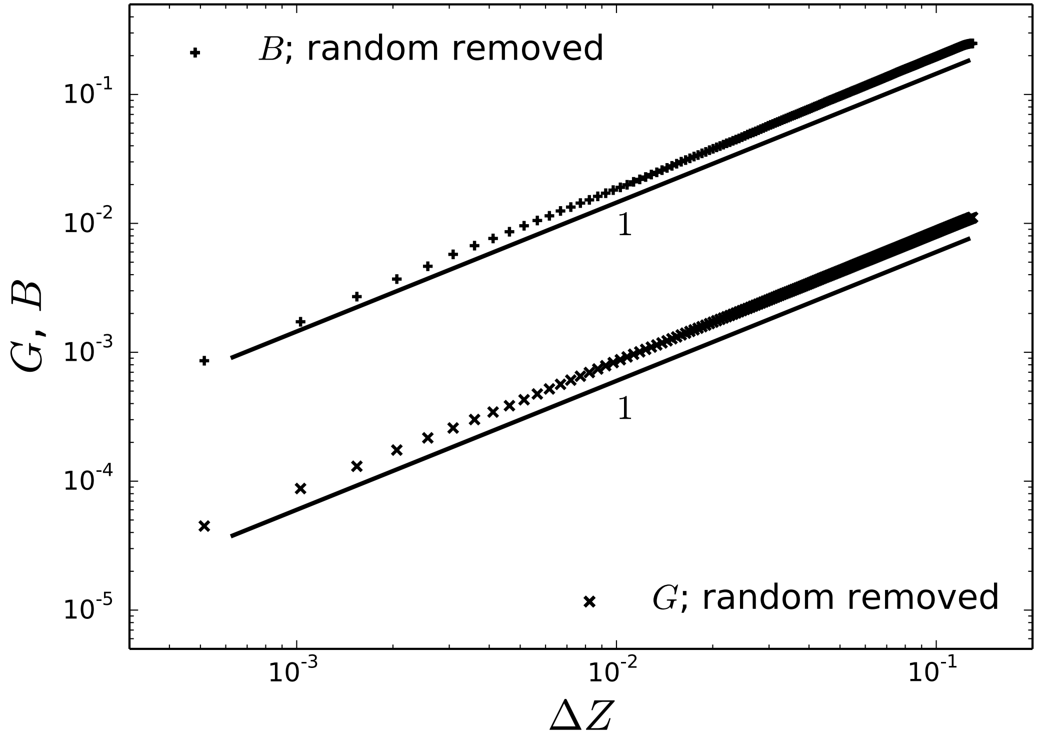
$G \sim$

$B \sim$

<u>prune bonds with largest G_i</u>

$G \sim$

$B \sim$



Tuning by pruning

<u>random</u>

$G \sim \Delta Z$

$B \sim \Delta Z$

<u>prune bonds with smallest B_i</u>

$G \sim \Delta Z$

$B \sim$

<u>prune bonds with largest B_i</u>

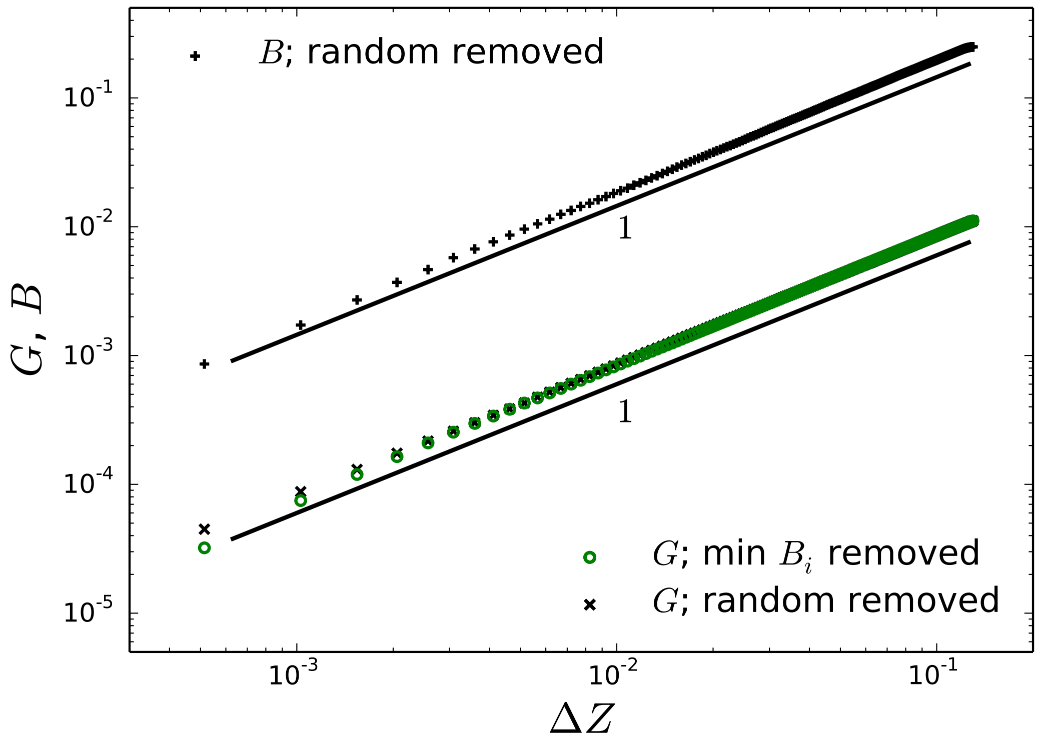
$G \sim$

$B \sim$

<u>prune bonds with largest G_i</u>

$G \sim$

$B \sim$



Tuning by pruning

random

$$G \sim \Delta Z$$

$$B \sim \Delta Z$$

prune bonds with smallest B_i

$G \sim \Delta Z$

$B \sim$

prune bonds with largest B_i

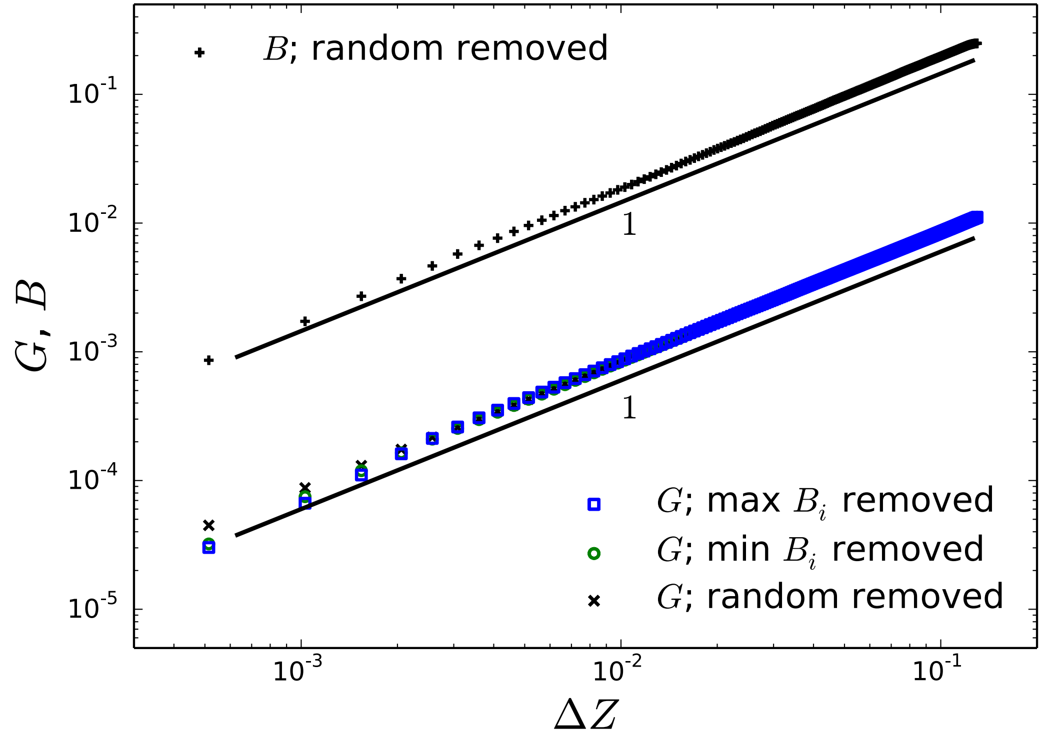
$G \sim \Delta Z$

$B \sim$

prune bonds with largest G_i

$G \sim$

$B \sim$



Tuning by pruning

prune bonds with smallest B_i

$G \sim \Delta Z$

$B \sim$

random

$G \sim \Delta Z$

$B \sim \Delta Z$

prune bonds with largest B_i

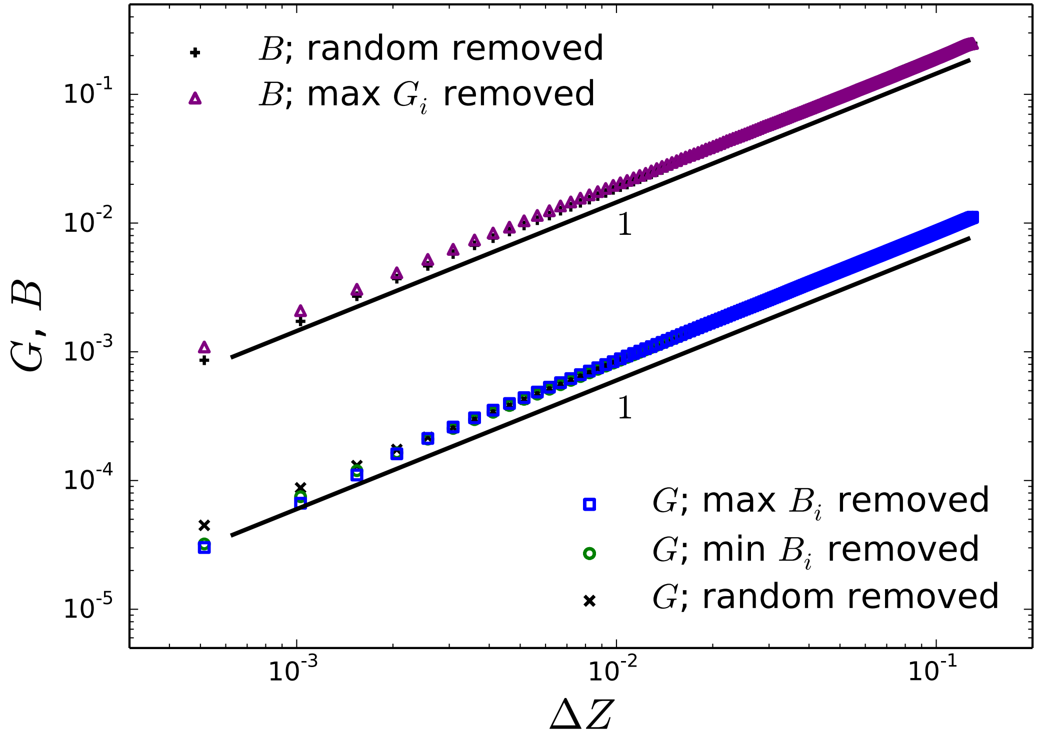
$G \sim \Delta Z$

$B \sim$

prune bonds with largest G_i

$G \sim$

$B \sim \Delta Z$



Tuning by pruning

prune bonds with smallest B_i

$$G \sim \Delta Z$$

$$B \sim$$

random

$$G \sim \Delta Z$$

$$B \sim \Delta Z$$

prune bonds with largest B_i

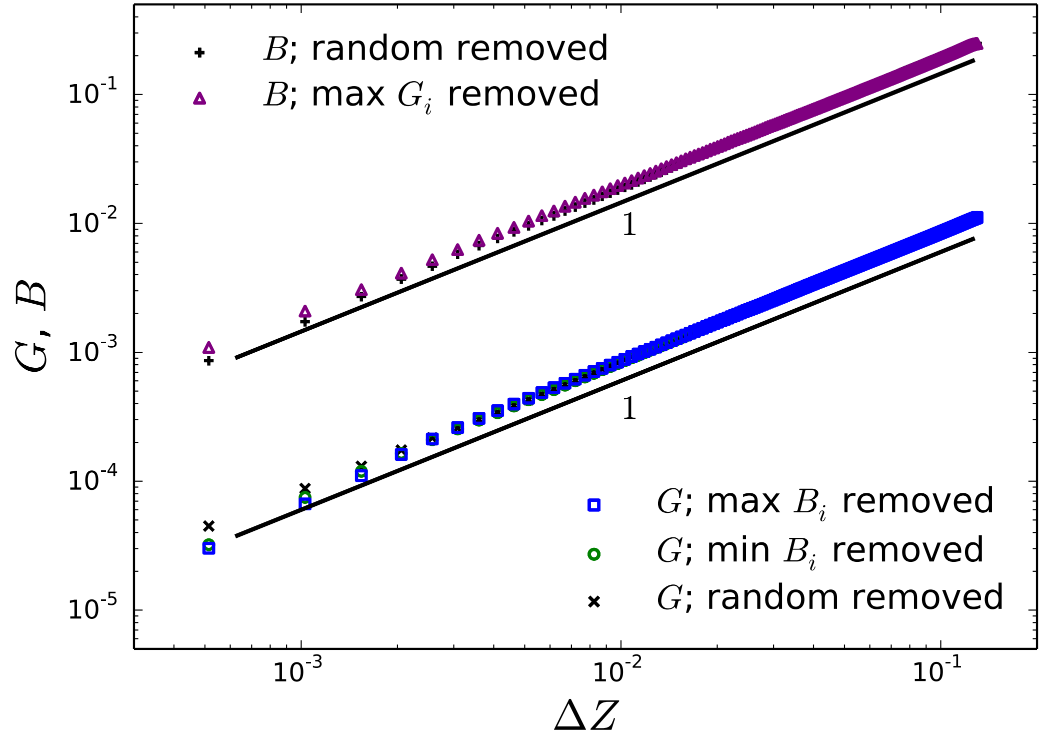
$$G \sim \Delta Z$$

$$B \sim$$

prune bonds with largest G_i

$$G \sim$$

$$B \sim \Delta Z$$



Independence of bond-level response!

Tuning by pruning

prune bonds with smallest B_i

$$G \sim \Delta Z$$

$$B \sim$$

prune bonds with largest B_i

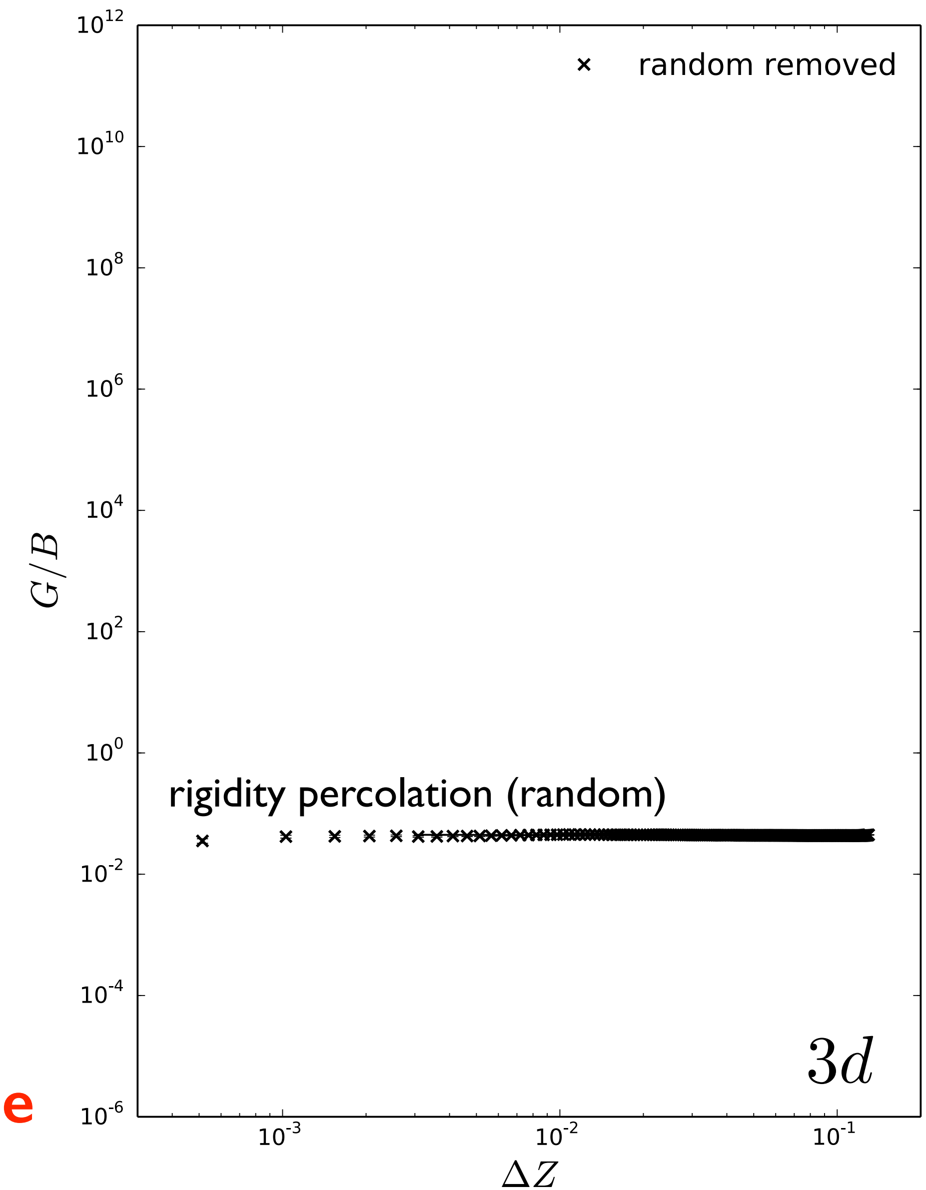
$$G \sim \Delta Z$$

$$B \sim$$

prune bonds with largest G_i

$$G \sim$$

$$B \sim \Delta Z$$



Tune G/B 18 orders of magnitude by pruning 2% of bonds

Tuning by pruning

prune bonds with smallest B_i

$$G \sim \Delta Z$$
$$B \sim 1$$

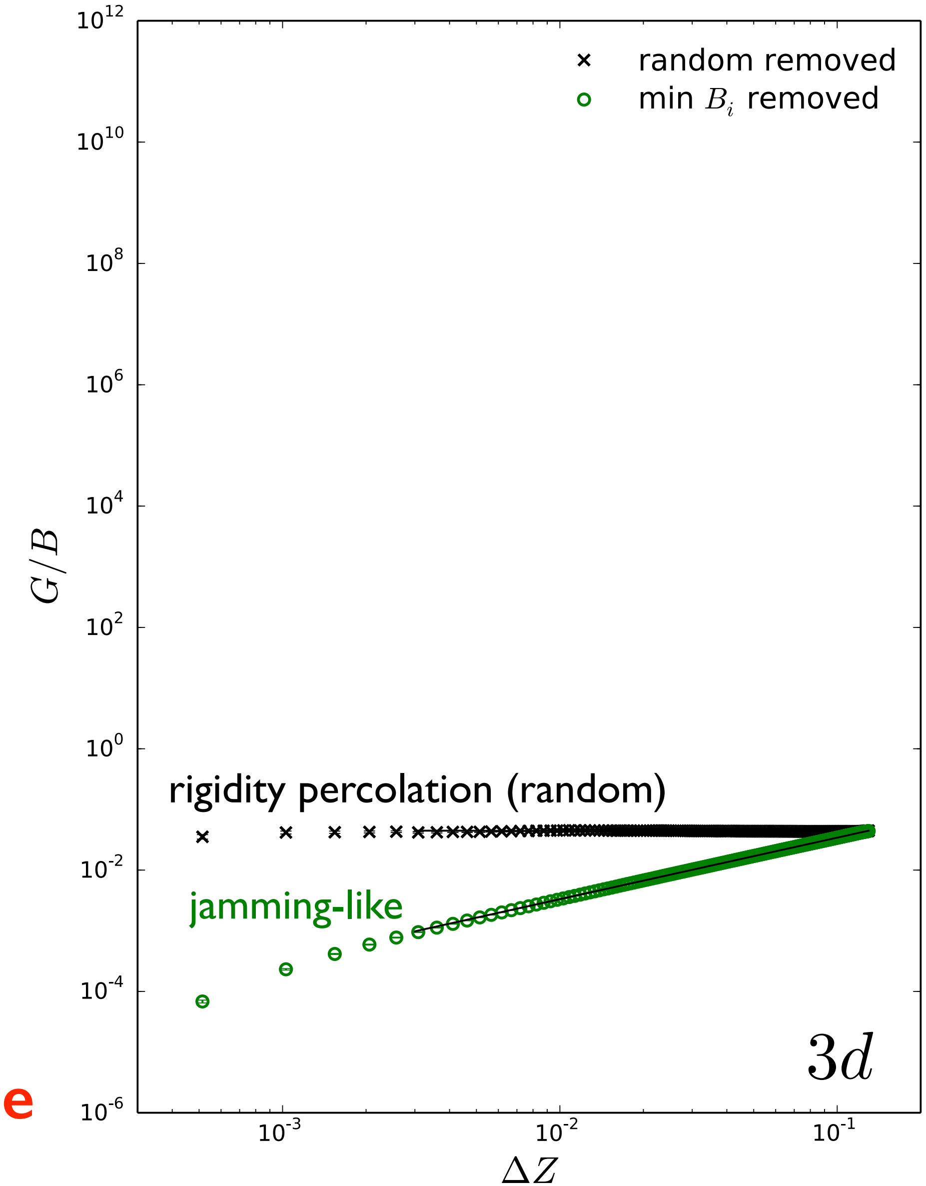
$$G/B \sim \Delta Z$$

prune bonds with largest B_i

$$G \sim \Delta Z$$
$$B \sim$$

prune bonds with largest G_i

$$G \sim$$
$$B \sim \Delta Z$$



Tune G/B 18 orders of magnitude by pruning 2% of bonds

Tuning by pruning

jamming scaling!

prune bonds with smallest B_i

$$G \sim \Delta Z$$
$$B \sim 1$$

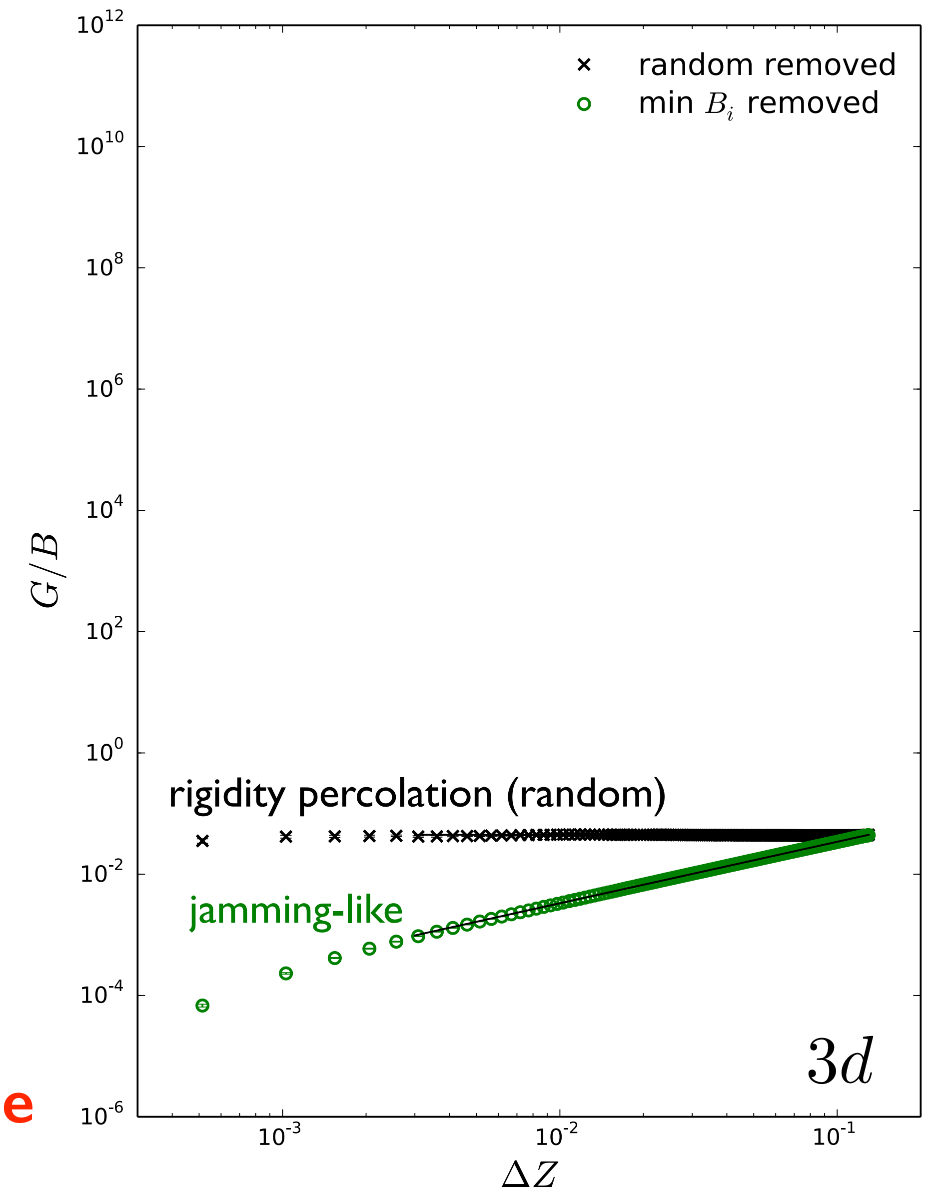
$$G/B \sim \Delta Z$$

prune bonds with largest B_i

$$G \sim \Delta Z$$
$$B \sim$$

prune bonds with largest G_i

$$G \sim$$
$$B \sim \Delta Z$$



Tune G/B 18 orders of magnitude by pruning 2% of bonds

Tuning by pruning

jamming scaling!

prune bonds with smallest B_i

$G \sim \Delta Z$

$B \sim 1$

$G/B \sim \Delta Z$

prune bonds with largest B_i

$G \sim \Delta Z$

$B \sim \Delta Z^{\sim 9}$

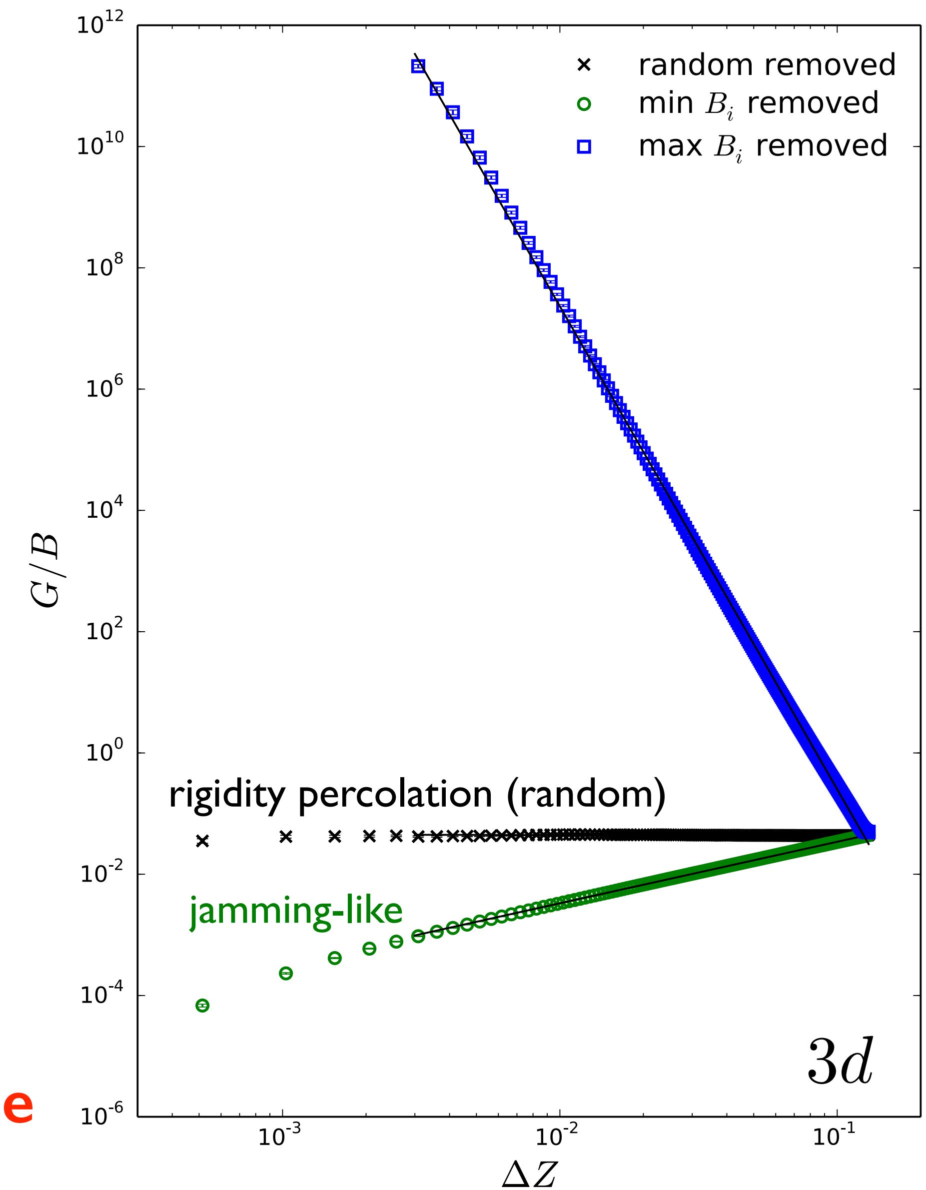
$G/B \sim \Delta Z^{\sim -8}$

prune bonds with largest G_i

$G \sim$

$B \sim \Delta Z$

Tune G/B 18 orders of magnitude by pruning 2% of bonds



Tuning by pruning

jamming scaling!

prune bonds with smallest B_i

$$G \sim \Delta Z \qquad B \sim 1 \qquad G/B \sim \Delta Z$$

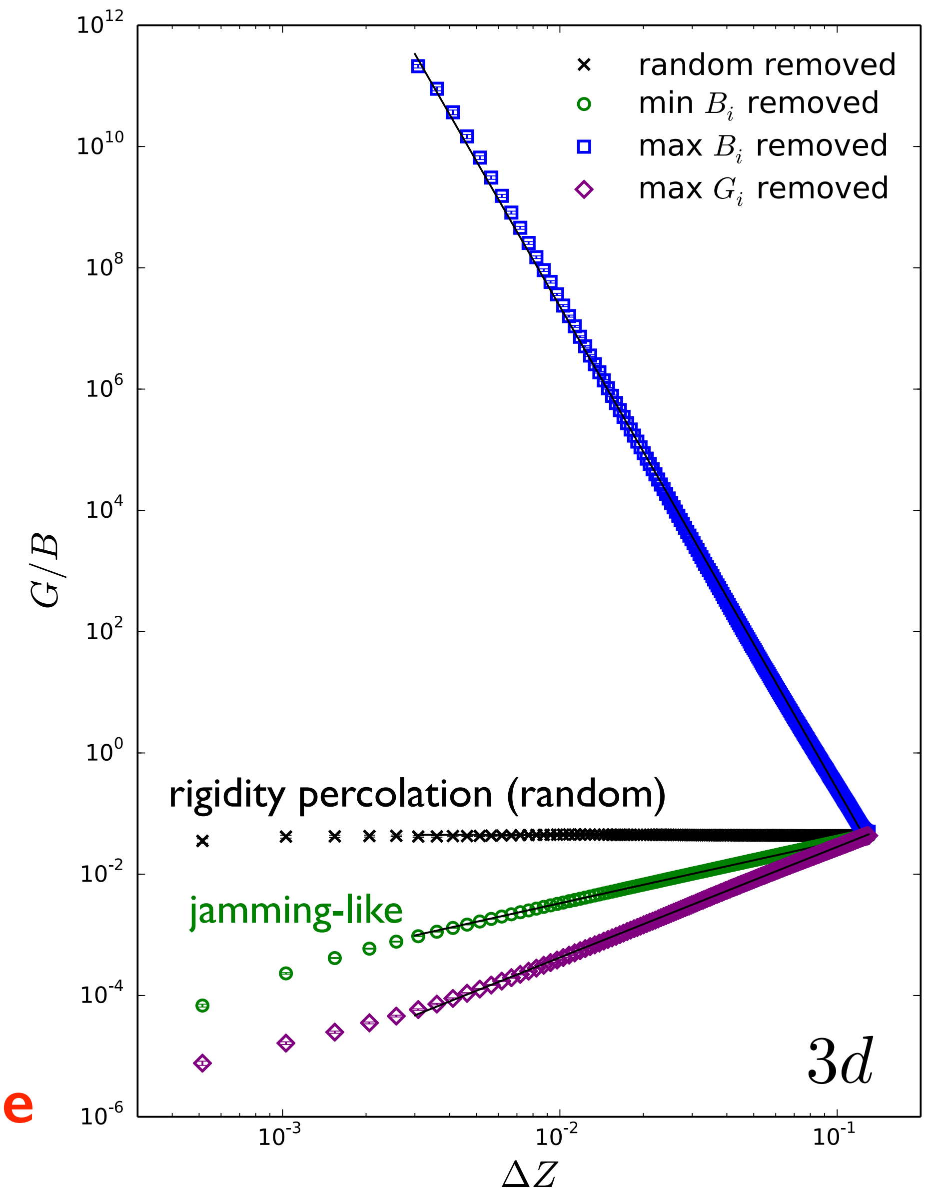
prune bonds with largest B_i

$$G \sim \Delta Z \qquad B \sim \Delta Z^{\sim 9} \qquad G/B \sim \Delta Z^{\sim -8}$$

prune bonds with largest G_i

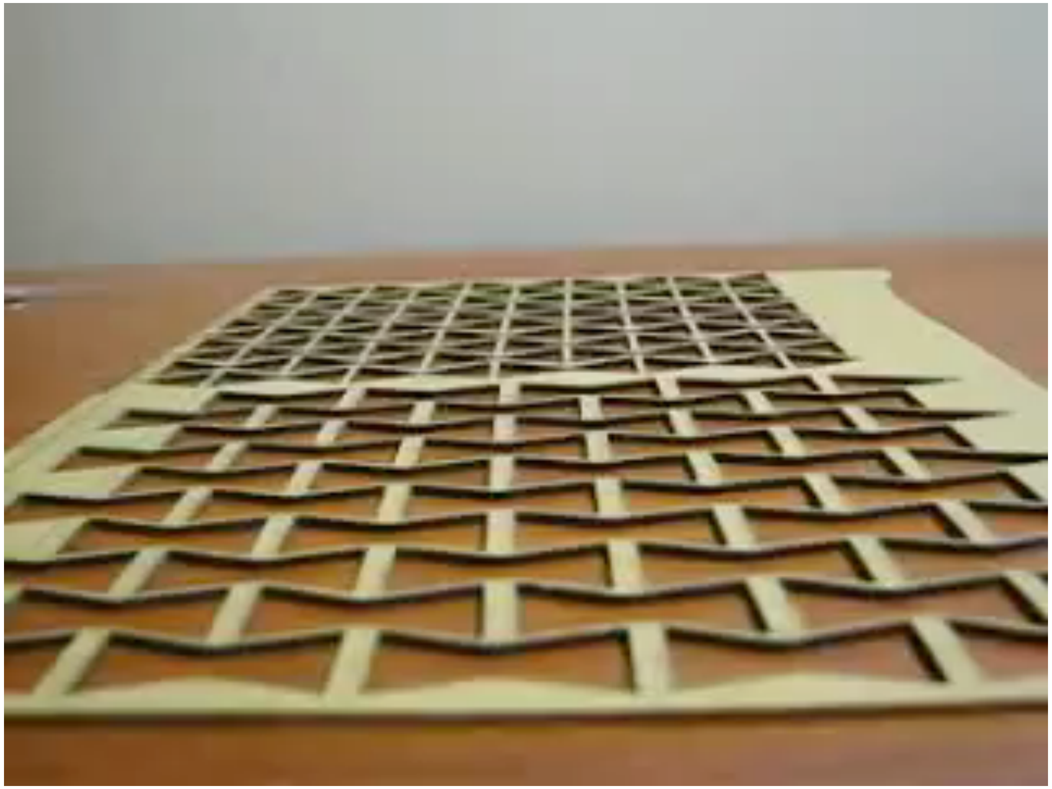
$$G \sim \Delta Z^{\sim 3} \qquad B \sim \Delta Z \qquad G/B \sim \Delta Z^{\sim 2}$$

Tune G/B 18 orders of magnitude by pruning 2% of bonds



Auxetic Materials

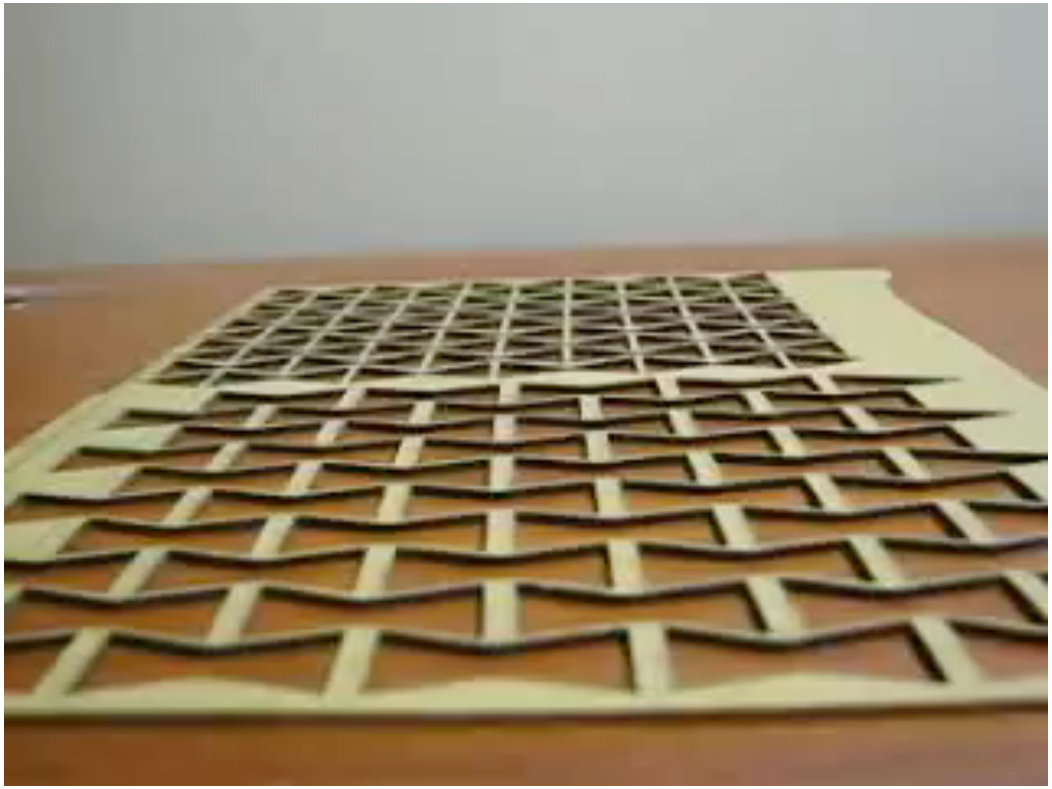
- Materials with G/B > 2/d in d dimensions are auxetic



https://www.youtube.com/watch?v=nDuR9hHIpZM

Auxetic Materials

- Materials with $G/B > 2/d$ in d dimensions are auxetic

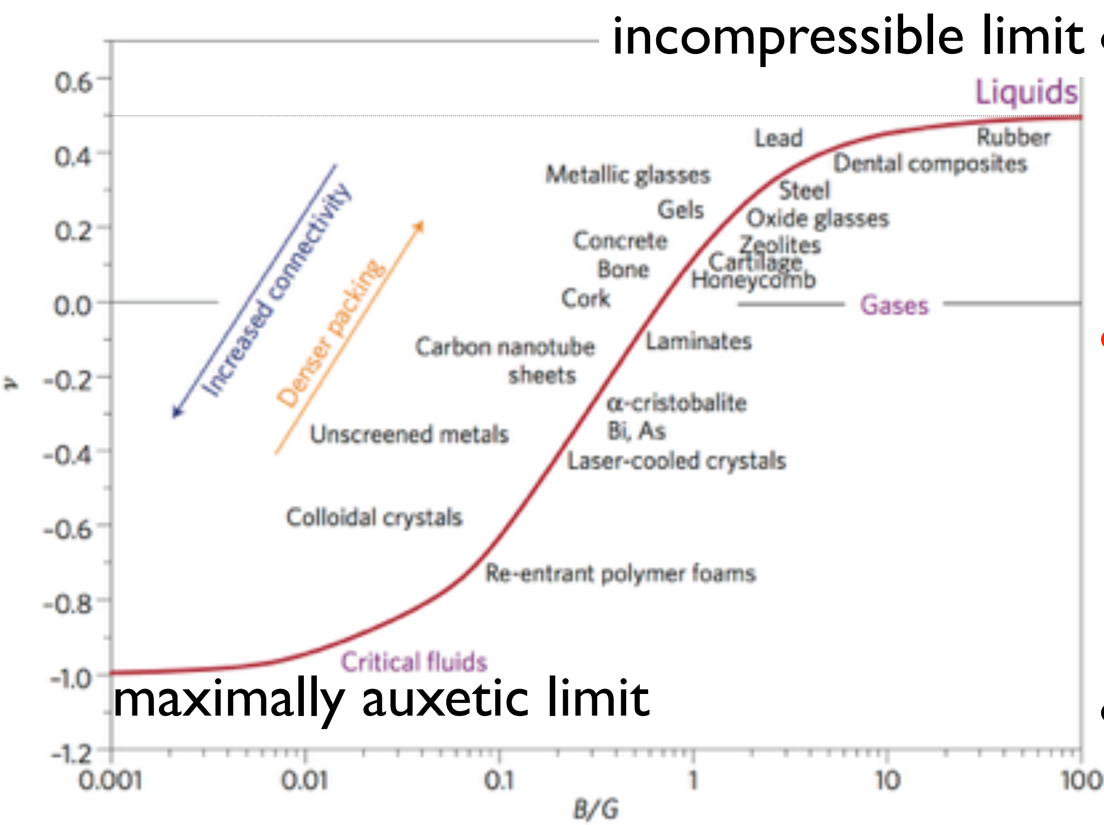


https://www.youtube.com/watch?v=nDuR9hHIpZM

From incompressible to auxetic

Poisson's ratio

$$\nu = \frac{d - 2G/B}{d(d-1) + 2G/B} \qquad -1 \leq \nu \leq 0.5 \text{ (in } 3d)$$



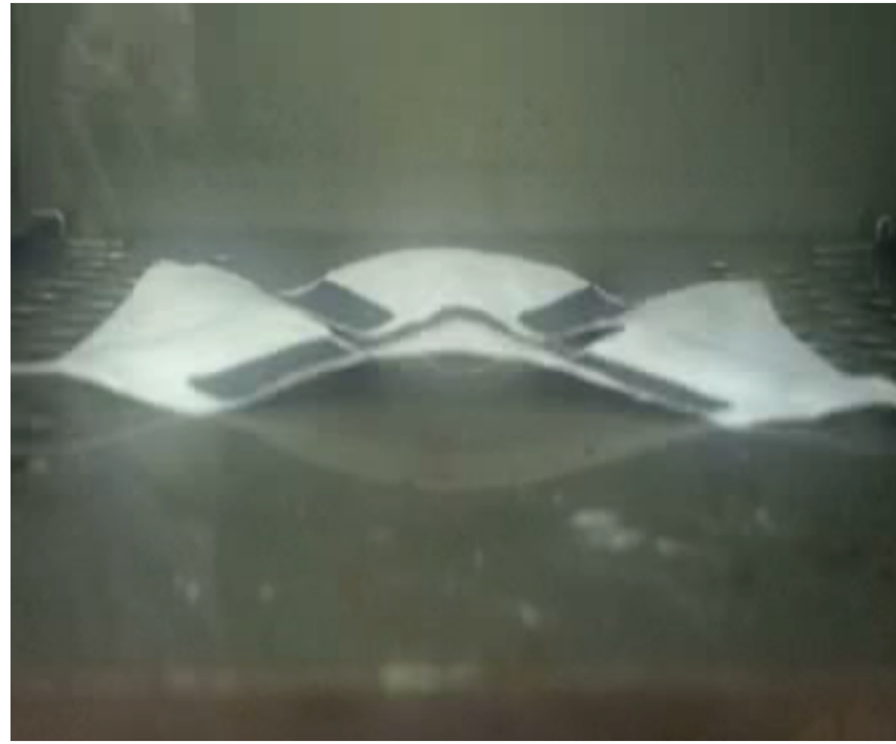
Greaves et al. *Nature Materials* (2011)

- Disordered networks can cover the entire range of allowed values
- Same density and connectivity at auxetic and incompressible limits—new physics
- procedure is experimentally natural

Macroscopic Origami/Kirigami Materials

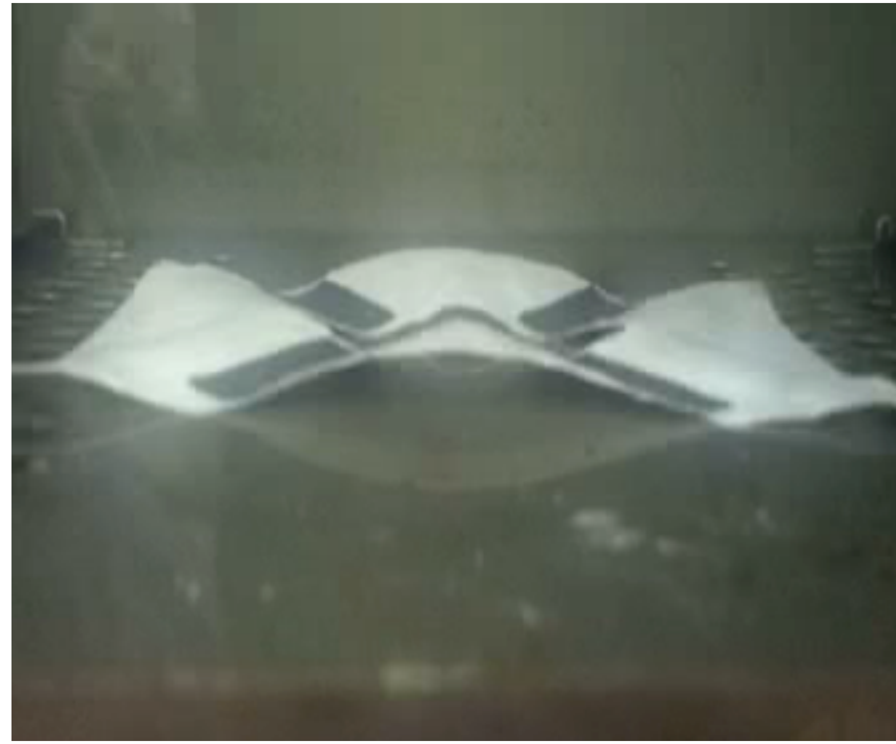
https://www.youtube.com/watch?v=CjfhfqAv1mI

Liu, et al. Soft matter, 2011



Castle, et al PRL (2014)

Macroscopic Origami/Kirigami Materials



https://www.youtube.com/watch?v=CjfhfqAv1mI

Liu, et al. Soft matter, 2011

Castle, et al PRL (2014)

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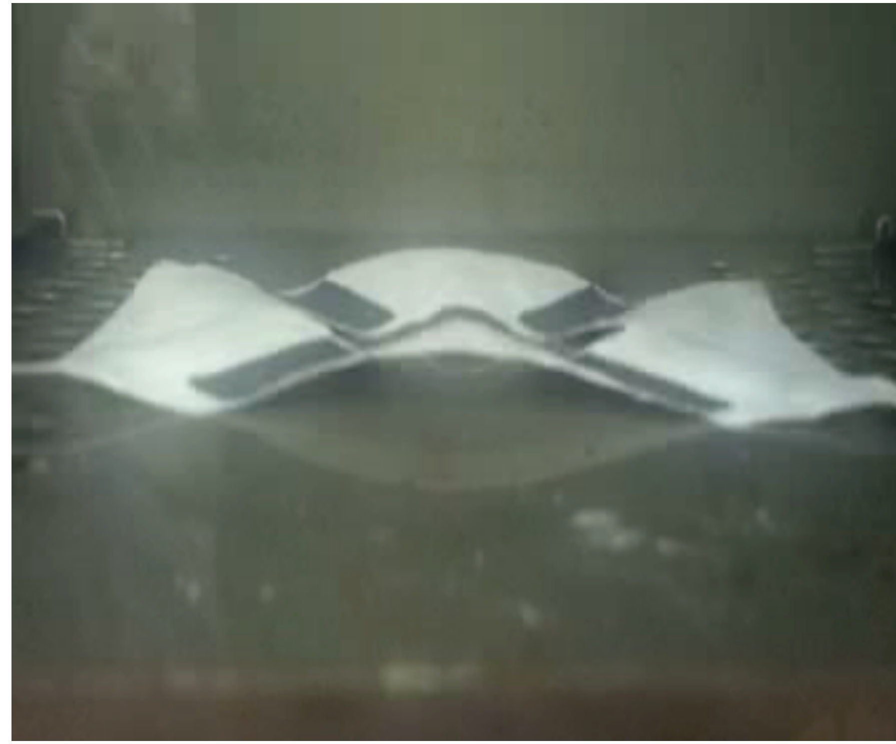
https://www.youtube.com/watch?v=CjfhfqAv1mI

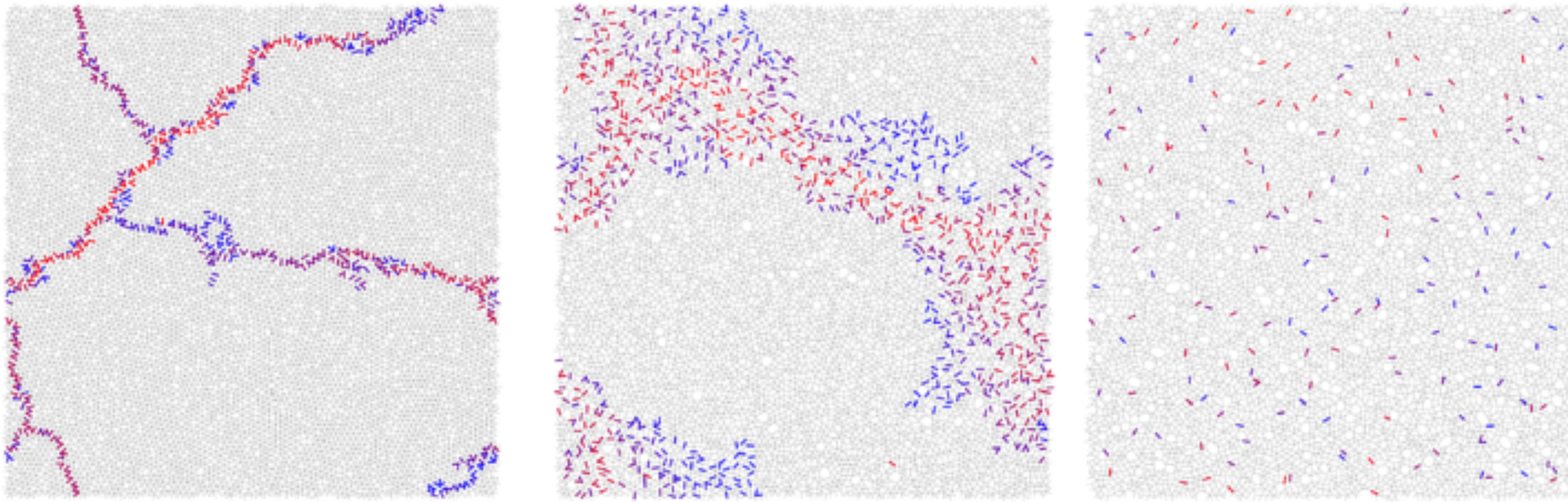
Liu, et al. Soft matter, 2011



Castle, et al PRL (2014)

Spatially Textured Response

$\Delta Z_{initial}=1.52$ $\Delta Z_{initial}=0.53$ $\Delta Z_{initial}=0.046$



- Can create low or zero G or low or zero B strips for origami/kirigami materials
- Can target any quantity that can be written as sum over bond-level contributions, e.g. thermal expansion coefficient

Summary

- Jamming scenario provides "solid" T=0 starting point for understanding mechanical/thermal properties of disordered solids
  - jamming transition is mixed 1st/2nd order transition
  - jammed state is more robust starting point than perfect crystal
  - rationale for commonality in glasses, granular matter, colloidal glasses, foams, emulsions, ….
  - starting point for designing disordered mechanical metamaterials

Thanks to

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Sid Nagel

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Matthieu Wyart	NYU
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Zorana Zeravcic	Rockefeller
Wouter Ellenbroek	Eindhoven
Ke Chen	UPenn
Tim Still	UPenn
Doug Durian	UPenn
Arjun Yodh	UPenn

Bread for Jam:

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