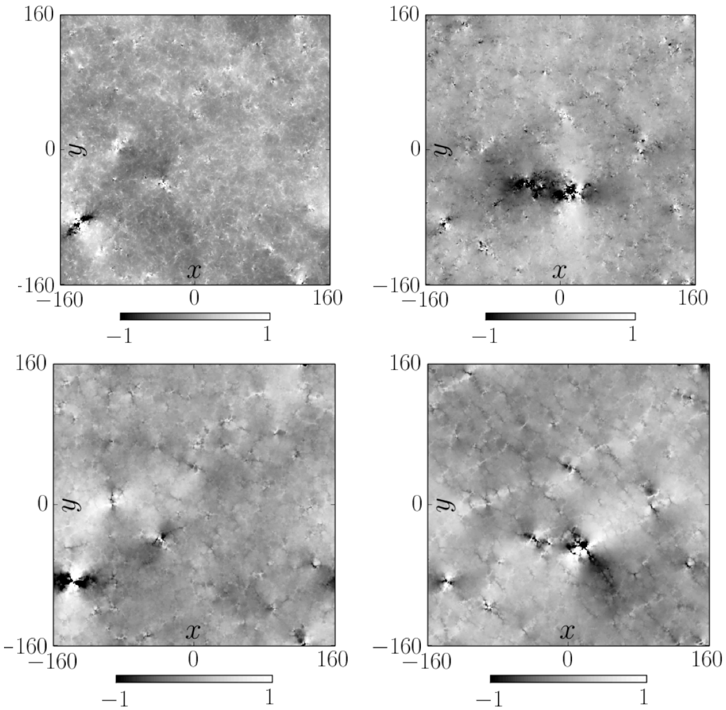
Elasticity in particle packings near jamming



- Finite shear modulus and yield stress above a critical volume fraction, ϕ_J.
- Linear response of static packings anomalous near ϕ_J beyond a lengthscale that diverges at ϕ_J.
- Different characteristic lengths control longitudinal and transverse components of the point response.
- Rigid shear: Modulus dependent on scale
- Free shear: Surprisingly invariant with respect to jamming.

KITP Program Seminar.

November 2014

Northeastern University

Craig Maloney
Soft and Nanoscale Mechanics

Acknowledgements

- Arka Roy
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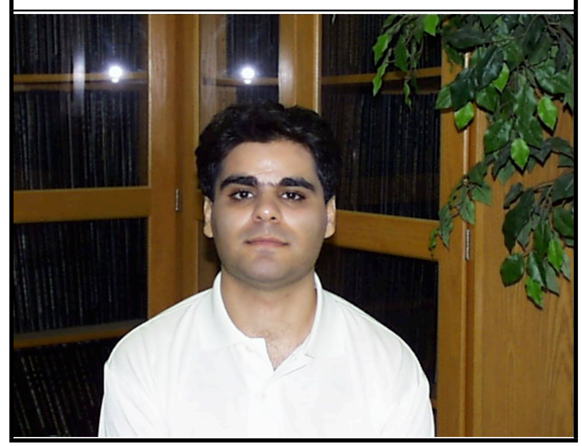
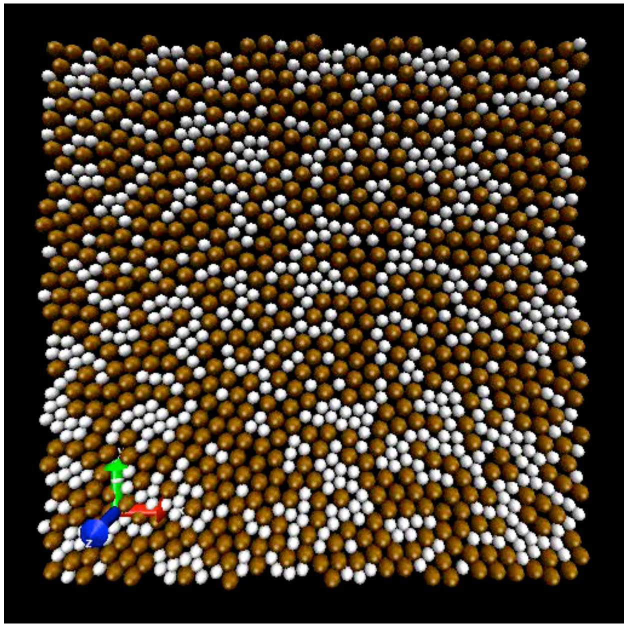


Outline

- Background and overview
  - Soft particle suspensions
  - Jamming and random close packing
  - Elasticity: Development of shear modulus
  - Plasticity: Development of yield stress
  - Simple models

- Elasticity
  - Scaling laws, (criticality?) and emergent lengthscales
  - Point response
  - Constrained homogeneous deformation
  - Unconstrained homogeneous deformation

- Plasticity:
  - Shear transformations, slip avalanches, and diffusion
  - Short-time intermittency
  - Long time diffusion
  - Plastic strain correlations



Soft glasses

- Particles suspended in liquids can behave like glasses or other conventional amorphous solids.

- Particles can be:
  - solid like in a paste
  - liquid like in an emulsion
  - air like in a foam or mousse

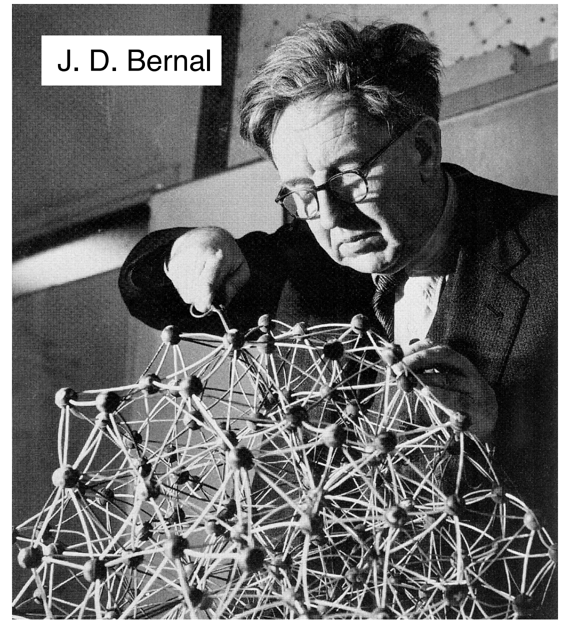
- Technological applications:
  - Device fabrication/assembly
  - Oil / Gas drilling/production
  - Food / personal care
  - Bio-related

- This work:
  - Athermal
  - Deformable
  - Jammed

Jamming: random close packing

A brief history of jamming:

- Key quantities: volume fraction, φ; contact #, z.
- Jamming: “Random close packing version 2.0”
- JD Bernal (1960): spheres “pack randomly” at φ~0.64, z~6.
- Donev et. al. (2004): M&M’s do better. φ~0.71 z~10.
- Maxwell constraint counting (frictionless spheres):
  - dN translational DOFs
  - there are zN/2 contacts in the system
  - z/2>d is a necessary condition for rigidity



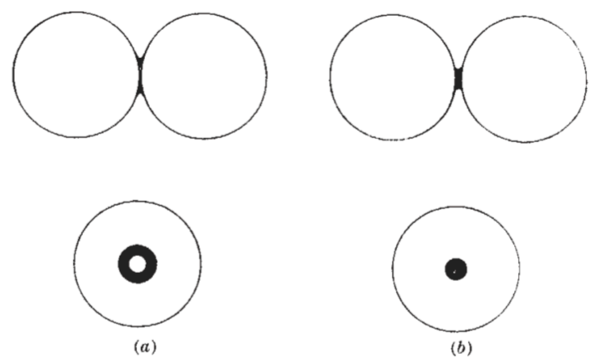


Fig. 4. Diagram of method of marking (a) close and (b) near contacts between spheres. The areas of adherent black paint are marked

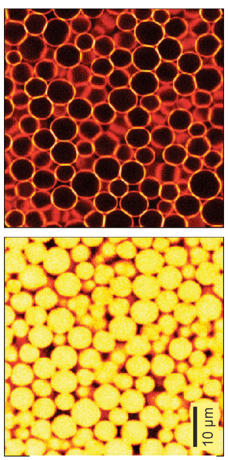
Jamming: development of a static shear modulus

- Mason et. al. Phys. Rev. Lett. 1995.
- Monodisperse oil-in-water emulsion
- Viscosity vs. concentration
- Shear modulus jumps by 4 orders of magnitude at ϕ_{rcp}
- Analagous to rigidity percolation?

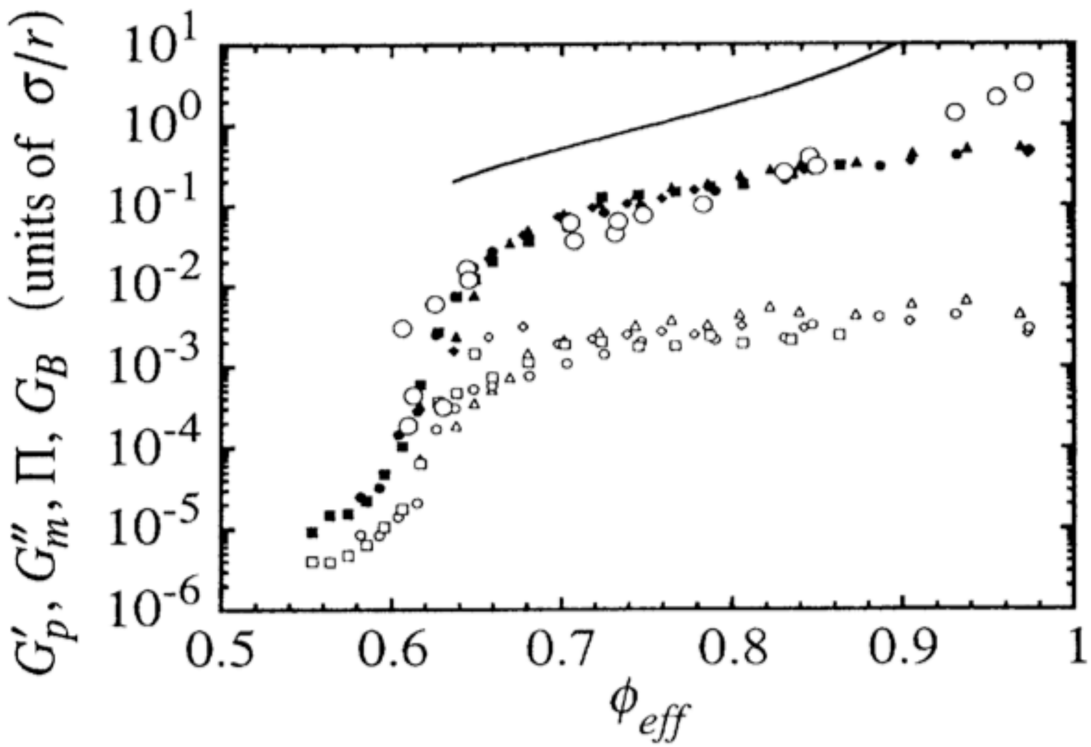
10 PHYSICAL REVIEW LETTERS

Elasticity of Compressed Emulsions

T. G. Mason,[1,2] J. Bibette,[3] and D. A. Weitz[1]

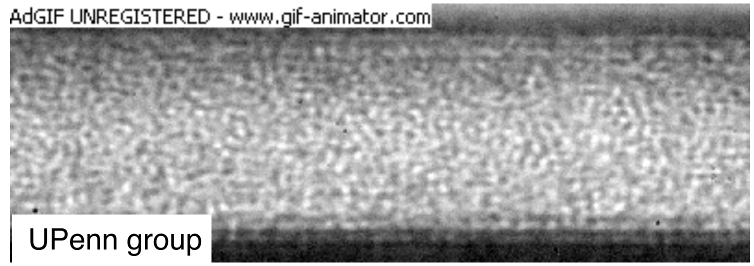


Blair lab. Georgetown



Jamming: development of yield stress

- Nordstrom et. al. Phys. Rev. Lett. 2010.
- μ-gel suspension
- $\phi > \phi_{rcp}$: yield stress
- $\phi < \phi_{rcp}$: viscous fluid



B.R. Saunders, B. Vincent Adv. Colloid Interface Sci. 80 (1999) 1–25 5

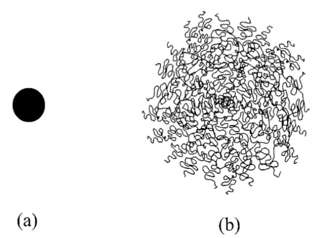
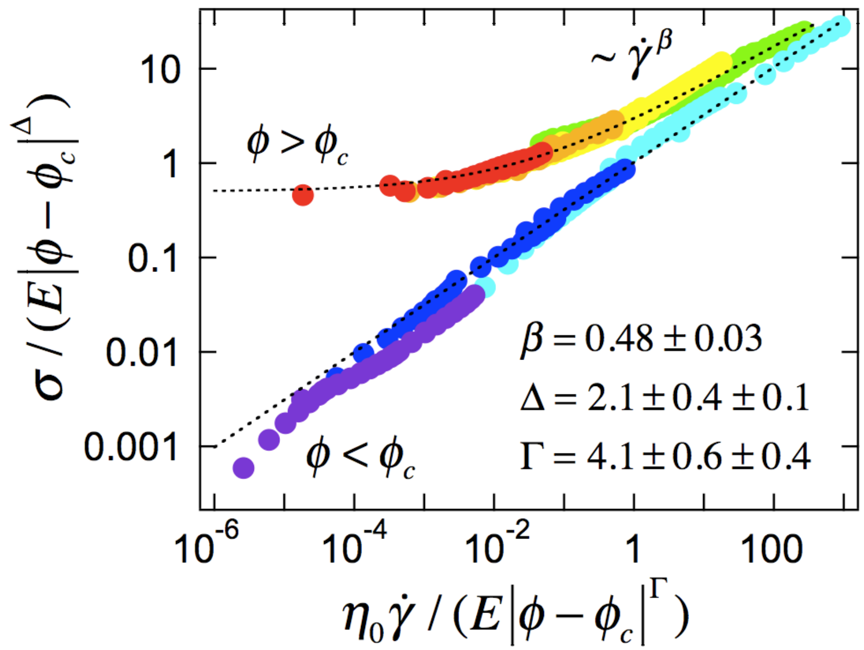
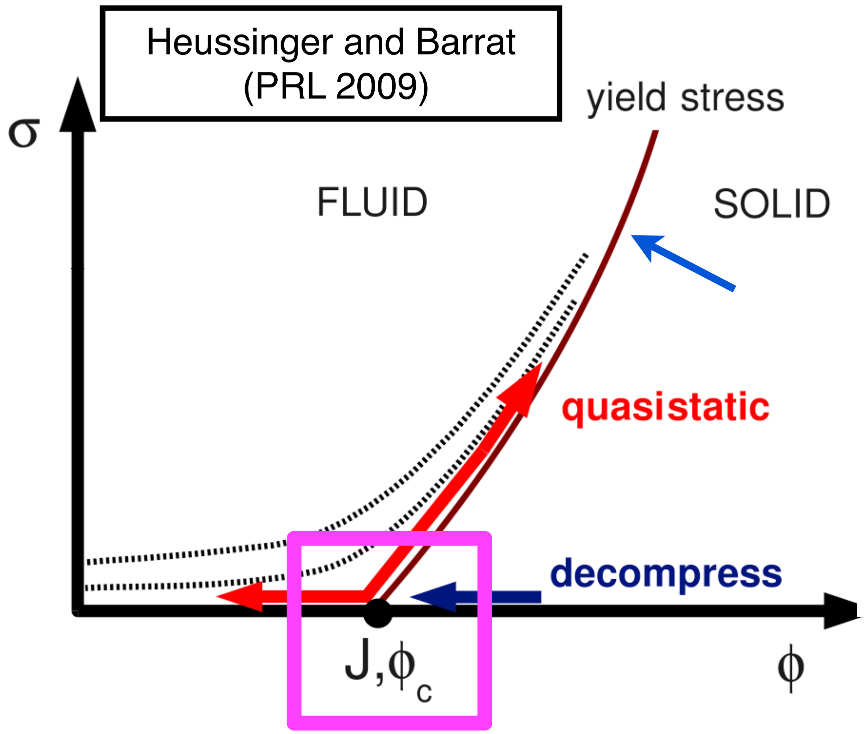
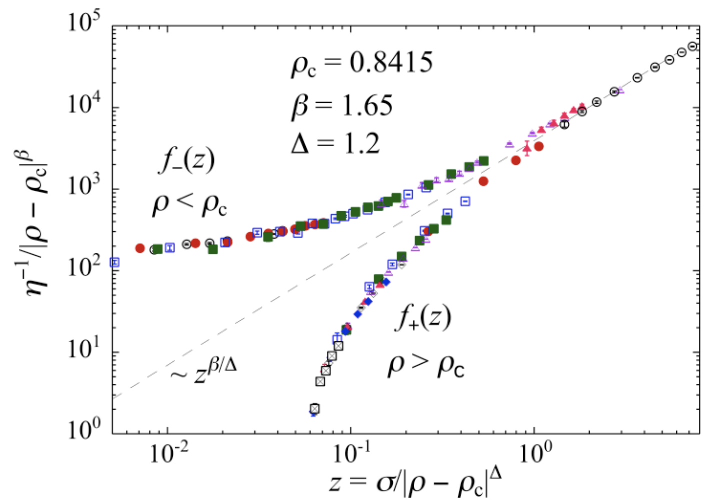


Fig. 2. Diagram depicting a microgel particle in a poor (a, $\chi_{12} > 0.5$) and good (b, χ_{12} 0) solvent, respectively.



Jamming: critical scaling at φc



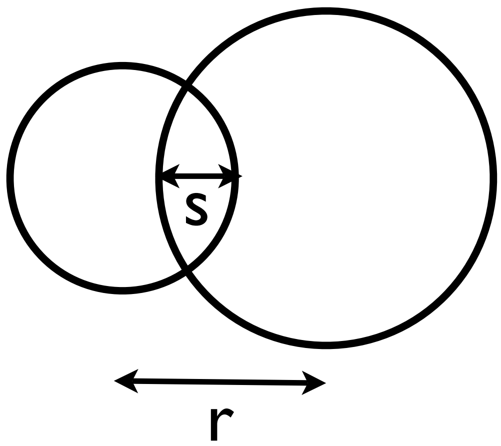


•Olsson and Teitel PRL 2008

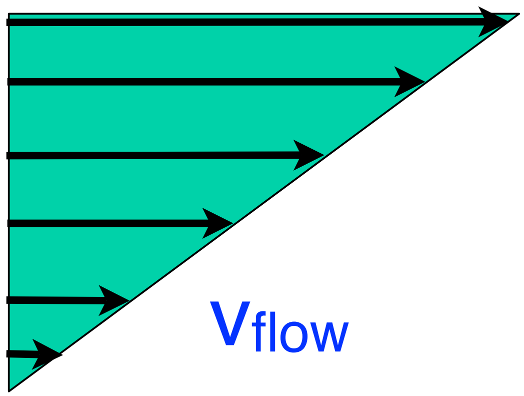
- φ,σ rheology scaling near "point J"
- Olsson and Teitel (bubbles), Hatano (grains)...

•Depinning-like transition (dynamical criticality) at yield surface: (CEM and Robbins -- Vandembroucq et. al.)

Bubble model (Durian)



- 50:50 bidisperse
- $R_{Small} = 1.4\ R_{Big}$



- Repulsion, F_{rep}, linear in overlap, s:
  - $F_{rep}=ks$
  - (could be arbitrary power of s)
- Drag, F_{drag}, w/r/t imposed flow:
  - $F_{drag}=b\ (v_{bubble}-v_{flow})$
- For (massless) bubbles, $F_{rep}=F_{drag}$
  - $v_{bubble}=F_{rep}/b + v_{flow}$
- Single timescale: $\tau_D=bR^4/k$
- Dimensionless shearing rate:
  - $De=(d\gamma/dt)\ \tau_D$
    (Deborah number)

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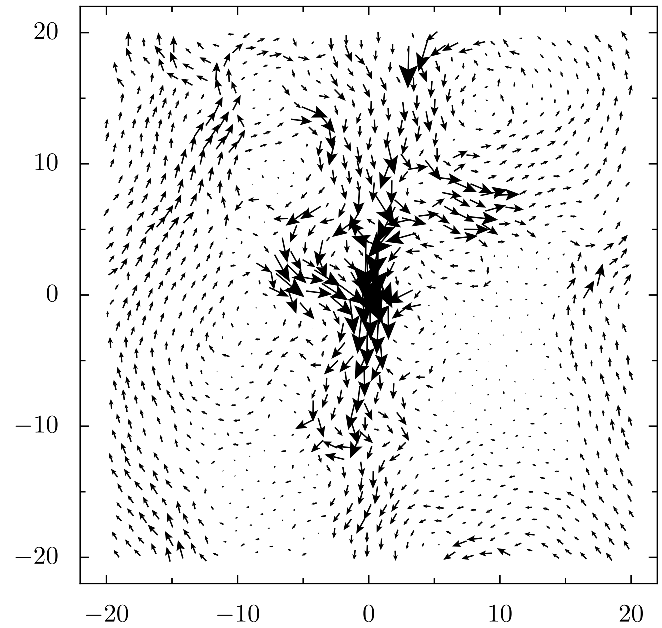
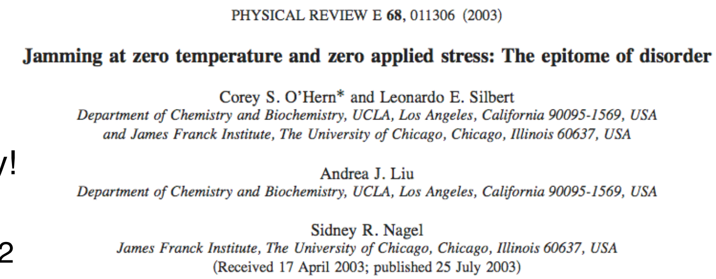


Elasticity near jamming: z, P, K, G

- $F = s^{\alpha}$; Harmonic: $\alpha=1$; Hertz: $\alpha=3/2$
- Previous results from simple models:
  - Excess contacts: $\Delta z = z - z_{Maxwell} \sim \Delta\phi^{1/2}$
    - Independent of force law, dimension, and polydispersity!
    - Related to Bernal's "almost-contacts"
  - Pressure, $P \sim \Delta\phi^{\alpha} \sim \langle s\rangle^{\alpha}$ e.g. Harm: $P \sim \Delta\phi \sim \Delta z^2$
    - Naive expectation
    - Implies compression modulus: K
    - $K = \delta P/\delta \ln V \sim \delta P/\delta\phi \sim \Delta\phi^{\alpha-1} \sim \langle s\rangle^{\alpha-1}$
  - Shear modulus, $G \sim \Delta\phi^{\alpha-3/2} \sim \langle s\rangle^{\alpha-3/2}$
    - So $G/K \sim \Delta z \sim \Delta\phi^{1/2}$
    - Particle packings are incompressible at jamming!


PHYSICAL REVIEW E **68**, 011306 (2003)

Jamming at zero temperature and zero applied stress: The epitome of disorder

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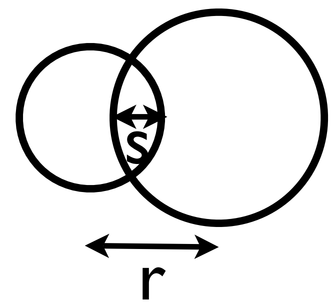
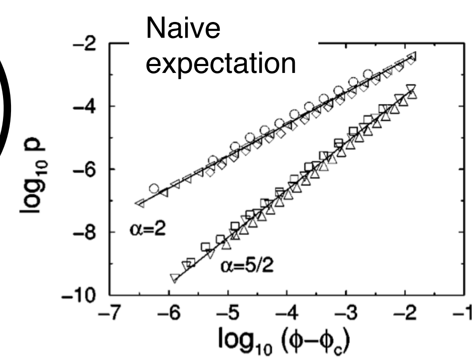
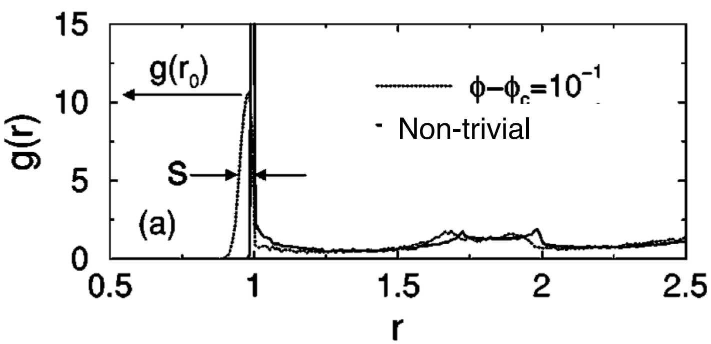
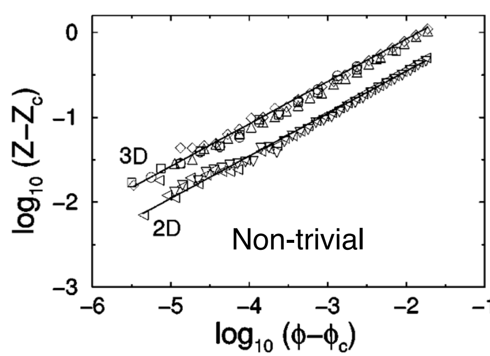
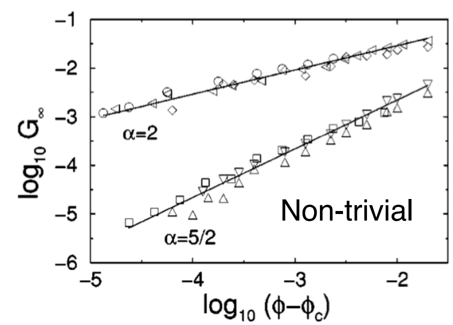










Diverging lengthscales and criticality at Φ_J

- ϕ_J critical point? Analogy to rigidity percolation? Diverging lengthscale?

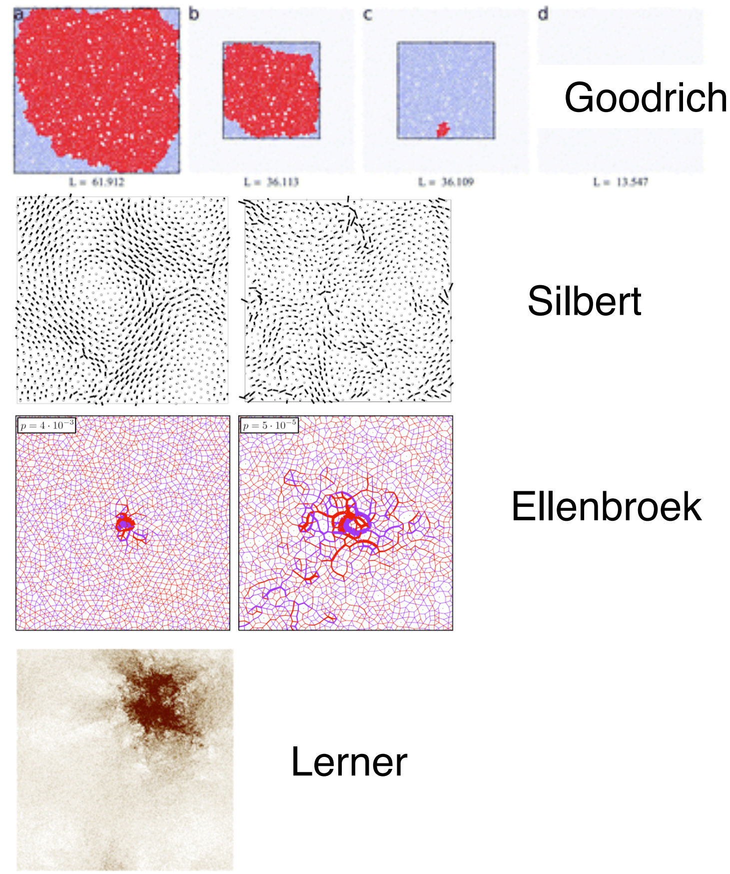
- Goodrich et. al. (Soft Matter 2014): rigidity length $l^* \sim 1/\Delta z \sim \delta\phi^{-1/2}$.
  - $O(L^d \Delta z)$ excess geometrical constraints
  - Free surface: release $O(L^{d-1})$ of them
  - For some $l^* \sim \Delta z^{-1}$, $L < l^*$ underconstrained

- Silbert et. al. (PRL 2005): dynamical structure factor at ω^*. $\xi_T \sim \delta\phi^{-1/4}$

- Ellenbroek et. al. (PRE 2009): longitudinal force fluctuations in response to local dilation. $l^* \sim \delta\phi^{-1/2}$

- Lerner et. al. (Soft Matter 2014): single bond extension $\xi_T \sim \delta\phi^{-1/4}$

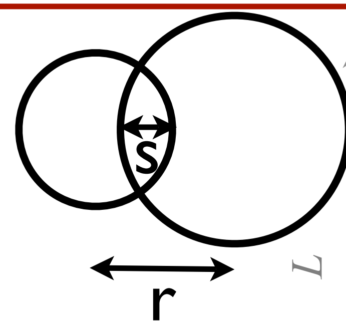
- Our goal: measure **both lengths** in a single, simple, **experimentally realizable** procedure

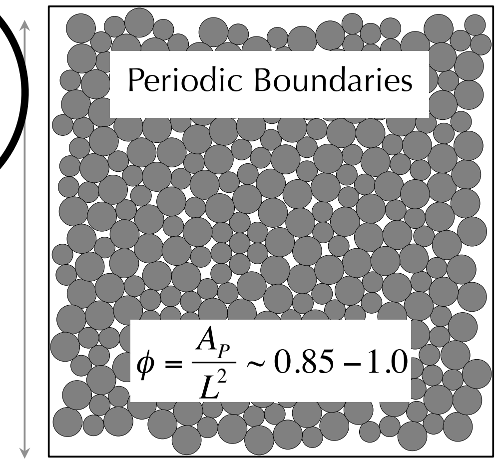


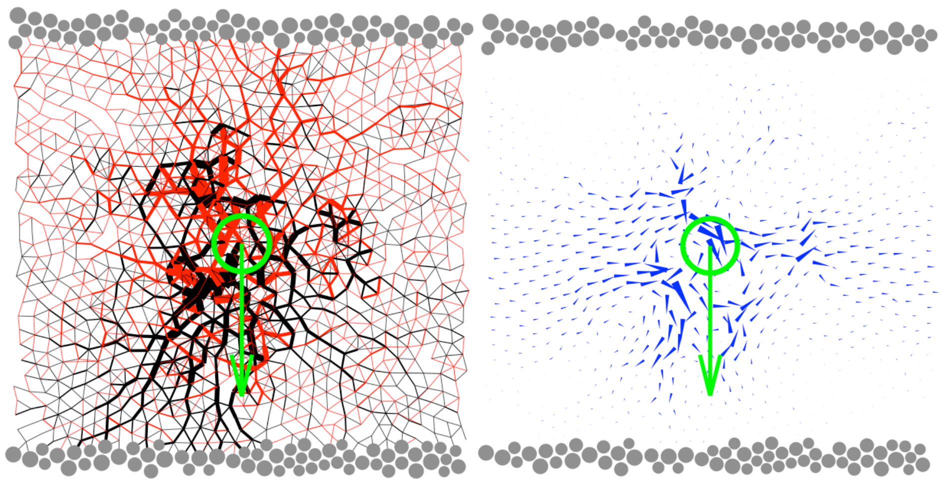
Measurement 1: Point response

$$(\lambda + G)\nabla(\nabla.\mathbf{u}) + G\nabla^2\mathbf{u} = 0$$

- Standard model and prep. protocol
- harmonic, 50:50, R_{big}=1.4R_{small}
- Infinitesimal point load on single particle
- (Slight difference with both Ellenbroek et. al. and Lerner et. al.)





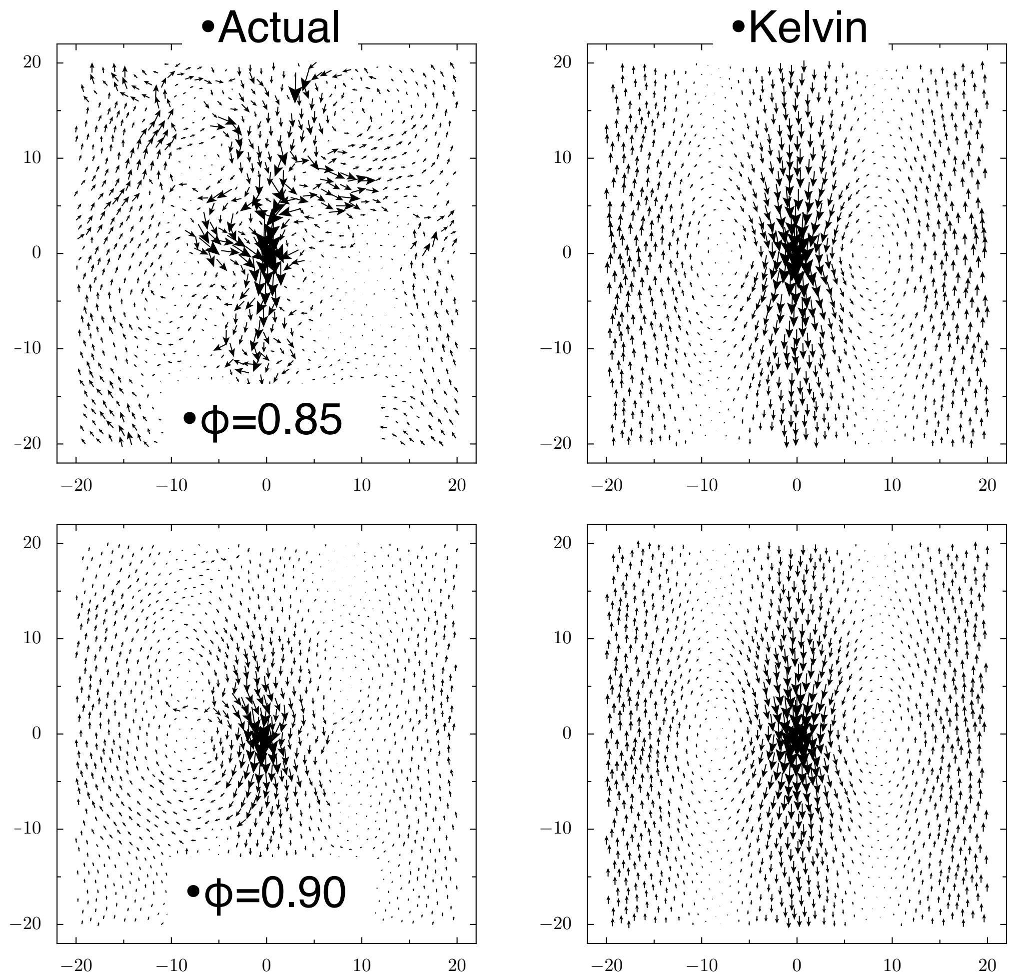


- Motivation: Leonforte et. al. PRB 2004 (Lennard-Jones)

Measurement 1: Point response

$$(\lambda + G)\nabla(\nabla.\mathbf{u}) + G\nabla^2\mathbf{u} = 0$$

- Elasticity: Lame'-Navier equation.
- Singular solution: Kelvin
- Lame' coefficients, G (shear modulus) and λ determined by homogeneous loading of large system with PBCs.
- "Continuum" solution computed at particles using Debye-like cutoff and linear dispersion ($\omega^2 \sim k^2$)
- Slight dependence on Poisson ratio.
- **Point response becomes less and less Kelvin-like near ϕ_J**



Measurement 1: Point response

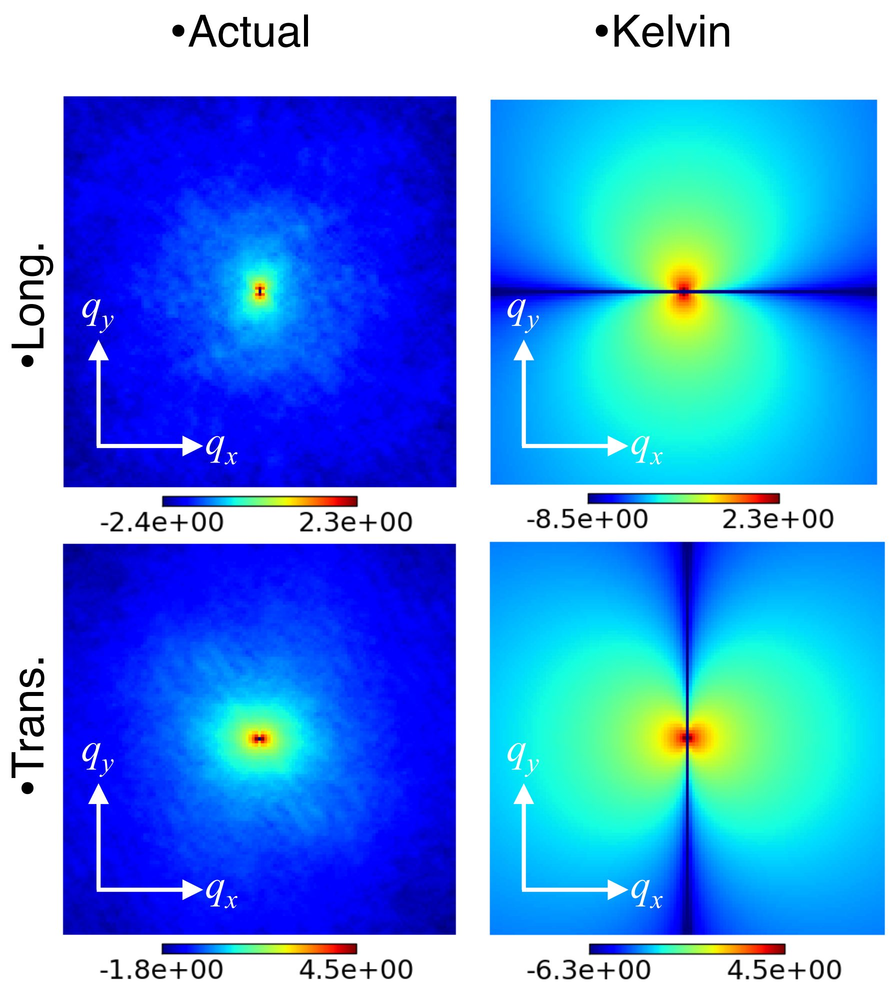
$$(\lambda + G)\nabla(\nabla.\mathbf{u}) + G\nabla^2\mathbf{u} = 0$$

- Averaged power spectrum at ϕ=0.85
- Look at Longitudinal and Transverse contribution separately.
- Kelvin:

$$u_L(\mathrm{q}) = \frac{\sin(\theta)}{(K+G)q^2}$$

$$u_T(\mathrm{q}) = \frac{\cos(\theta)}{Gq^2}$$

- Note: u_L should be zero along θ=0 and u_T should be zero along θ=π/2.



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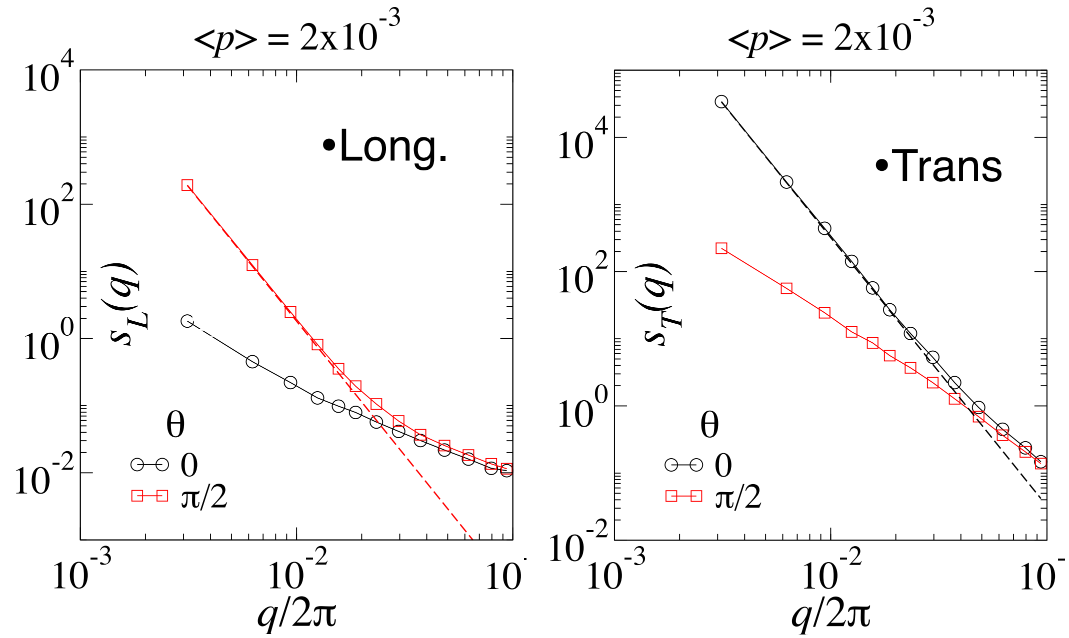
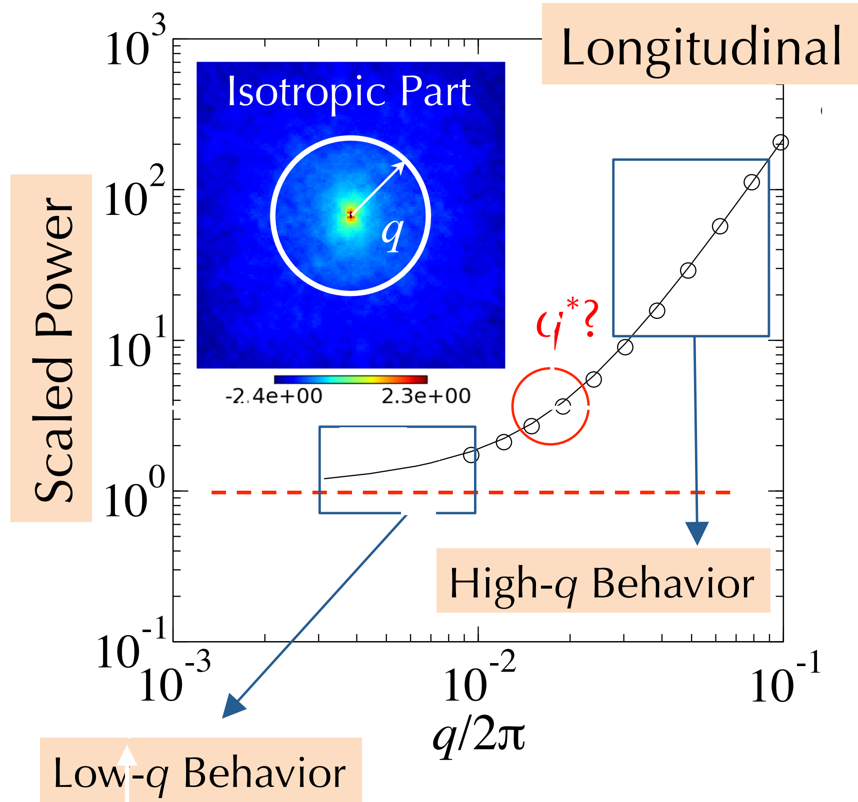


- Note: u_L should be zero along θ=0 and u_T should be zero along θ=π/2.

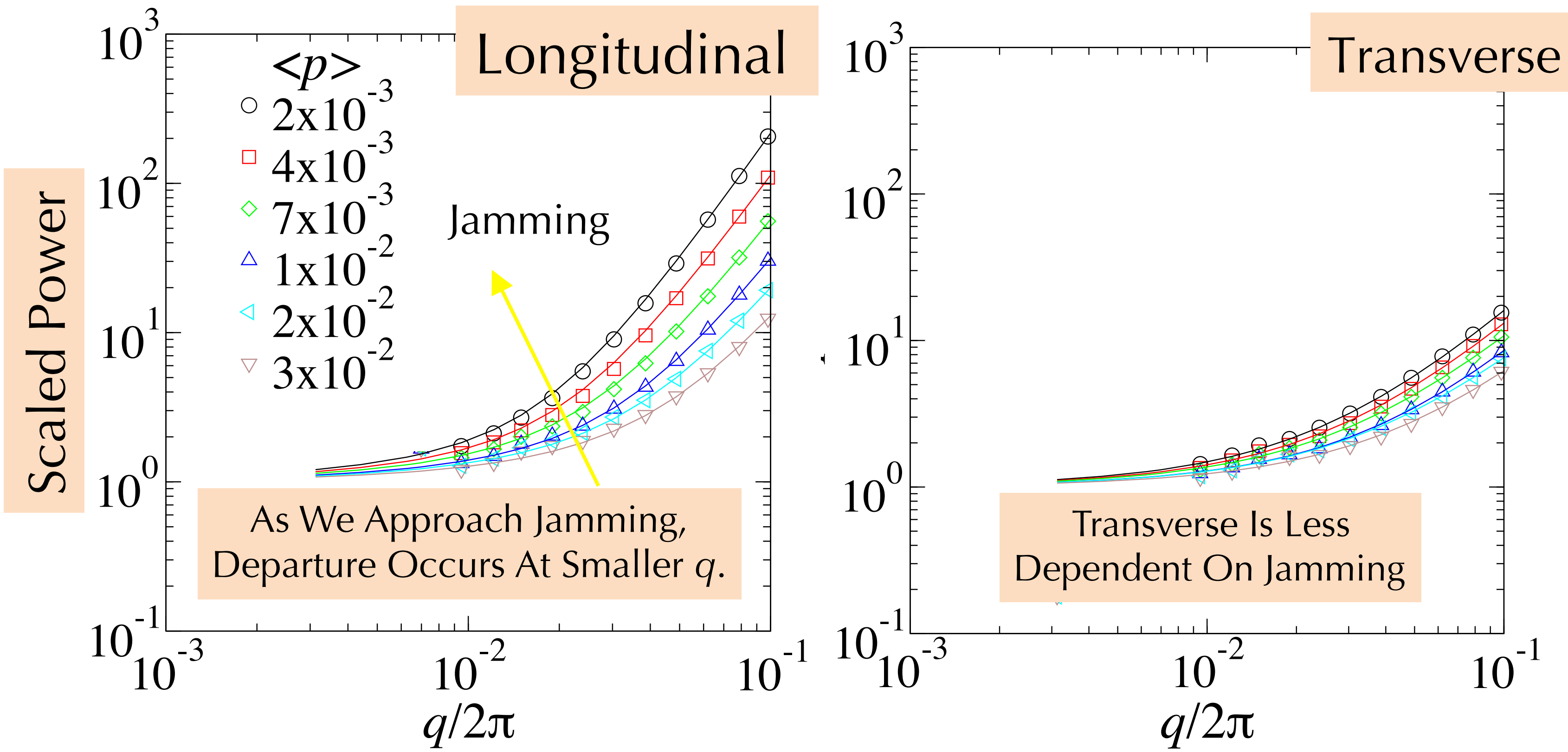
Measurement 1: Point response

$$(\lambda + G)\nabla(\nabla . \mathbf{u}) + G\nabla^2 \mathbf{u} = 0$$

- Take isotropic average of Log(S) for better statistics.
- S=1 means Kelvin.
- Note: long wavelength behavior determined by "macroscopically" measured G and K.
- No free parms. in fit to low-q.



Point response: scaling with pressure



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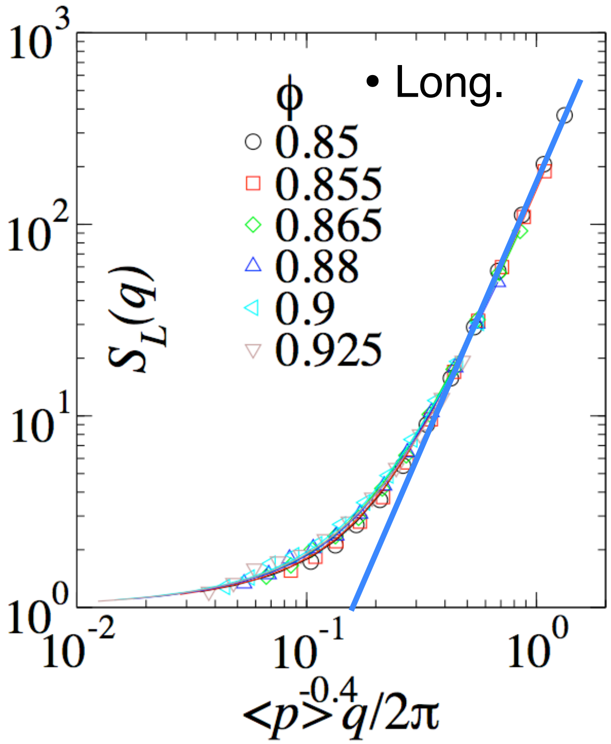
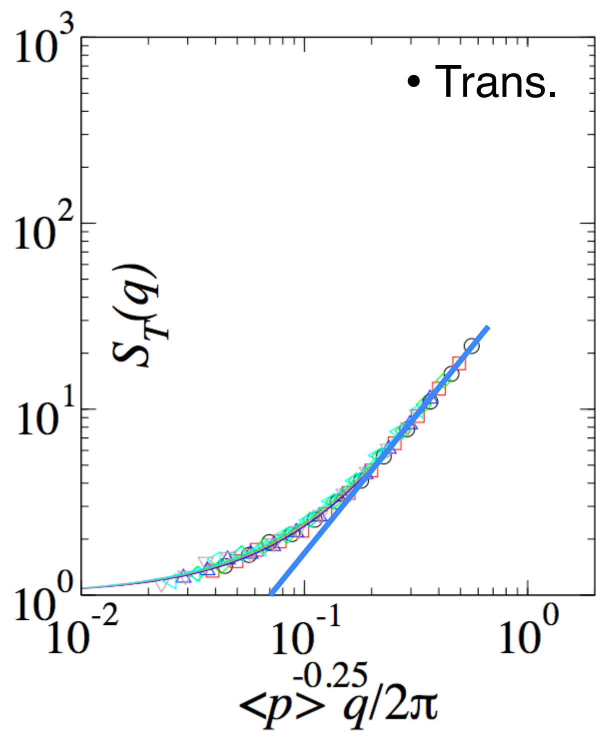


- $\xi_L \sim p^{-0.4}$



- $\xi_T \sim p^{-0.25}$

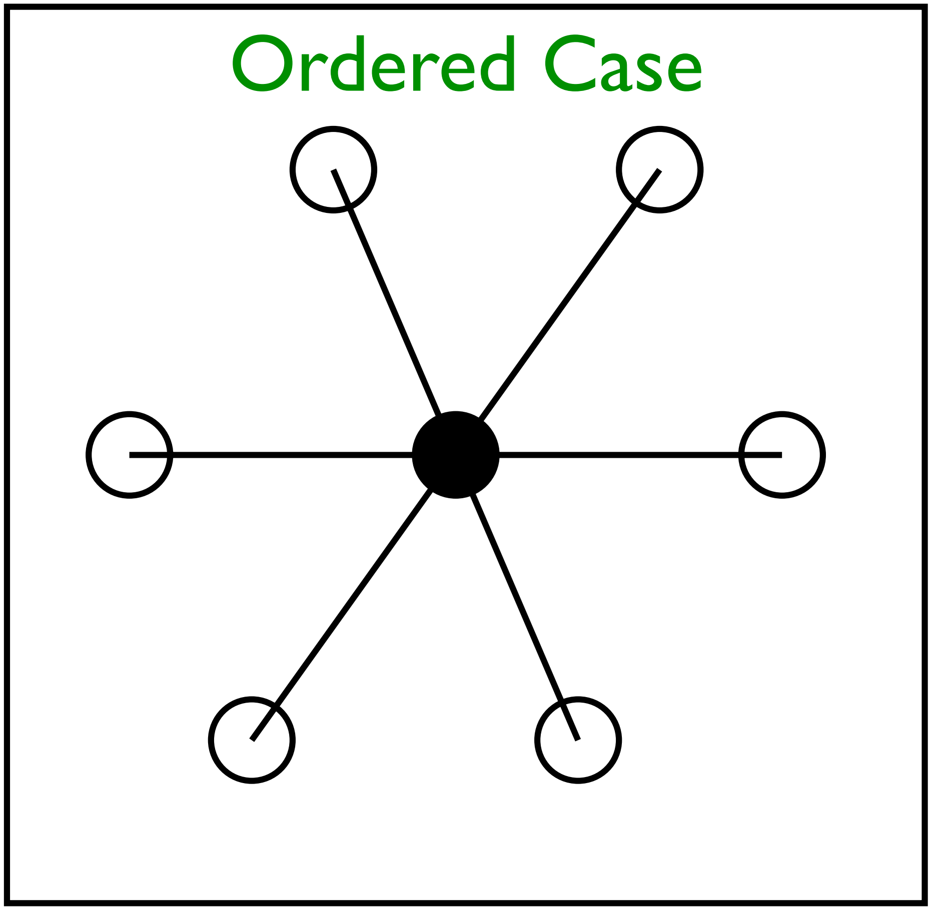
- Note: longitudinal scaling function more severe than transverse.
- $S_L \sim q^2$, $S_T \sim q^1$

Measurement 2: Constrained shear modulus

Detour: non-affine elastic formalism

Aside: non-affine elastic formalism

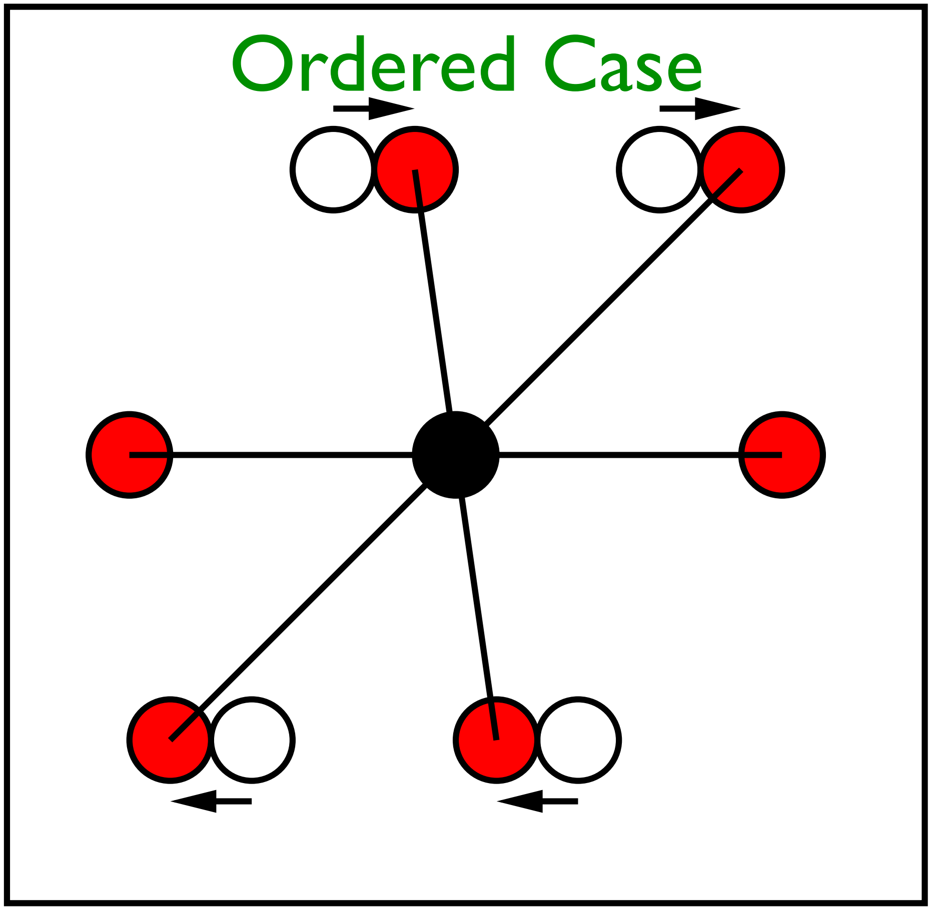
- Single particle toy problem:
  - Start at F=0



- Lutsko (J. App. Phys. 1988)
  CEM+Lemaître (PRL 2004)

Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at F=0
  - Apply affine shear
  - Forces remain zero
  - No correction necessary



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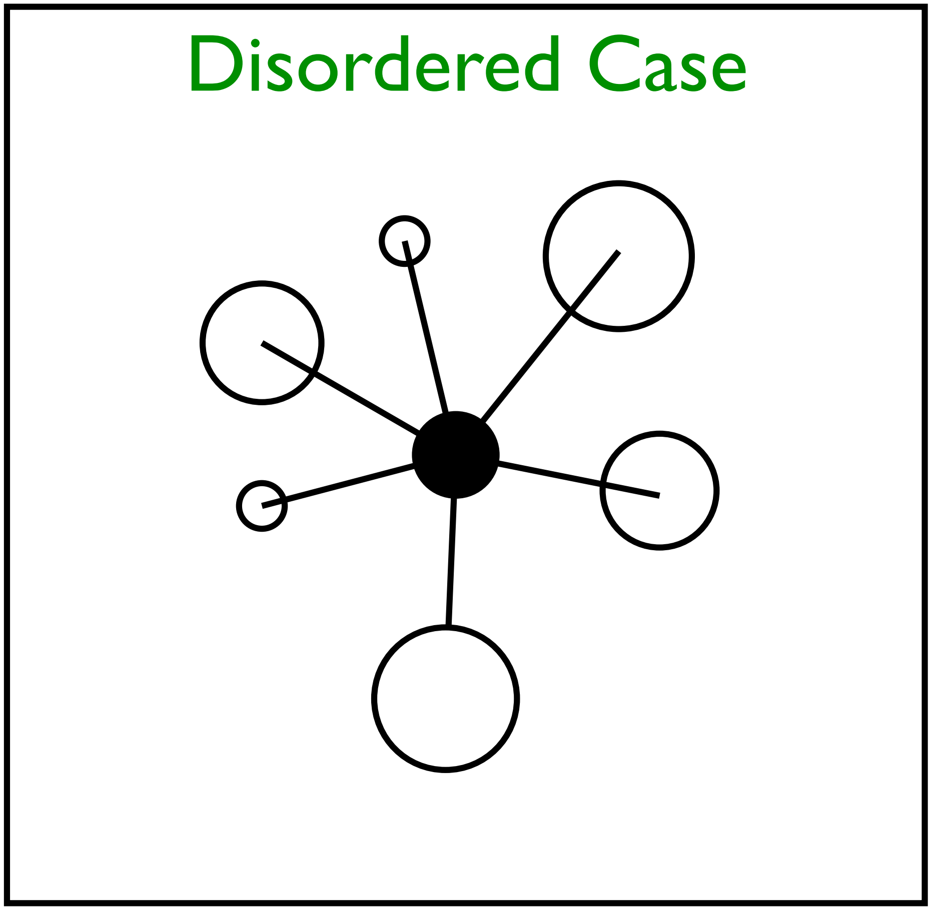
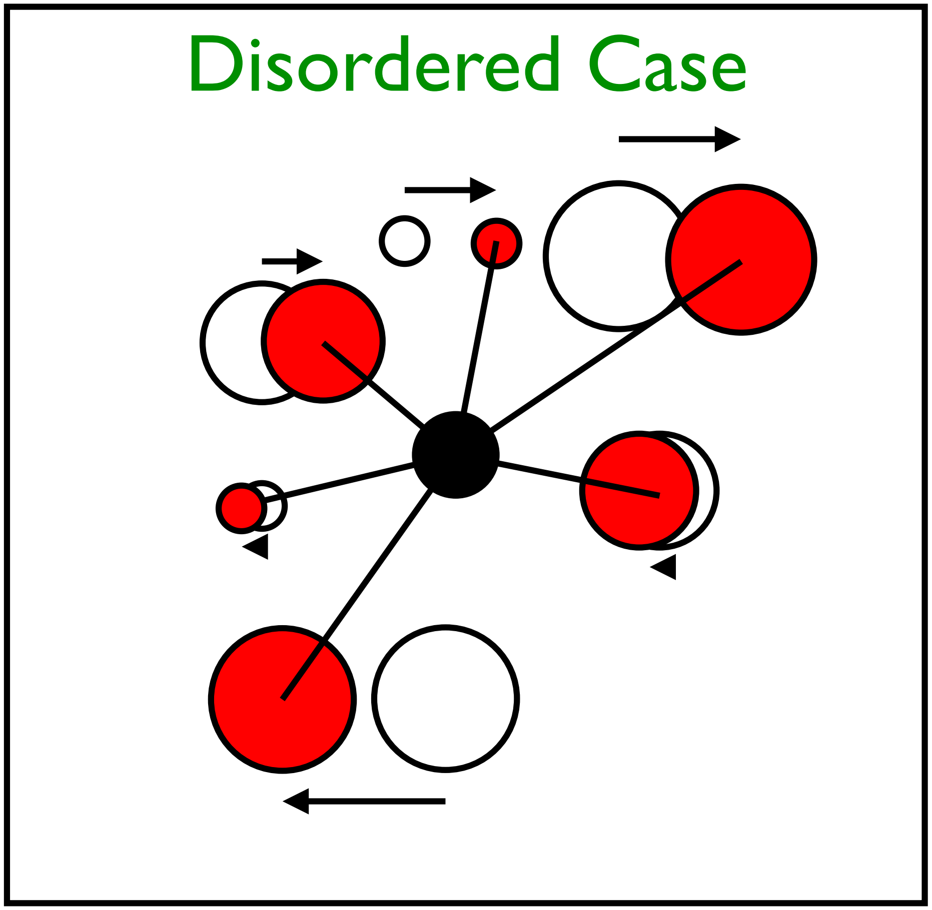


Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at F=0
  - Apply strain

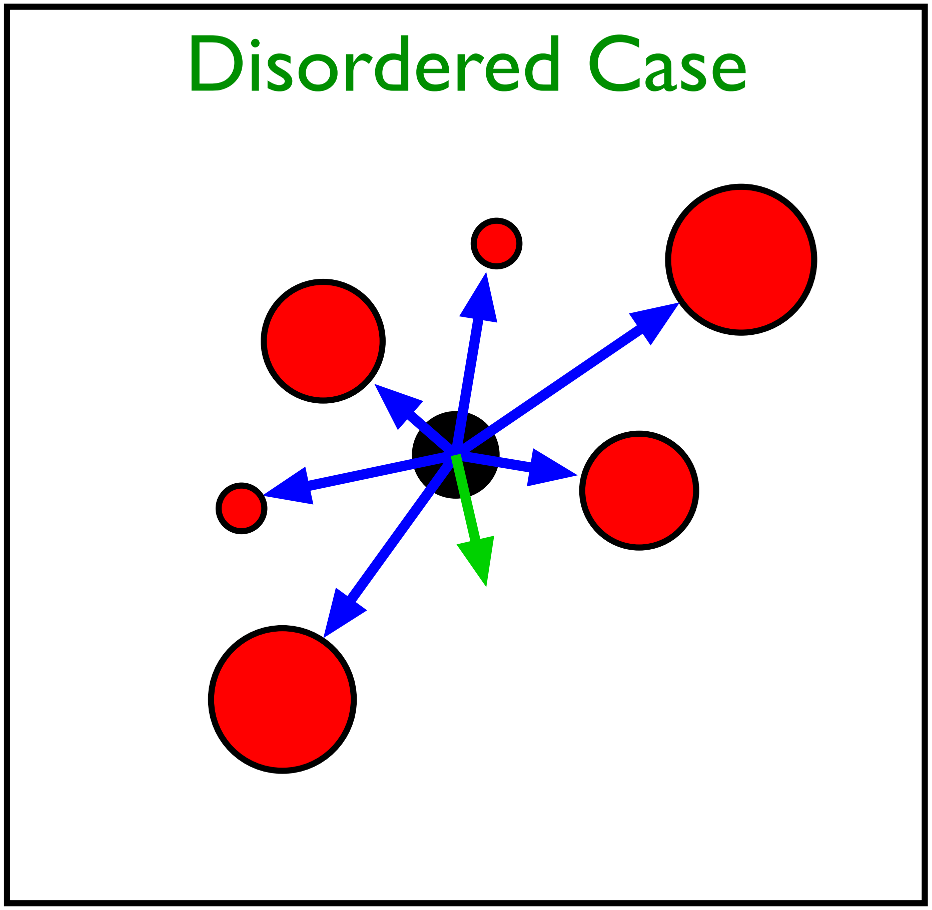


Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at F=0
  - Apply strain

Use Hessian to compute
"Affine force"

$$\vec{\Xi}_i = \gamma \sum_j \mathbf{H}_{ij} \hat{\mathbf{x}} \delta y_j$$



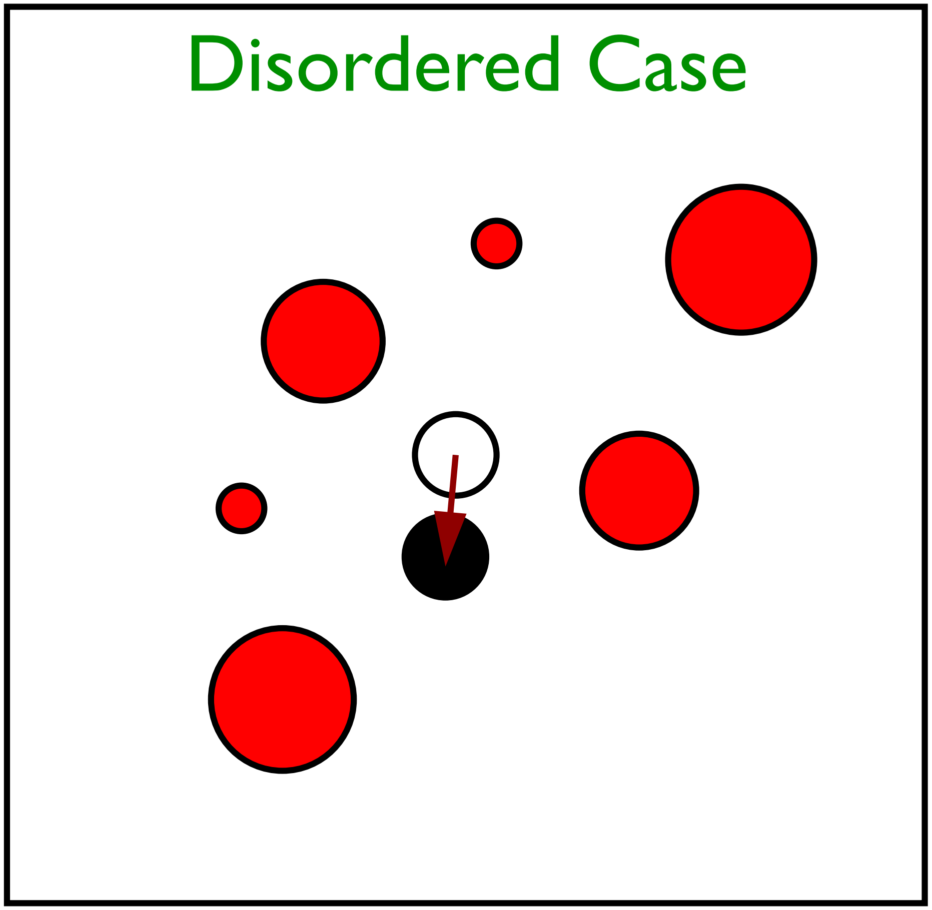
Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at F=0
  - Apply strain

  Use Hessian to find position correction

$$\vec{\Xi}_i = \mathbf{H}_{ii} \vec{dr}_i$$

$$\vec{dr}_i = \mathbf{H}_{ii}^{-1} \vec{\Xi}_i$$

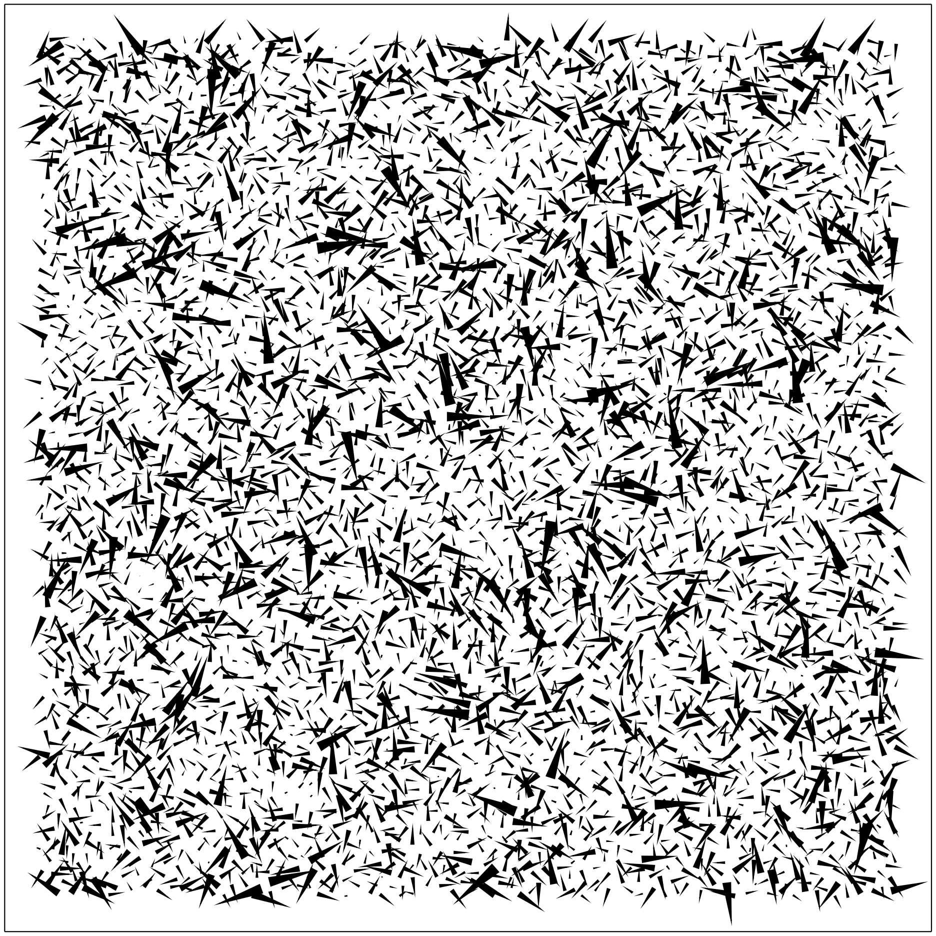


Aside: non-affine elastic formalism

- Back to full assembly:

$$\vec{\Xi}_i = \gamma \sum_j \mathbf{H_{ij}} \hat{\mathbf{x}} \delta y_{ij}$$

  - Measure of local disorder.
  - Only short range correlations in our samples.

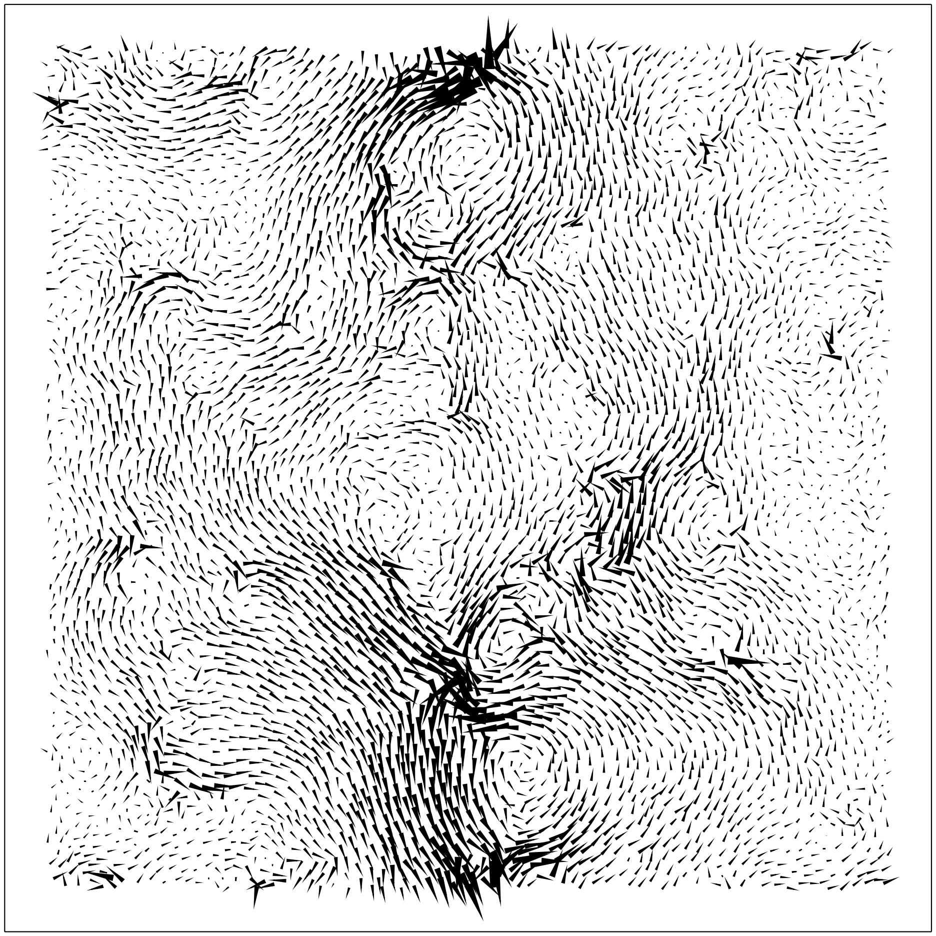


Aside: non-affine elastic formalism

- Back to full assembly:

$$\vec{dr}_i = \gamma \sum_j \mathbf{H_{ij}^{-1}} \vec{\Xi}_j$$

Force balance:
Affine forces, Ξ, must be balanced by correction forces, $H^{-1}{}_{ij} dx_j$

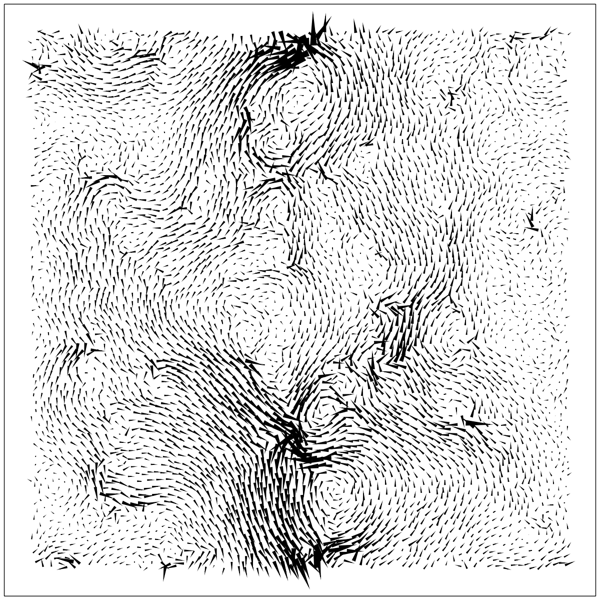


Aside: non-affine elastic formalism

- Tangent modulus

$$\sigma \doteq \frac{dU}{d\gamma} = \frac{\partial U}{\partial \mathring{r}_{i\alpha}} \frac{d\mathring{r}_{i\alpha}}{d\gamma} + \frac{\partial U}{\partial \gamma} = \frac{\partial U}{\partial \gamma}$$

$$\mu \doteq \frac{d\sigma}{d\gamma} = \frac{\partial^2 U}{\partial \gamma^2} - \Xi_{i\alpha} H^{-1}_{i\alpha j\beta} \Xi_{j\beta} = \mu_a - \mu_{na}$$



Crucial for this talk:
Non-affine motion gives negative definite correction to any physical modulus.
e.g. $\mu_{net} < \mu_{affine}$ and $K_{net} < K_{affine}$ (but not necessarily λ)

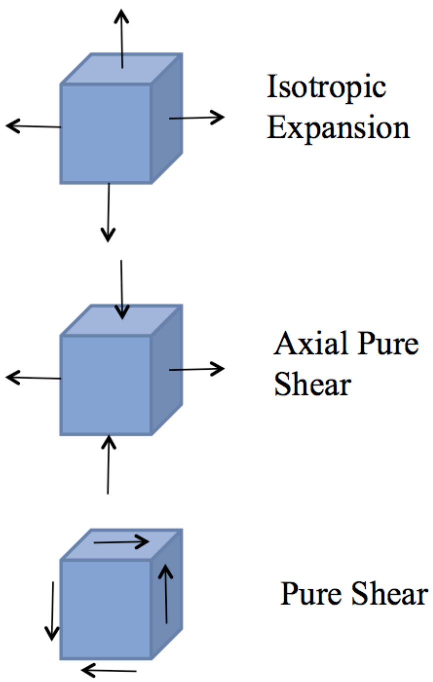
Parenthetical:
Tangent modulus goes to negative infinity at bifurcation points

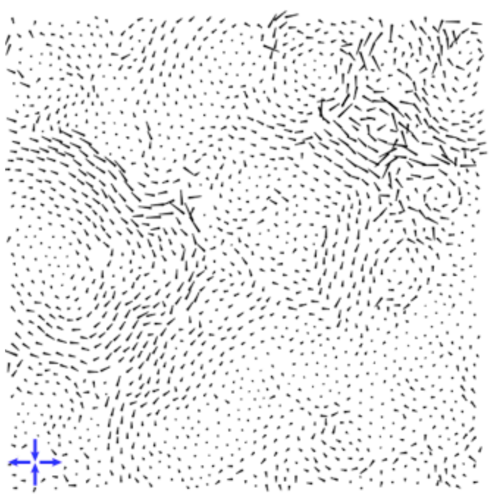
Measurement 2: Constrained shear modulus

Detour finished... back to results

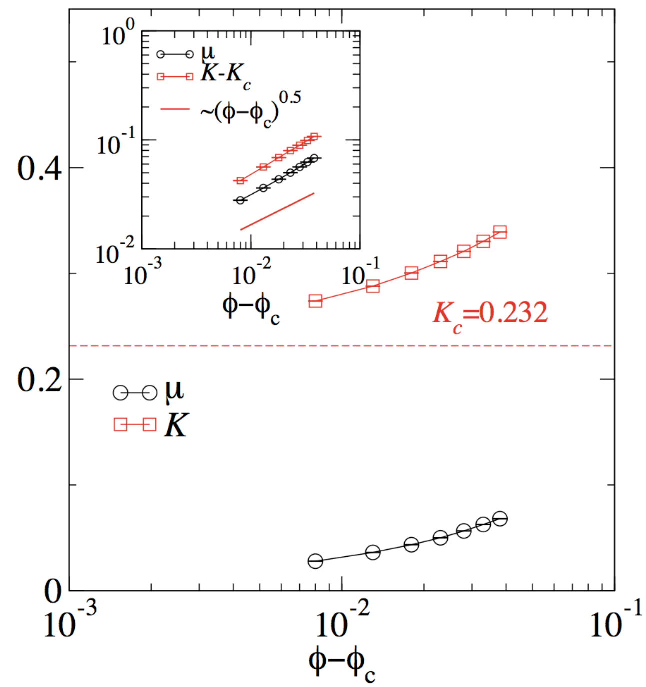
Measurement 2: Constrained shear modulus

- As usual: modulus, μ=Δstress/strain
- Apply homogeneous shear at boundaries, but material responds inhomogeneously in interior
- inhomogeneous motion always lowers μ relative to "naive" value
- Q) how big a chunk of material do I need before I converge to a well defined elastic modulus?



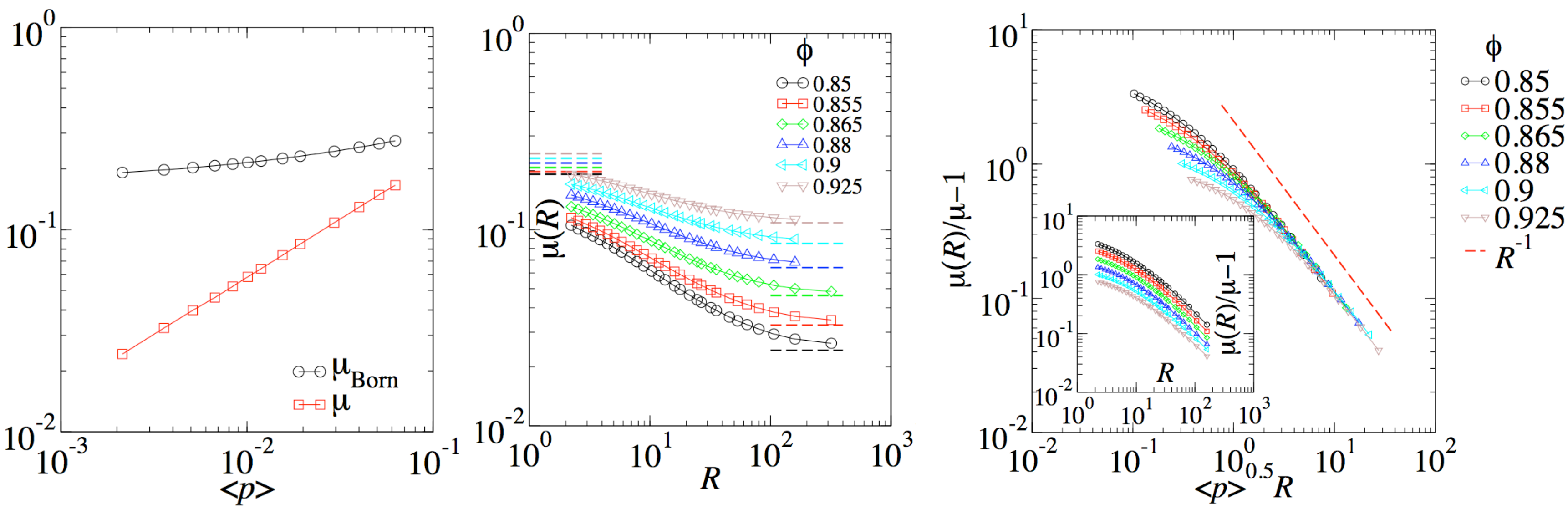


(b) $\delta\underline{\mathbf{v}}$ in axial pure shear



Measurement 2: Constrained shear modulus

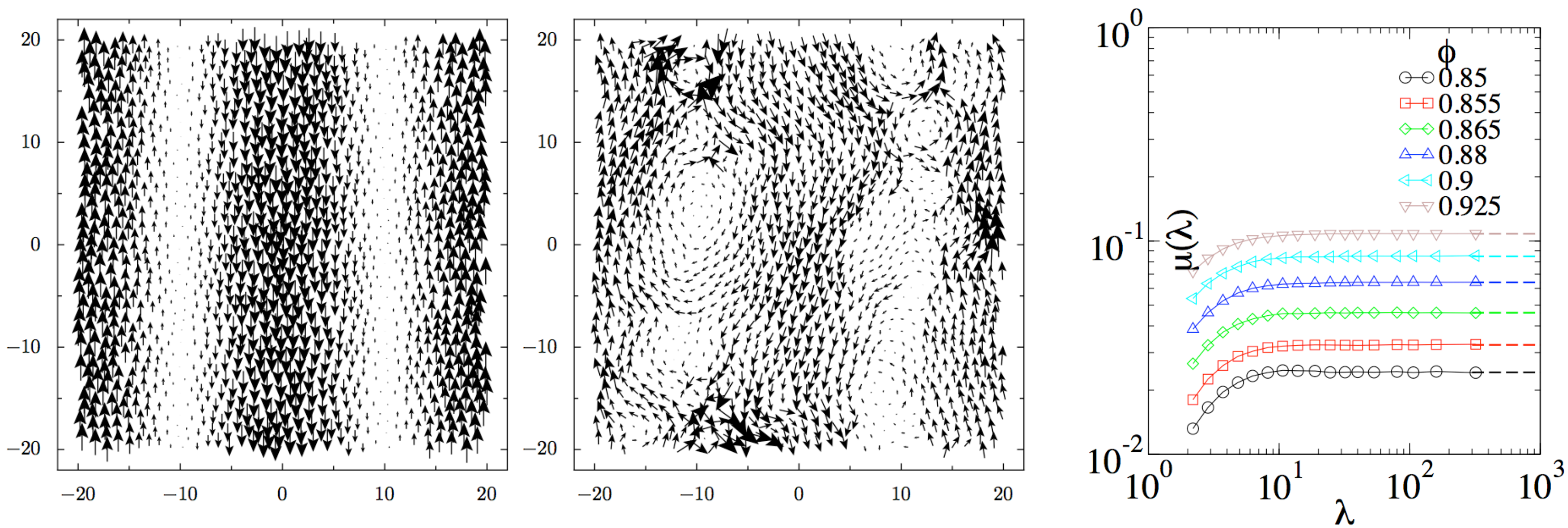
- Small R, inhomogeneous corrections are suppressed (Cauchy-rule enforced).
- μ decays to μ_∞ as R -> ∞
- known: near ϕ_{rcp} μ(R=0) -> constant and μ(R= ∞) goes to zero.
- so what?: at φ=0.88 R=100 gives μ to 10%, at φ=0.85, need R=500!



- Simple scaling form: bulk vs. boundary says μ(R)/μ-1 ~ 1/R
- Collapse to 1/R form when R scaled by p-0.5.
- Reminiscent of Goodrich rigidity percolation procedure and l* ~ 1/Δz ~ $1/p^{1/2}$

Measurement 3: Unconstrained (wave)

- Wave forcing: Impose external field
- Measure projected response to infer modulus: μ(λ)



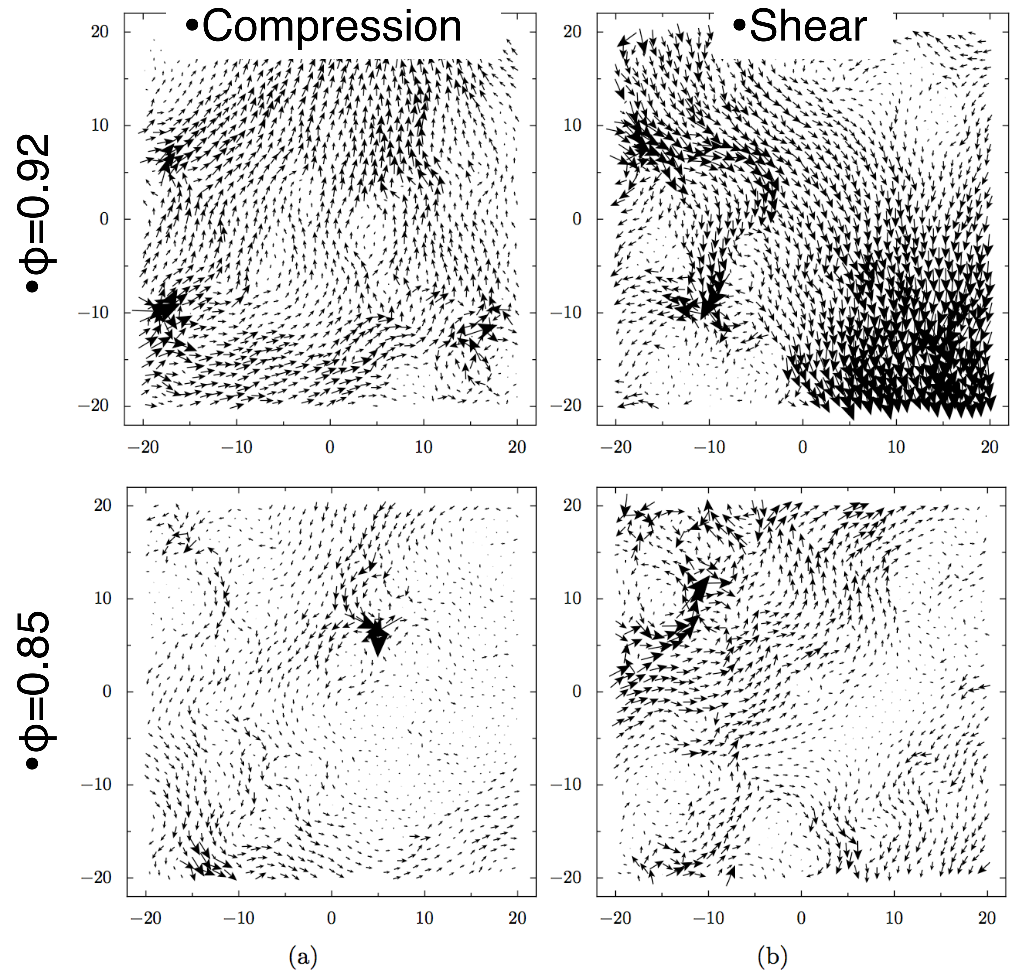
- Inferred μ(λ) rapidly approaches bulk value.
- Small λ error can be understood as pseudo-Brillouin-boundary effects
- **Move it along... nothing to see here...**
- **Recent update. Private conversation w/S Teitel... interesting scaling for K(λ)**

Measurement 3: Unconstrained deformation

• Unconstrained homogeneous deformation with periodic boundary conditions.

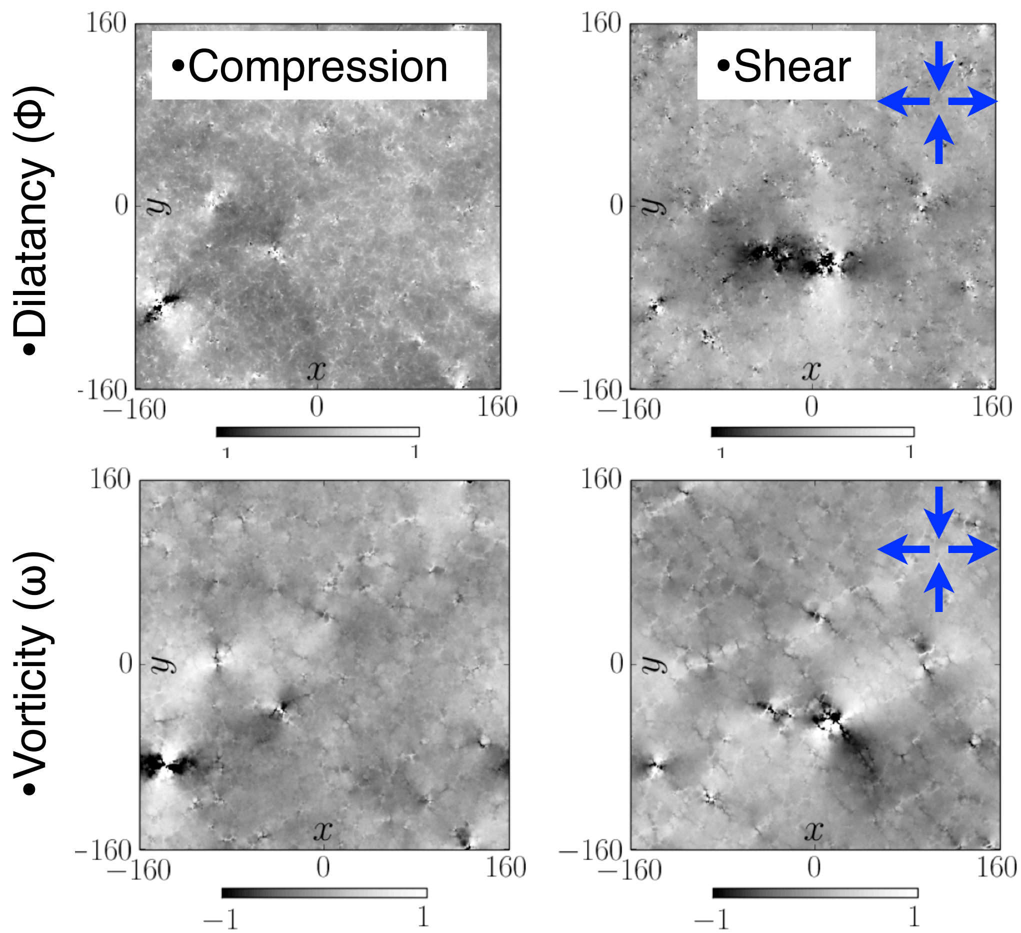
• Moduli (both K and G) rapidly converge with system size to bulk values.
(as in seminal work by O'Hern et. al. PRE 2003)

• Consistent with 2D Lennard-Jones (Tanguy et. al. PRB 2002)



Measurement 3: Unconstrained deformation (φ=92%)

• Measure local dilatancy (longitudinal), Φ, and local vorticity (transverse), ω in response to both compression (Φ_c,ω_c) and shear (Φ_s,ω_s).



• One or two dominant displacement quadrupoles ("STZ"s?) in a typical 320x320 box.

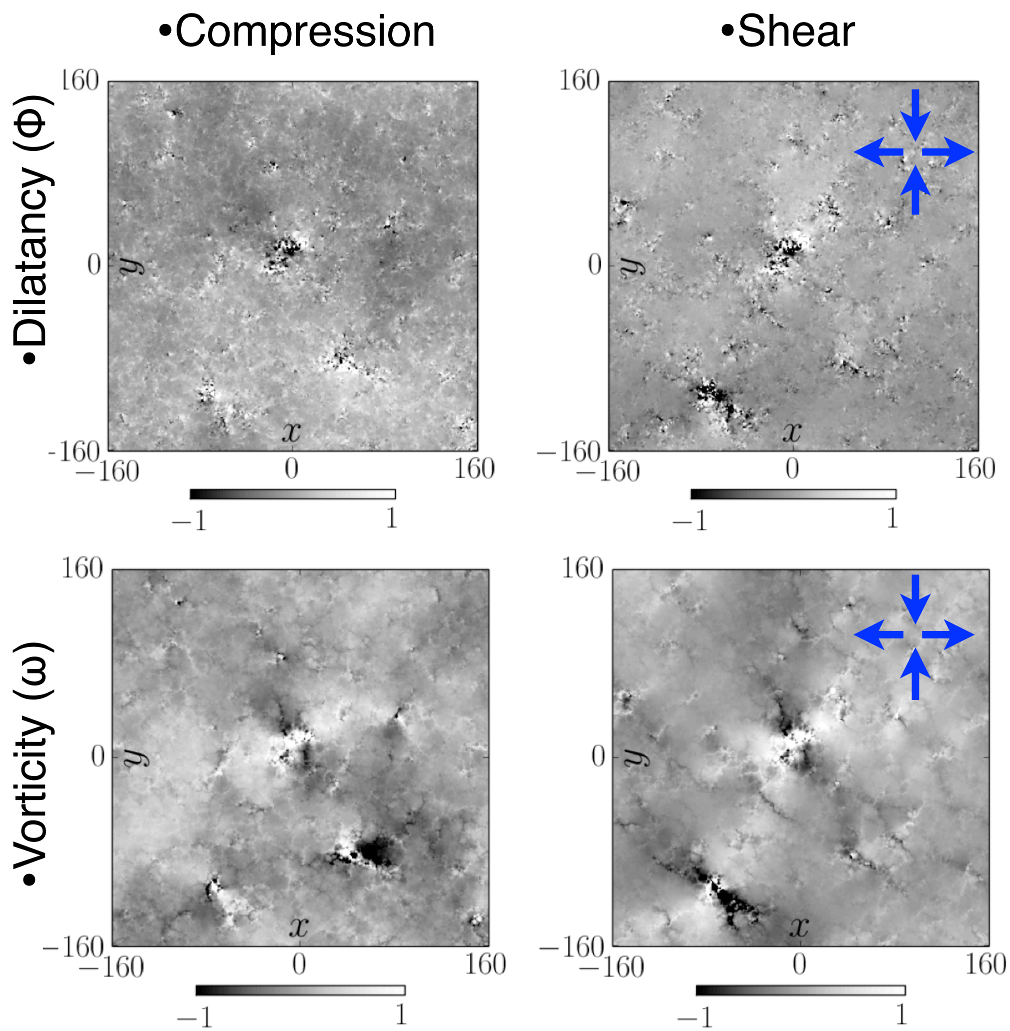
• shear: disp. quadrupoles align (vertical compression, horizontal extension)

• compression: quadrupoles random orient.

• Φ=92% just like Lennard-Jones

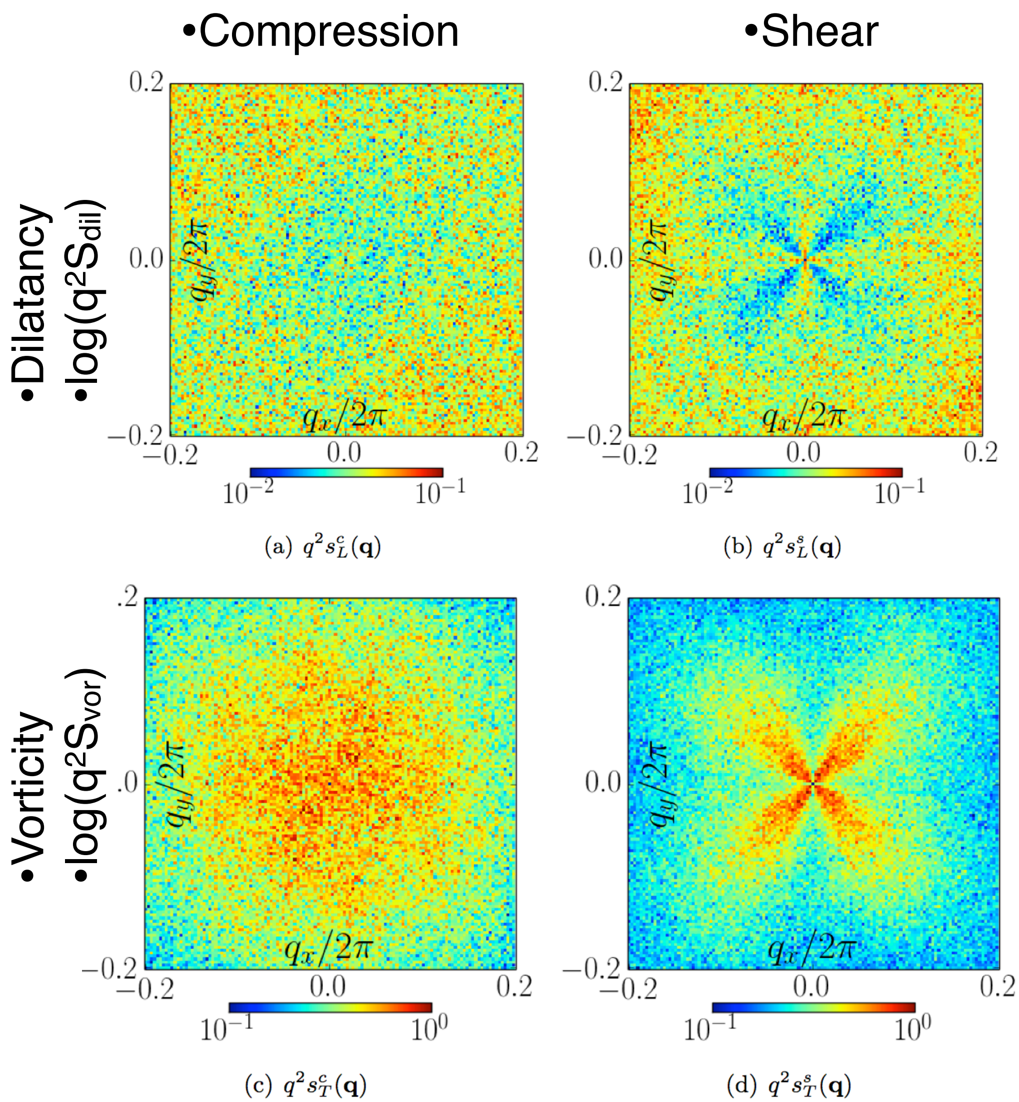
•Effective-medium-like calculations (Didonna & Lubensky PRE 2005, Maloney PRL 2006) imply Gaussian random whitenoise for both Φ and ω fields. (Obvious: not strictly true)

Measurement 3: Unconstrained deformation (φ=85%)



- At φ=85%, dilatancy is less "coherent" in both compression and shear.
- Shear induced vorticity very similar to φ=92%. **VERY SURPRISING!** (Related to Ellenbroek, et. al. "sliding only" result?)
- Shear induced quadrupoles are no longer visible in long-range dilatancy field.
- Very small hint of compression induced quadrupoles in the vorticity (but not dilatancy)
- Idea: dilatancy must vanish outside STZ cores, but may be non-zero inside.

Measurement 3: Unconstrained deformation (φ=92%)



(a) $q^2 s_L^c(\mathbf{q})$

(b) $q^2 s_L^s(\mathbf{q})$

(c) $q^2 s_T^c(\mathbf{q})$

(d) $q^2 s_T^s(\mathbf{q})$

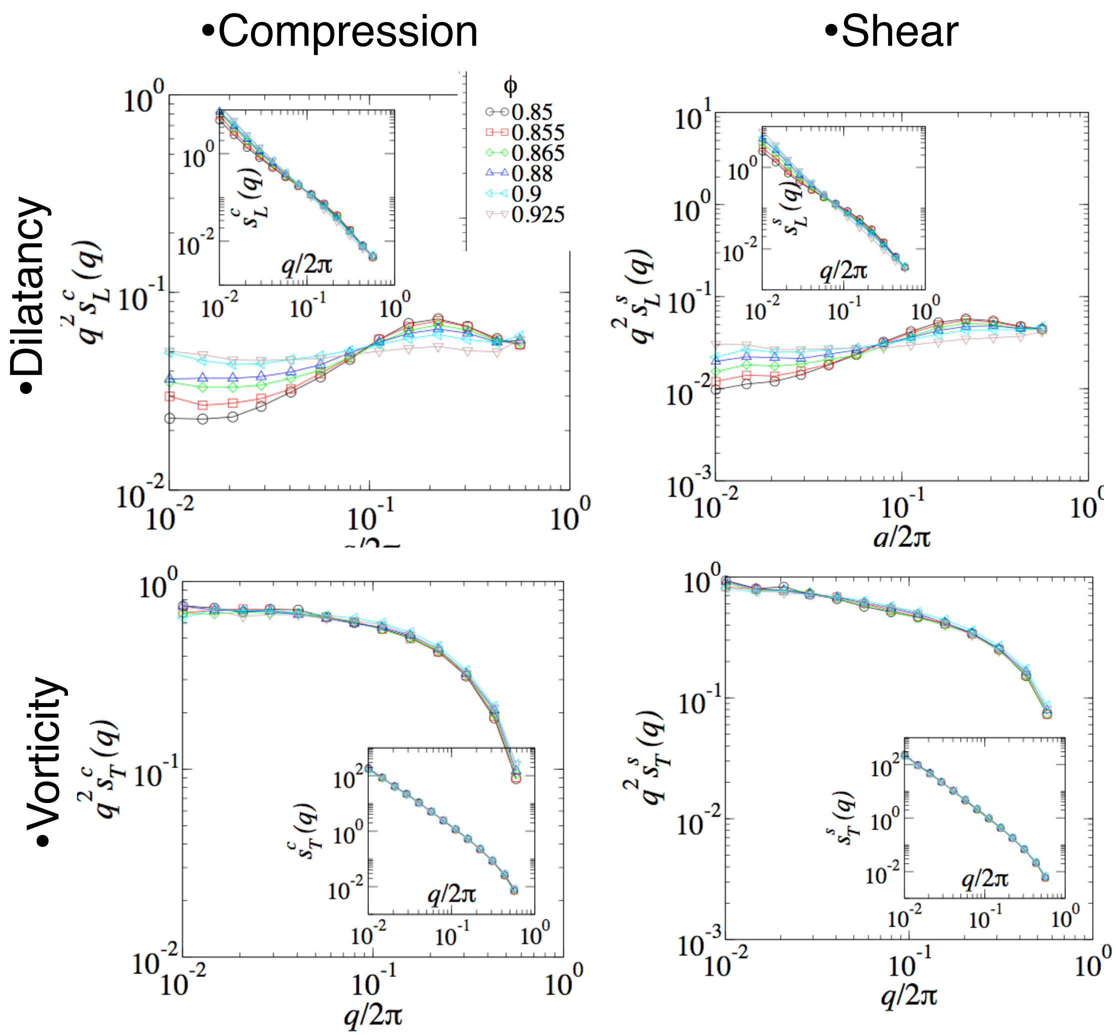
- Power spectra for dilatancy (longitudinal) and vorticity (transverse)

- EMT says $q^2S(q)$ should be flat and isotropic for both dilatancy and vorticity

- Clear deviations from both $S\sim q^{-2}$ and isotropy (compression response is isotropic by **construction** for qL_{cell}>>1)... that is: quadrupoles align with the shear.

- Anisotropy much more pronounced in dilatancy than vorticity (agreement with impression from real-space images).

Measurement 3: Unconstrained deformation



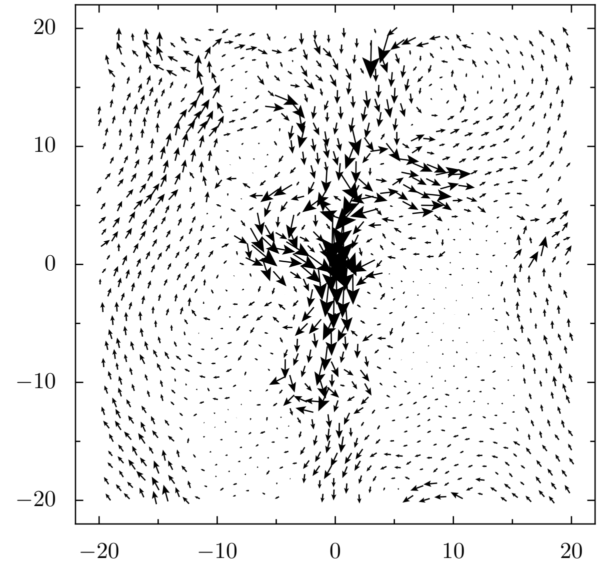
- Take isotropic average of log($q^2S(q)$)

- EMT says $q^2S(q)$ should be flat and isotropic for both dilatancy and vorticity

- Clear deviations from both $S \sim q^{-2}$ and isotropy (compression response is isotropic by **construction** for $qL_{cell} >> 1$)... that is: quadrupoles align with the shear.

- Anisotropy much more pronounced in dilatancy than vorticity (agreement with impression from real-space images).

Conclusions (Elasticity)



- Method 1) Point response:
  - $\xi_L \sim p^{-0.4}$, $\xi_T \sim p^{-0.25}$
  - hard to see ξ_L since G/K -> 0 so $S_L/S_T \sim 0$
  - shape of scaling function $S(\xi q)$?

- Method 2) Constrained deformation:
  - $\mu(R)/\mu - 1 \sim 1/(Rp^{-0.5})$
  - analogous to rigidity-based approaches and l*

- Method 3) Unconstrained deformation:
  - "Wave method" $G(\lambda)$
    - quick convergence G_∞ beyond $\lambda \sim 5$
    - insensitive to ϕ_J
    - (Should also check K)!
  - S_T
    - effective medium (uncorrelated strains) good approx
    - puzzle: insensitive to ϕ!
  - S_L
    - effective medium only OK approx
    - details depend on ϕ
    - "incoherent" beyond "shear zone size".
    - peak position independent of ϕ
    - shear transformation zones / soft spots???