The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2254-2

Workshop on Sphere Packing and Amorphous Materials

25 - 29 July 2011

Growing Correlations at Unjamming of Sphere Packings

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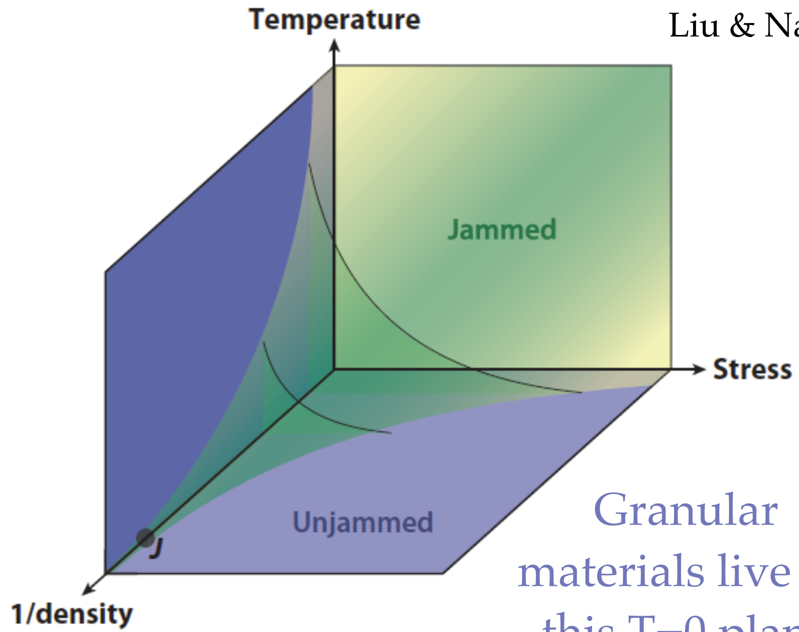
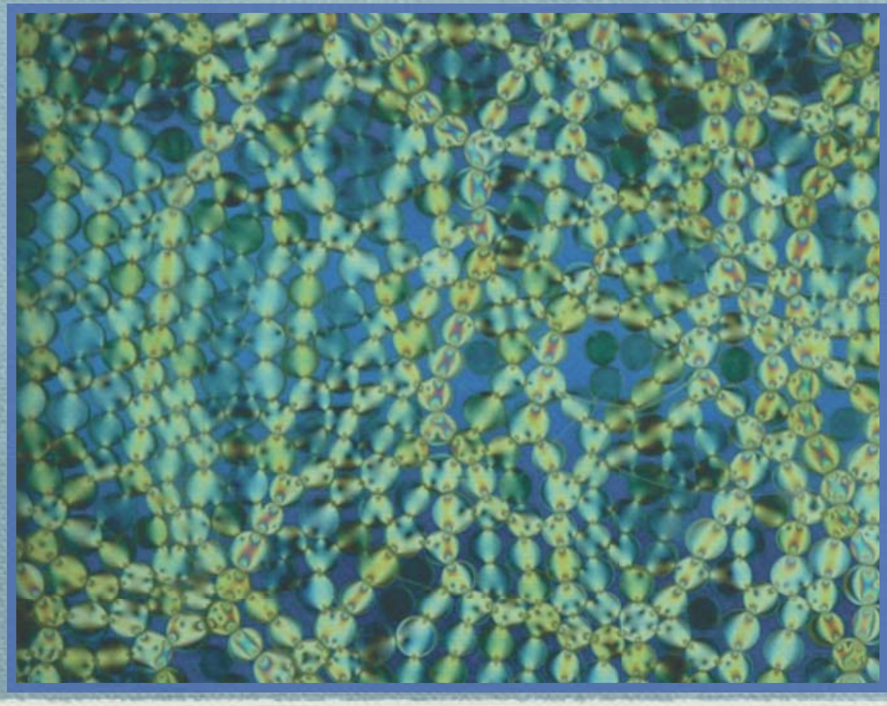
Liu & Nagel Annu. Rev. Condens. Matter Phys. 2010. 1:347–69



Granular materials live on this T=0 plane

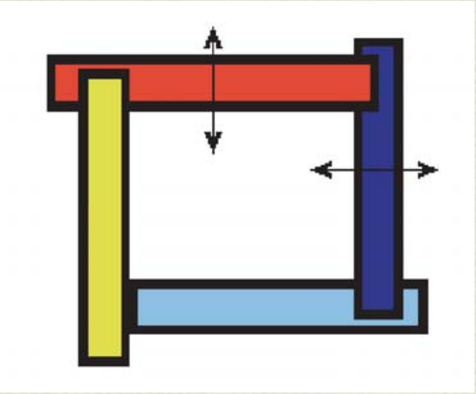
J-Point is a non-equilibrium critical point



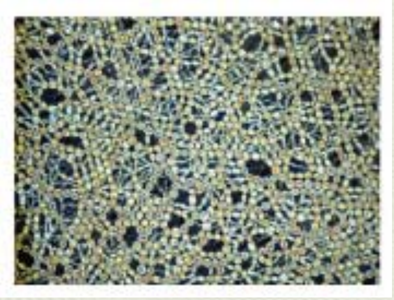
Growing Correlations at Unjamming of sphere packings

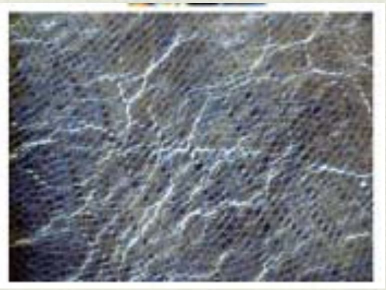
Dry Granular Materials

❖No cohesive interaction
❖Grains are nearly rigid
❖Unjammed side: Hard spheres
❖Jamming : Increasing density leads to states that are jammed
❖ Deformable grains beyond Point J: states of mechanical equilibrium
❖Unjamming: Falling apart because there is not enough imposed stress to impart rigidity



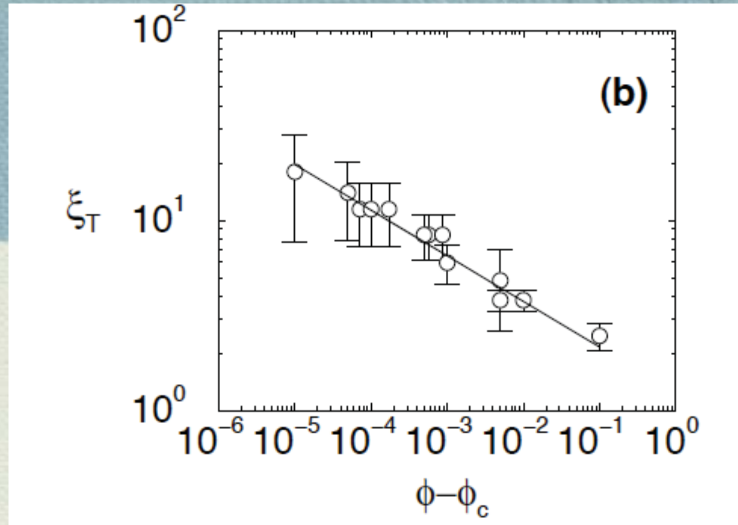
Put in N grains
Change shape
and/or size of box



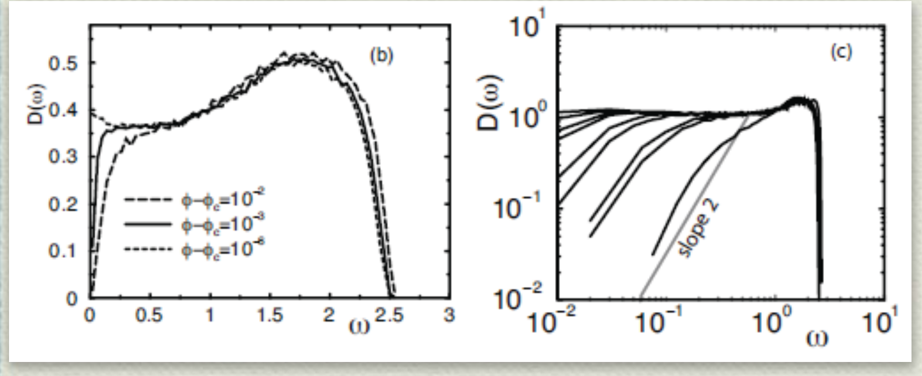


Length Scales

Silbert, Liu & Nagel, PRL 95, 098301 (2005)



Soft Modes and *l**

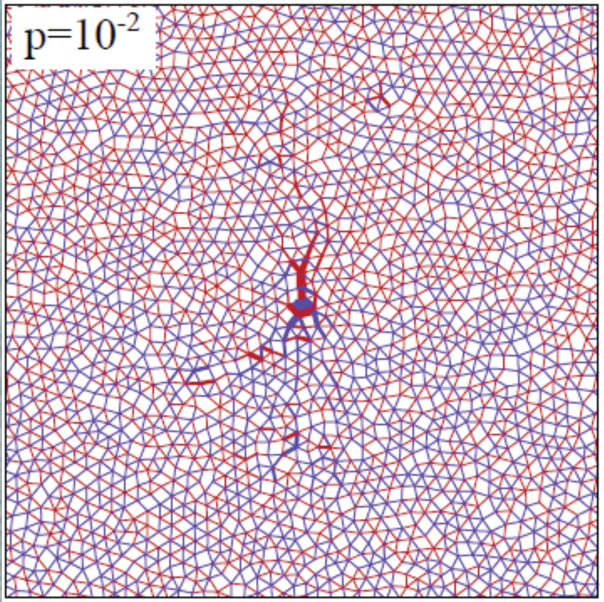


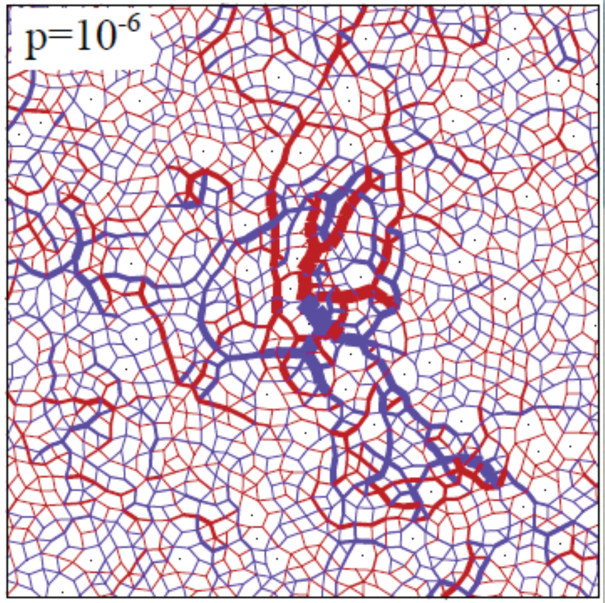
O'hern et al, PRE 68 (2003) 01130

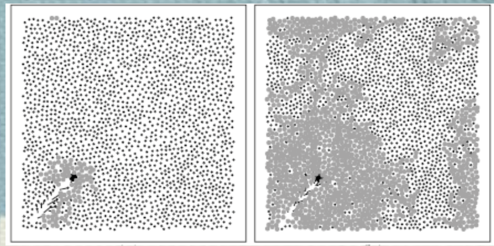
Exponent = $1/4$

- Onset of unjamming associated with emergence of "anomalous modes."
- Plateau defines crossover frequency ω^*.
- Bulk-surface argument: ⇨ $l^* \sim 1/\delta z$ ⇨ Exponent = $1/2$
  (M. Wyart, T. Witten)

MEASURING LENGTH SCALES FROM RESPONSE

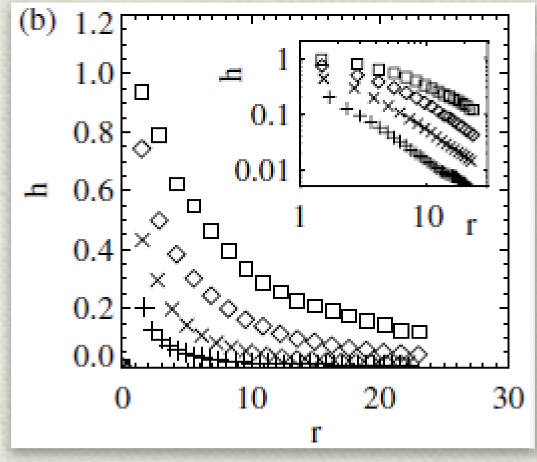


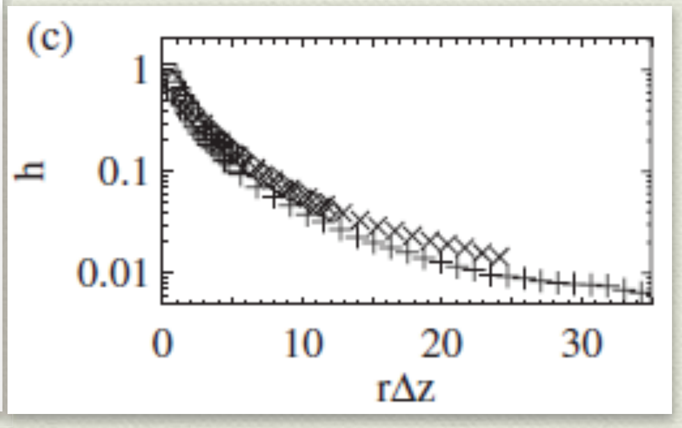




J.A. Drocco et al., PRL **95** 088001 (2005)

A growing length scale is observed as a result of perturbations in simulation.





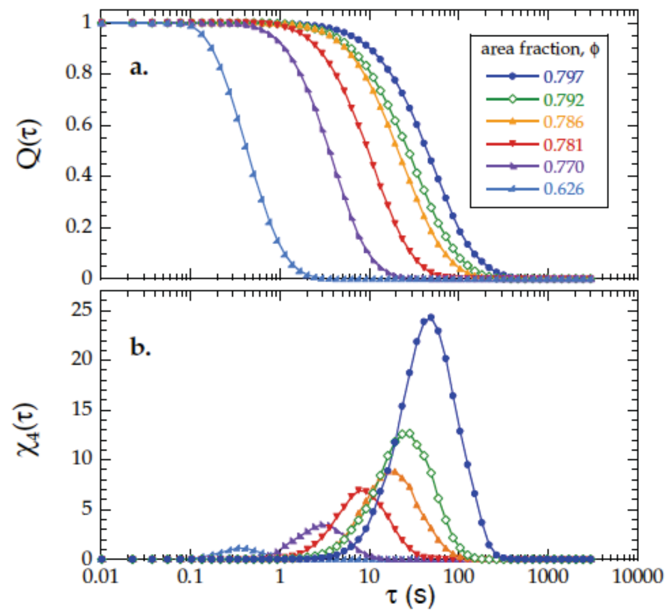
l scaling verified from force response*

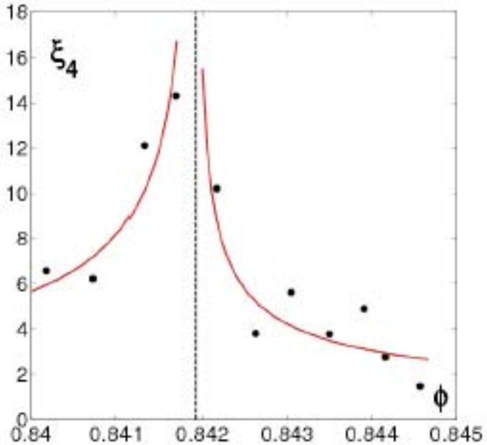
Ellenbroek W. G. et al, PRL 97 (2006) 258001

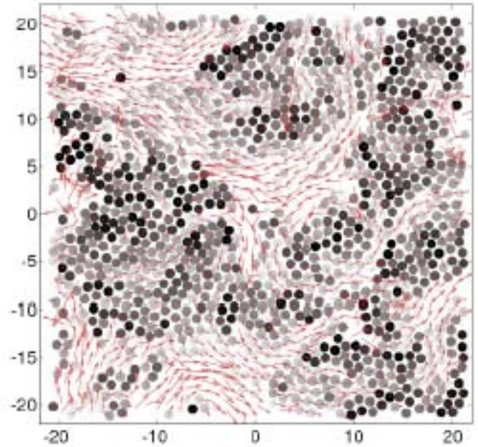
Dynamical Heterogeneity

F. Lechenault et al., Europhys. Lett. 83, 46003 (2008)

Fluidized Monolayer



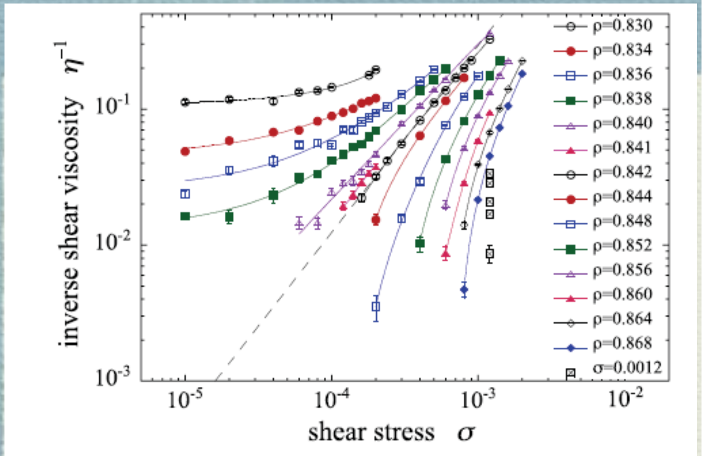




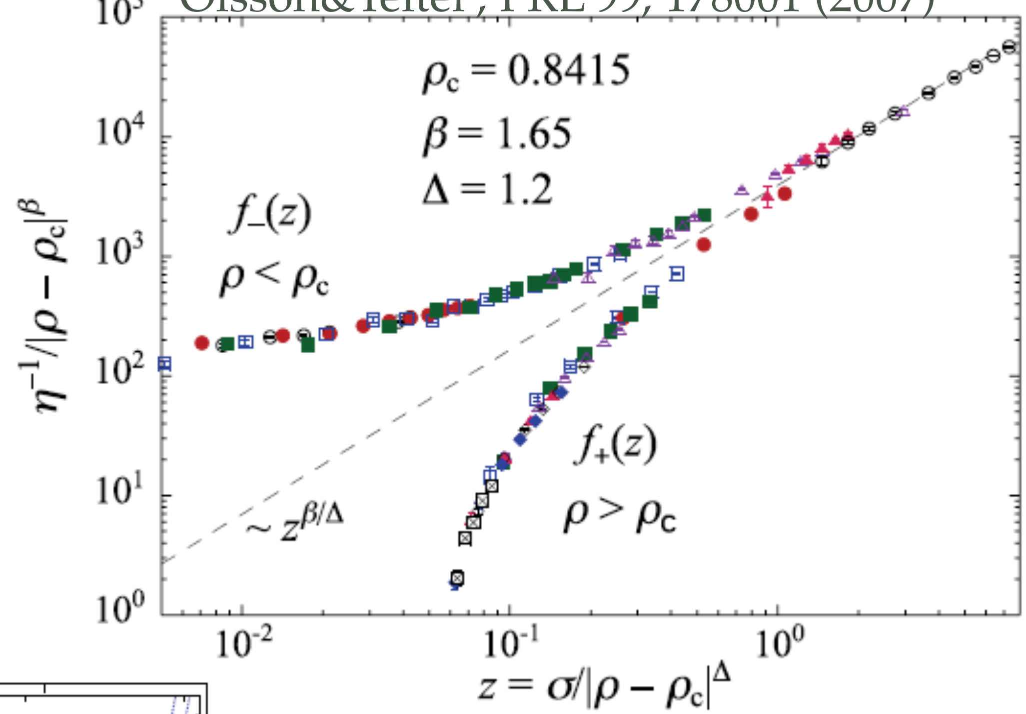
Vibrated Monolayer

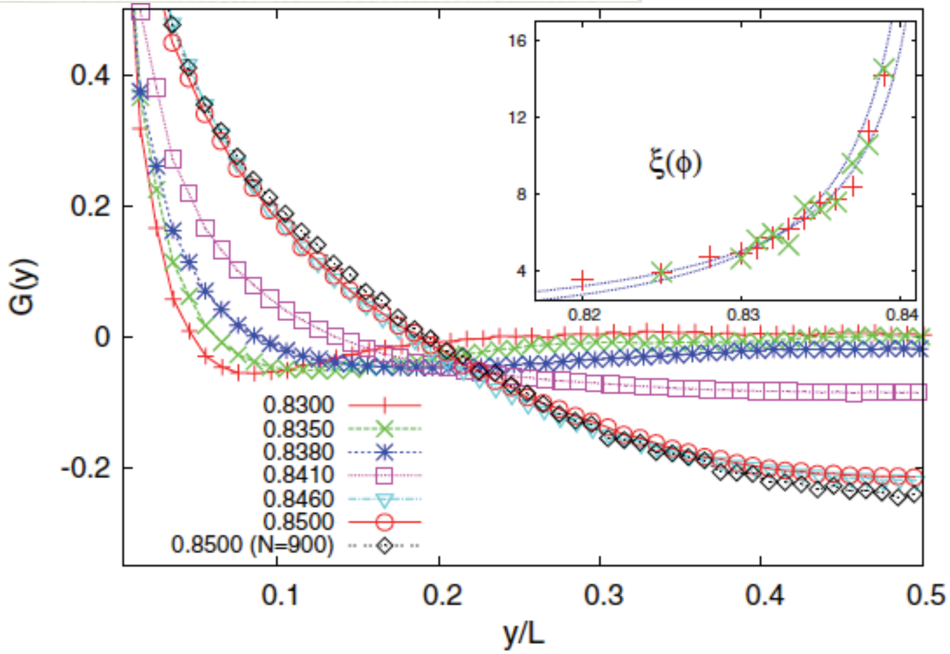
Abate and Durian, PRE 76, 021306 (2007)

Scaling under shear



Olsson&Teitel , PRL 99, 178001 (2007)



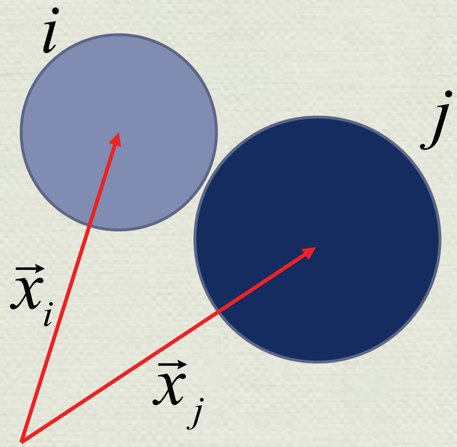


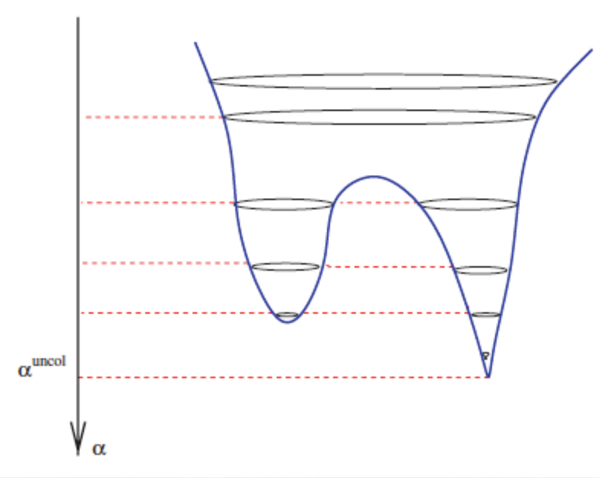
Two-point correlations: no growing length scale on jammed side

Heussinger &Barrat , PRL 102, 218303 (2009)

Is there a Static Measure that detects a growing length scale?

- Two types of constraint satisfaction:
  - Jamming: Packing Problem
  - Unjamming: Mechanical stability constraints
- Many Solutions
- Entropy Crisis
- Mapping to Energy Landscape
- Connection to statistical mechanics of glassy systems





Krzakala &Kurchan , PRE 76, 021122 (2007)

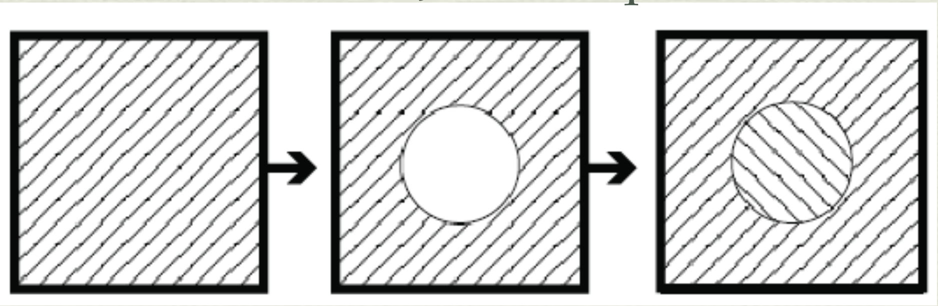
POINT-TO-SET CORRELATIONS

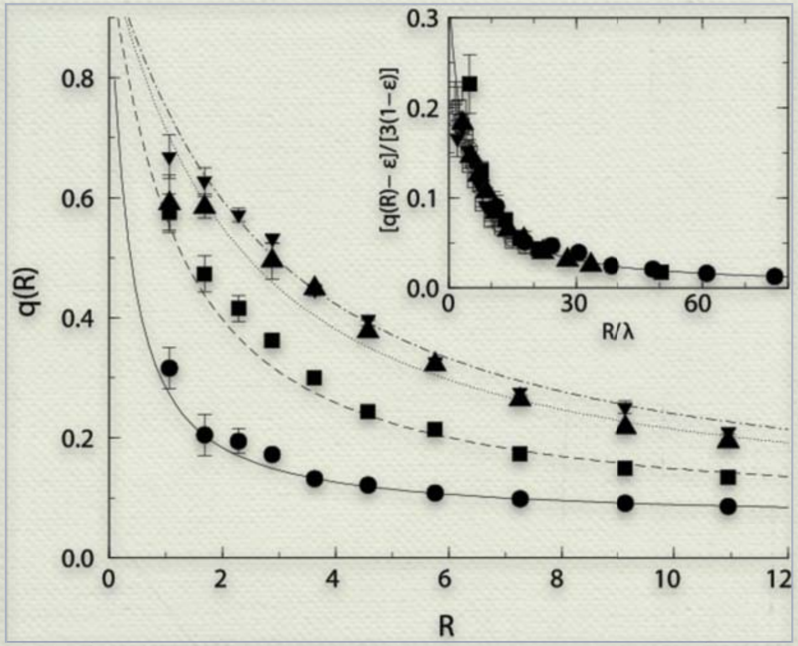
Probes boundary effects:

near a critical point, effects of boundaries should become long-ranged

Random-First-Order Theory: Entropic droplets

Lennard-Jones Liquids

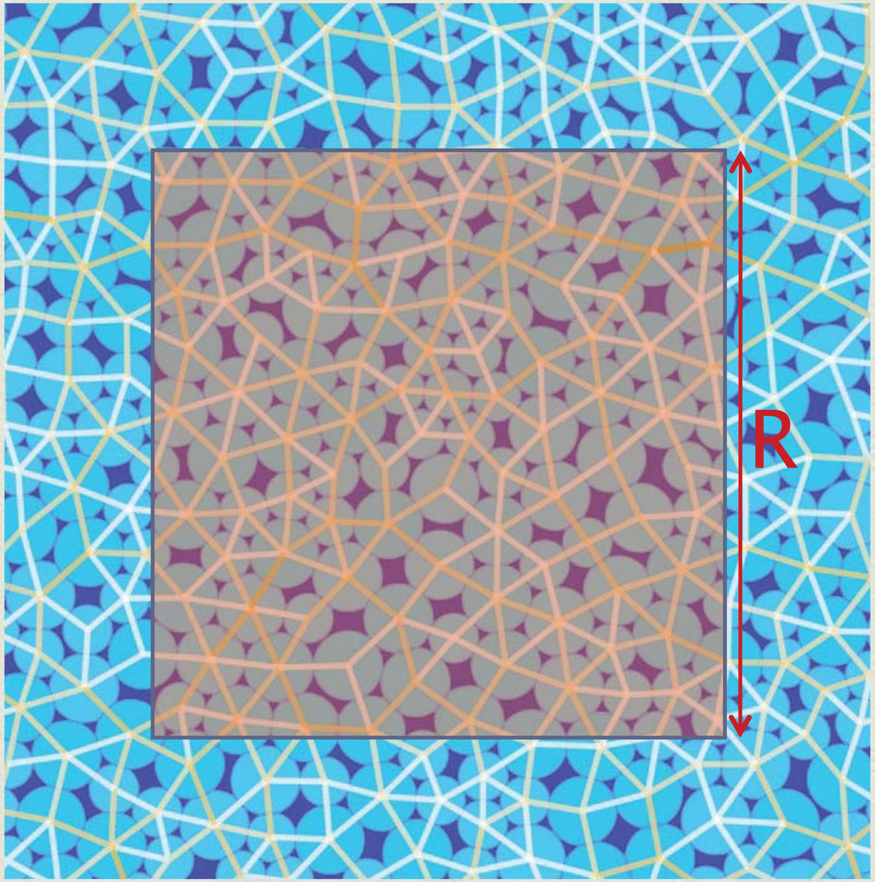




A. Cavagna et al., PRL 98 (2007) 187801,
A. Montanari and G. Semerjian, J. Stat. Phys. 125 (2006)
G. Biroli et al Nature Physics, 4, 771, (2008)

Formulation of PTS In Force Space

M. Mailman, Thesis & M. Mailman and BC JSTAT L07002, (2011)



- Generate configurations at a given compression using quench protocol
- Keep grain configuration fixed outside of B(R).
- Find another configuration in ME by only reconfiguring the interior.

Force network image originated at:http://jamming.research.yale.edu/multimedia/soft/gallery.htmlR

INDETERMINISM OF CONTACT FORCES: Force-network Ensemble (Leiden Group)

Brian P. Tighe, Jacco H. Snoeijer, Thijs J. H. Vlugt and Martin van Hecke , ***Soft Matter***, 2010, **6**, 2908-2917

- Soft Spheres (M in d dimensions, z contacts/ grain):
  - dM constraints from mechanical equilibrium (ME).

$$\sum_{j \in contacts\ of\ i} \left|\vec{f}_{ij}\right| \frac{\vec{r}_{ij}}{\left|\vec{r}_{ij}\right|} = 0$$

  - Mz/2 equations associated with contact forces.

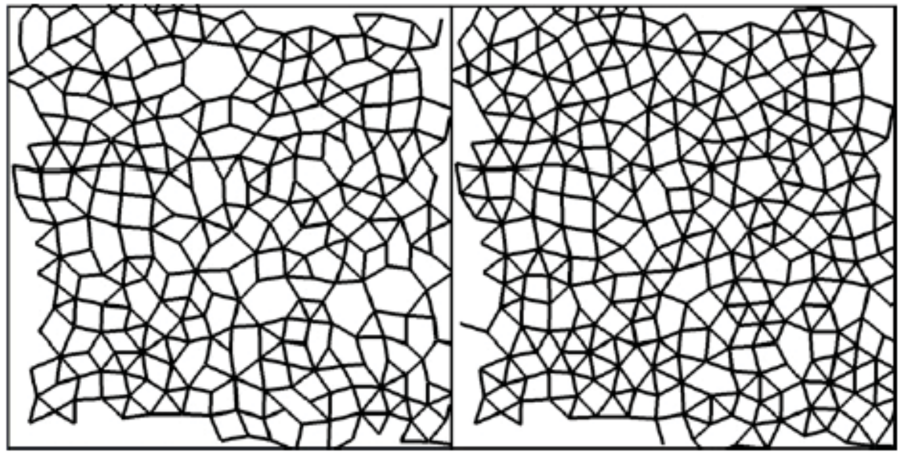
$$\vec{f}_{ij} = \vec{f}_{ij}\left(\vec{r}_i, \vec{r}_j; d_i, d_j\right)$$

Force magnitude decouples from deformations if grains are hard enough.

  - Force magnitudes are still constrained by the ME equations : Linear problem characterized by a geometry matrix, A

Constructing force-networks

- Construct overcompressed packings of soft spheres using the O'Hern protocol (Packings are different from elastic network)
- Obtain the geometry matrix A, and the stress tensor
- Create multiple force networks on this geometry, keeping the same stress tensor



$$A\hat{g} = 0$$

Random walk with reflecting boundary conditions in null space of matrix A

$$\vec{f} = \vec{f}(P_0) + \sum_{i=1}^{\delta z} c_i \hat{g}_i$$

BOUNDARY CONDITIONS AND THE CONSTRUCTION OF PTS

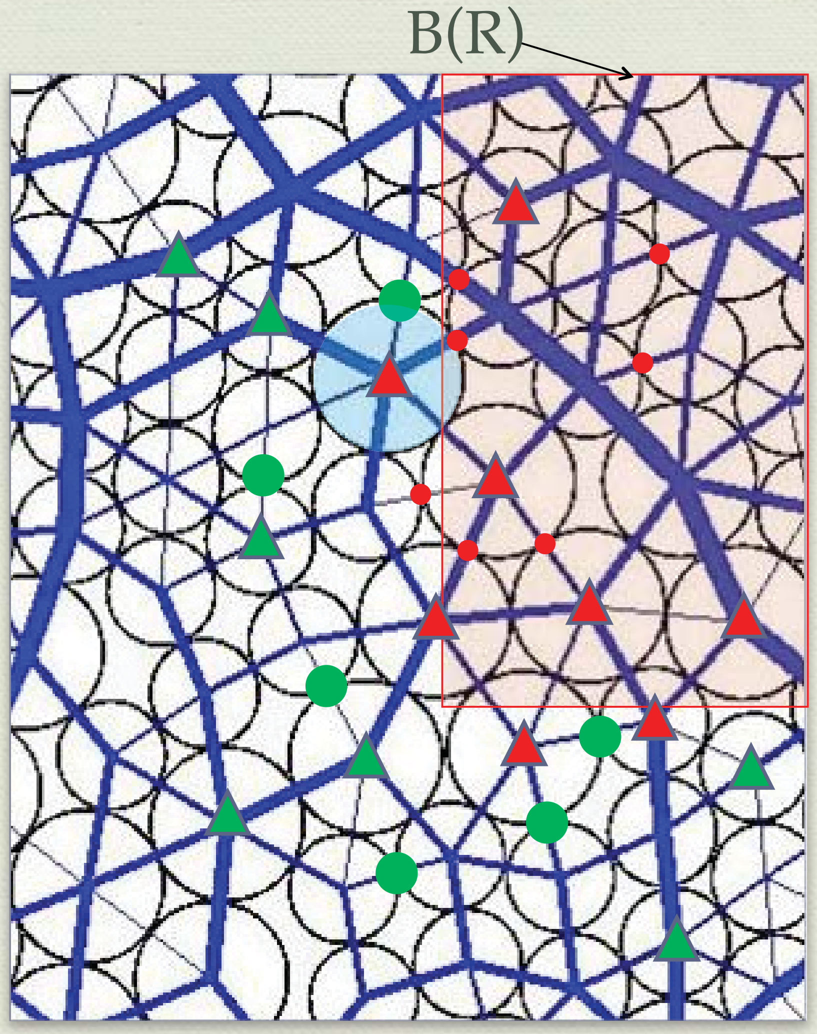
- Begin with static packing and $\vec{f}_0$
- PTS is the overlap with an equivalent force network
- Freeze force variables outside of boundary B(R): $C(R) = \hat{f}_0 \cdot \hat{f}(R)$

Grains contribute 2 ME constraints.

No additional constraints.

Fluctuating DOF.

Frozen DOF.

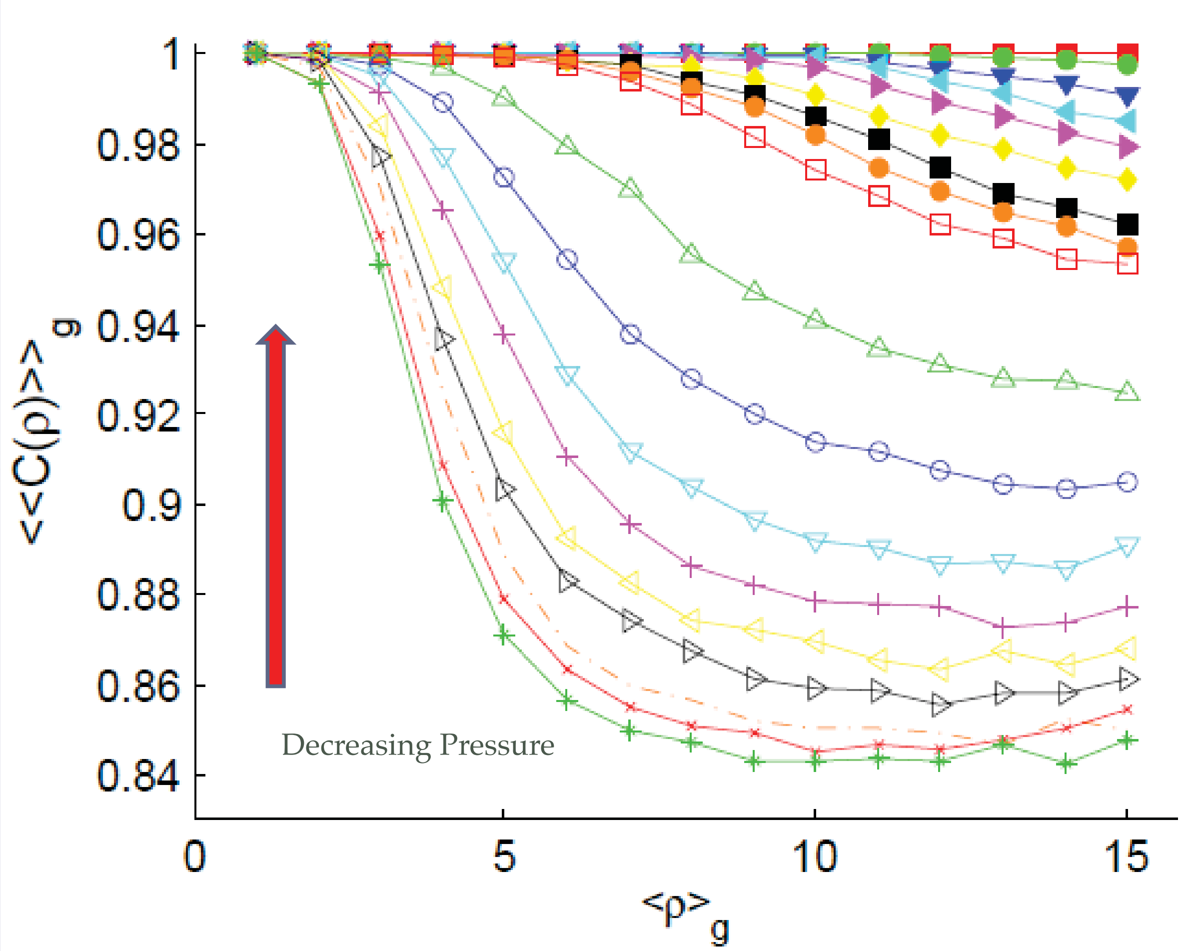


RESULTS FOR PTS

- 900 grains, 2D, bidisperse.
- Packing fraction from 10^{-3} to 10^{-1}.
- 40 packing geometries.

$\rho = R/D$

Scaled Box size

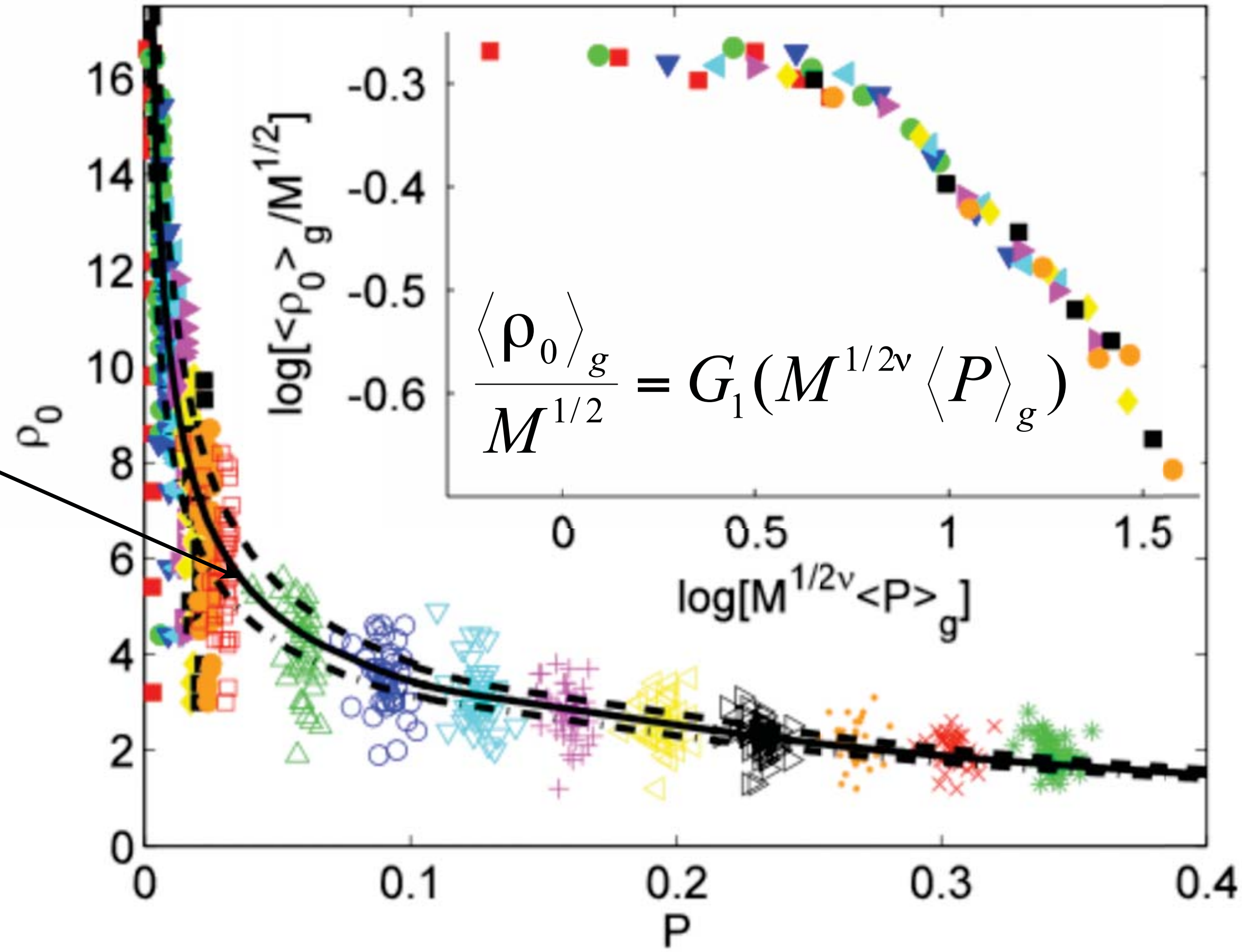


FINITE SIZE SCALING

Fit:

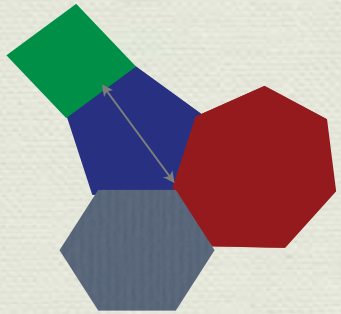
$\nu = 0.46 \pm 0.01$

Wyart argument



Summary so far

- PTS correlation length in force space measures how far boundary forces propagate into the interior.
- PTS exhibits a growing length scale as packings are decompressed
- Finite size scaling hints at divergence
- PTS is the natural correlation function that should capture the length scale emerging from bulk-surface arguments of Wyart-Witten



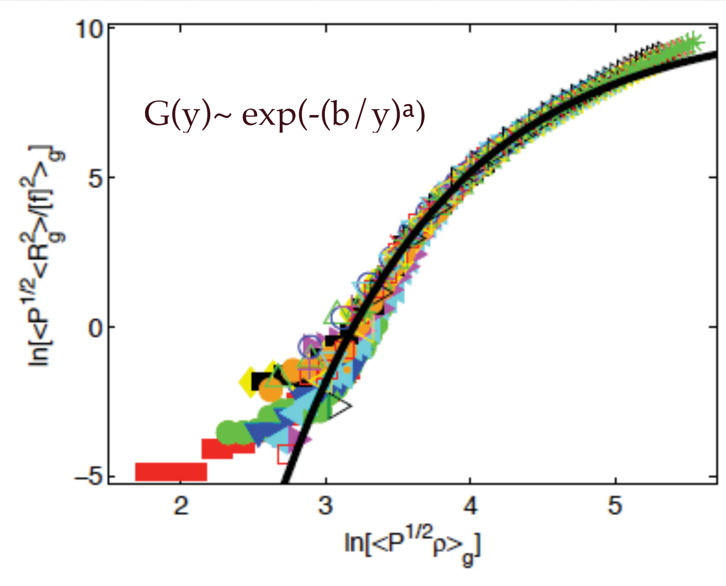
mosaic of force tiles

CONFIGURATIONAL ENTROPY

- Relation to PTS

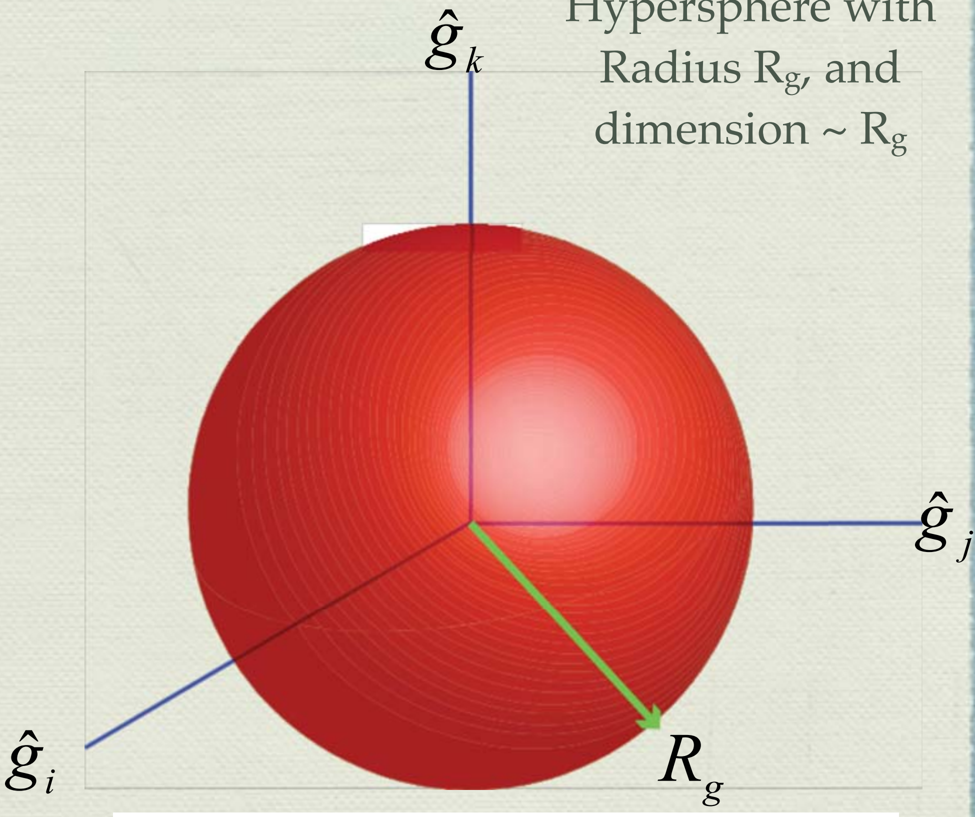
$$C(\rho) = p_{\alpha=\beta} q_1 + p_{\alpha\neq\beta} q_0$$

- Equal probability of each network is built into our sampling: $p_\alpha = \dfrac{1}{V_{\delta n}}$



Logarithmic corrections to meanfield

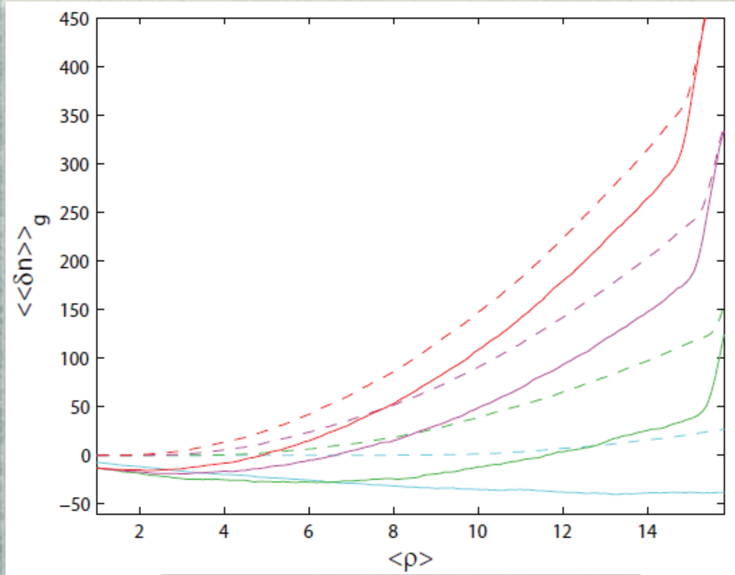
Hypersphere with Radius R_g, and dimension ~ R_g

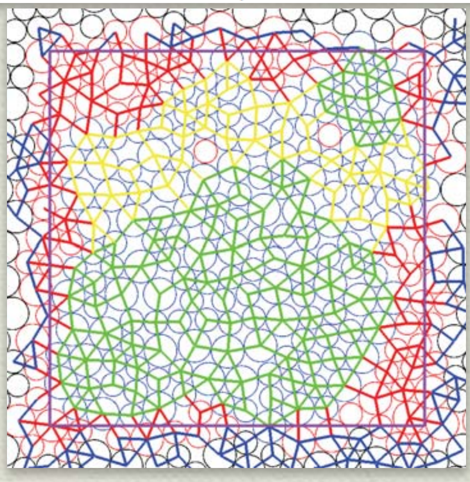


$$\langle \rho_0 \rangle_g^{-1} = \frac{\langle P \rangle_g^{1/2}}{b} \left(\ln \frac{G_0}{\eta_0} - \frac{\ln \langle P \rangle_g}{2} \right)^{1/\alpha}$$

CORRECTIONS TO MEAN FIELD

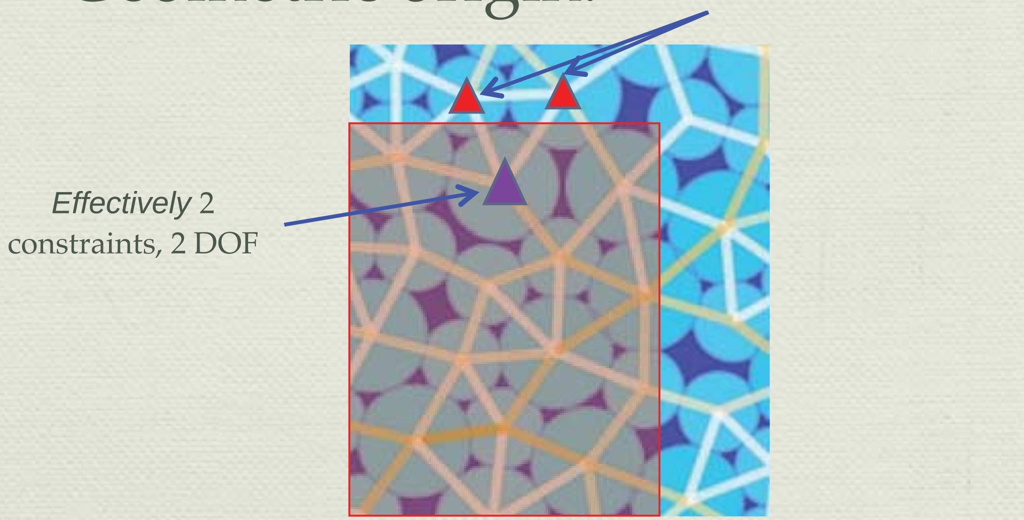
Dashed line: nullity
Solid line: counting

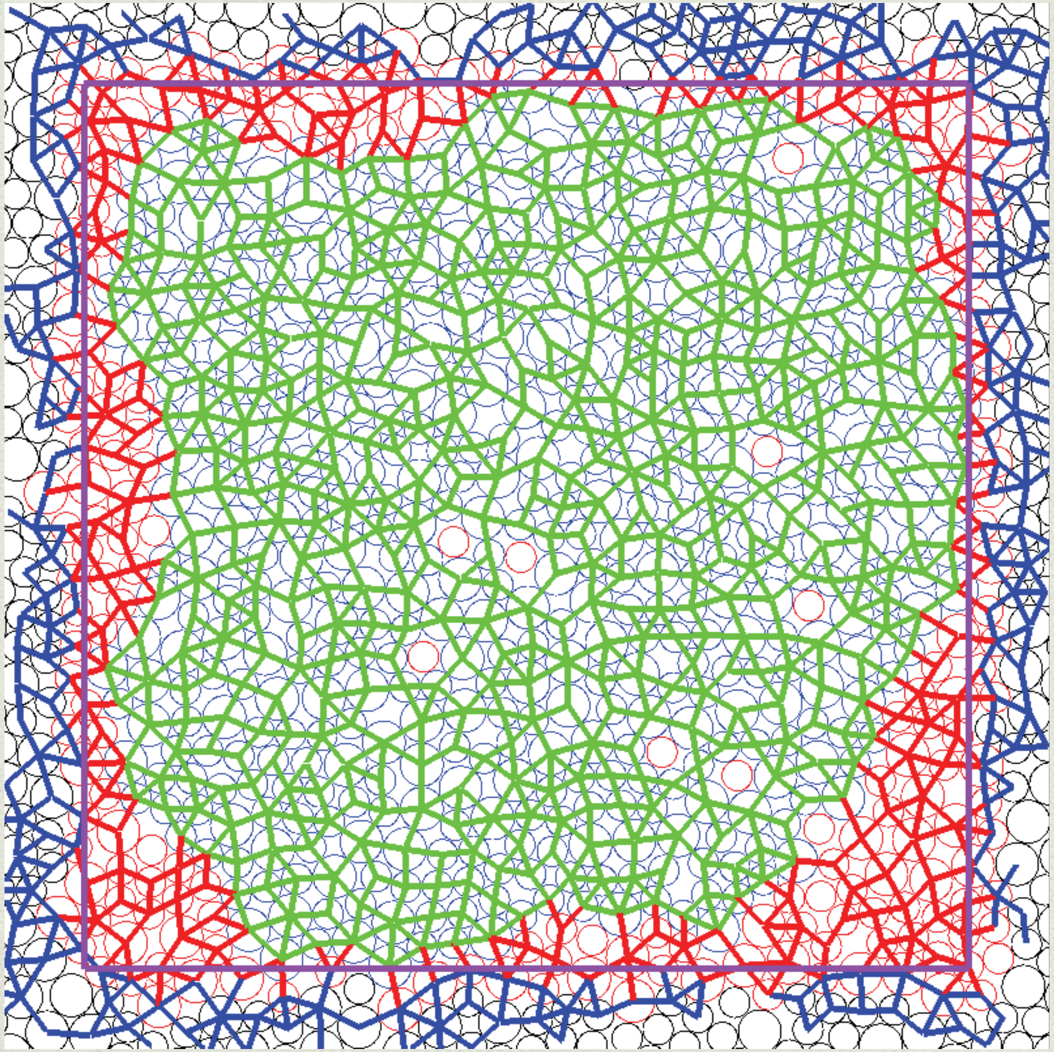




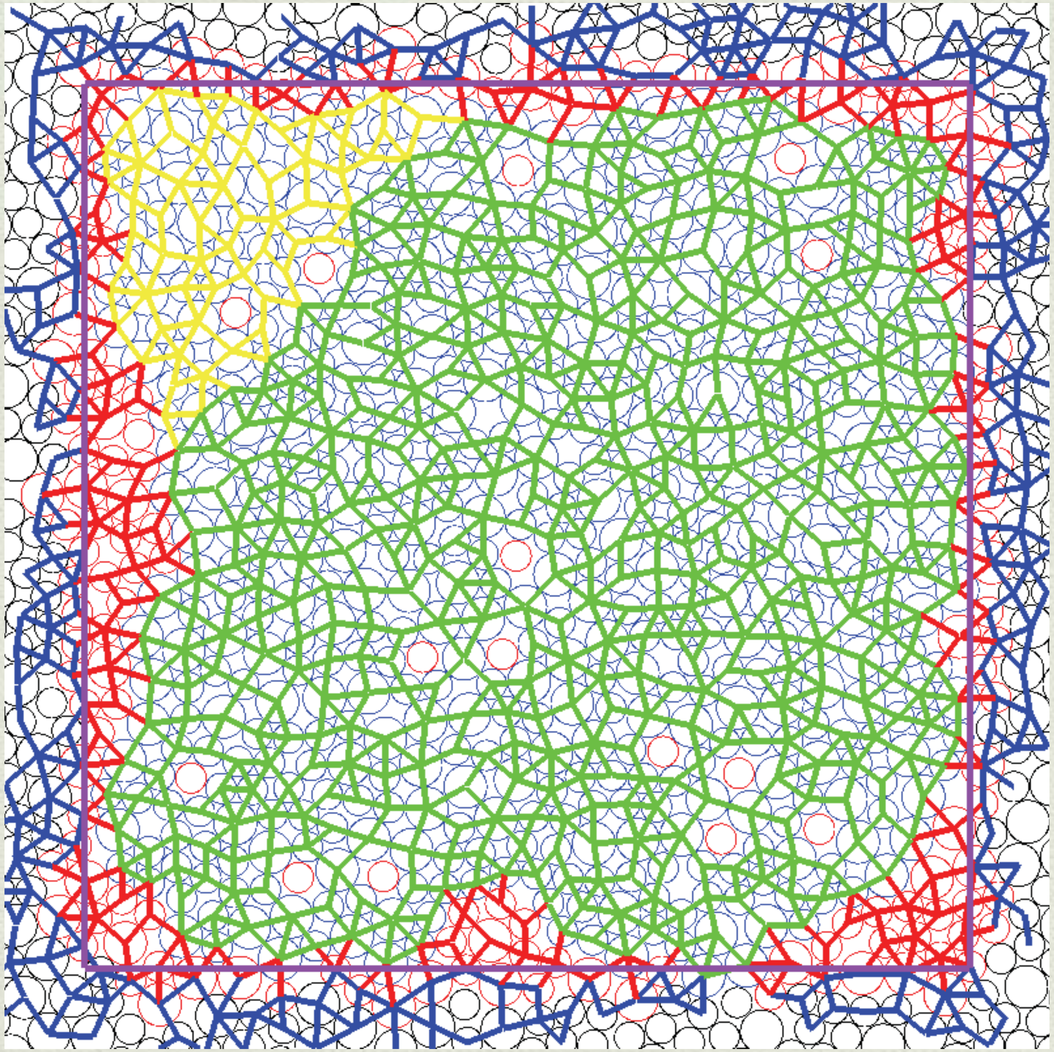
- Discrepancy between excess number of DOF and the nullity

- Geometric origin:

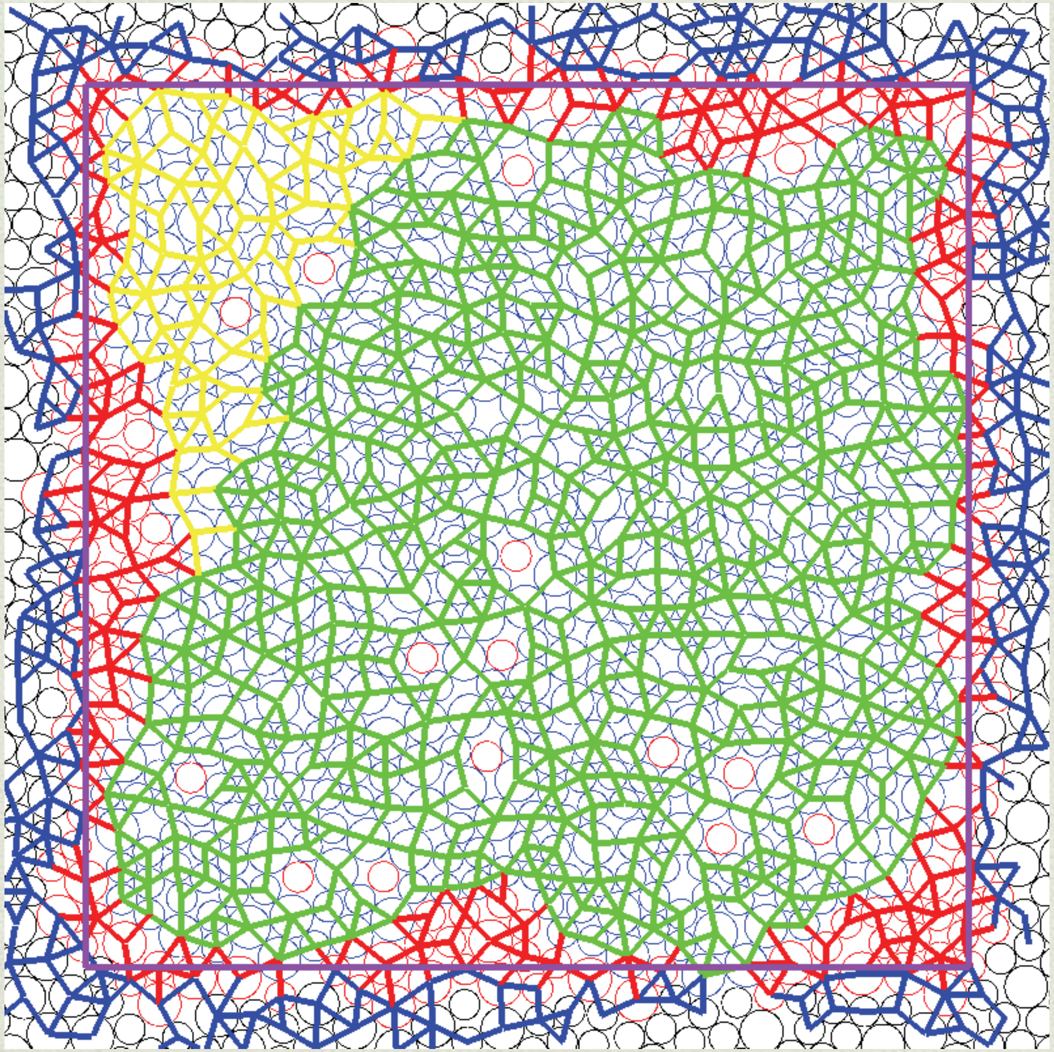




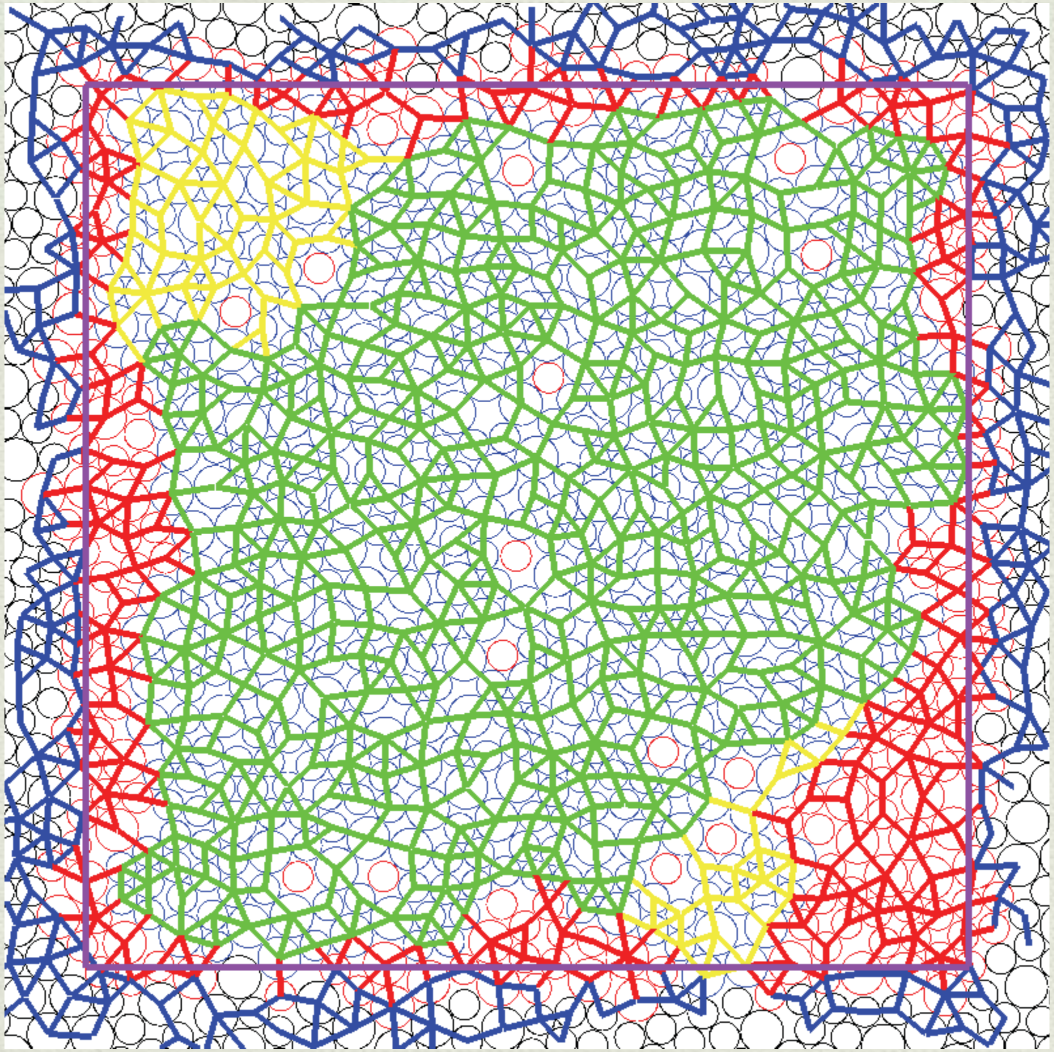
$\delta\phi = 0.007$



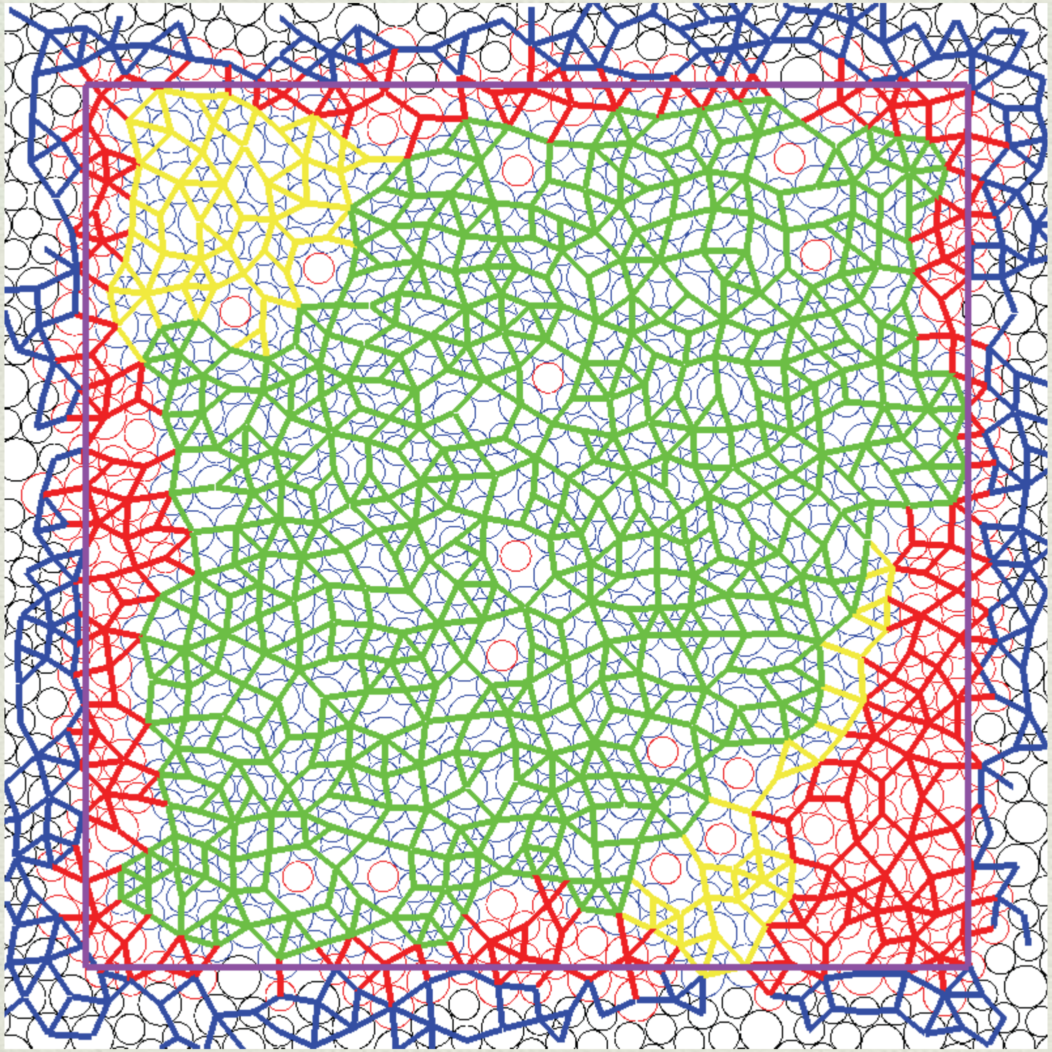
$\delta\phi = 0.006$



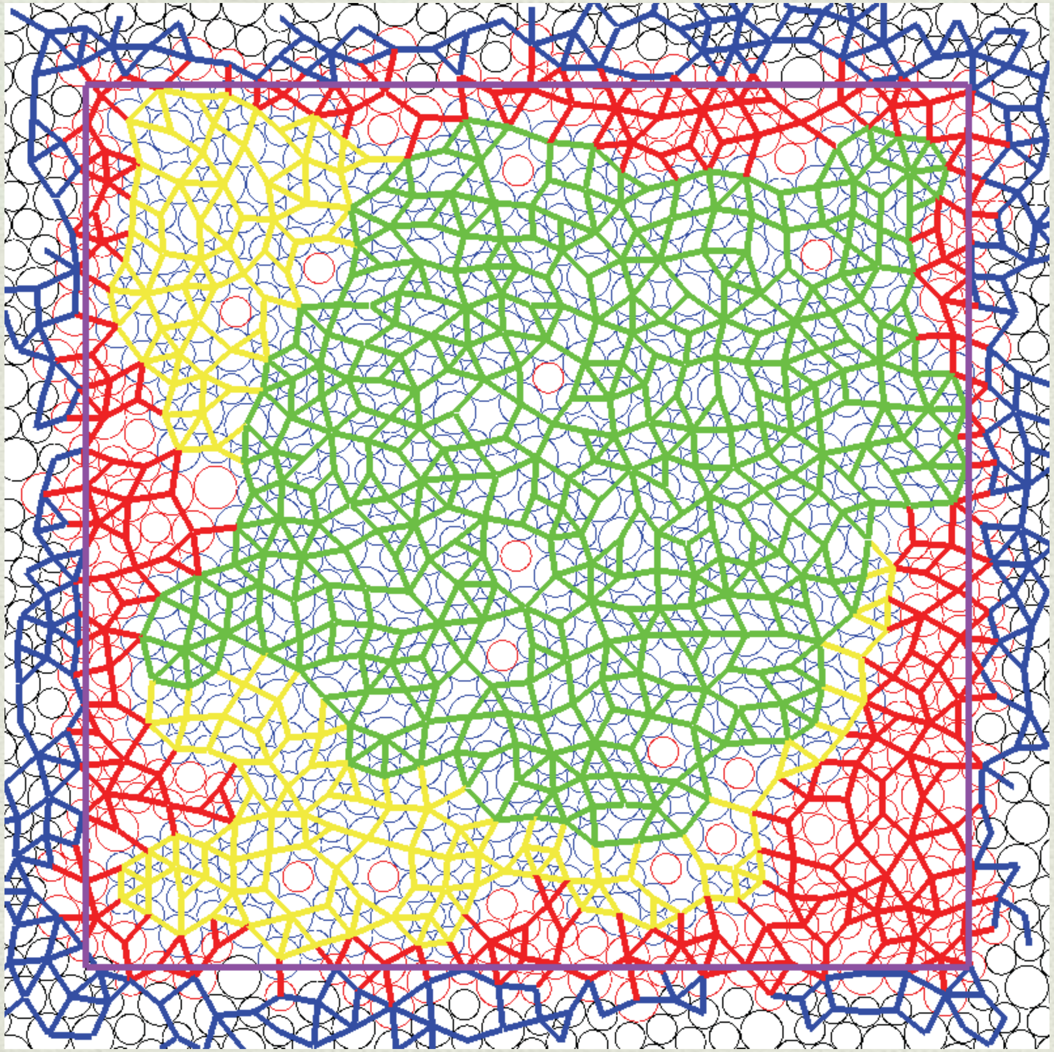
$\delta\phi = 0.005$



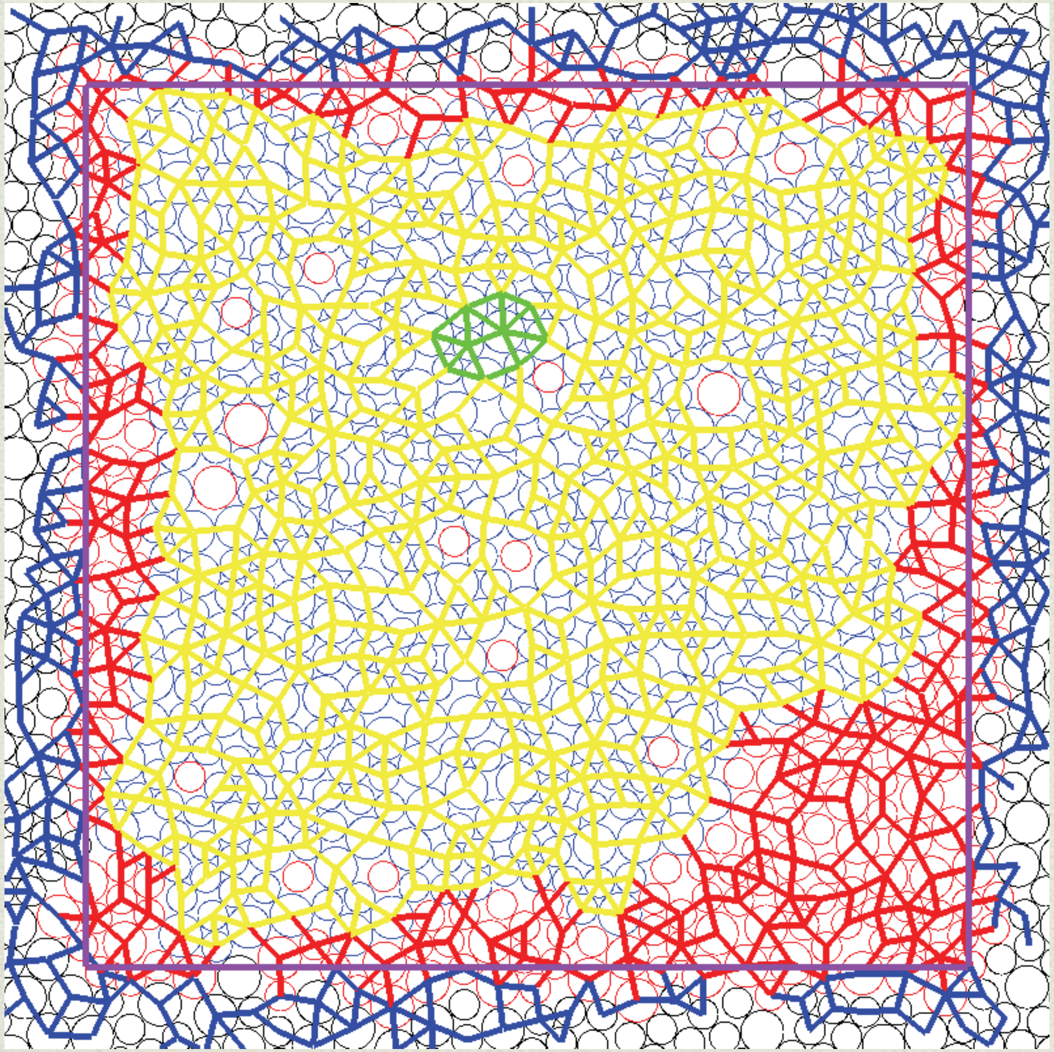
$\delta\phi = 0.004$



$\delta\phi = 0.003$



$\delta\phi = 0.002$



$\delta\phi = 0.001$

Questions and Future Work

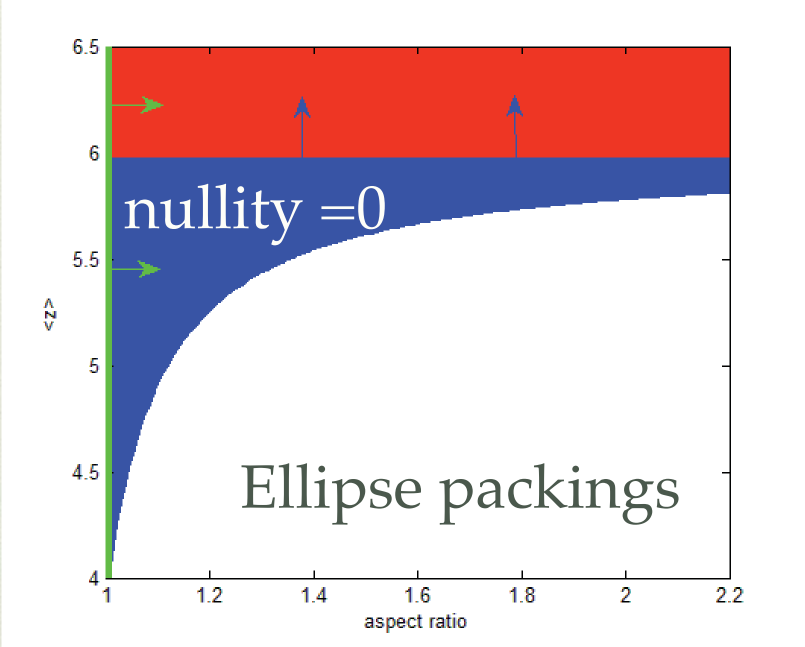
◆Are the corrections to mean-field only relevant for one-sided spring networks?

◆Stress fluctuations close to jamming, related to mesoscopic regions that fluctuate ?

◆Relation to response, dynamical heterogeneities?

◆Can the PTS length scale be measured experimentally?

◆Anisotropic grains ? Hypostatic packings



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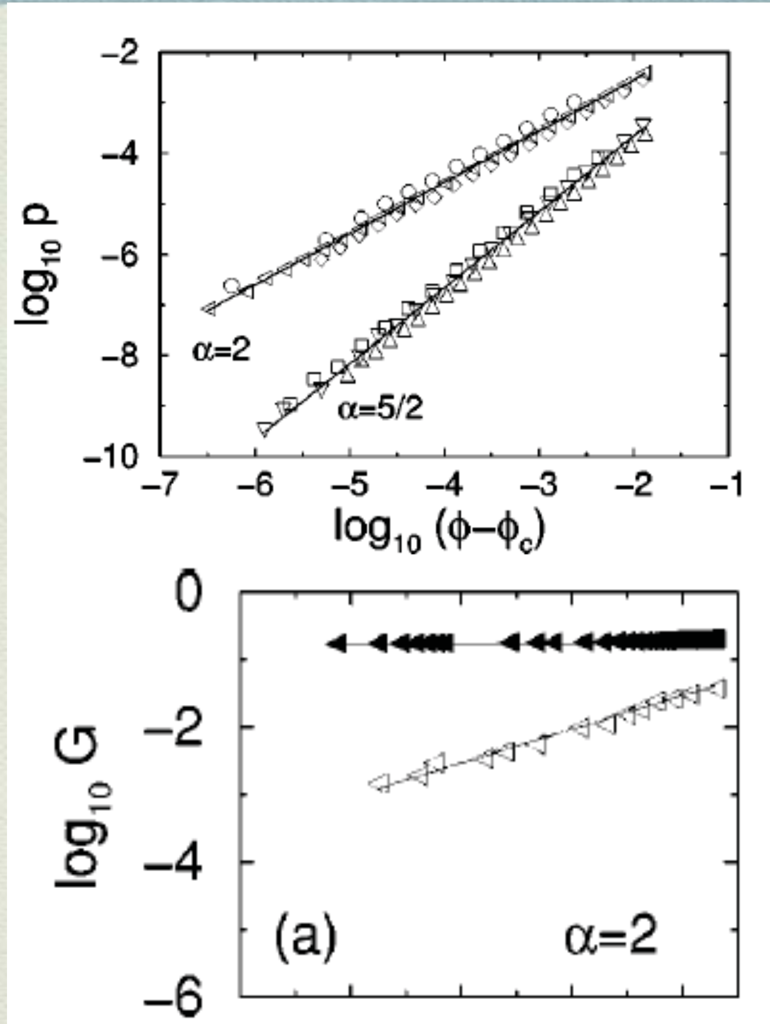
F. Krzakala

Funding: NSF

Nature of Jamming/Unjamming Transition

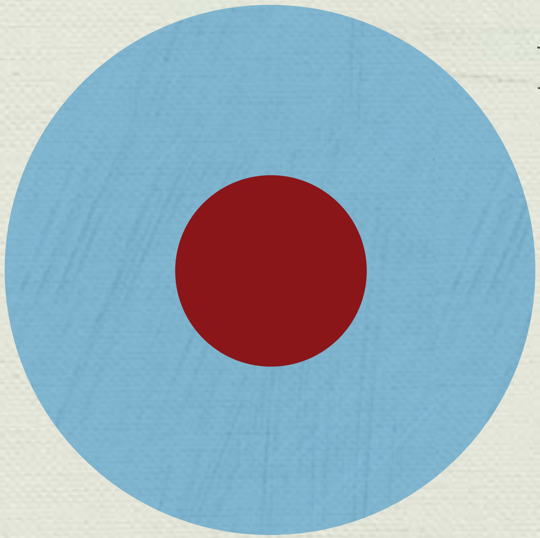
Signatures of a critical point

- Power law relationships
  - O'hern et al, PRE 68 (2003) 01130
- Long-ranged correlations on .
- Scaling
- Symmetry Breaking
- Possibility of First order transition



RFOT: Entropic Nucleation

$$\tau \propto \exp\left[B\left(\frac{\Delta F}{k_B T}\right)^{\psi}\right] \qquad \xi^{\theta} \approx \frac{\Delta F}{k_B T} \qquad \xi \approx \left(\frac{1}{TS_c}\right)^{\frac{1}{d-\theta}}$$



Entropy Gain: $TS_c(T)\xi^d$

Surface Tension: $\Gamma\xi^{\theta} : \theta \leq d-1$

Fragility ~ Related to Configurational Entropy

To get Vogel-Fulcher: Mosaic length scale has to diverge	Fragility is related to how strongly the mosaic length scale diverges