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Workshop on Sphere Packing and Amorphous Materials

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Random Spring Networks vs. Soft Sphere Packings: Jamming Meets Percolation

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Random spring networks vs. soft sphere packings: jamming meets percolation

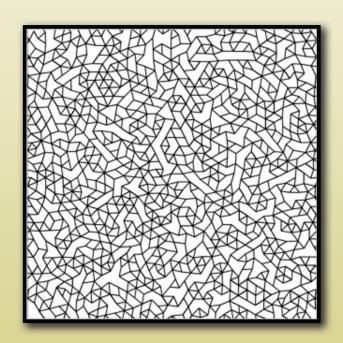
Wouter G. Ellenbroek

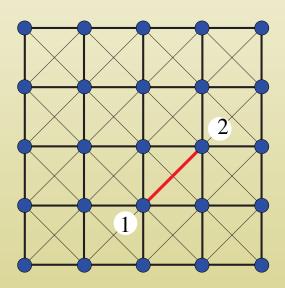
Eindhoven University of Technology

Department of Applied Physics

&

Institute for Complex Molecular Systems

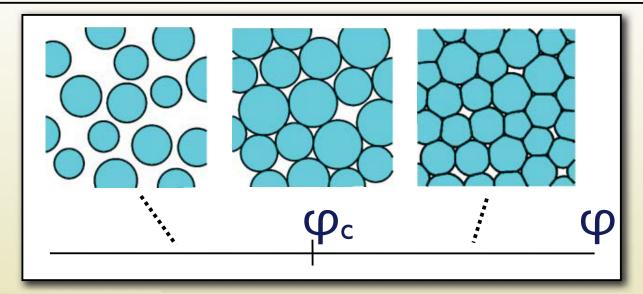


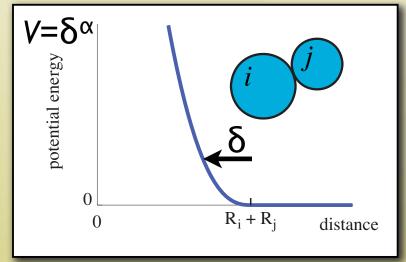






Soft sphere packings

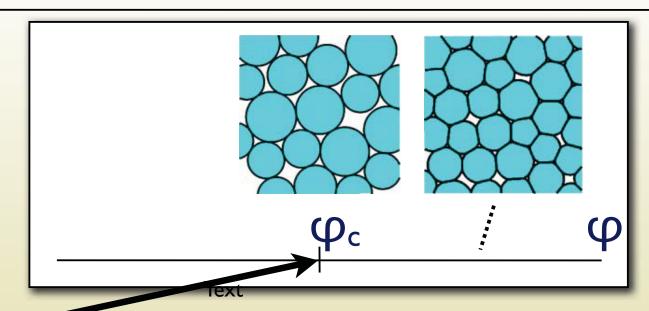




2D polydisperse disk packings: disordered solids with properties determined by $\Delta \phi {=} \phi {-} \phi_c$



Marginal stability and scaling away from it

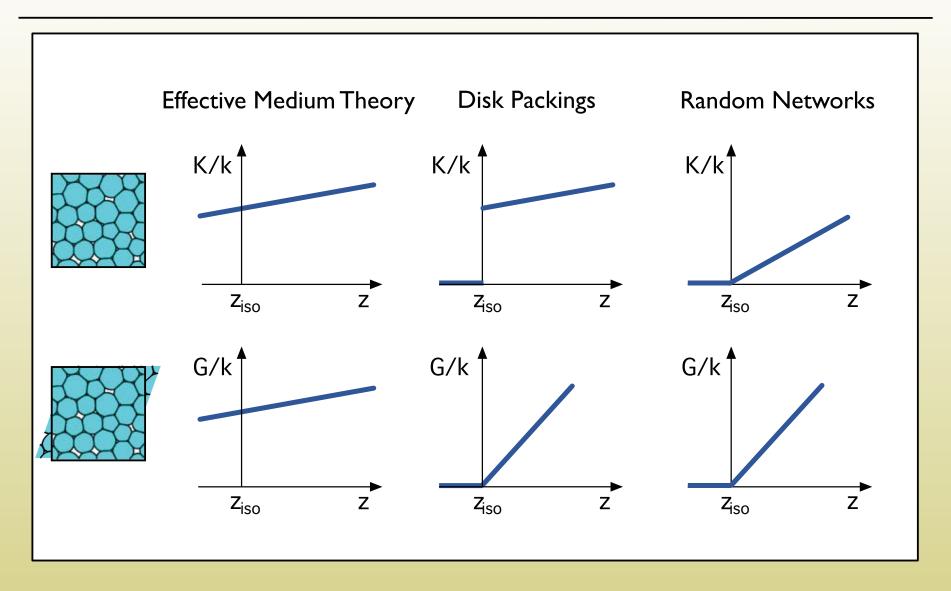


at
$$\phi = \phi_c$$
:
 $p=0$
 $z=z_c=2d$

overlap
$$\delta \sim \phi - \phi_c$$
 pressure $p \sim \delta^{\alpha-1}$ contact number $z = z_c \simeq \delta^{1/2}$ elastic moduli $G/K \sim \delta^{1/2}$ length scale $\psi \sim \delta^{-1/2}$

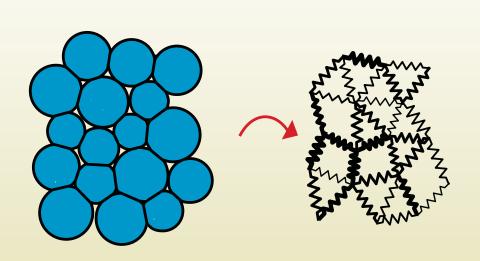


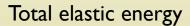
Which is the odd one out?



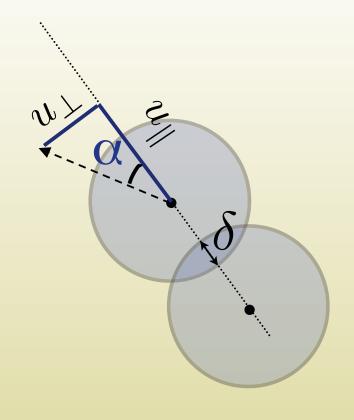


Elastic network description of packings





$$E = \sum_{i \neq j} V(r_{ij})$$



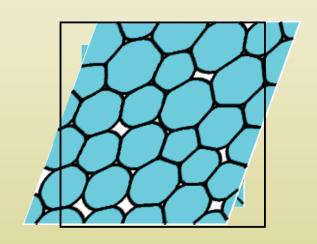
Change in elastic energy due to displacements u

$$\Delta E = \frac{1}{2} \sum_{i \neq j} k_{ij} u_{\parallel}^2 - \frac{f_{ij}}{r_{ij}} u_{\perp}^2$$



Effective Medium Theory?

EMT assumes that the map from old to new positions is affine





assuming affine deformation:

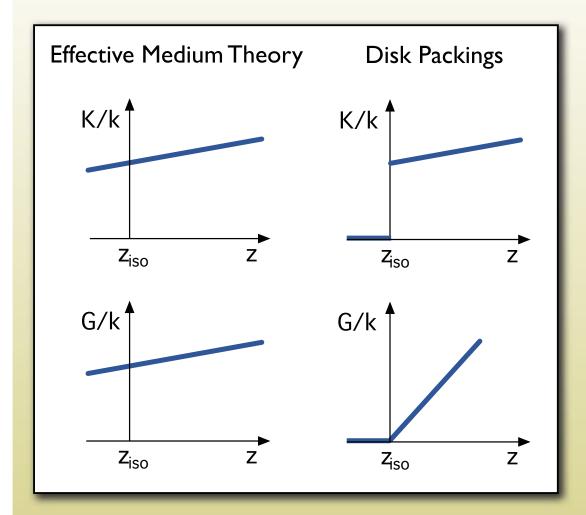
$$u_{\parallel} \sim \epsilon$$

$$u_{\perp} \sim \epsilon$$

$$\Delta E \sim kz\epsilon^{2}$$



Effective Medium Theory?

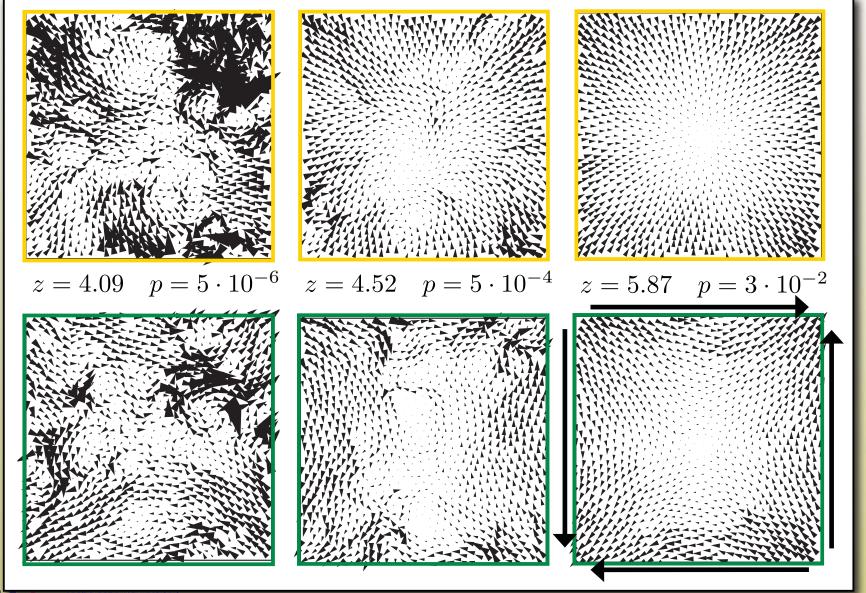


Why does EMT fail?

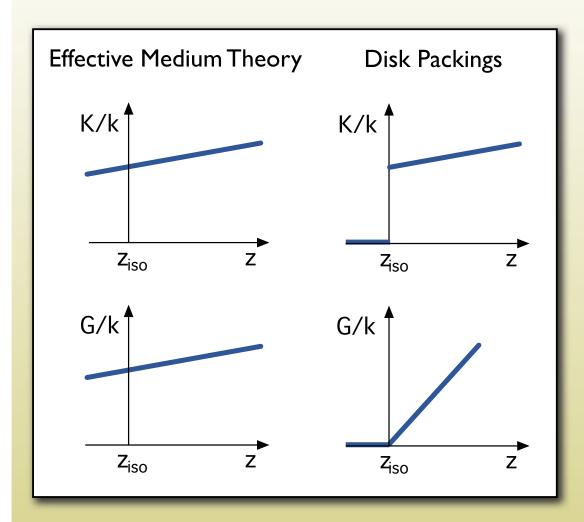
Makse et al., PRL 1999



Non-affinity!



EMT's main assumption fails horribly near ϕ_c



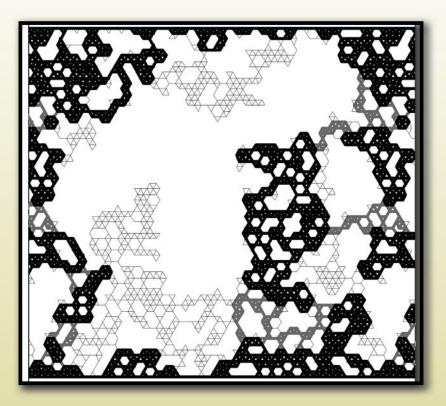
Why does EMT fail?

Makse et al., PRL 1999

Why does EMT seem to work? Ellenbroek et al., EPL 2009



Rigidity percolation



Traditional example:

Diluted triangular lattice
Each bond present with probability p
Threshold value p_c
Fractal rigid backbone
Second order transition
Elastic moduli vanish at the transition

Moukarzel, 1999 Jacobs and Thorpe, 1995

What can we learn from rigidity percolation models that are closer to soft disk packings?

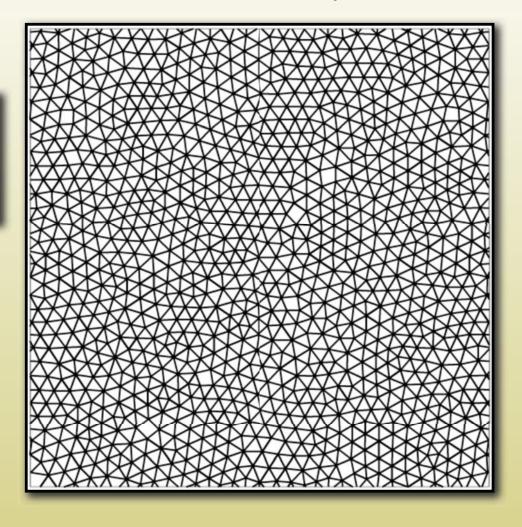


Random Networks

Packings are almost like random networks... but not quite!

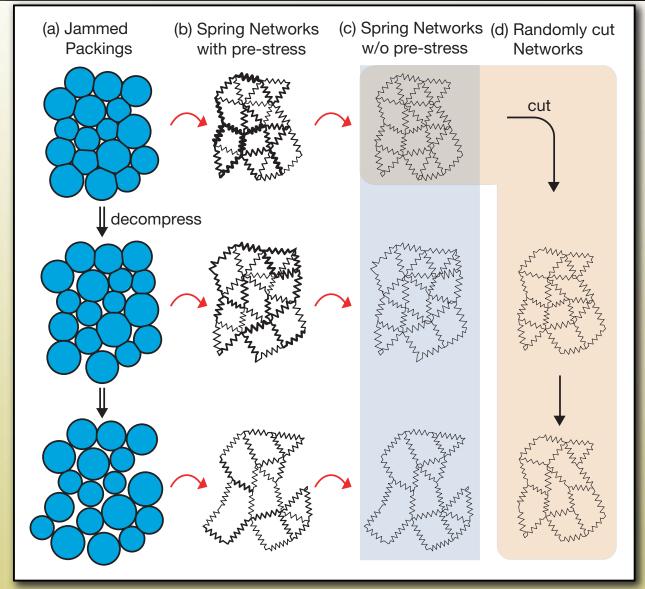
Start from high density packing

Randomly delete/cut bonds while keeping at least 3 bonds per node



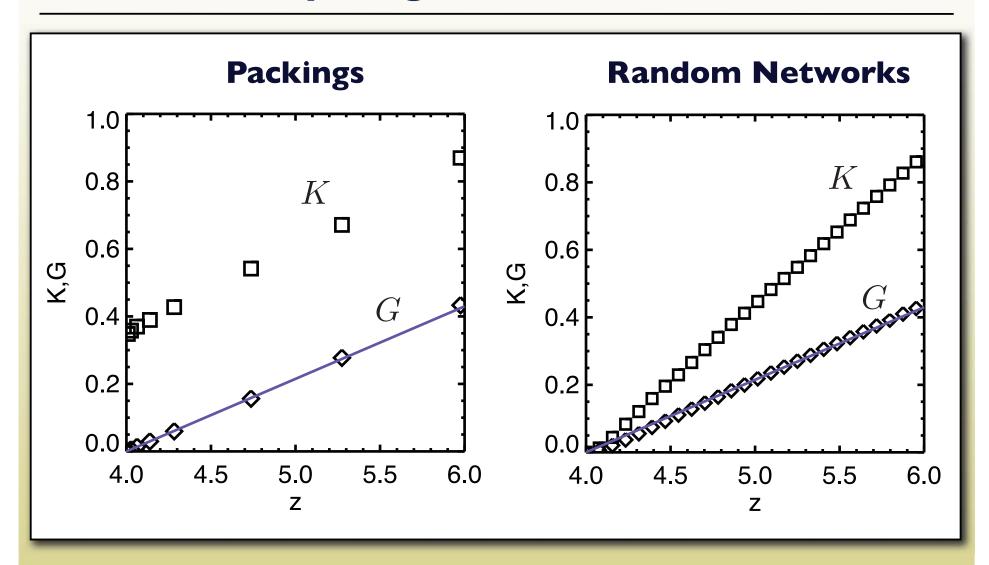


Families of networks



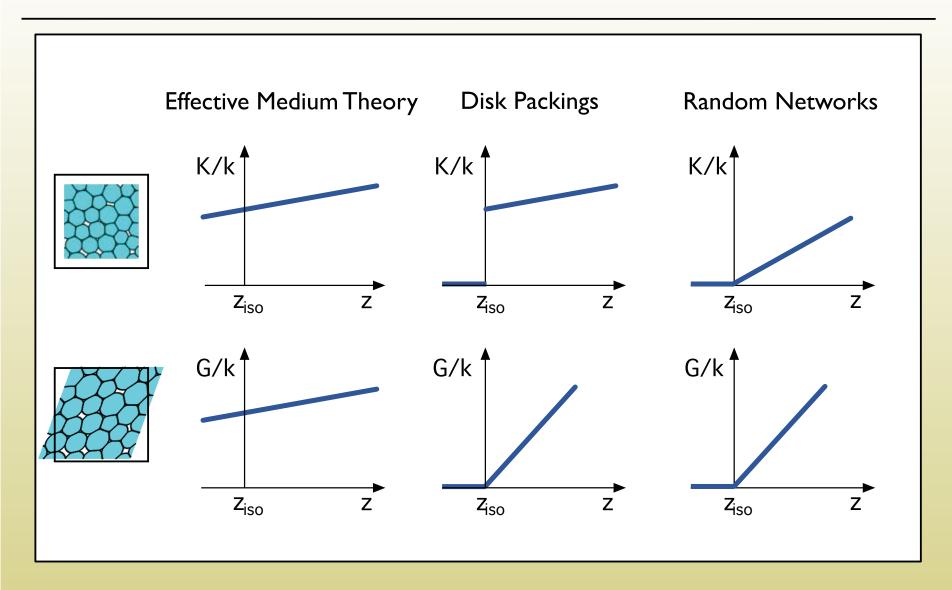


Comparing the elastic moduli





What else can we learn from this?



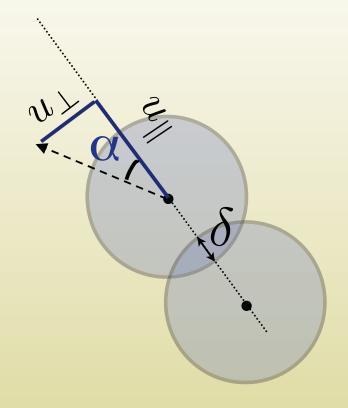


Characterizing non-affinity

Change in elastic energy due to displacements u

$$\Delta E = \frac{1}{2} \sum_{i \neq j} k_{ij} u_{\parallel}^2 - \frac{f_{ij}}{\gamma_{ij}} u_{\perp}^2$$

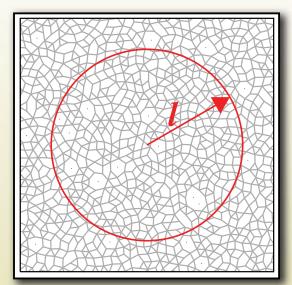
Note that we can vary dN coordinates to minimize zN/2 energy contributions



Study statistics of the "displacement angle" α while varying z

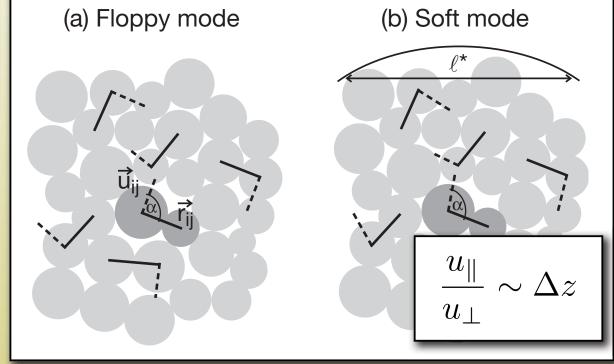


What α do we expect?



$$\ell^* \sim \frac{1}{\Delta z}$$

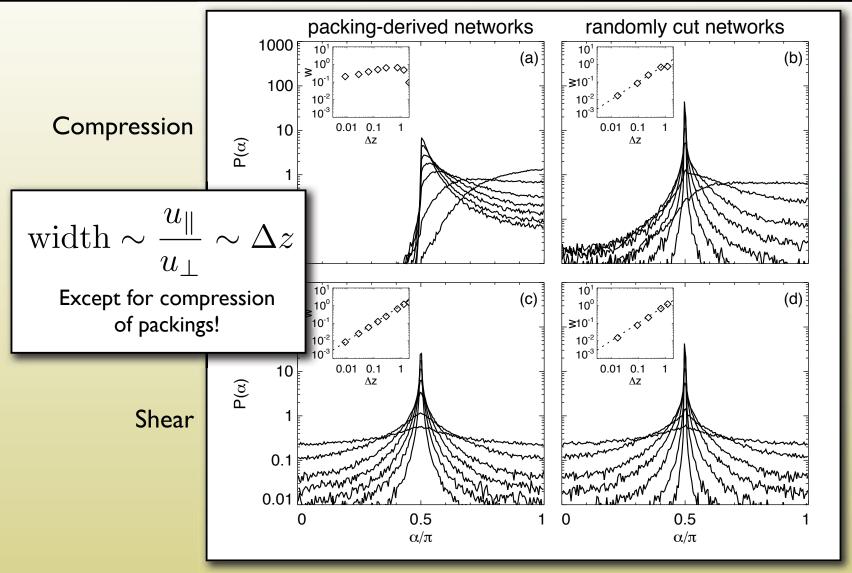
Cutting out this piece will give something floppy if there are more boundary bonds than excess bulk bonds





Wyart et al., EPL (2005), PRL (2008) Ellenbroek et al., EPL (2009)

Probability densities of α



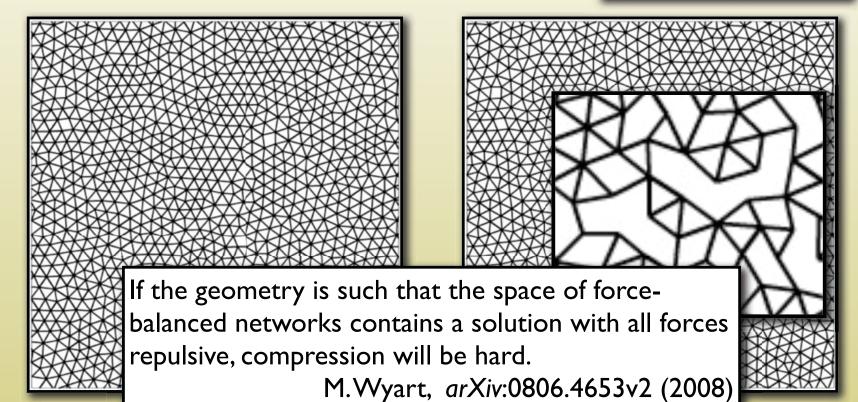


Ellenbroek et al., EPL (2009)

What's behind this?

$$\Delta E = \frac{1}{2} \sum_{i \neq j} k_{ij} u_{\parallel}^2 = \frac{1}{2} \sum_{i,j=1}^{dN} u_i M_{ij} u_j$$

With all spring constants identical, the dynamical matrix M is purely geometric



Summary (moduli)

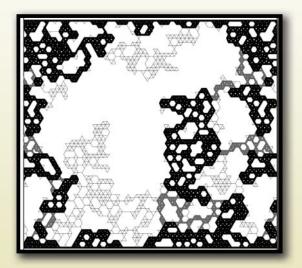
Non-affinity diverges as unjamming is approached.

Elastic behavior of random networks is the same as that of sheared packings.

The compression response of packings is anomalous.

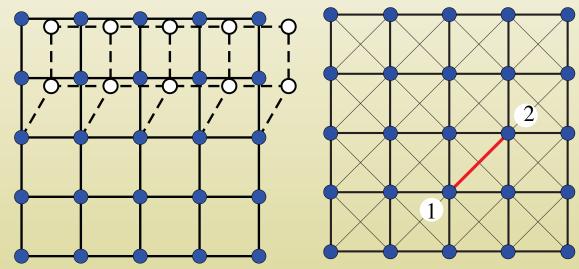


How to theorize more?



Learning about jamming from rigidity percolation: What are suitable models?

- we want a non-fractal structure at the transition
- we want isostaticity at the transition

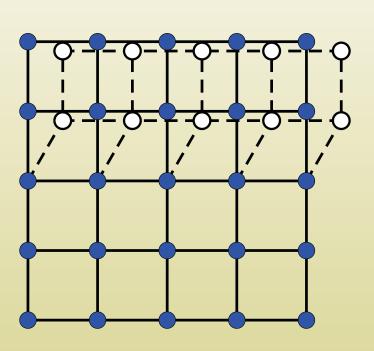


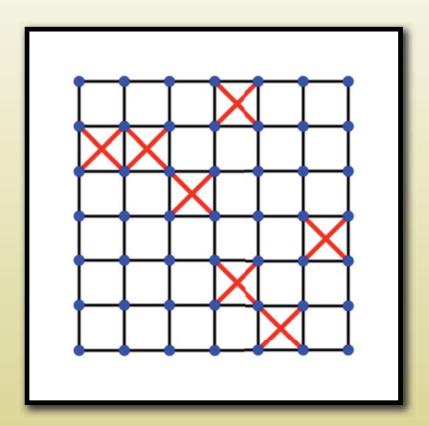
Square lattice with randomly added next-nearest-neighbor bonds



Rigidity transition

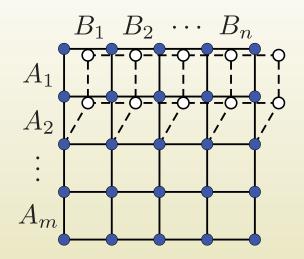
For what *p* is the resulting structure rigid? How does this *p* depend on system size?



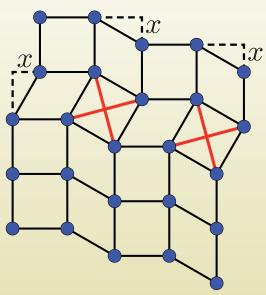




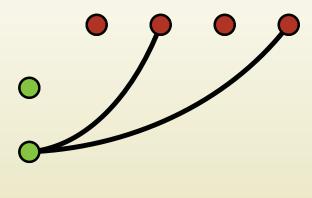
Defining variables and mapping



(n+m)-dimensional space of floppy modes



Each crosslink sets two coordinates to be equal



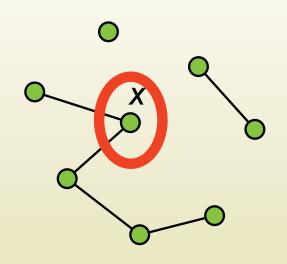




A connected graph represents a rigid configuration



Connectivity of simple random graph



illustrating k=5 term

$$\mathcal{F}_1(n,p) = \text{P[random graph with } n \text{ vertices and edge probability } p \text{ is connected]}$$

Construct recurrence relation by considering all possible sizes k of the cluster that node x belongs to

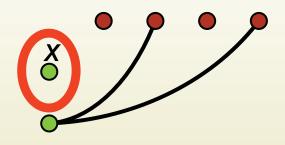
$$1 - \mathcal{F}_1(n, p) = \sum_{k=1}^{n-1} {n-1 \choose k-1} \mathcal{F}_1(k, p) q^{k(n-k)}$$

$$q = 1 - p$$

Gilbert, Ann. Math. Statist. (1959)



Connectivity of bipartite random graph



 $\mathcal{F}(m,n,p) = \text{P[random graph with } m \text{ green and } n \text{ red vertices and edge probability } p \text{ is connected]}$

Generalize recurrence relation by considering all possible sizes k,l of the cluster that node x belongs to

$$1 = \sum_{k=1}^{m} \sum_{l=0}^{n} {m-1 \choose k-1} {n \choose l} \mathcal{F}(k,l,p) q^{k(n-l)} q^{l(m-k)}$$



Connectivity of bipartite random graph

$$1 = \sum_{k=1}^{m} \sum_{l=0}^{n} {m-1 \choose k-1} {n \choose l} \mathcal{F}(k,l,p) q^{k(n-l)} q^{l(m-k)}$$

in the limit $m=n\to\infty$

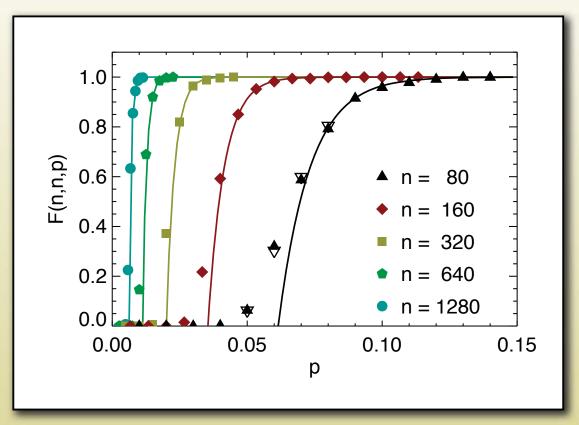
Upper bound on **F** from I-**F** $(n,n,p) \ge P[graph contains at least I isolated node]$ Lower bound on**F** $from <math>F(k,l,p) \le I$

Bounds coincide to lowest order in I/n: $\mathcal{F}(n,n,p)
ightarrow 1-2nq^n$



Testing the limiting form of F

$$\mathcal{F}(n,n,p) \to 1 - 2nq^n$$



Closed symbols: numerical test of graph connectivity Open symbols: evaluation of recurrence formula Lines: Limiting form of **F**



Scaling of the threshold probability

Define critical p as function of system size through

$$\mathcal{F}(n, n, p_{\mathbf{R}}(n)) = 1/2$$

From our work, rigorously
$$p_{\mathrm{R}} \geq \frac{\ln 2n}{n}$$

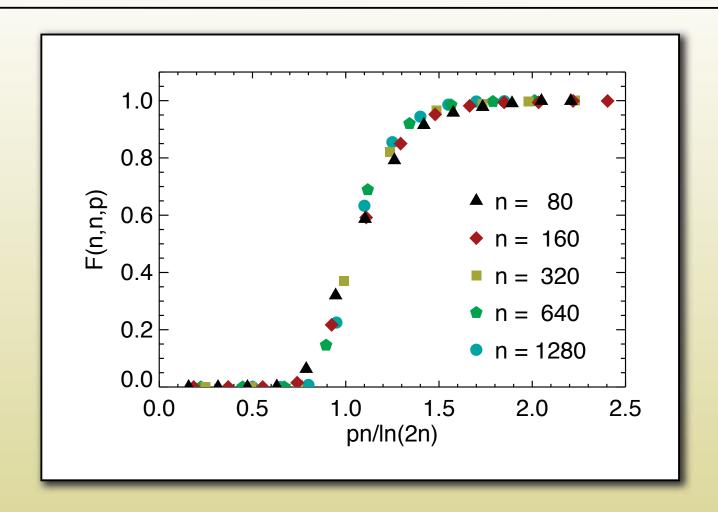
and numerically
$$p_{\mathrm{R}} \lesssim \frac{\ln 4.93n}{n}$$

From Palásti (1963) it can be derived that
$$p_{\mathrm{R}} = \frac{\ln(2n/\ln 2)}{n} \approx \frac{\ln 2.89n}{n}$$

$$p_{\rm R} = \frac{\ln n}{n} + \mathcal{O}(1/n)$$
 as $n \to \infty$



Finite size scaling of the numerical data





Generic rigidity?

If we move away from the perfect square lattice to something with the same topology but with disordered positions...

- having one crossbar in each row and column is still not sufficient, and no longer necessary for rigidity
- the structure can be rigid even for non-connected graphs
- the order of the rows becomes important (not all green nodes are equivalent anymore)
- graph mapping used so far becomes pretty hopeless

...but numerically we can use the pebble game! Jacobs and Thorpe, PRL (1995), PRE (1996)



Conclusion (square lattice)

The threshold p for NNN rigidity percolation on the square lattice goes to zero with increasing system size \Rightarrow transition at isostatic point

$$p_{\rm R} = \frac{\ln n}{n} + \mathcal{O}(1/n)$$
 as $n \to \infty$

Now what if we want to learn about jamming from this? ⇒

Recent work by Xiaoming Mao, Anton Souslov, Tom Lubensky, Andrea Liu

Mao et al., PRL 104, 085504 (2010)

Souslov et al., PRL 103, 205503 (2009)



Summary

Effective medium theory has nothing to say about elasticity of packings close to unjamming.

Random networks tell us that what's special about packings is that they resist compression so strongly.

It's fun to link together bits of known math to write down an exact expression, even if the relevant asymptotics were already known.

Ellenbroek, Zeravcic, Van Saarloos, Van Hecke, EPL 87, 34004 (2009) Ellenbroek, Mao, arXiv: I 107:3933 (2011) and references therein



Thank you so much...









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