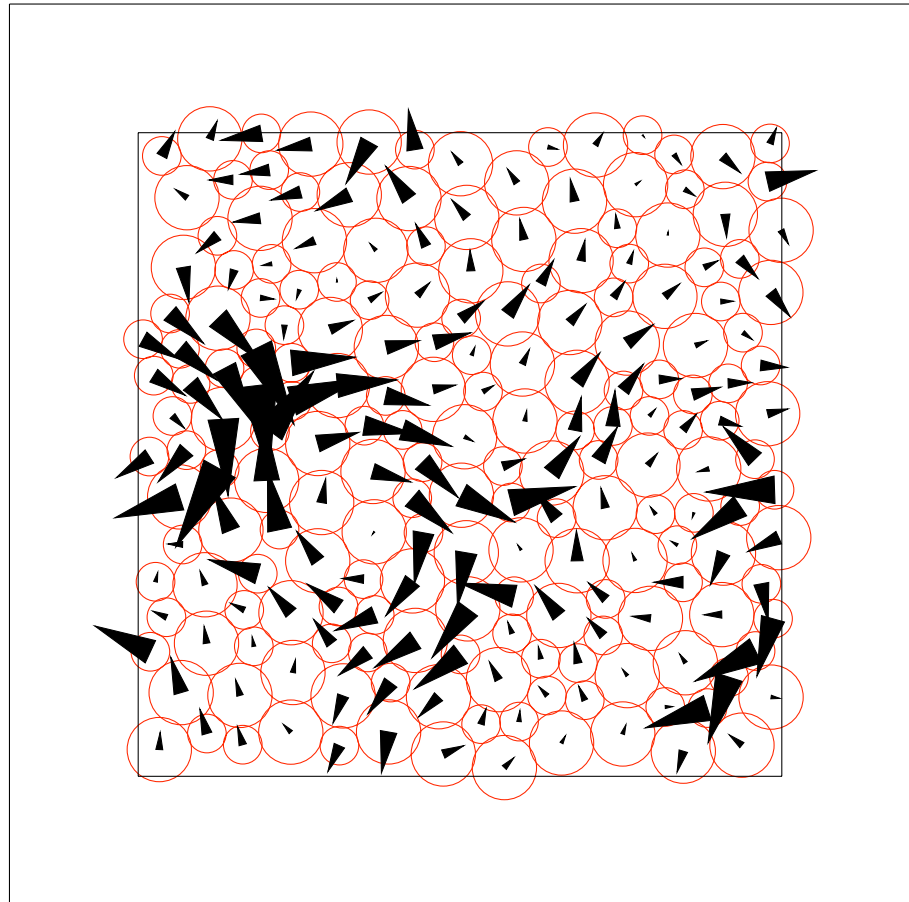


Non-affine Elasticity in Jammed Systems

Craig Maloney
JHU/KITP

APS March
Meeting
2006
Baltimore, MD

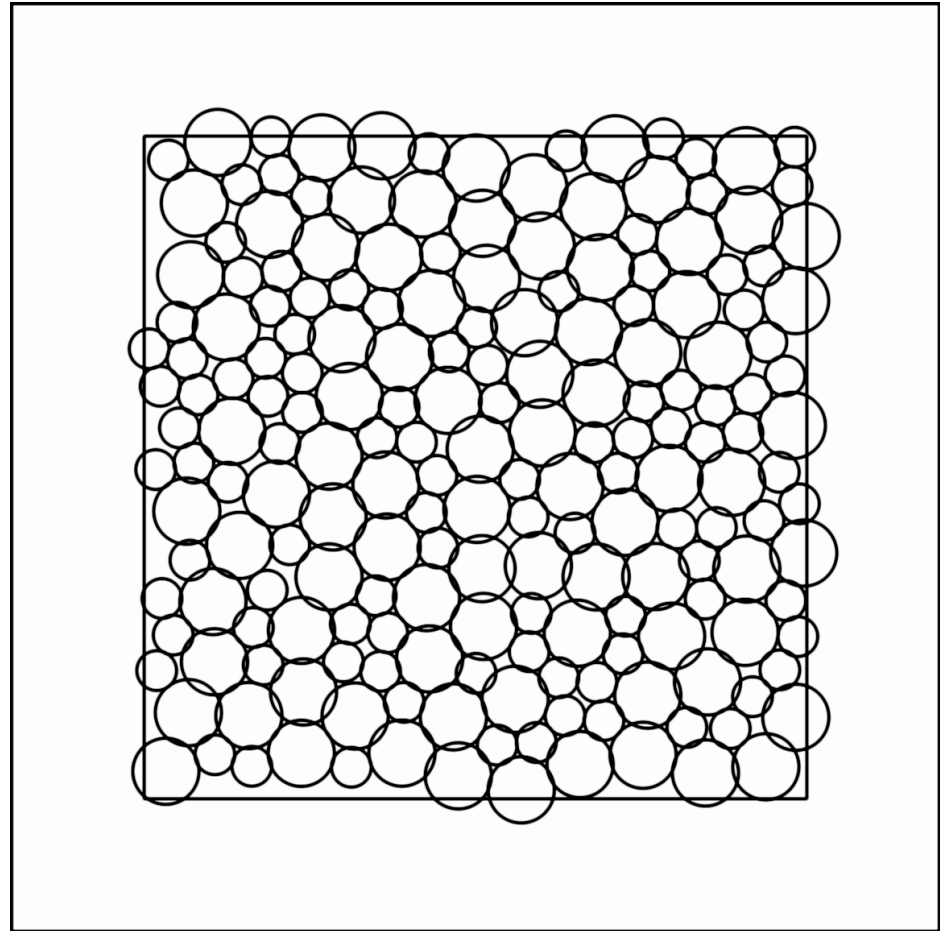


Acknowledgments

- A. Lemaître, Institut Navier
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- M.O. Robbins, JHU
- Funding: LLNL University Relations

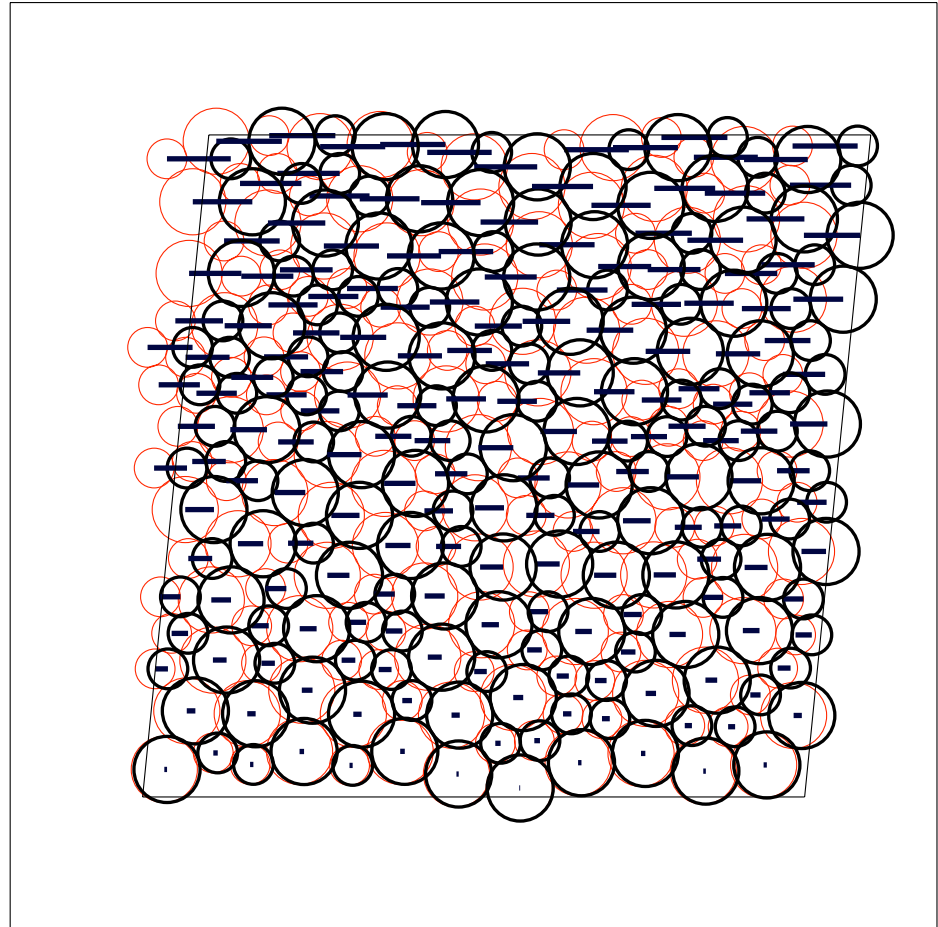
Non-affine Response

- Sequence:
 - Initial packing, $F=0$
- What is this stuff?
 - Bubbles or
 - Grains or
 - Atoms



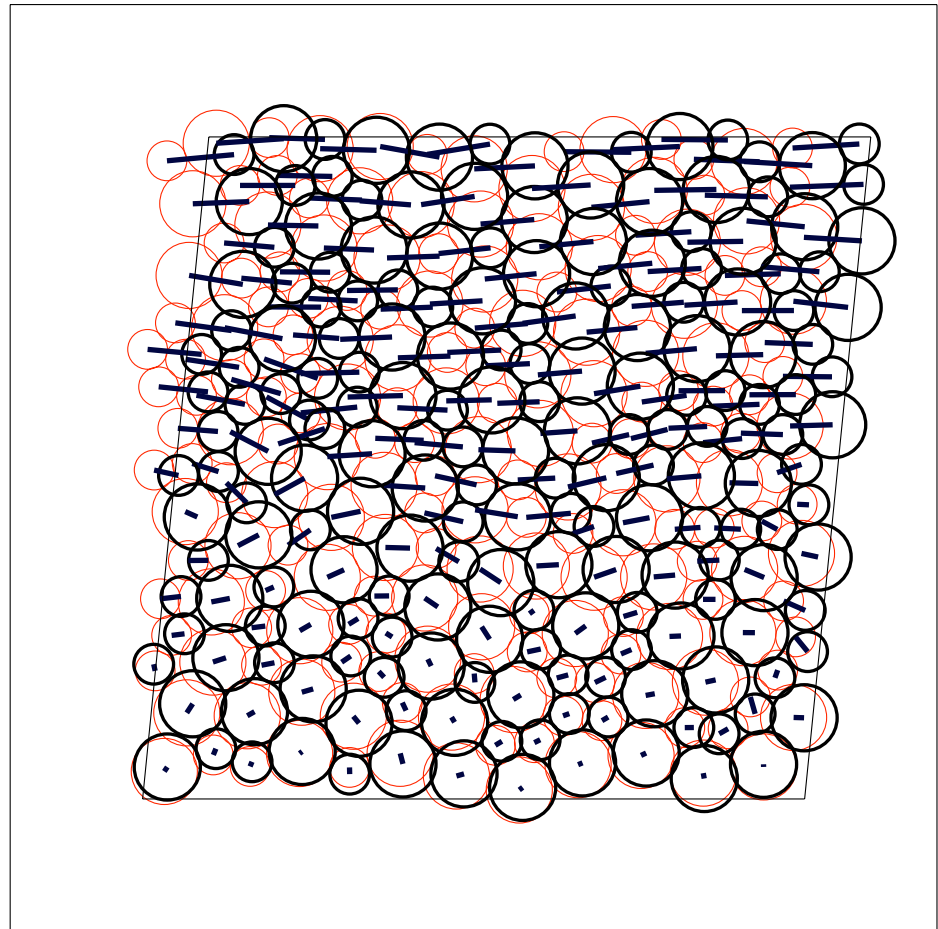
Non-affine Response

- Sequence:
 - Initial packing, $F=0$
 - Sheared state, $F \neq 0$



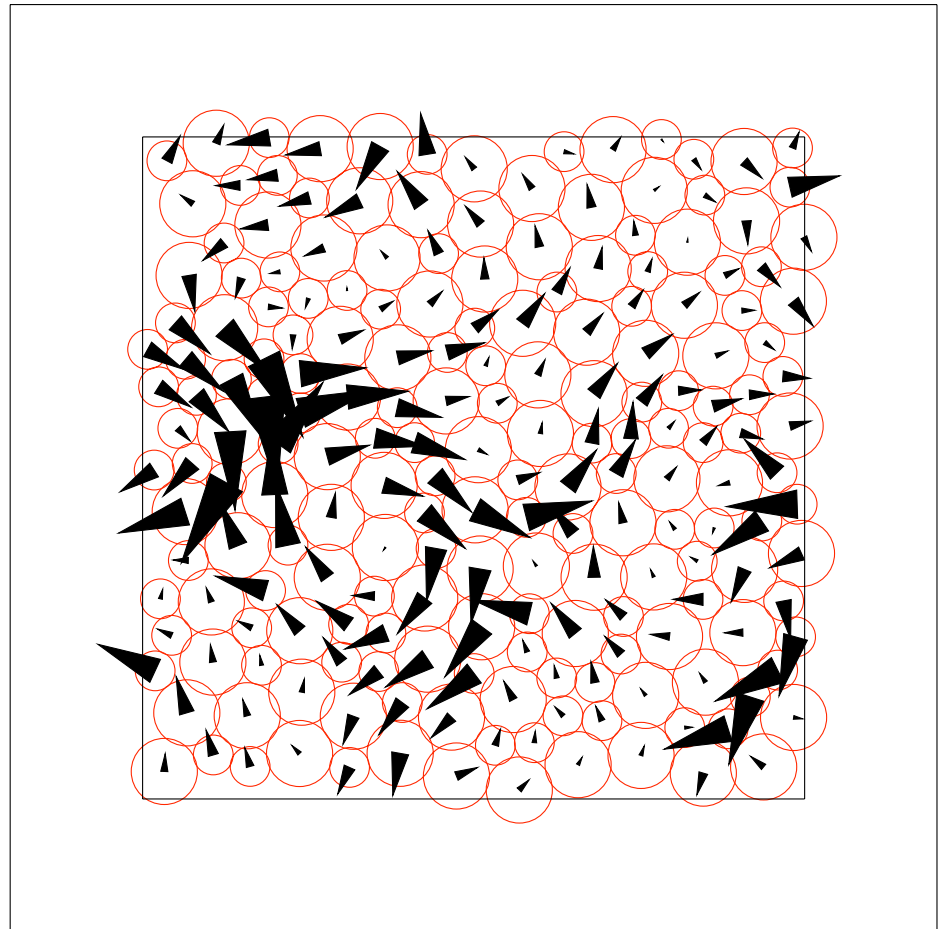
Non-affine Response

- Sequence:
 - Initial packing, $F=0$
 - Sheared state, $F \neq 0$
 - Allow correction so $F=0$ again.



Non-affine Response

- Sequence:
 - Initial packing, $F=0$
 - Sheared state, $F \neq 0$
 - Allow correction so $F=0$ again.
 - Subtract affine piece.



Motivation:

Q) How to characterize the local disorder?

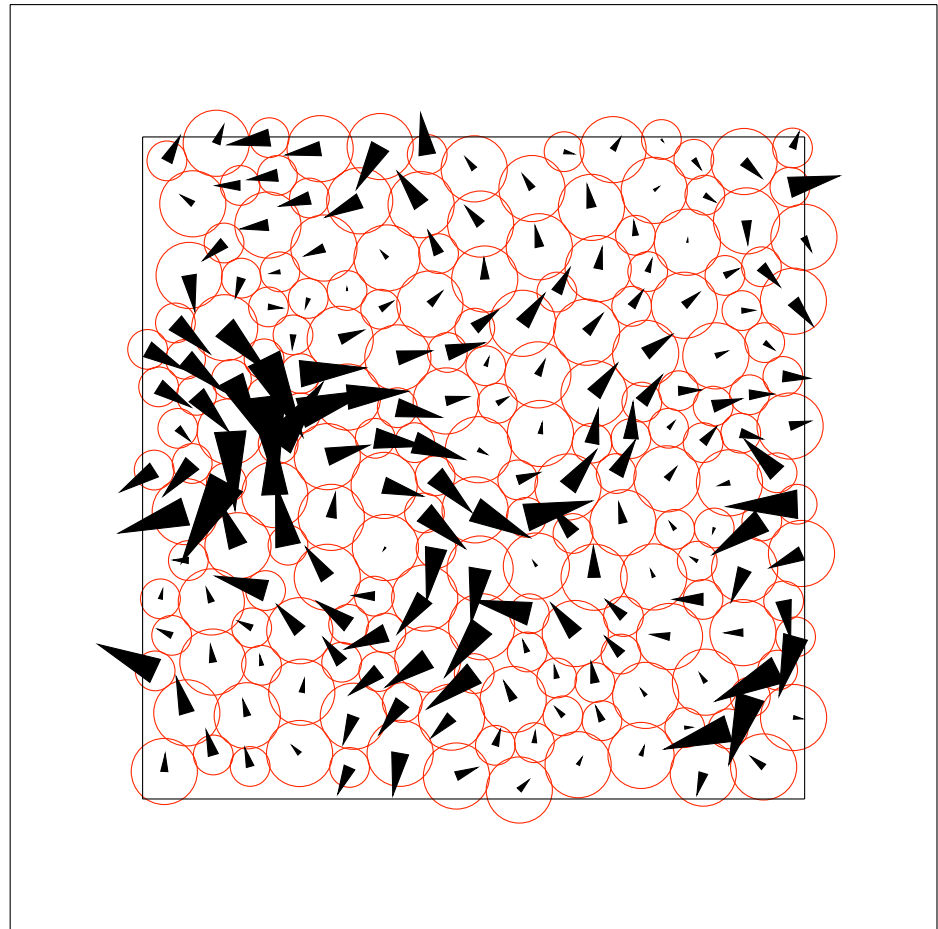
A) The “affine forces”, Ξ

Q) Can a characteristic length be defined?

A) No. Vortices scale with system size.

Q) How do heterogeneities in the elasticity initiate plasticity?

A) Elastic response localizes into a shear zone



Motivation:

Q) How to characterize the local disorder?

A) The “affine forces”, Ξ

Q) Can a characteristic length be defined?

A) No. Vortices scale with system size.

Q) How do heterogeneities in the elasticity initiate plasticity?

A) Elastic response localizes into a shear zone

- Leonforte, et. al., find a characteristic vortex size.
- DiDonna and Lubensky develop a framework which exhibits log divergences.
- We develop a similar framework, but conclude that vortices are scale free.
- Can get good quantitative agreement with the data.

Motivation:

Q) How to characterize the local disorder?

A) The “affine forces”, Ξ

Q) Can a characteristic length be defined?

A) No. Vortices scale with system size.

Q) How do heterogeneities in the elasticity initiate plasticity?

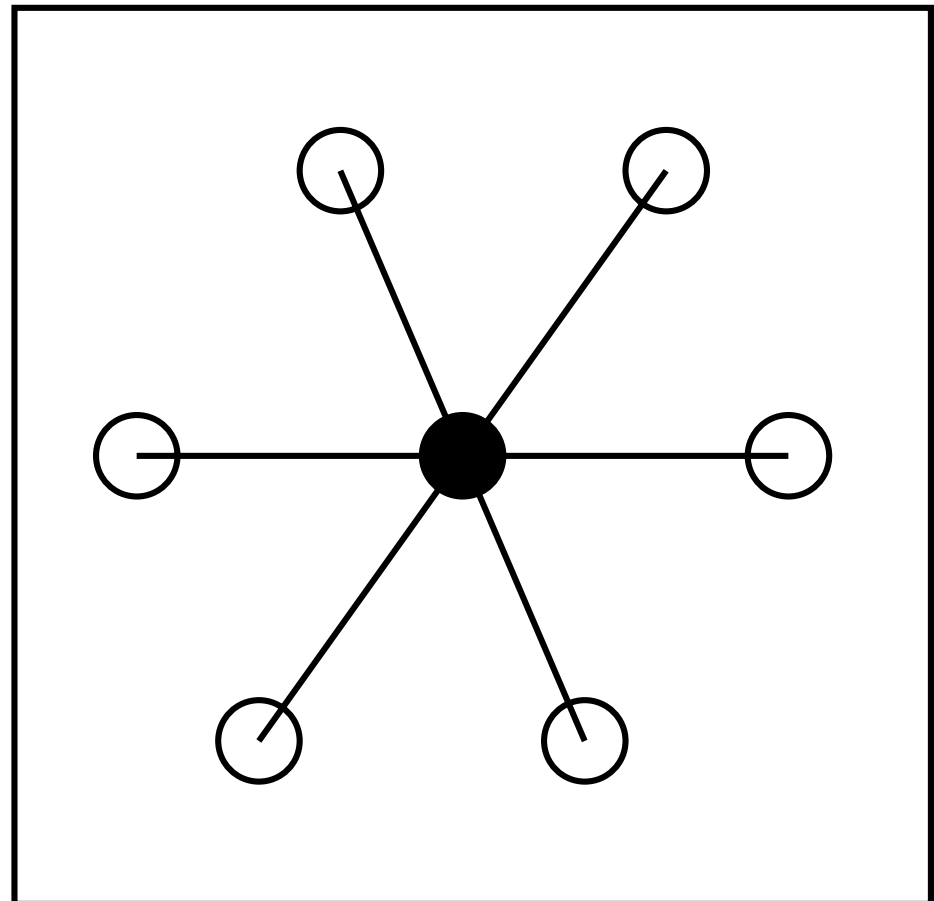
A) Elastic response localizes into a shear zone

- Older studies [Srolovitz et. al. Acta Metal. 1981] find that plasticity is nucleated near stress concentrations.
- In our systems, plasticity is instead nucleated at regions of large non-affine elasticity.
- We derive analytical expressions for this nucleation process.

Computing the response

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

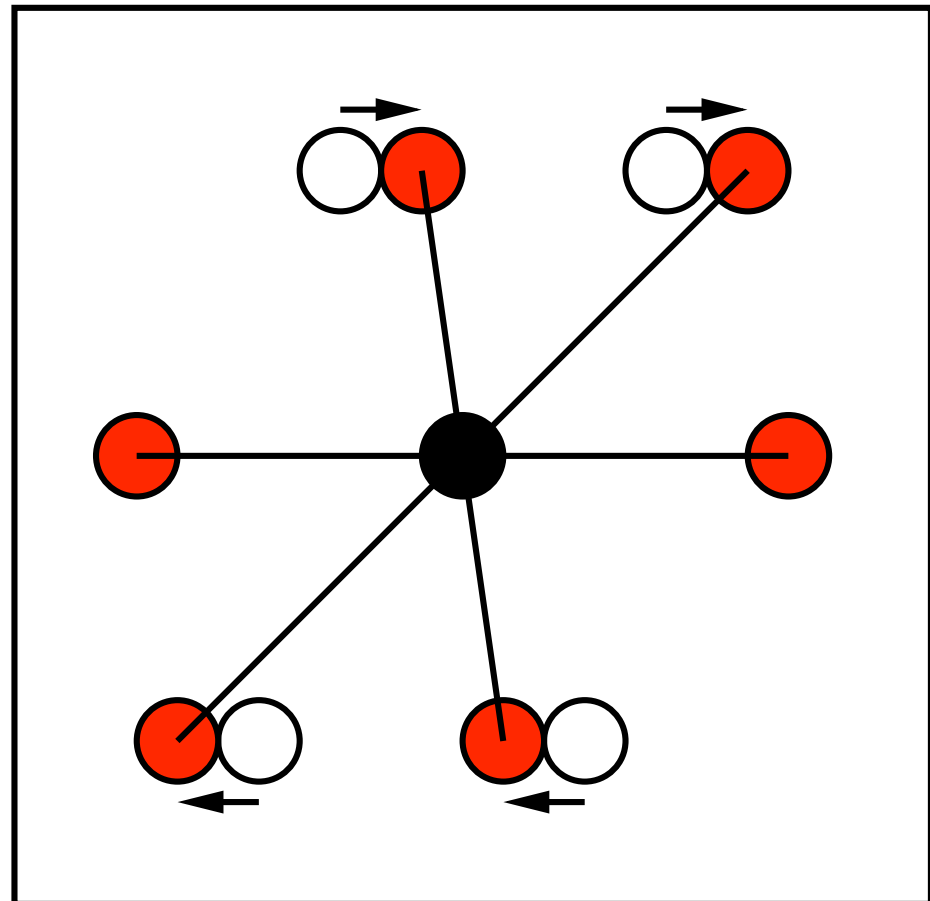
Ordered Case



Computing the response

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

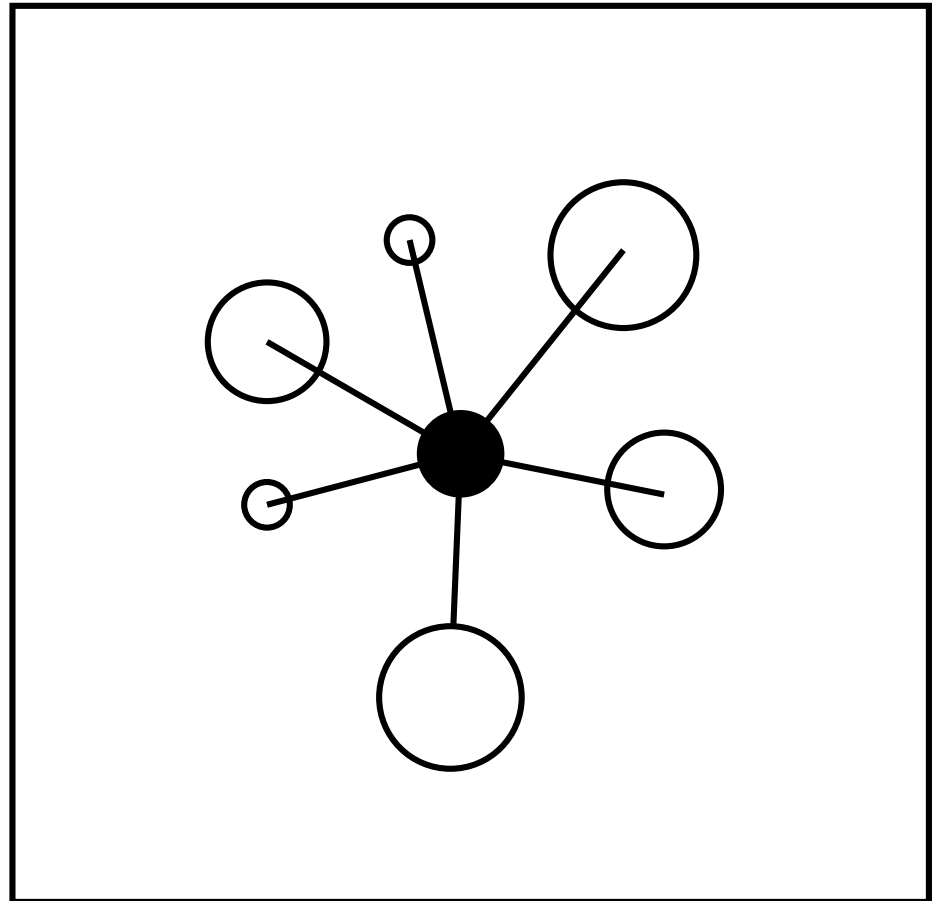
Ordered Case



Computing the response

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

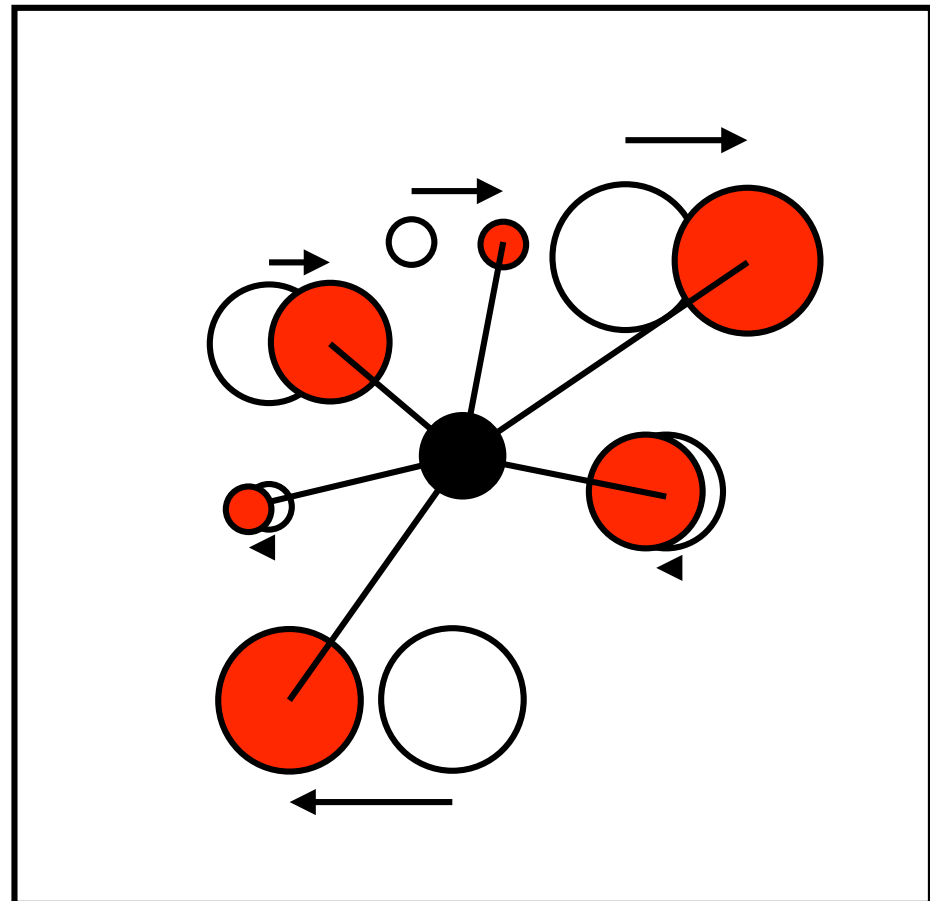
Disordered Case



Computing the response

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

Disordered Case



Computing the response

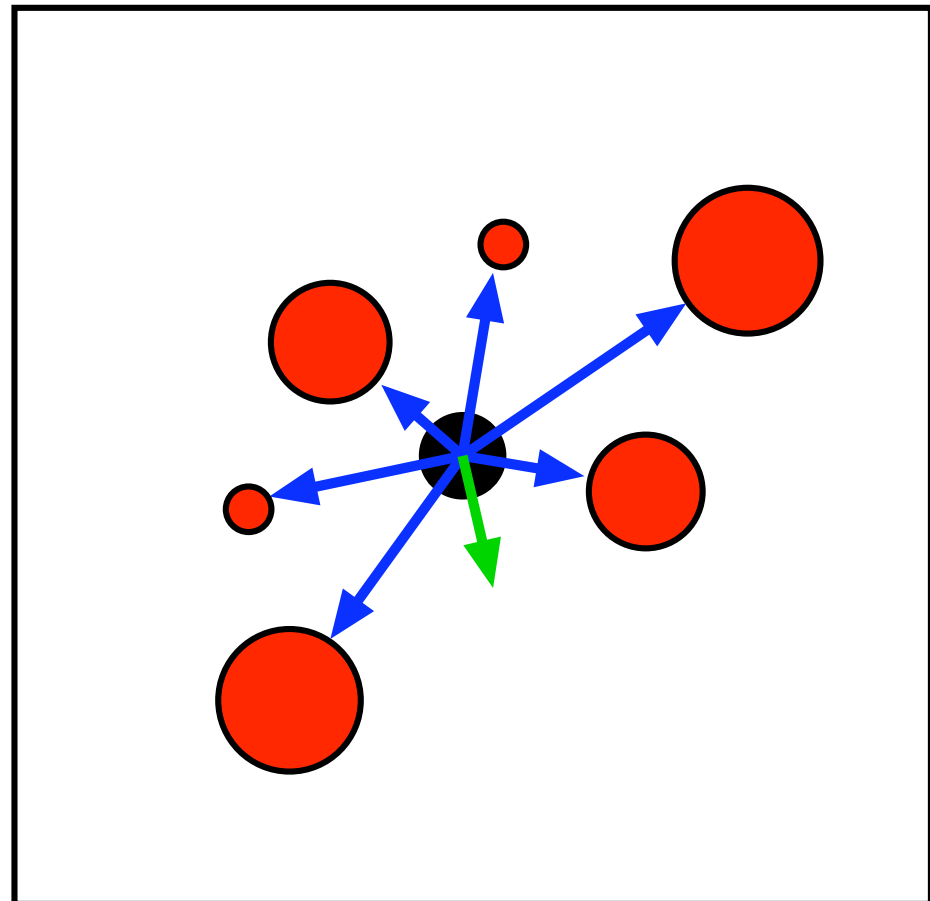
- Single particle toy problem:
 - Start at $F=0$
 - Apply strain

Use Hessian to compute “Affine force”

$$\vec{\Pi}_i = \sum_j \mathbf{H}_{ij} \vec{d}r_j$$

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

Disordered Case



Computing the response

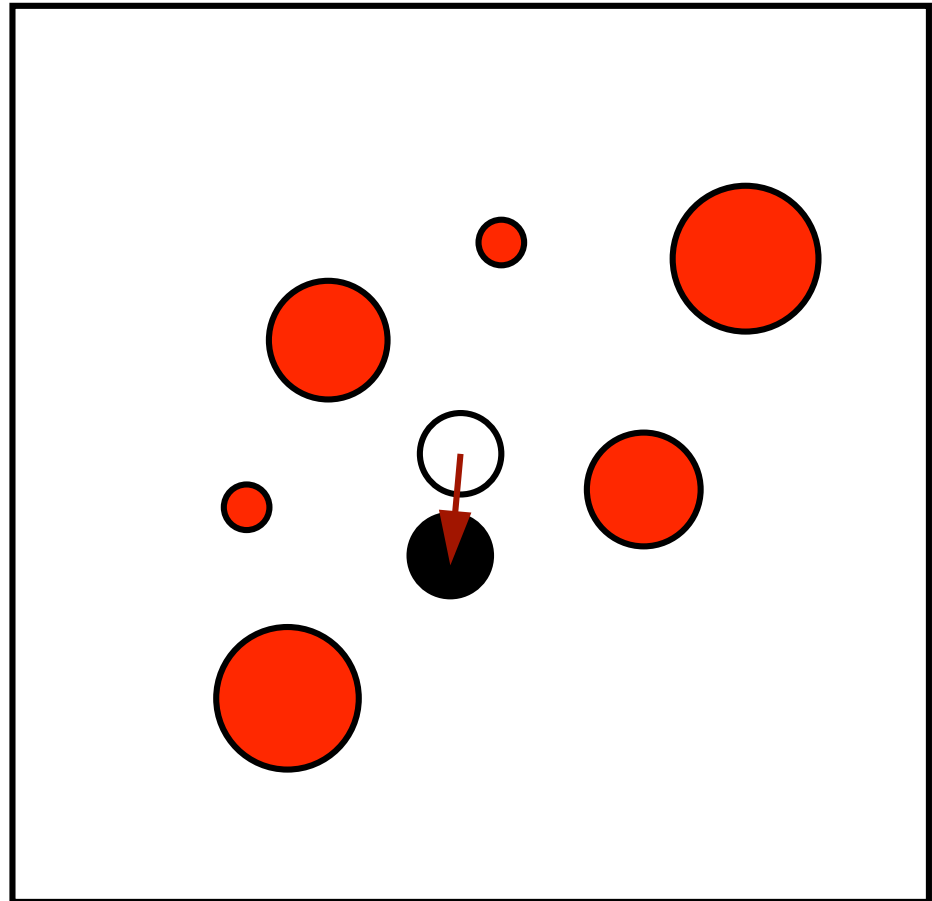
- Single particle toy problem:
 - Start at $F=0$
 - Apply strain

Use Hessian to find position correction

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

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

Disordered Case

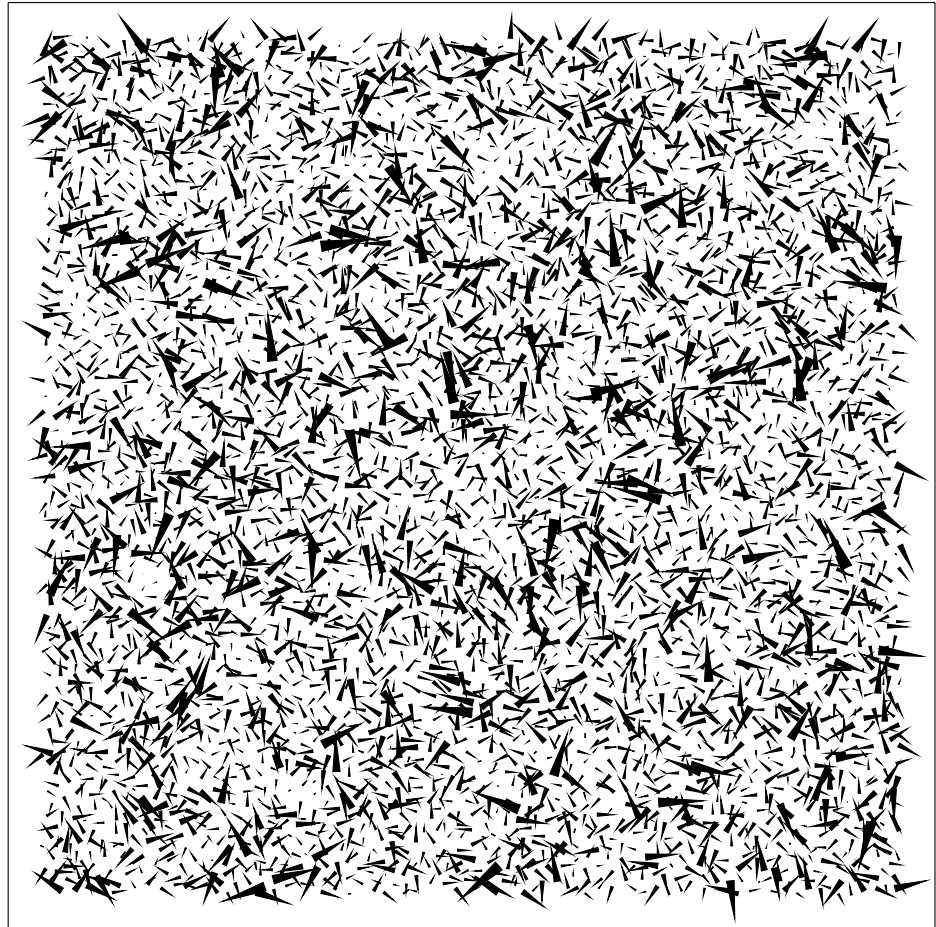


Computing the response

- Back to full assembly:

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

- Measure of local disorder.
- No spatial correlations in our samples.



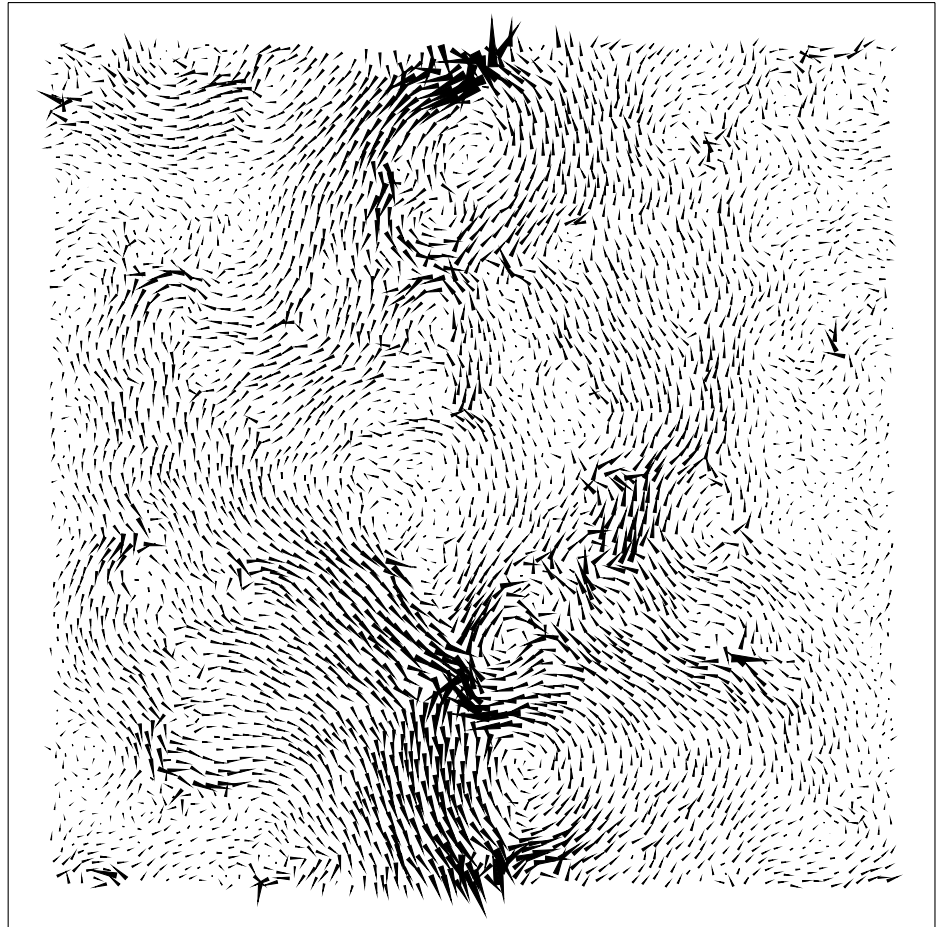
Computing the response

- Back to full assembly:

$$\vec{d}r_i = \gamma \sum_j \mathbf{H}_{ij}^{-1} \vec{\Xi}_j$$

Force balance:

Affine forces, $\vec{\Xi}$, must
be balanced by
correction forces,
 $\mathbf{H}^{-1} dx_j$



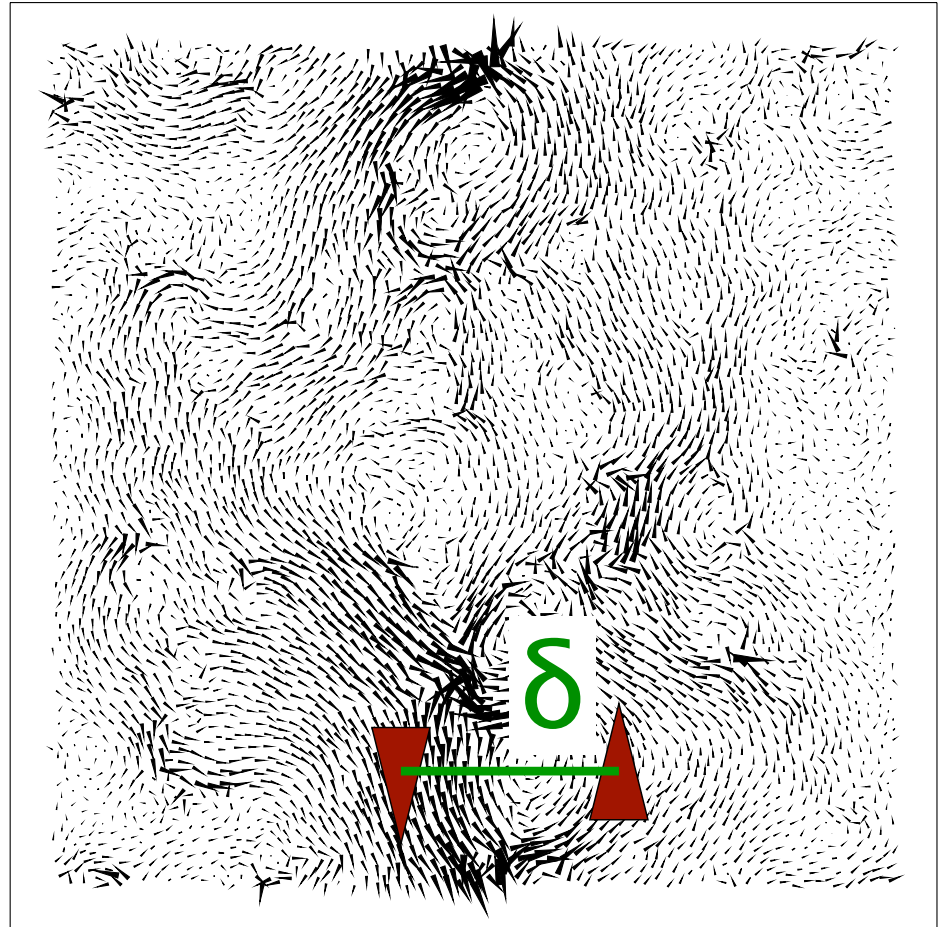
Outline

- Overview
- **Scale free vortices:** (CEM [PRL submitted?])
 - Autocorrelation $g(r)$
 - Normal-mode decomposition
- Plastic nucleation
- Outlook

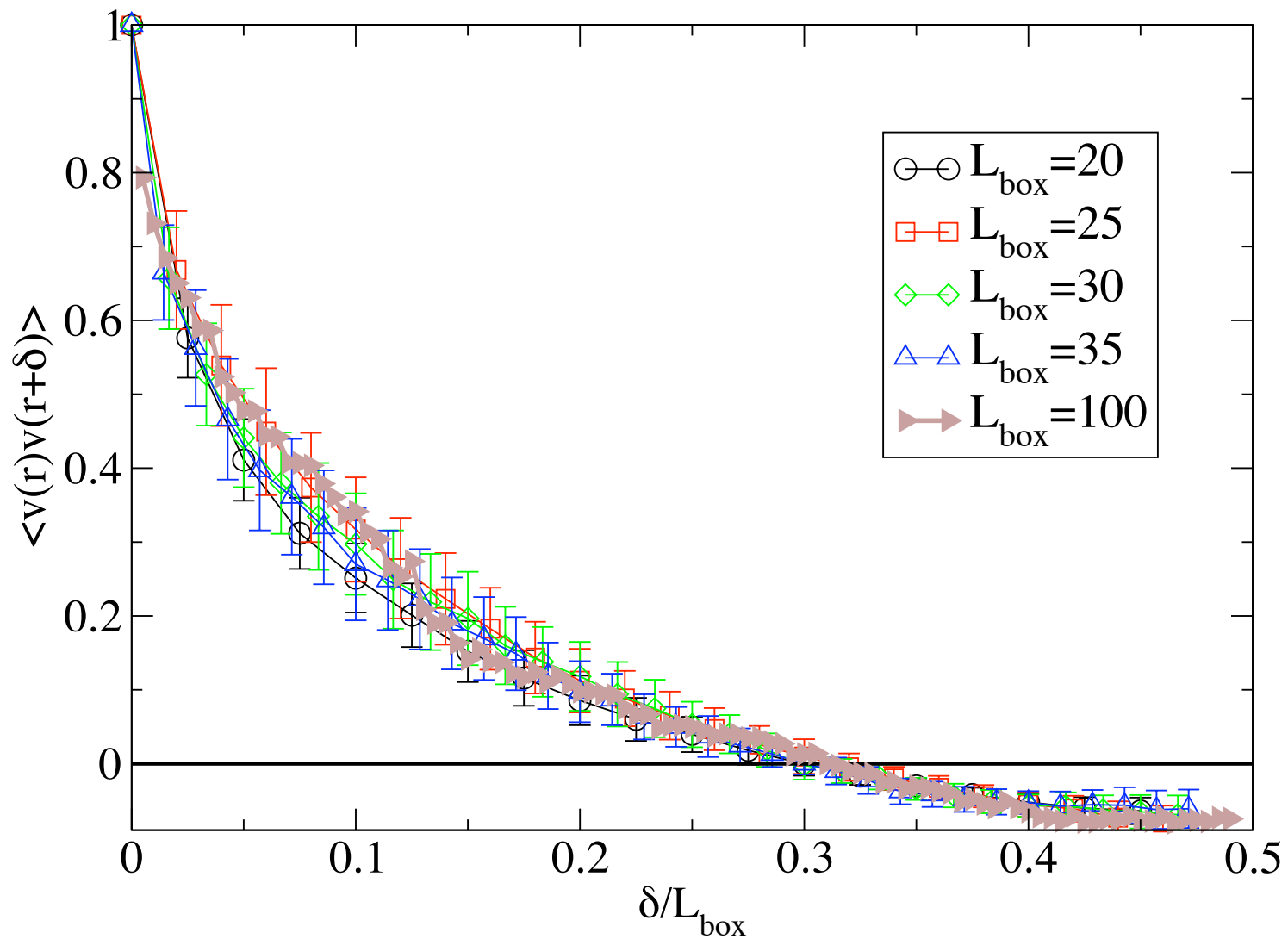
Autocorrelation, $g(\delta)$

$$g(\vec{\delta}) \doteq \int \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r} + \vec{\delta}) d\vec{r}$$

- Usual autocorrelation
- Measures “vortex size”
- Characteristic length?



Autocorrelation, $g(\delta)$



$g(\delta)$: Theoretical form

Recall:

$$\vec{d}r_i = \gamma \sum_j \mathbf{H}_{ij}^{-1} \vec{\Xi}_j$$

Then:

$$\vec{d}r_i = \gamma \sum_p \left(\frac{\vec{\Xi}_p}{\lambda_p} \right) \vec{\psi}_{ip}$$

• **Note:**

- $\vec{\Xi}_p$ are random
- Ψ_p are plane waves to first order in $\vec{\Xi}$

$g(\delta)$: Theoretical form

Recall:

$$\vec{d}r_i = \gamma \sum_j \mathbf{H}_{ij}^{-1} \vec{\Xi}_j$$

Then:

$$\vec{d}r_i = \gamma \sum_p \left(\frac{\Xi_p}{\lambda_p} \right) \vec{\psi}_{ip}$$

• **Note:**

- Ξ_p are random
- Ψ_p are plane waves to first order in Ξ

Approximate $d\mathbf{r}_i$ as random sum of plane waves:

$$\vec{d}r_i \sim \sum_{k=(m,n)} \phi_{mn} \frac{e^{2\pi i \vec{k} \cdot \vec{x}_i / L}}{|\vec{k}|}$$

Then $g(\delta)$ is:

$$g(\vec{\delta}) \sim \sum_{k=(m,n)} \frac{\cos(2\pi \vec{k} \cdot \vec{\delta} / L)}{k^2}$$

Simulation and Theory

$$g(\vec{\delta}) \sim \sum_{k=(m,n)} \frac{\cos(2\pi \vec{k} \cdot \vec{\delta}/L)}{k^2}$$

Similar to DiDonna
+Lubenksy,

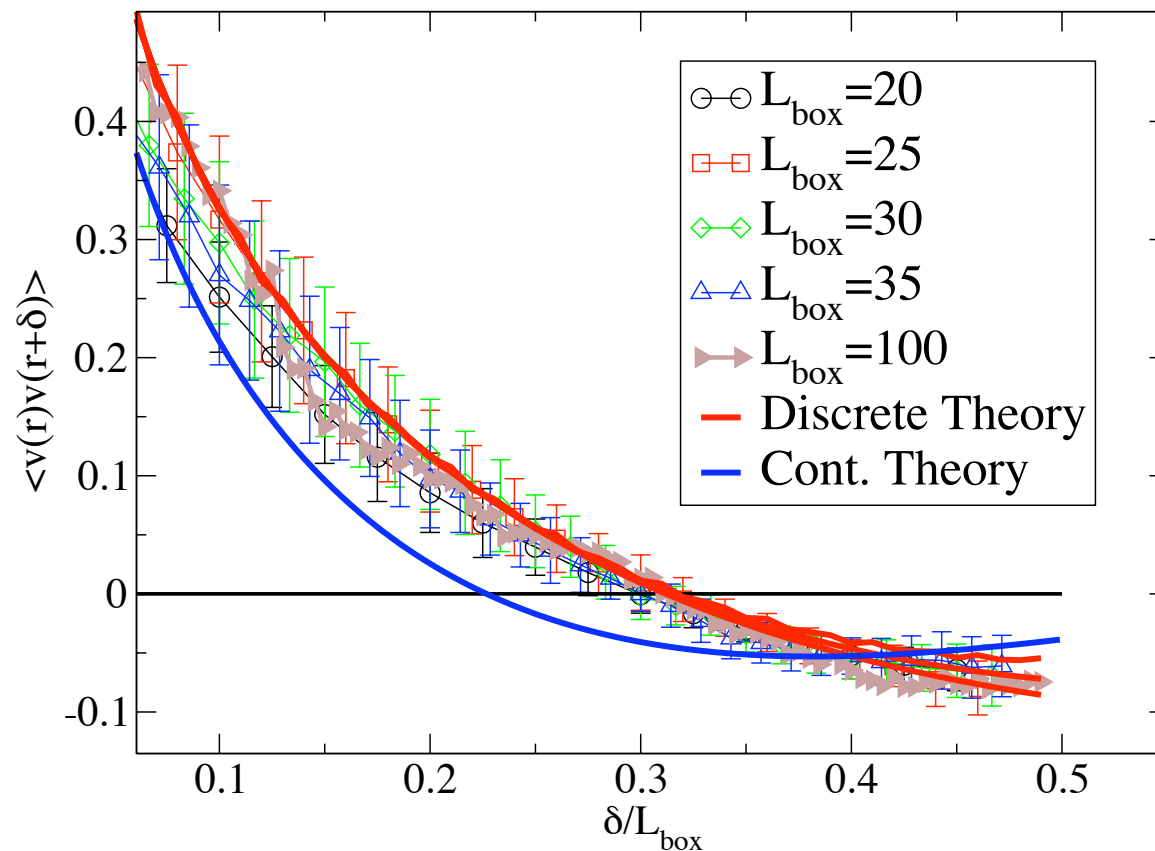
- $g(k) \sim 1/k^2$

but:

- Fully discrete derivation

Blue curve:
Semi-continuum

Red curve(s):
Partial sum (n=40)
3 different angles



Outlook

Summary:

- Displacement field from random forces on a homogeneous sheet.
- Predicts “vortex length” $\sim .32 L_{\text{box}}$
- No length scale comes out of data or theory.

Future Direction:

- When does the assumption of uncorrelated Ξ break down?
- Can this bring out a characteristic length?
- How to make systematic pert. expansion for H?

Outline

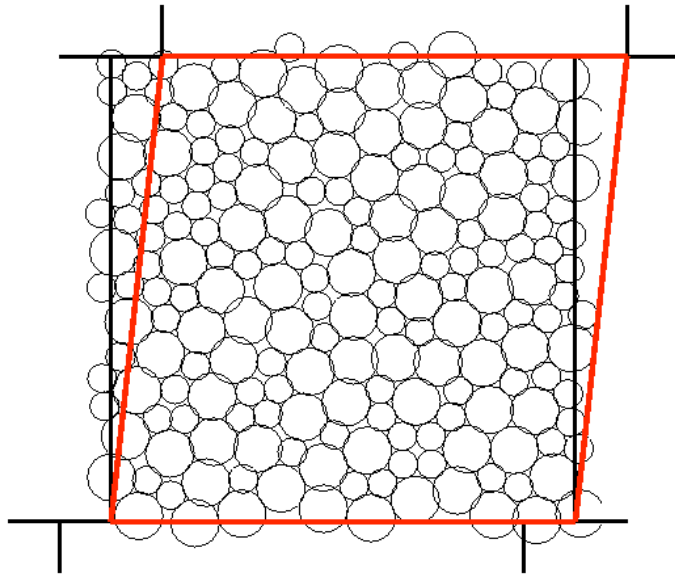
- Overview
- Scale free vortices
- **Plastic nucleation** (CEM+A. Lemaître [PRL 2004] [PRE submitted])
 - Energy Landscape Perspective
 - Breakdown of Elasticity in Real Space
- Outlook

Only if I have time.

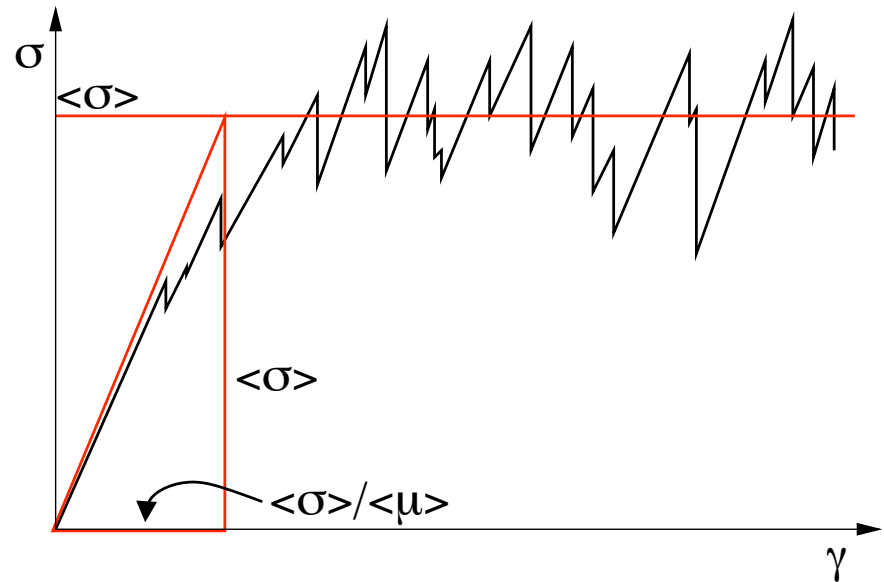
Large Strains

- Procedure:
- Minimize energy
 - Shear system
 - Repeat

- Procedure is:
 - Athermal, Quasi-static
 - “minimalist”



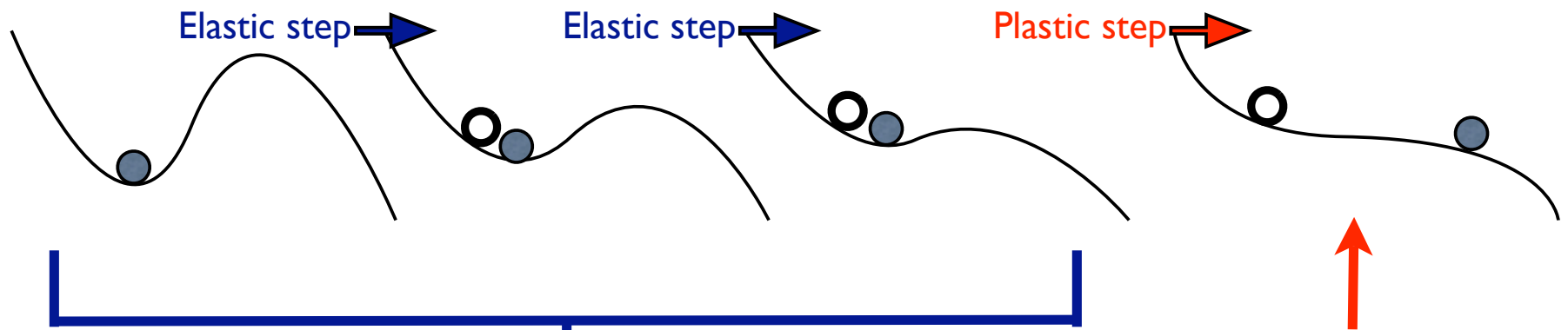
“Lees-Edwards” Cell



Typical Stress-Strain Curve

Landscape Perspective

Increasing strain \Rightarrow

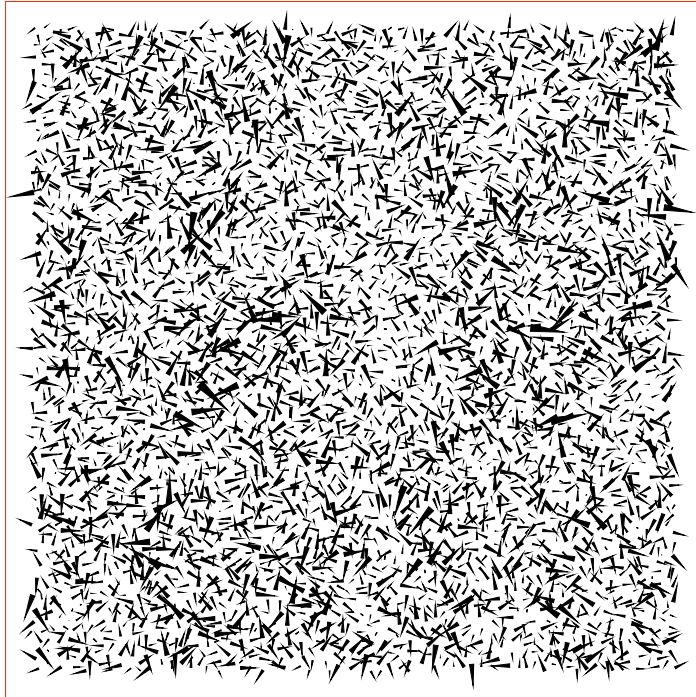


Response can be linearized.
Deformation is reversible (elastic).

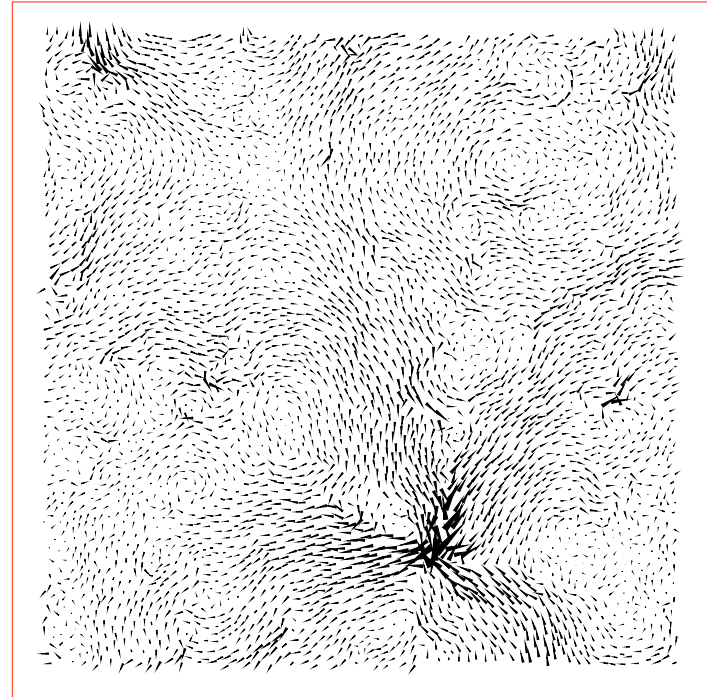
Response cannot be linearized.
Deformation is irreversible (plastic).

Recall:
$$d\vec{r}_i = \gamma \sum_j \mathbf{H}_{ij}^{-1} \vec{\Xi}_j$$

Singular Mode



Ξ

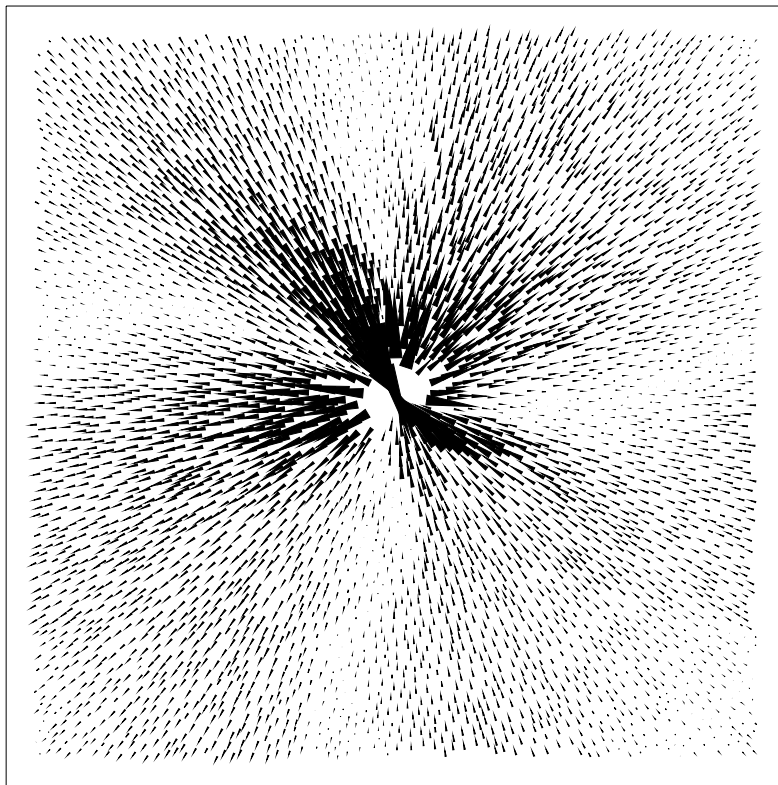


dr

Plastic nucleation is intrinsically non-local!
Cannot be detected via Ξ !

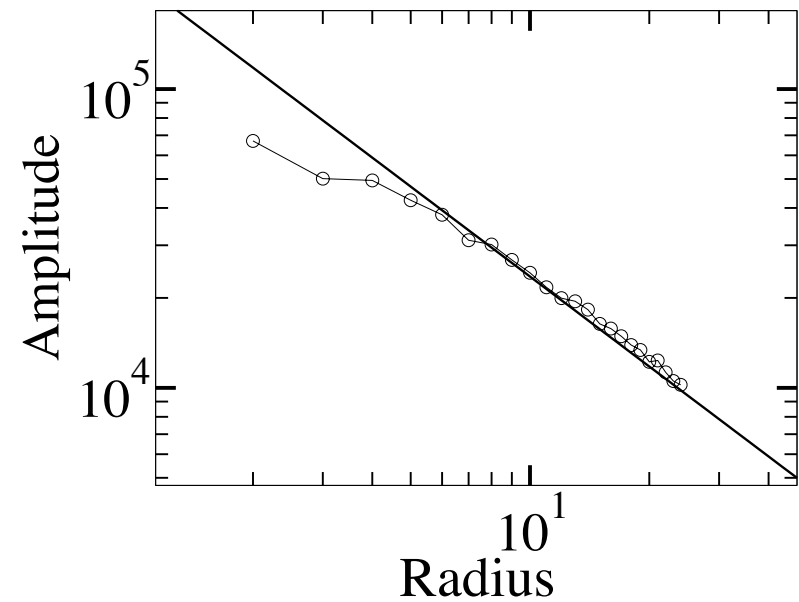
Singular Mode

Can critical mode be rationalized elastically?



Lamé-Navier predicts, for quadrupoles:

$$v_r(r) = \frac{2A}{r^3} + \frac{(1 + \kappa)B}{r}$$



Outlook

Summary:

- Diverging elastic displacement triggers plastic nucleation
- Onset of plasticity is NOT detectable via the local quantities ($\sigma, \bar{\epsilon}, \mu_{\text{Born}}$, etc)

Future Direction:

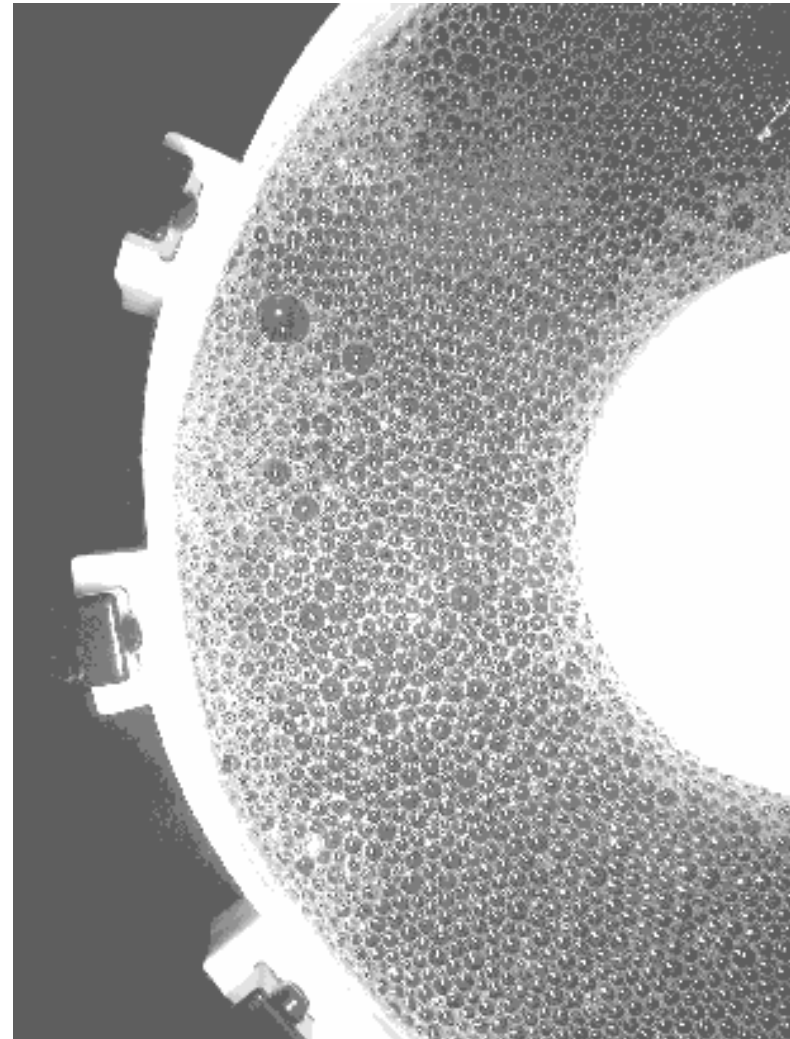
- Can a critical “core” region be defined?
- How might these core regions affect the non-critical elastic behavior?

Related APS talks:

- Majumdar (Behringer) B8
- Schall (Cohen, Spaepen, Weitz) B2 I
- Abate, D I
- Walder (Dennin, Levine) R8

Jammed Systems

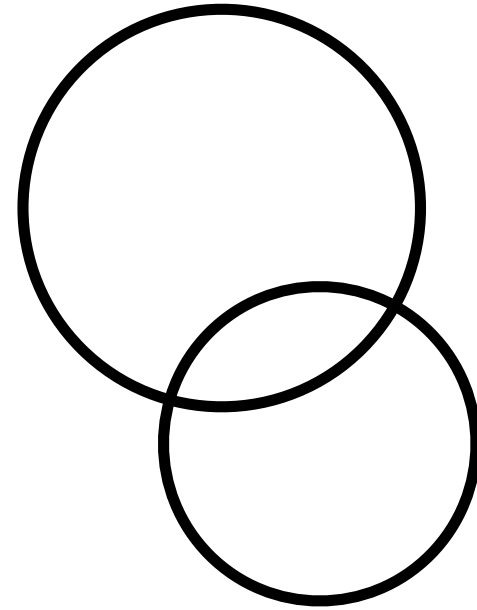
- **Examples:**
 - Bubbles/Emulsions
 - Grains
 - Glasses
- **Non examples:**
 - Suspensions / **Rigid** Grains
- **Differences:**
 - Inertia/Temp/Dissipation
- **Similarity:**
 - Geometry!
- **Issues:**
 - Characterizing disorder
 - Elasticity / Vibrations
 - Plasticity / Yielding



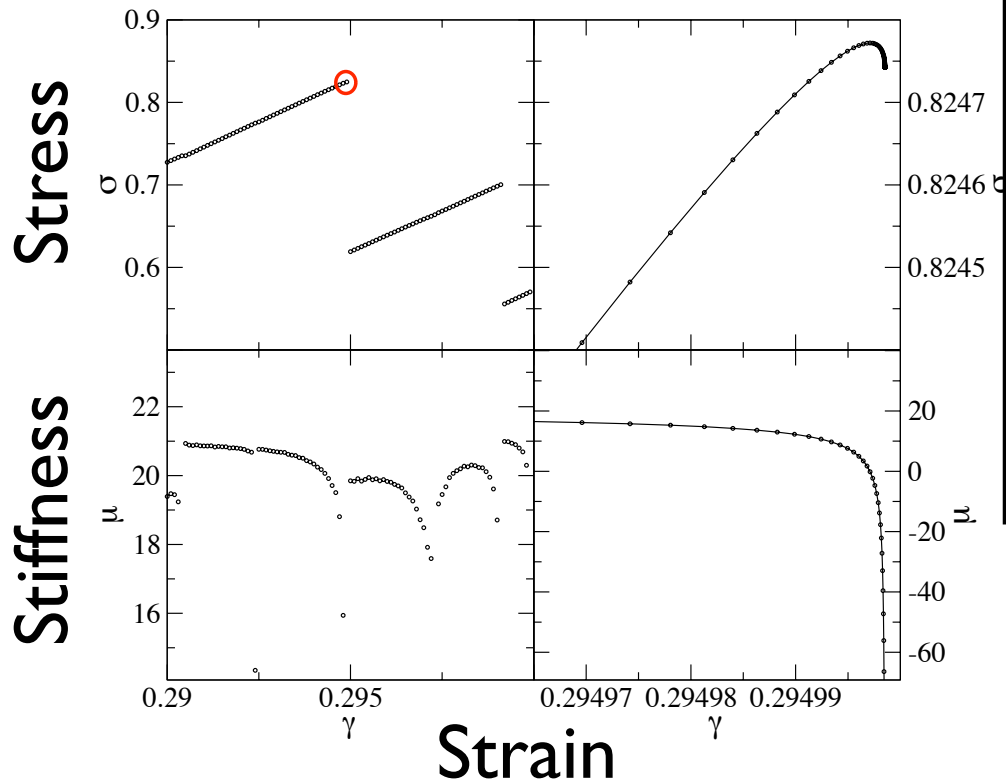
From (M Dennin)

Numerical protocol

- All results for 2D
- Binary mixtures to prevent crystallization
- Interactions:
 - Harmonic contact repulsion
 - Standard Lennard-Jones 6-12
- Preparation: “violent” quench from initial random state.



Approach to Singularity



Initiation of single plastic event

$$\begin{aligned}
 \frac{d\sigma}{d\gamma} &= \frac{\partial\sigma}{\partial\gamma} + \sum_i \frac{\partial\sigma}{\partial r_{i\alpha}} \frac{dr_{i\alpha}}{d\gamma} \\
 &= \frac{\partial\sigma}{\partial\gamma} - \sum_{ij} \Xi_{i\alpha} H_{i\alpha j\beta}^{-1} \Xi_{j\beta} \\
 &= \frac{\partial\sigma}{\partial\gamma} - \sum_p \frac{\Xi_p^2}{\lambda_p}
 \end{aligned}$$

Catastrophe Theory:

$$\begin{aligned}
 \lambda_0 &\sim \sqrt{\delta\gamma} \\
 \mu &\sim -(\delta\gamma)^{-1/2}
 \end{aligned}$$