Amorphous material in athermal quasistatic shear

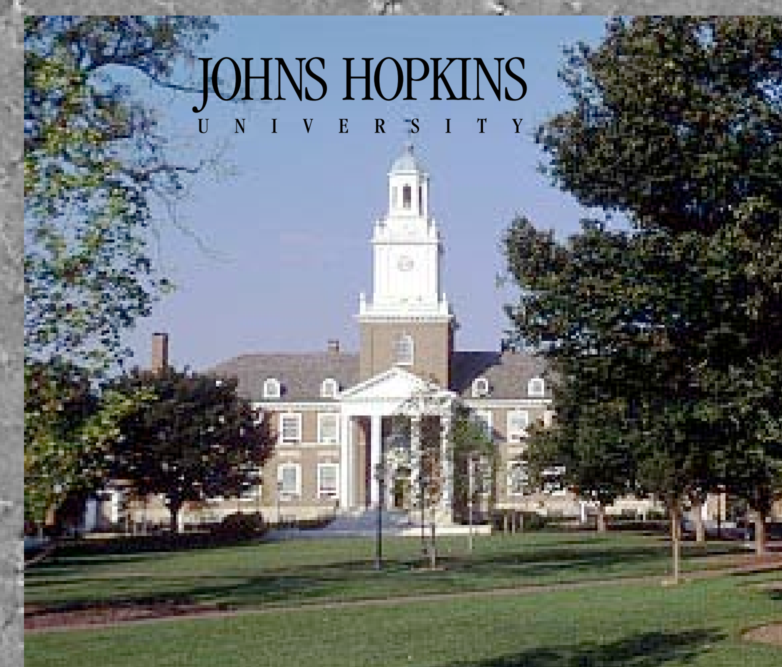
Pacific Institue of Theoretical Physics; July 2007

C.E.M. + A. Lemaître
PRL 2004, PRE 2006

C.E.M.
PRL 2006

LLNL University Relations Program
J.S. Langer, V.V. Bulatov

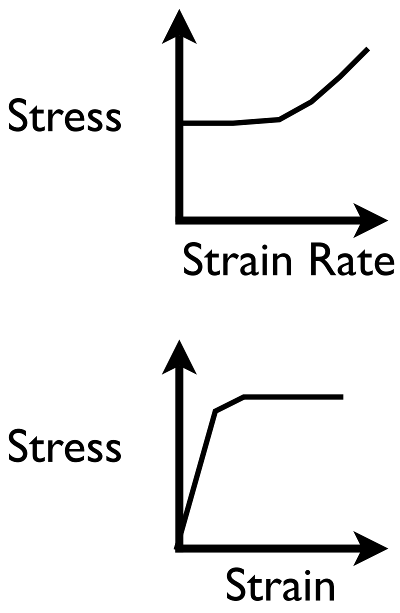
C.E.M. + M.O. Robbins
in preparation

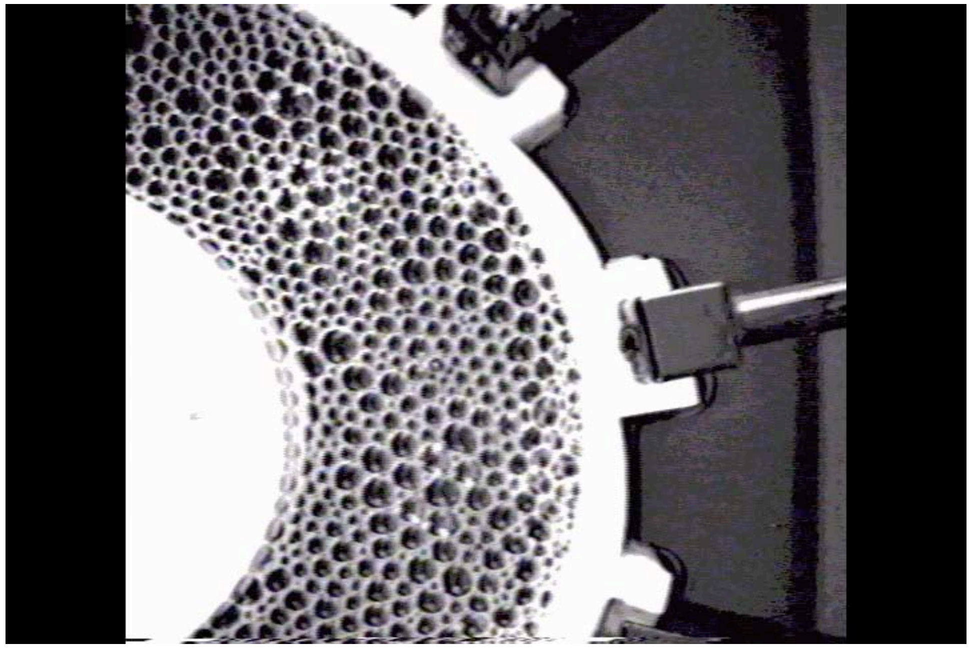


NSF DMR-0454947 and
PHY99-07949

Liquid or solid?

Many amorphous materials behave like solids below some yield stress, but fluids above.
"Yield stress fluid."
"Visco-plastic solid."

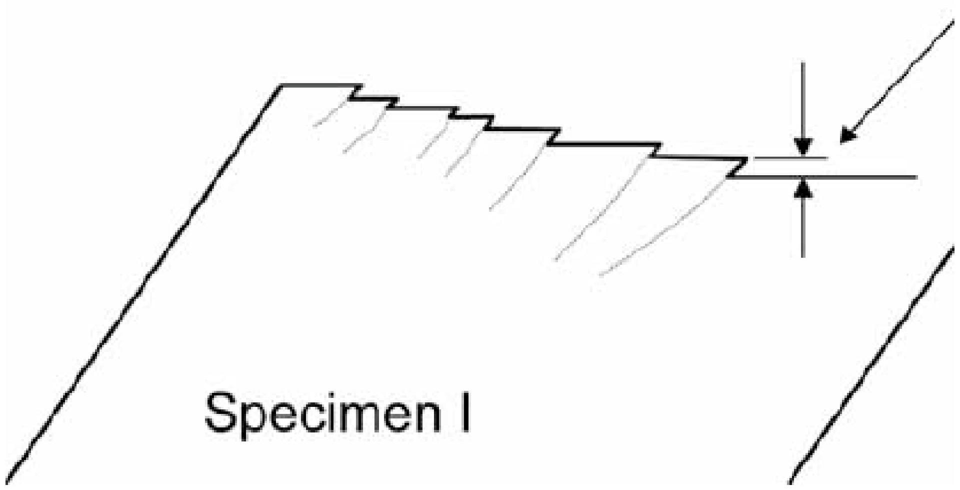




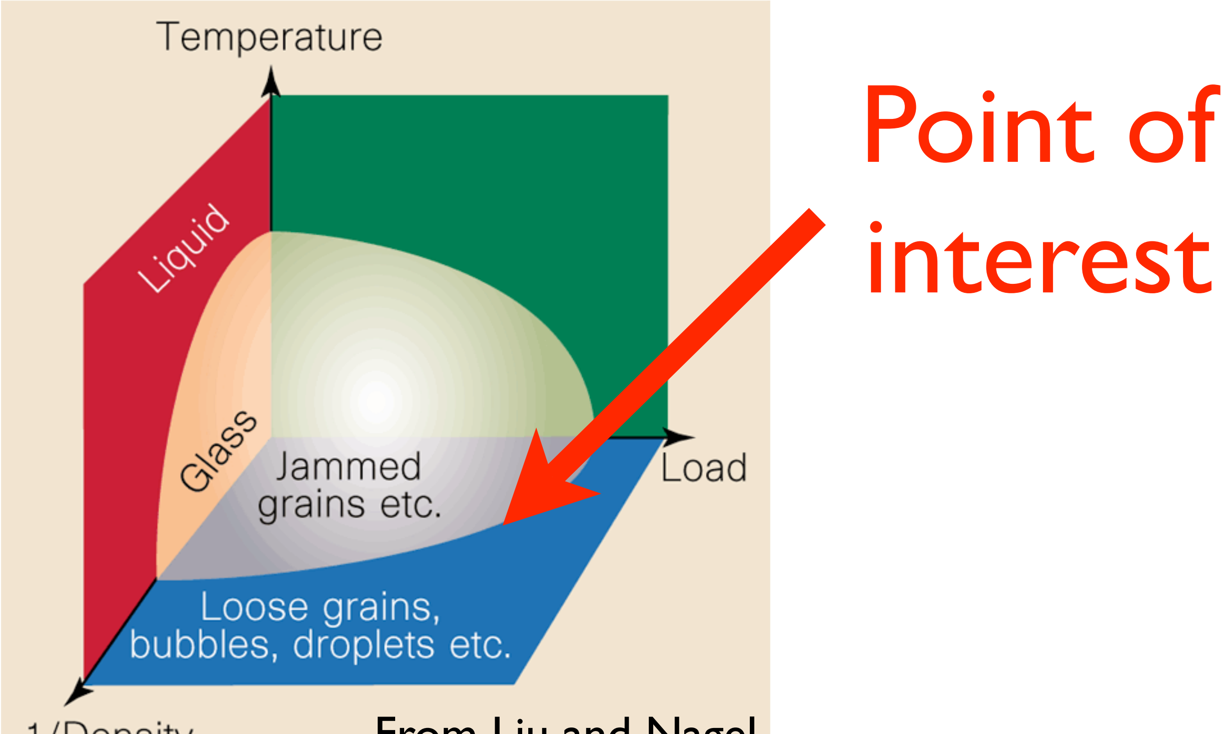
Raft of soap bubbles: From M. Dennin UCI

Examples:
- Emulsions, Suspensions,
- Granular materials
- Metallic glasses

Issues:
- Value of yield stress
- Localization of flow
- Intermittent behavior, etc.

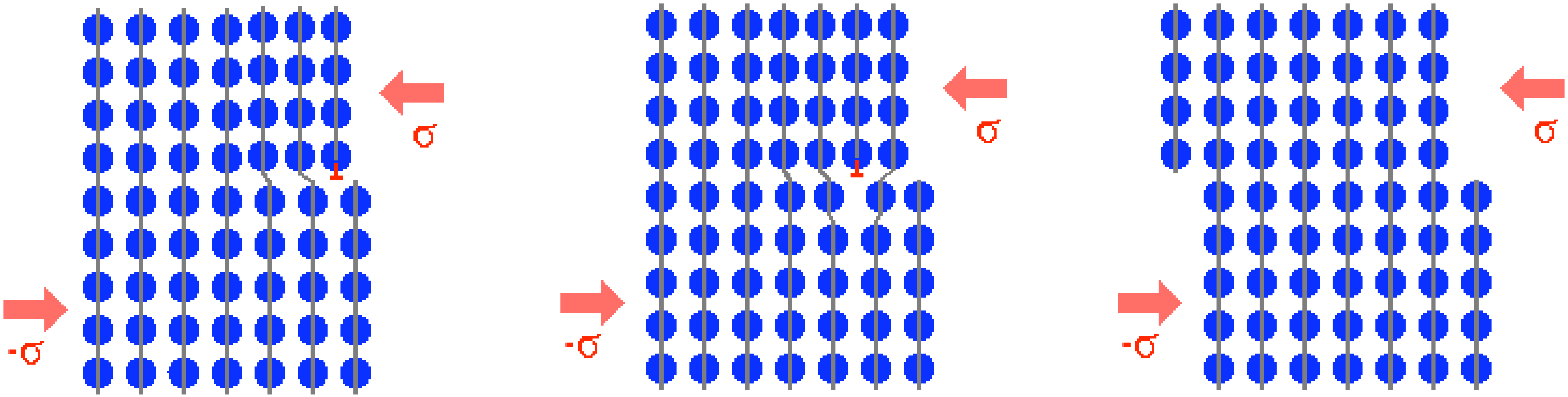


Nanoindentation of metallic glass:
From Moser et. al. ETH



From Liu and Nagel

Dislocations



- Responsible for plastic deformation in crystals
- Nucleated at boundary or in pairs in the interior
- "T" "points" toward extra material
- "Glide" mechanism leaves behind a line of slip
- Particular to crystals!

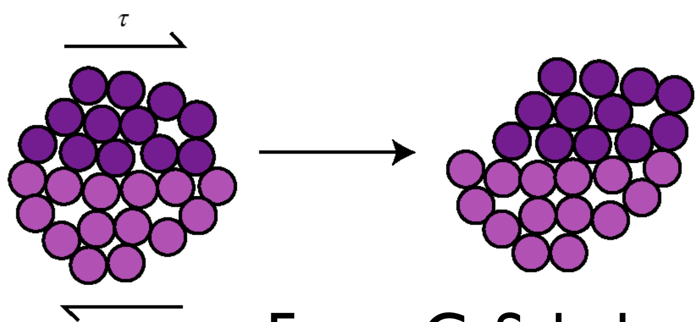
Elastic consequences:

Pressure Decrease

Shear Stress Increase | T | Shear Stress Increase

Pressure Increase

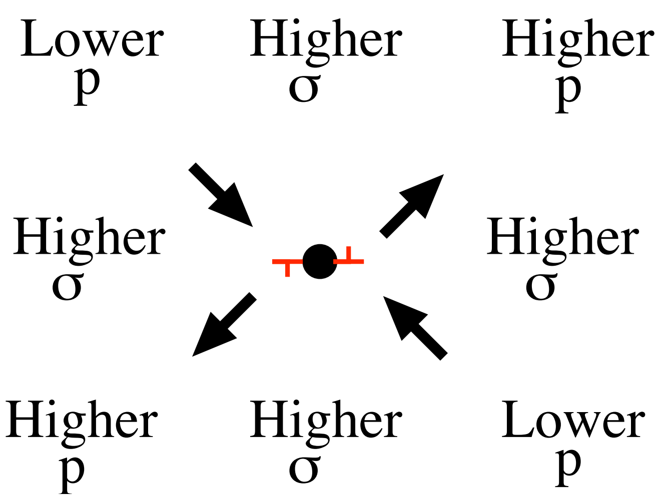
Shear Transformation Zones (STZs)



From C. Schuh

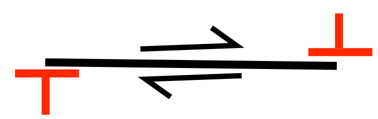
No crystal... no defects

Elastic consequences:

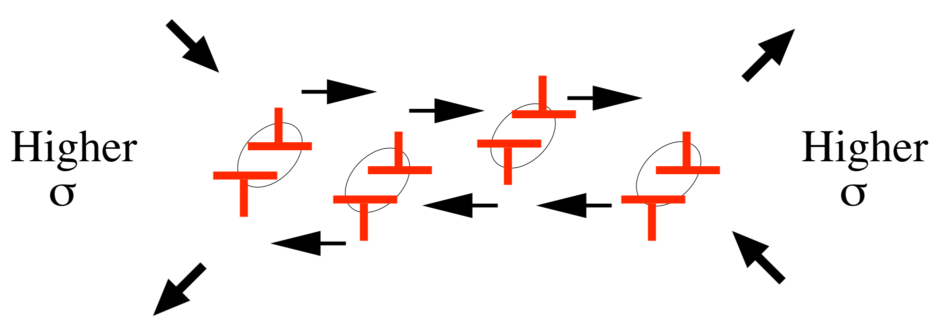


- Argon and Kuo: bubble raft experiments
- Maeda and Takeuchi: computer simulations
- Bulatov and Argon: banding mechanism
- Falk and Langer: mean field theory

Analogous to dislocation glide:



Cascade mechanism:



Look for STZ cascades in numerical model and measure statistical parameters

Outline

- Overview
- The Athermal Quasi-Static (AQS) limit
  - Spatial structure of plastic rearrangement events
  - Scaling with system size and interaction type
- Finite driving rates
  - Strain distributions
  - Spatial organization of strain
  - Direct measure of diverging ξ
  - Relation to thermally driven rearrangement
- Summary

Atomistic Numerical Model

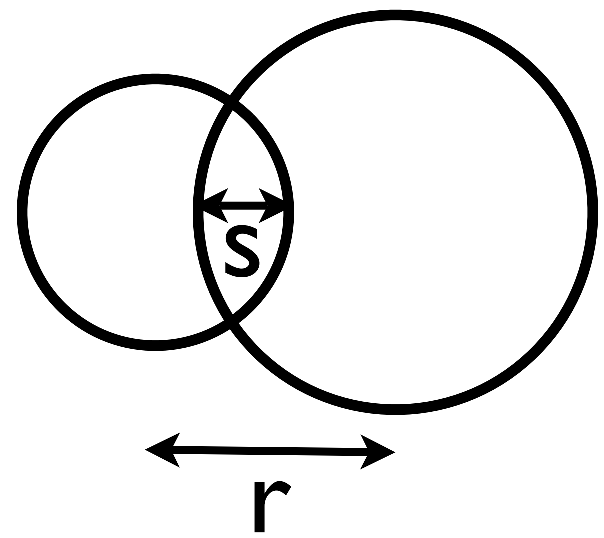
Various interaction potentials:

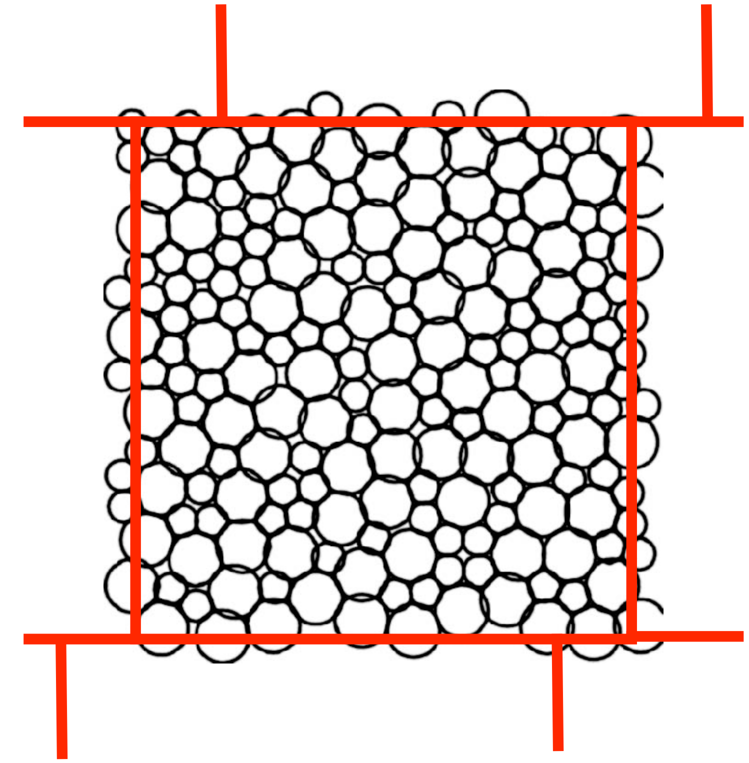
$U_{harm}=(\epsilon/2)\ s^2$

$U_{hertz}=\epsilon\ s^{5/2}$

$U_{Lennard\text{-}Jones}=\epsilon(r^{-12}-r^{-6})$

Binary distribution





Athermal, Quasistatic Procedure:

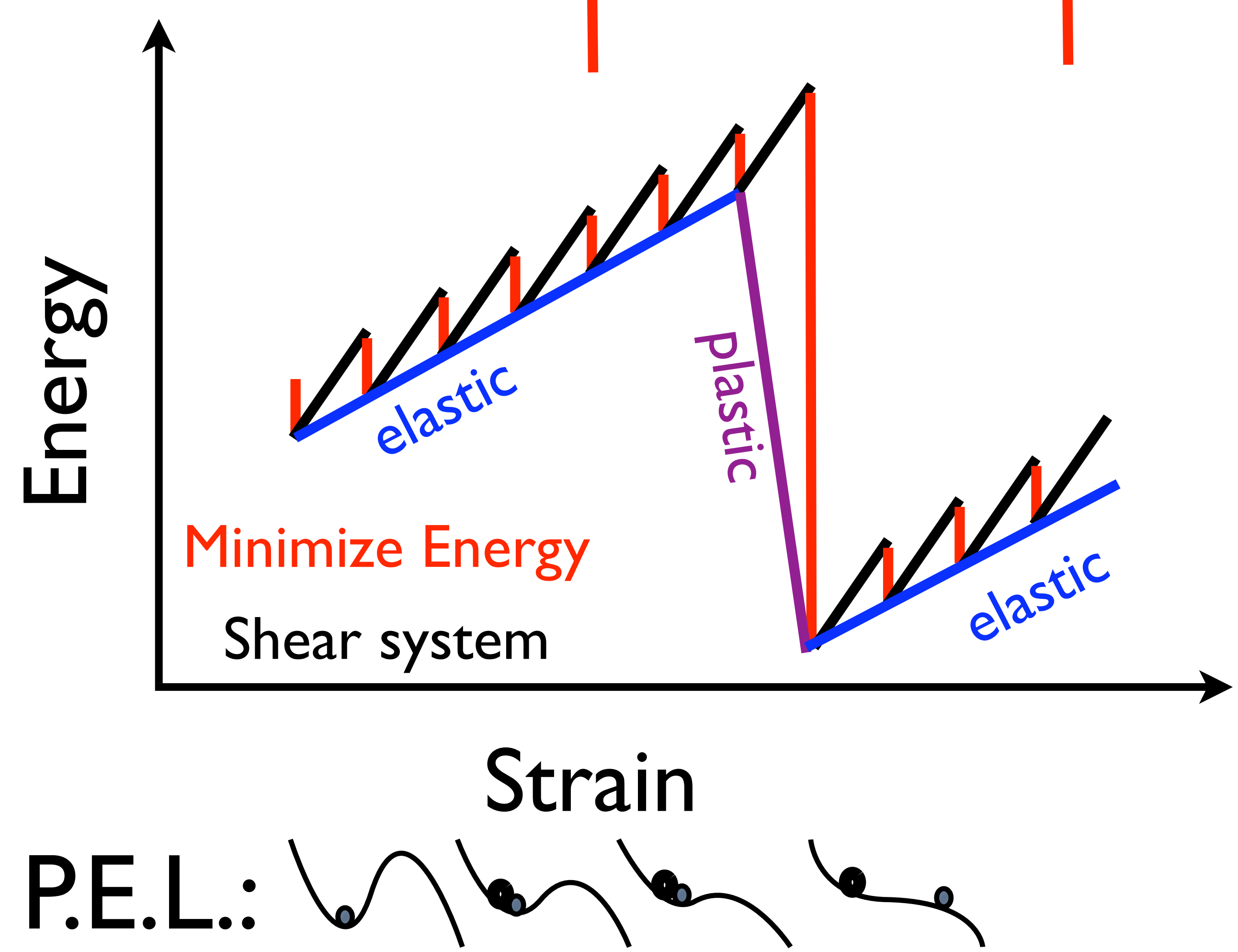
- Minimize potential energy
- Shear boundaries and particles
- Repeat

Represents: $\tau_{pl} << \tau_{dr} << \tau_{th}$

- Bulk metallic glass in the zero temperature, zero strain rate limit
- Granular material or emulsion in zero strain rate limit

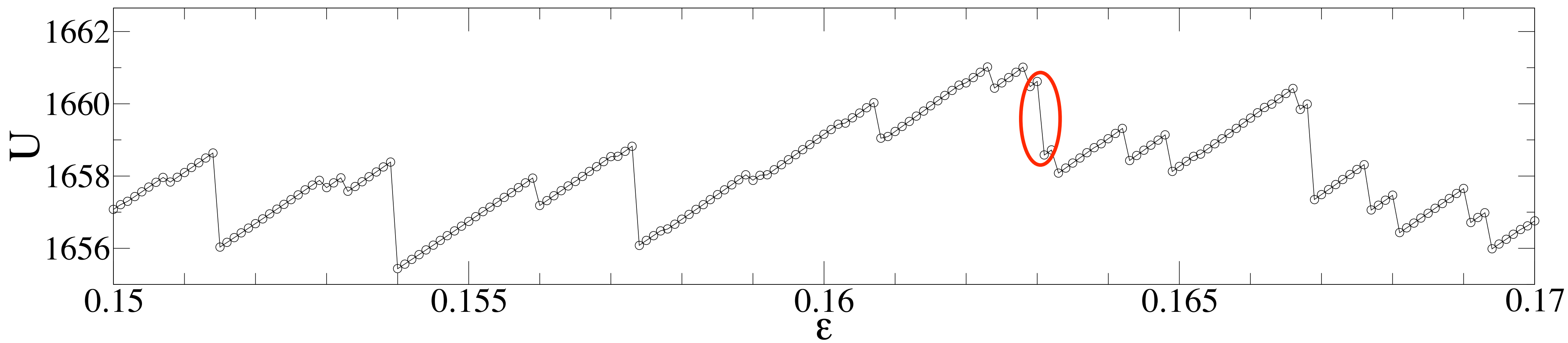
Behavior:

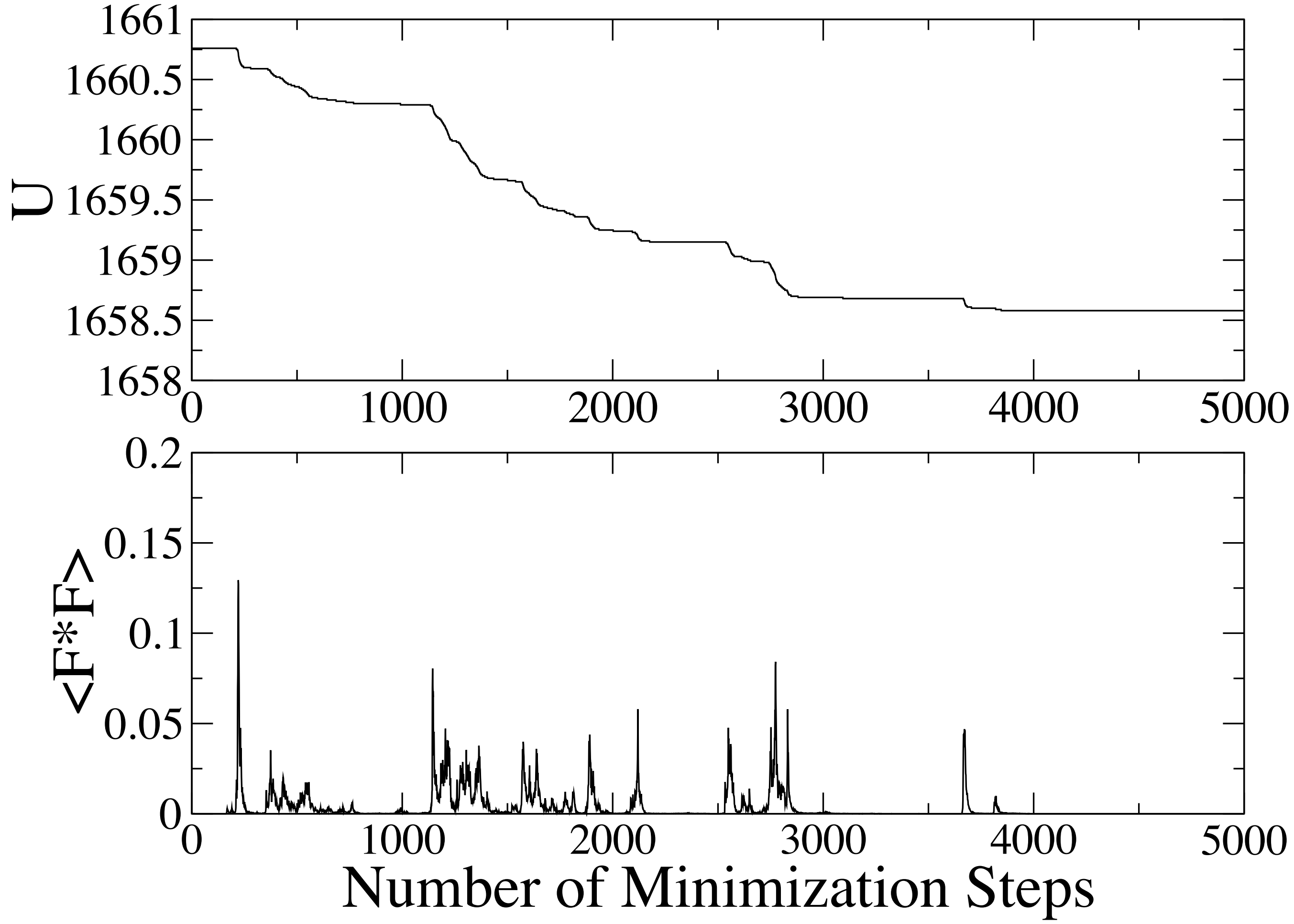
- Discrete plastic jumps separate smooth, reversible elastic segments



after Malandro and Lacks

A typical plastic event

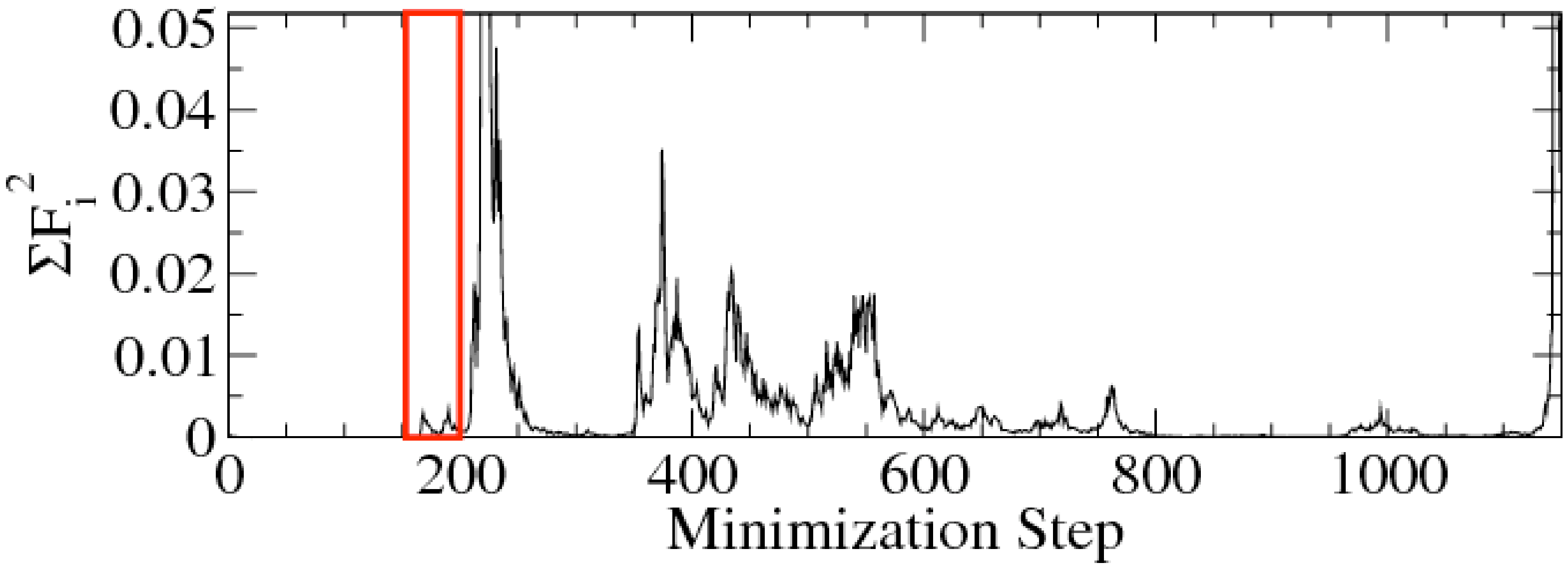




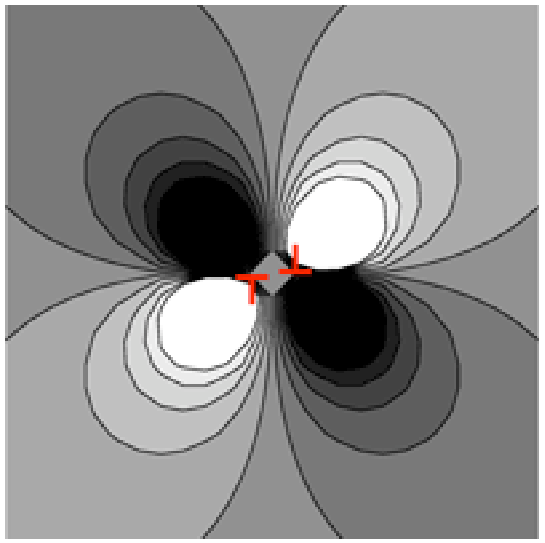
- Single typical plastic event
- All relaxation at one strain
- "Number of minimization steps" analogous to time <F*F>~dU/dt
- Descent is intermittent...

A typical plastic event

Initial portion of descent from previous slide:



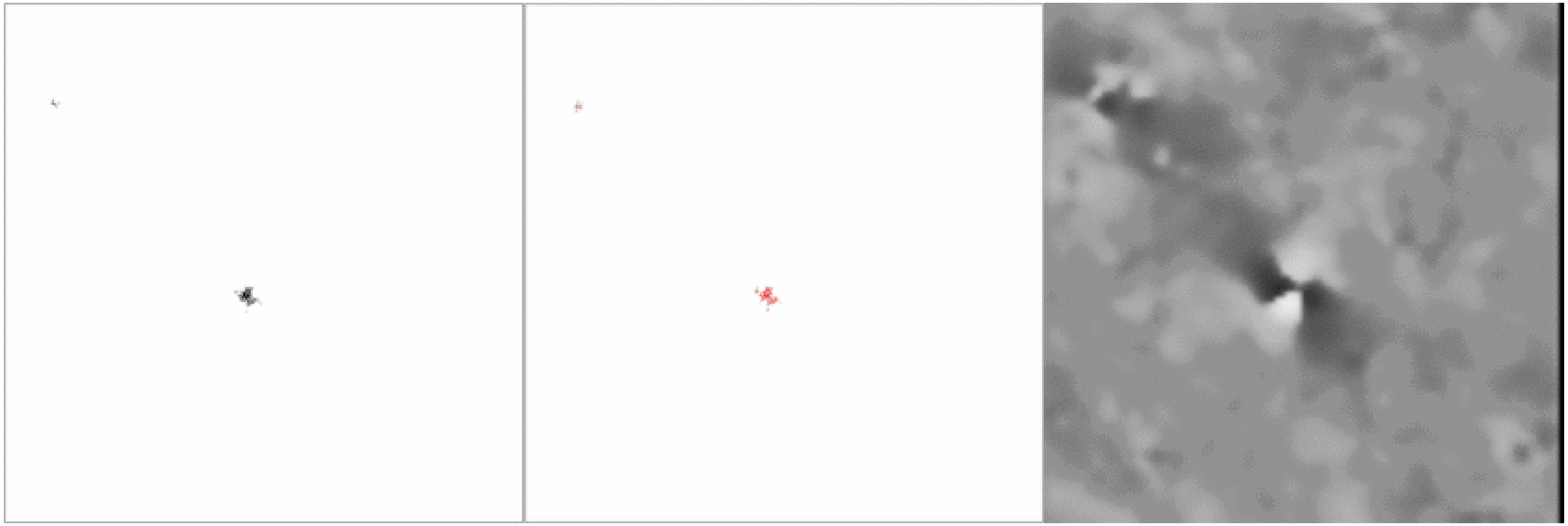
Expected energy change after nucleation of localized slip:



Incremental "slip": $\vec{u} - \langle \vec{u} \rangle$

Cumulative slip

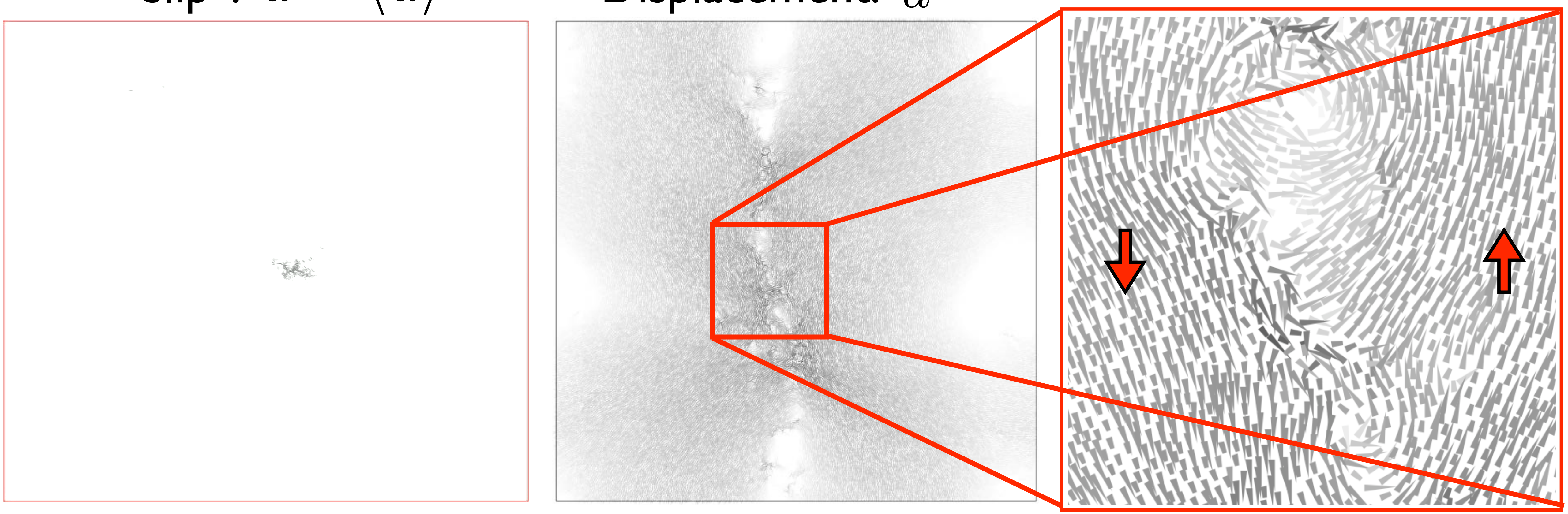
Incremental energy drop



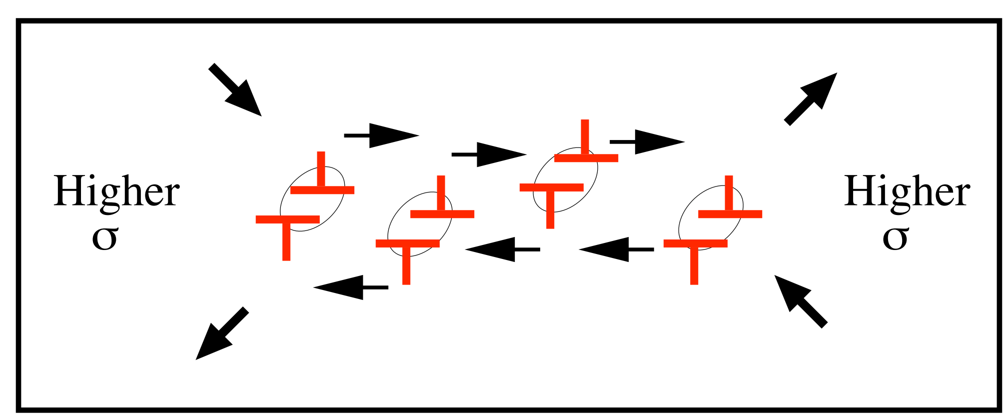
A typical plastic event

At the end of the whole cascade, we are left with a slip line:

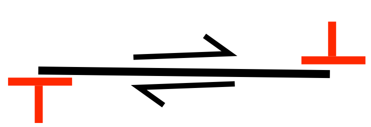
"Slip": $\vec{u} - \langle \vec{u} \rangle$ Displacement: $\vec{u}$



But with local shearing zones:



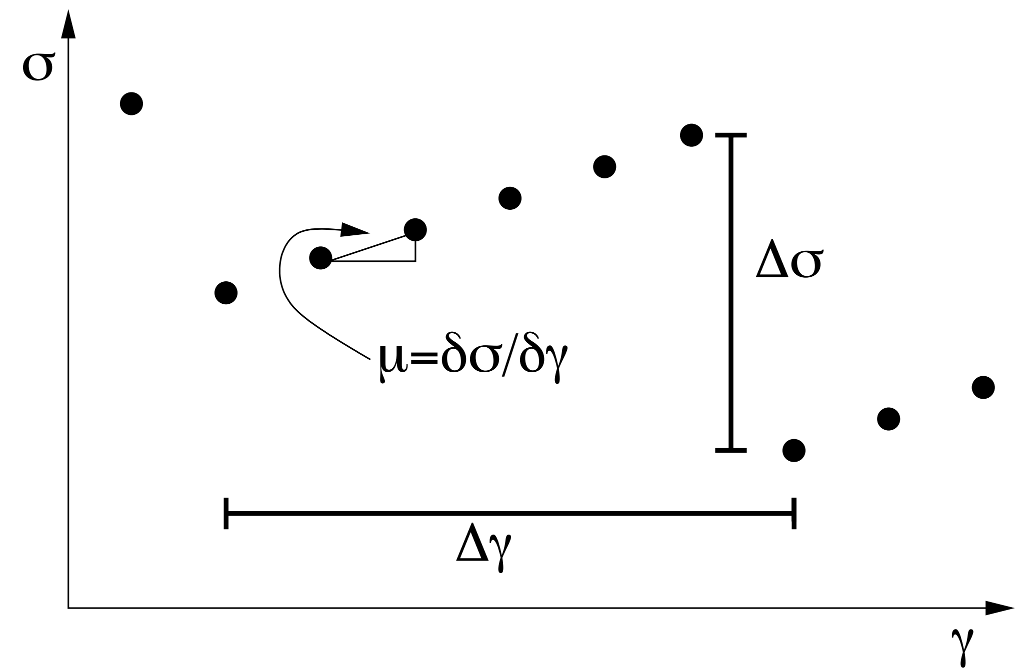
Analogous to dislocation glide:

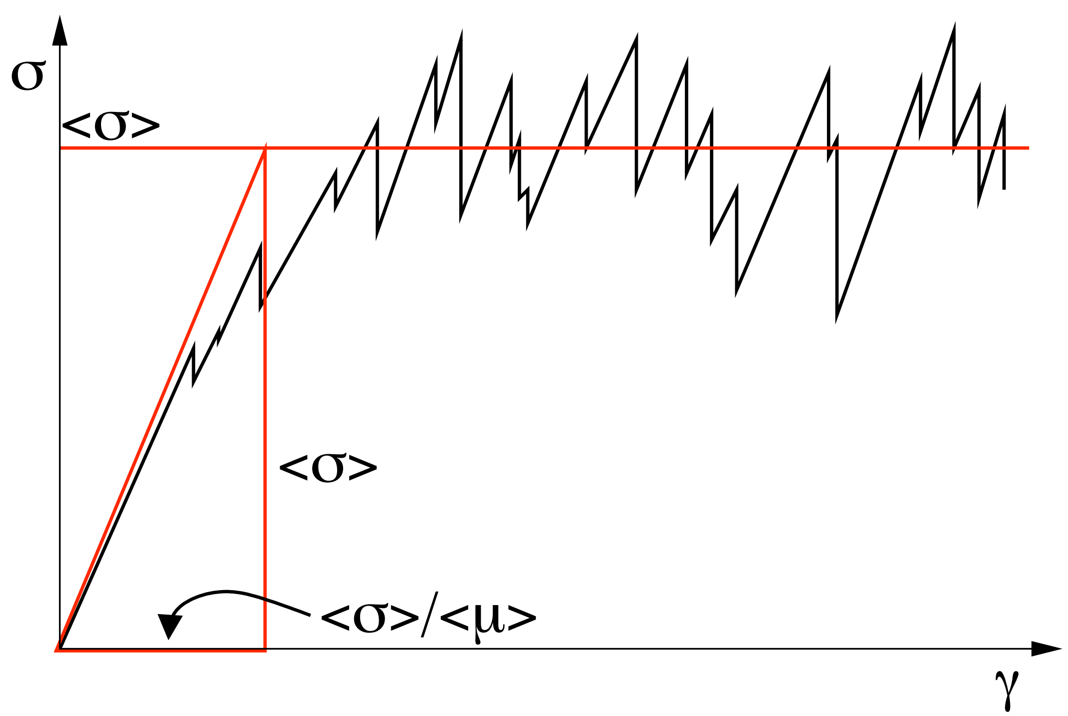


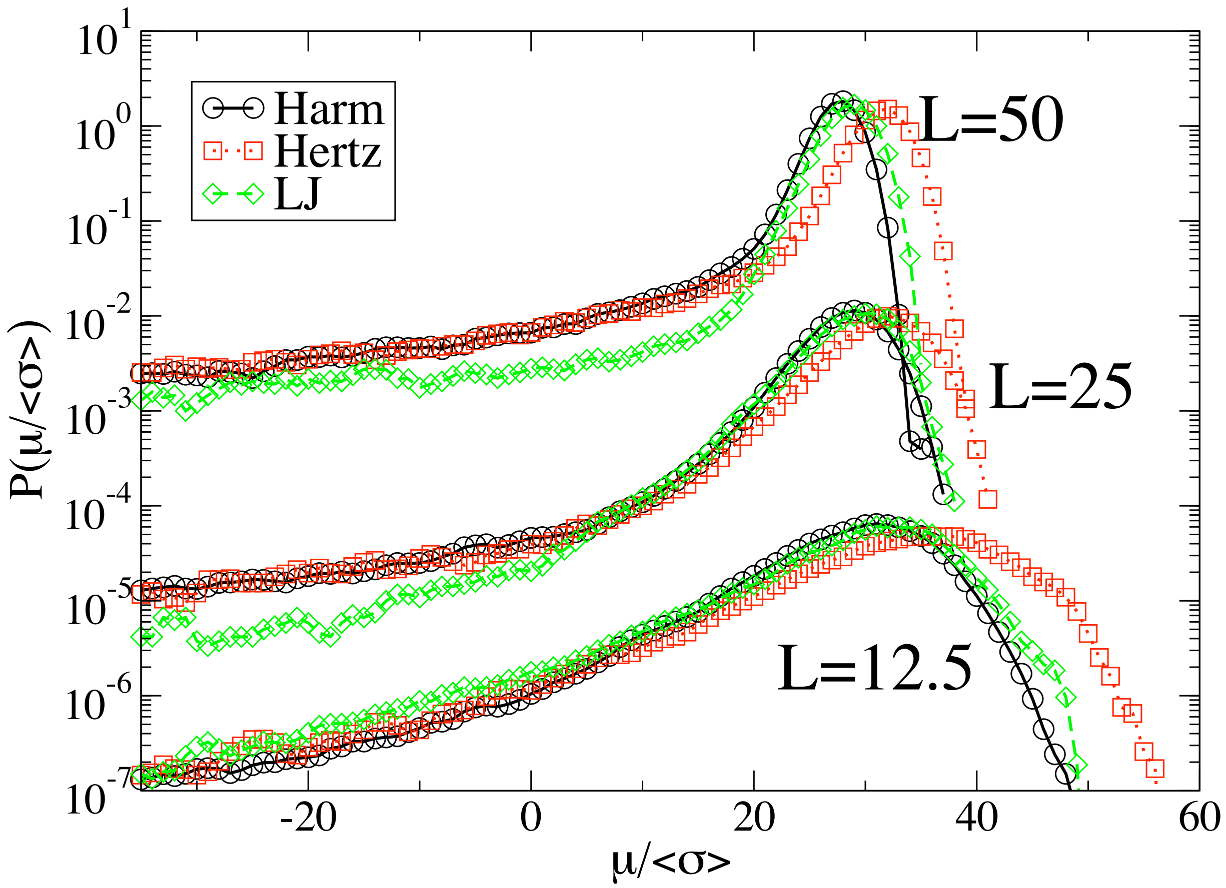
Statistics and size scaling

Collect statistics for different system size and interaction potentials:

- "Modulus"
- Elastic interval
- Stress drop
- Energy drop





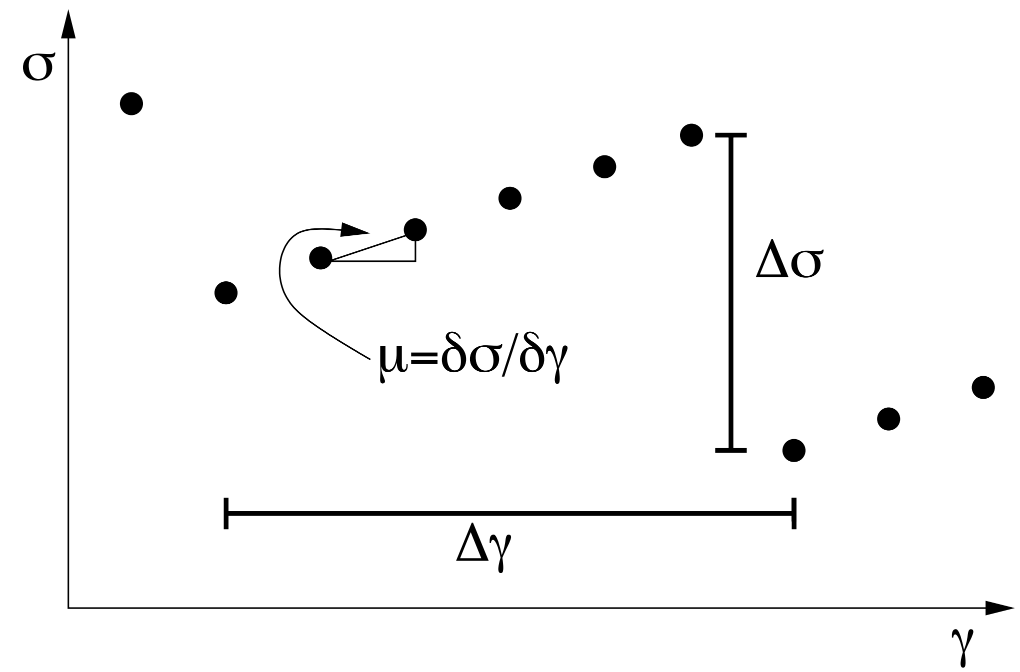


<σ>/μ is universal! ~ 3%

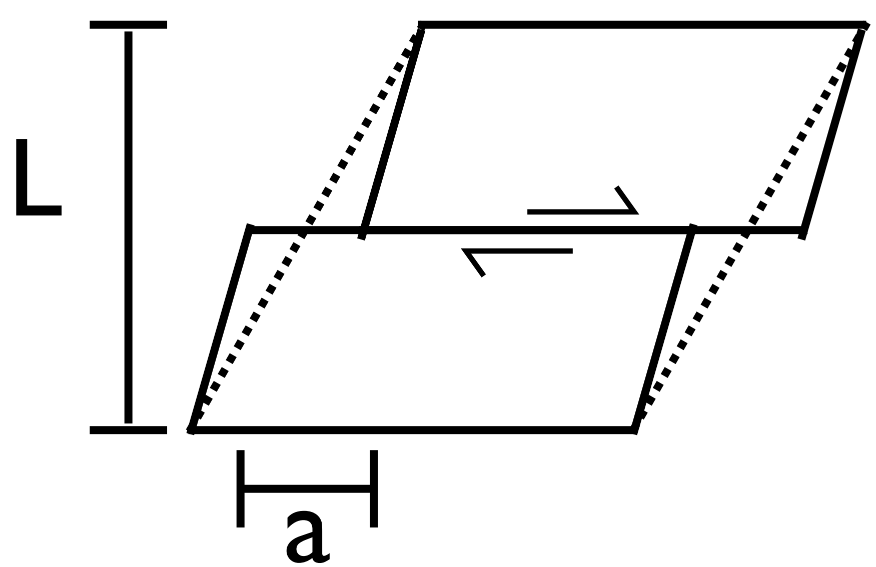
Statistics and size scaling

Collect statistics for different system size and interaction potentials:

- "Modulus"
- Elastic interval: $\Delta\gamma$
- Stress drop: $\Delta\sigma$
- Energy drop: ΔU



Scaling argument: slip by length "a"

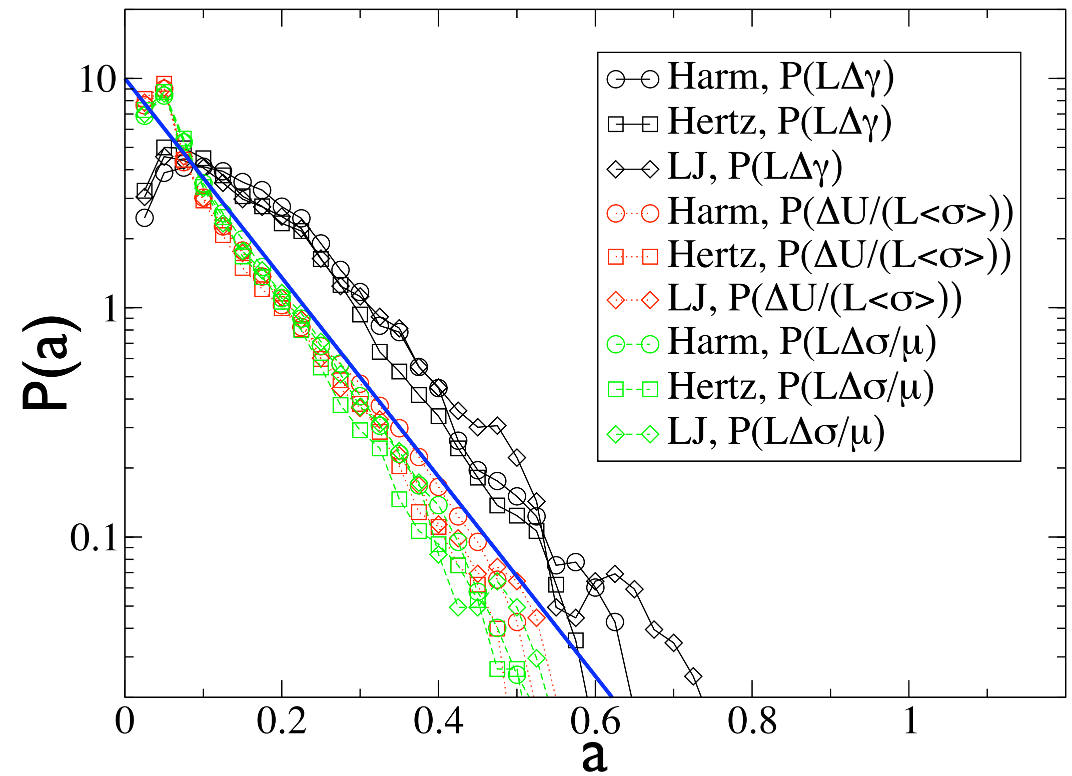


$\Delta\gamma \sim a/L$

$\Delta\sigma \sim \mu\Delta\gamma \sim \mu a/L$

$\Delta U \sim (L^2/\mu)\langle\sigma\rangle\Delta\sigma$
$\sim aL\langle\sigma\rangle$

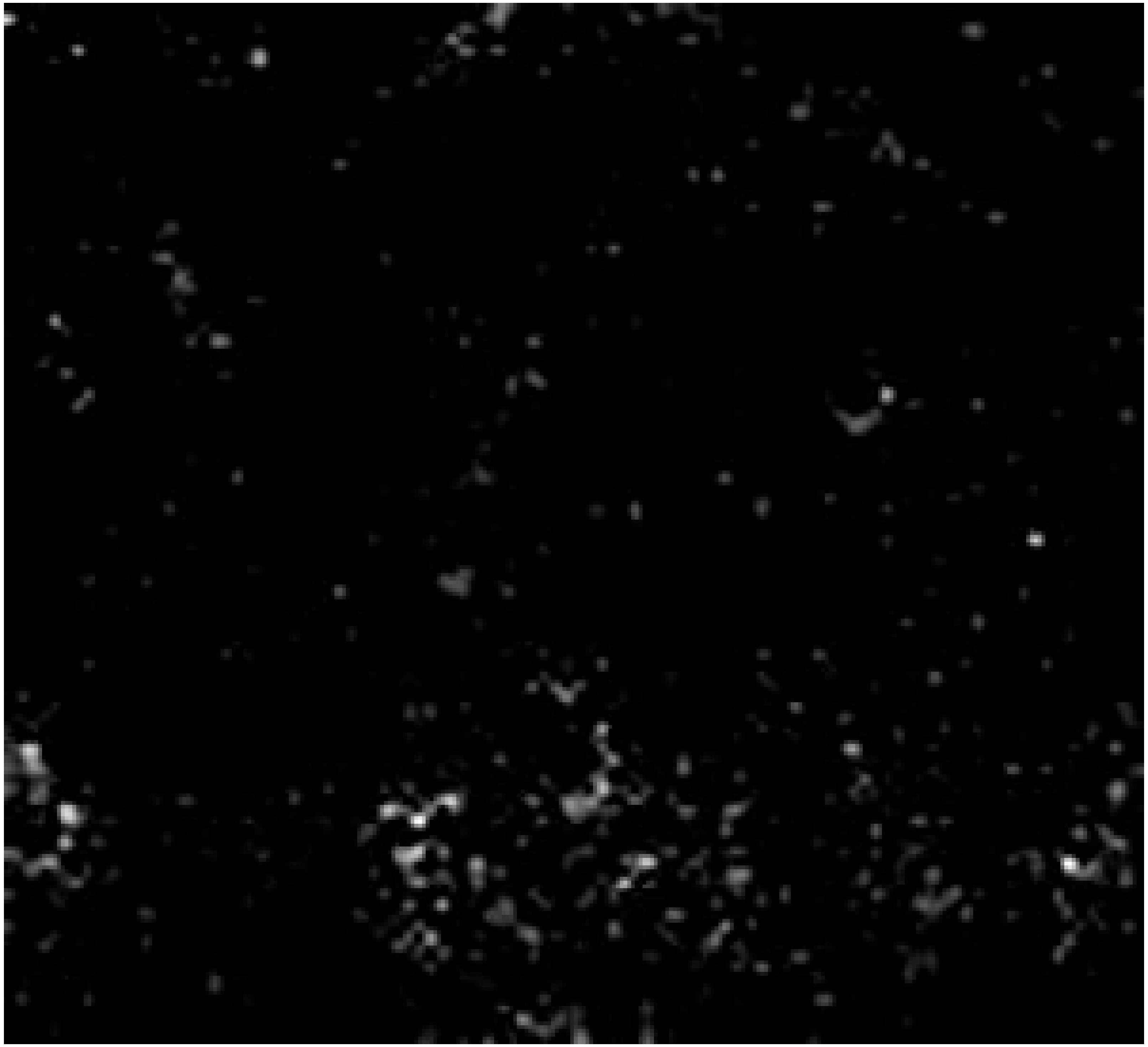
Scaled distributions of $\Delta\gamma$, $\Delta\sigma$, ΔU



Event size independent of potential and scales simply with system size!

Persistent localization?

Red: new slip. White: all slip in last 0.5% strain



- 200x200 sized binary LJ system shown
- Individual events localized.
- Inter-event correlation exists but short-lived.
- No persistent localization.

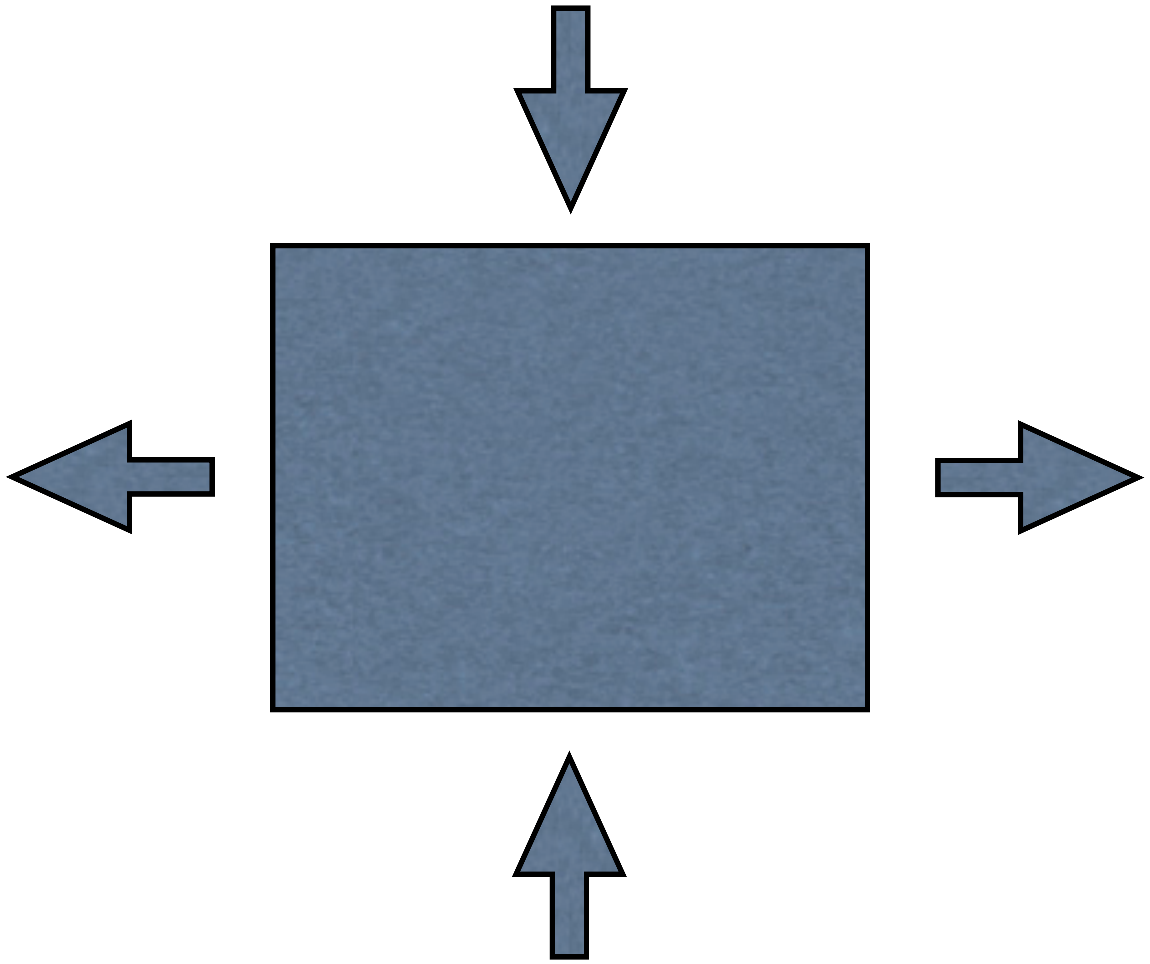
Finite Strain Rates

To address objections to AQS simulation protocol, do "plain old" Molecular Dynamics:

- binary Lennard-Jones system quenched at P=0
- local damping (Kelvin/DPD)
- uniaxial stress state
- bi-periodic boundaries
- system sizes up to 3000x3000 in QS regime (order 500 CPU days / run)

Note: switching deformation mode to uniaxial compression

prescribed $L_y(t)$
set $\sigma_{xx}=0$



What to measure?

For each triangle:

$$\frac{\partial u_i}{\partial x_j} = F_{ij}$$

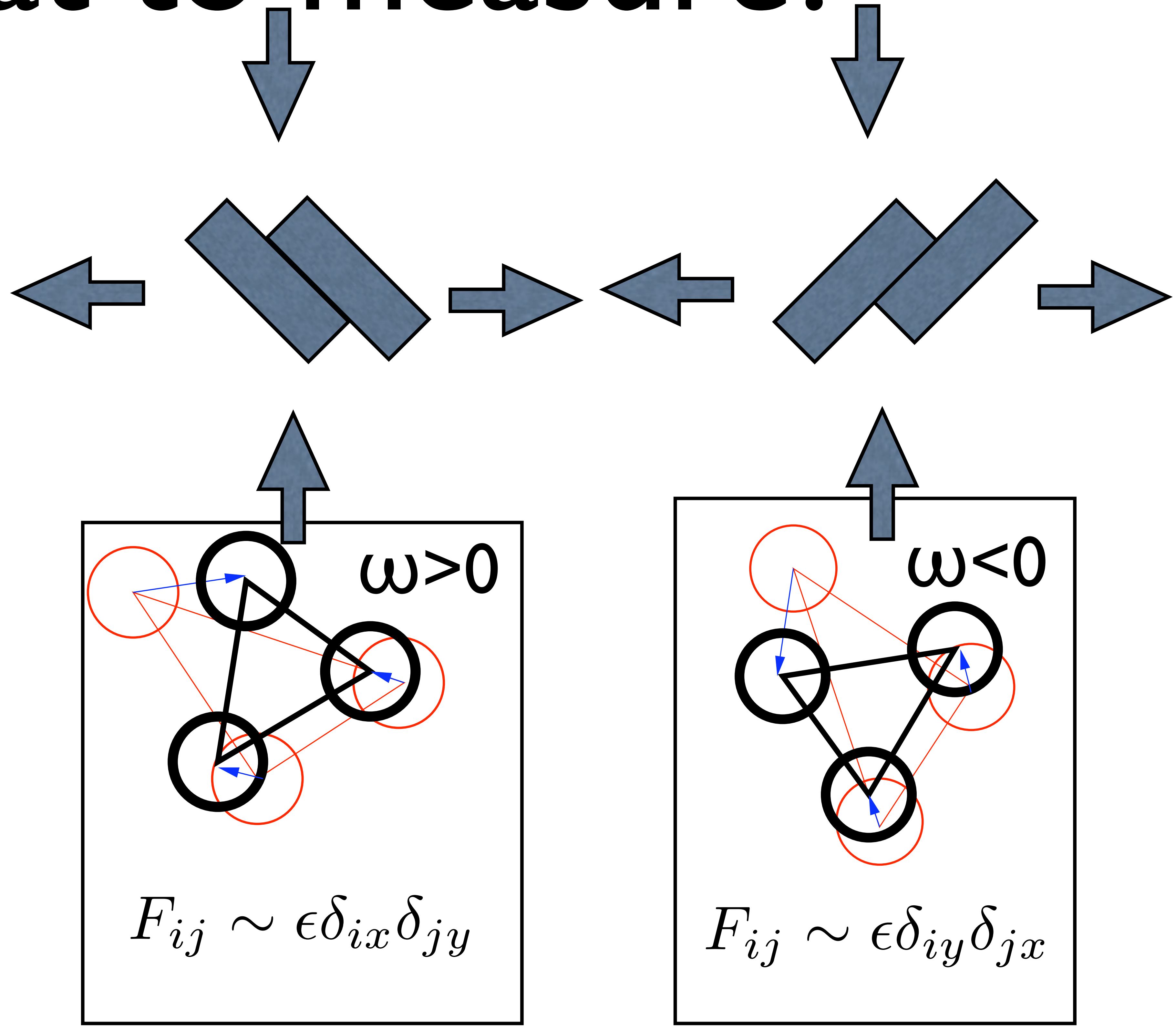
$$\epsilon_1 = \frac{F_{xx} - F_{yy}}{2}$$

$$\epsilon_2 = \frac{F_{xy} + F_{yx}}{2}$$

Invariants:

$$\epsilon = \sqrt{\epsilon_1^2 + \epsilon_2^2}$$

$$\omega = F_{xy} - F_{yx}$$

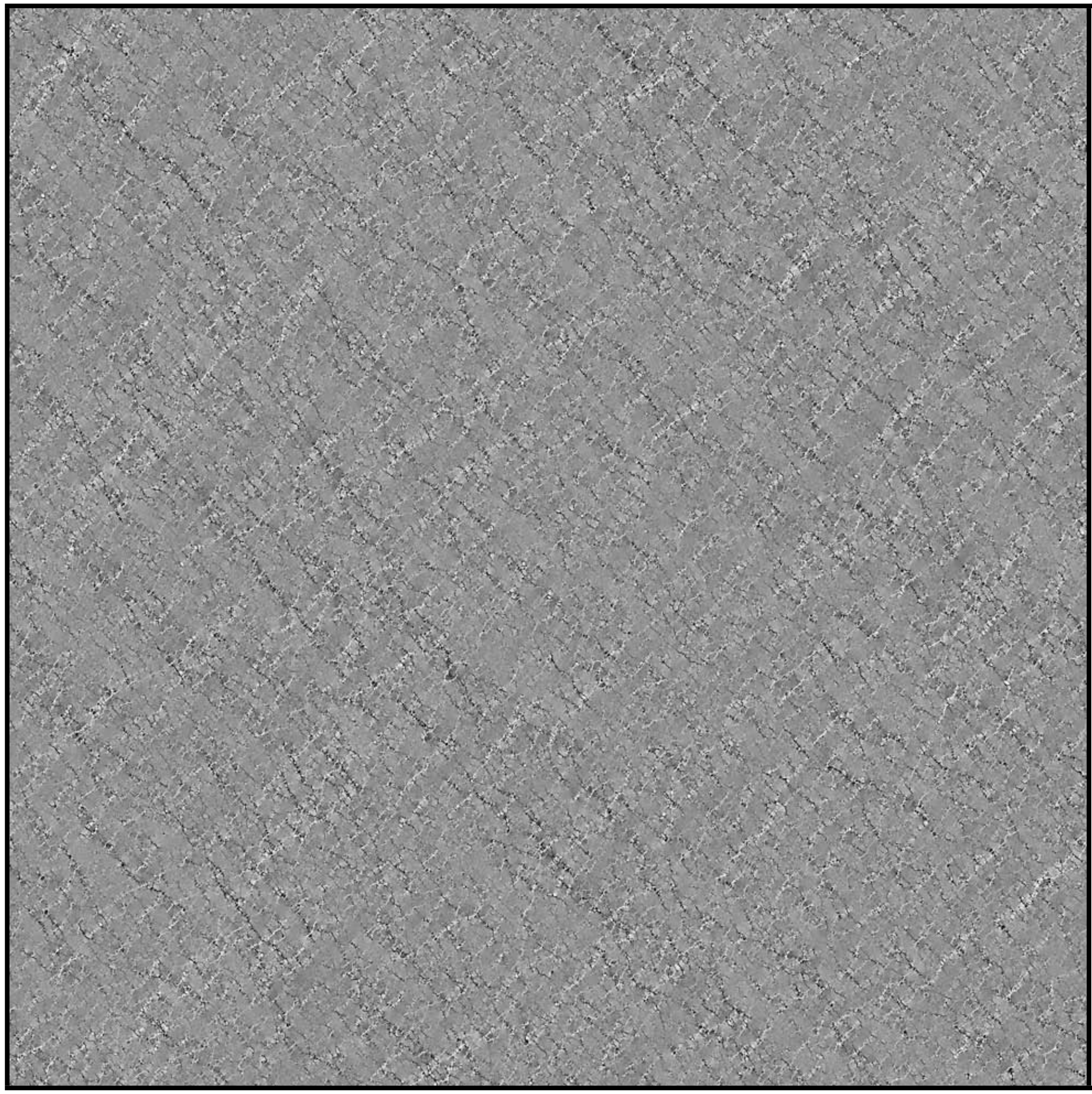


"Right Strain" "Left Strain"

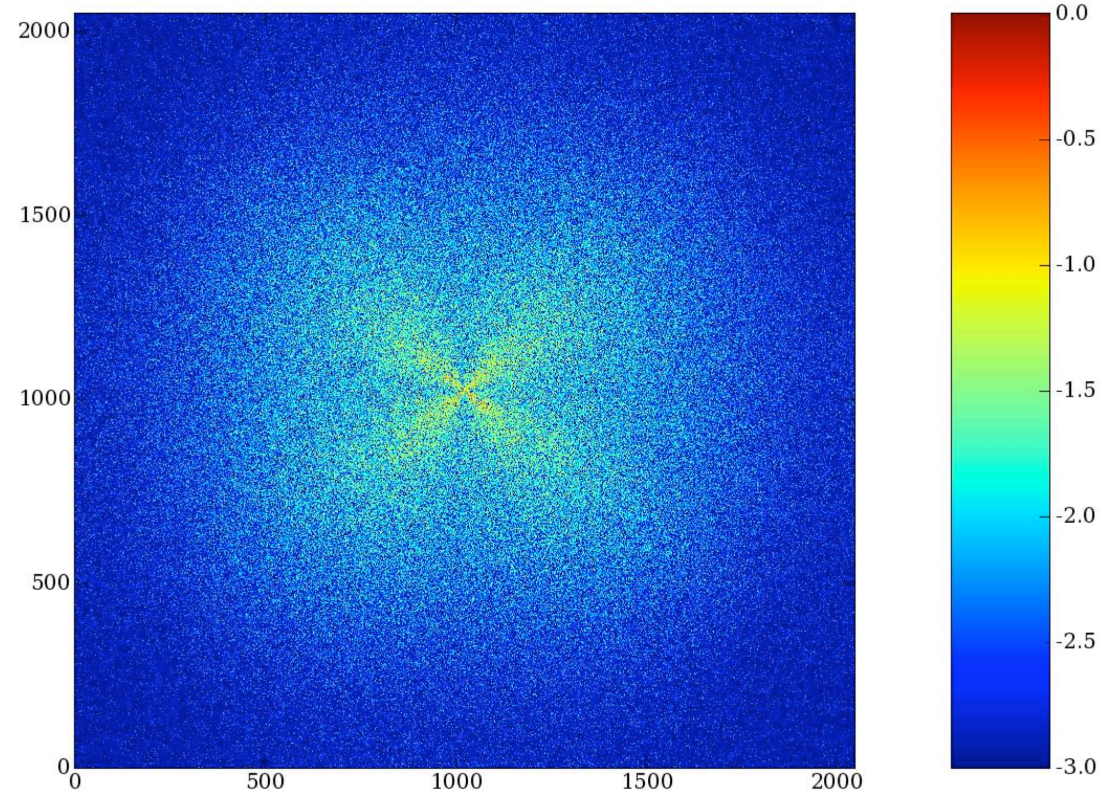
Local Strain (ω)

3% Strain

ω



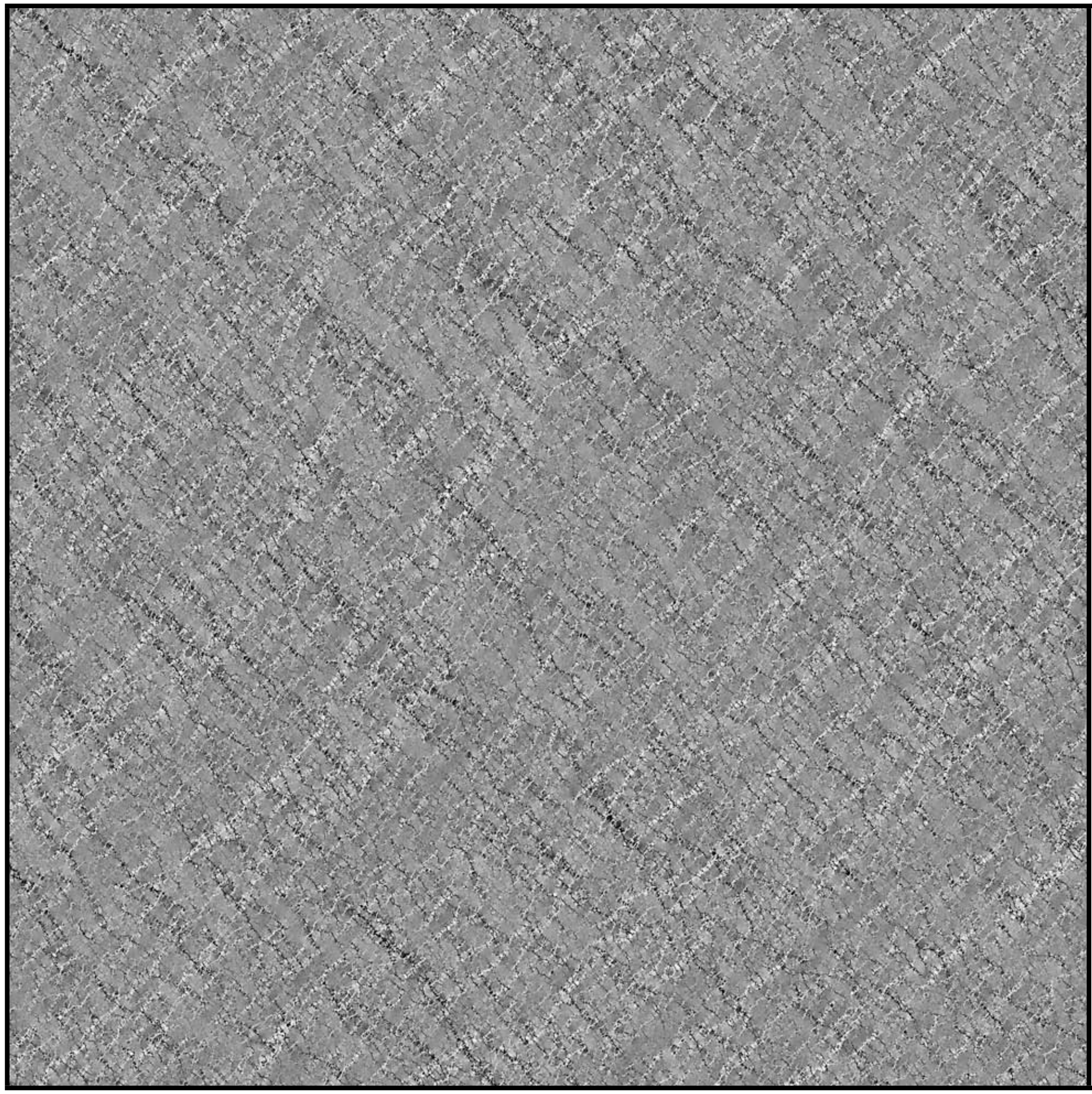
$\log_{10}[S(q_x,q_y)]$



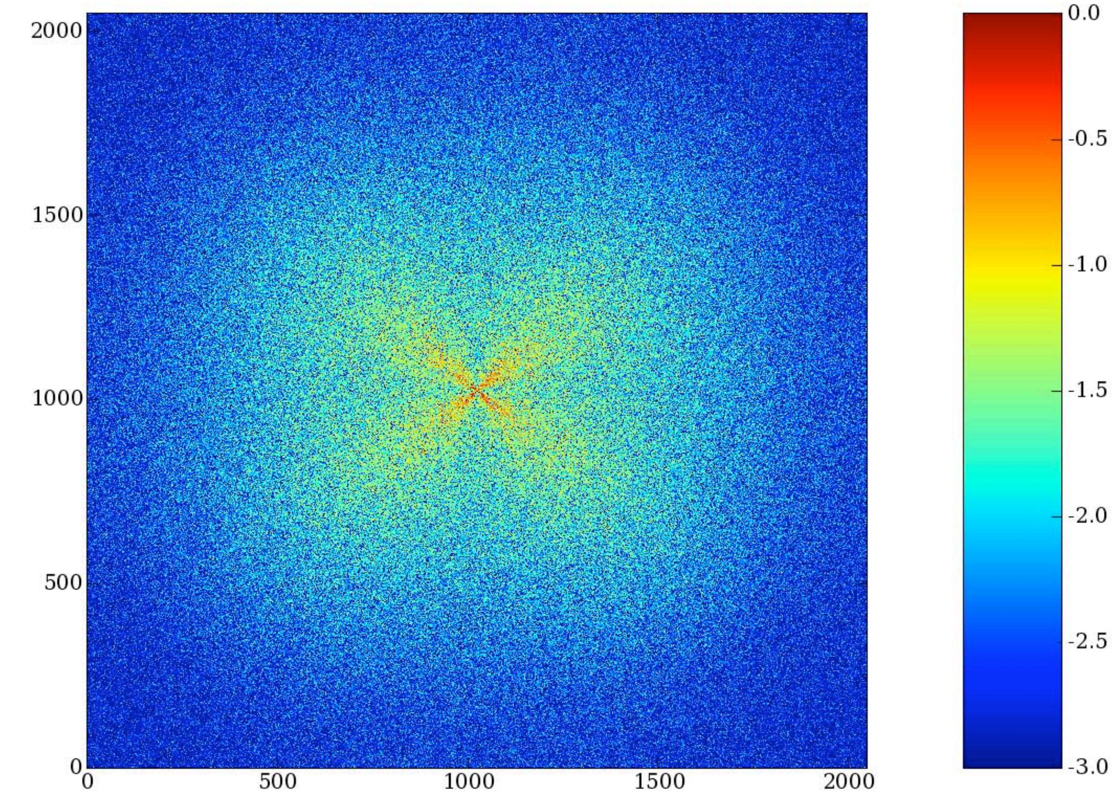
Local Strain (ω)

4% Strain

ω



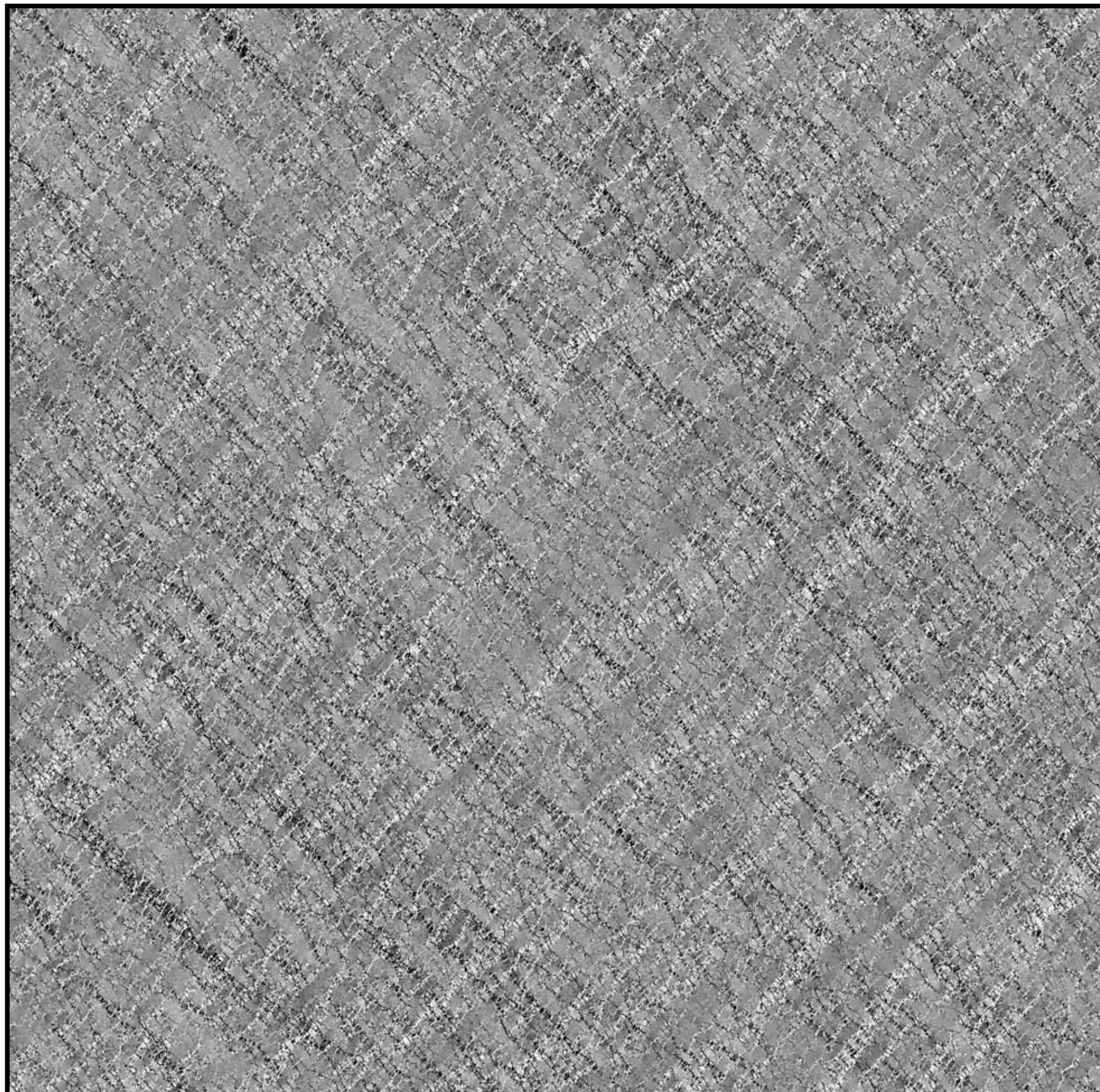
$\log_{10}[S(q_x,q_y)]$



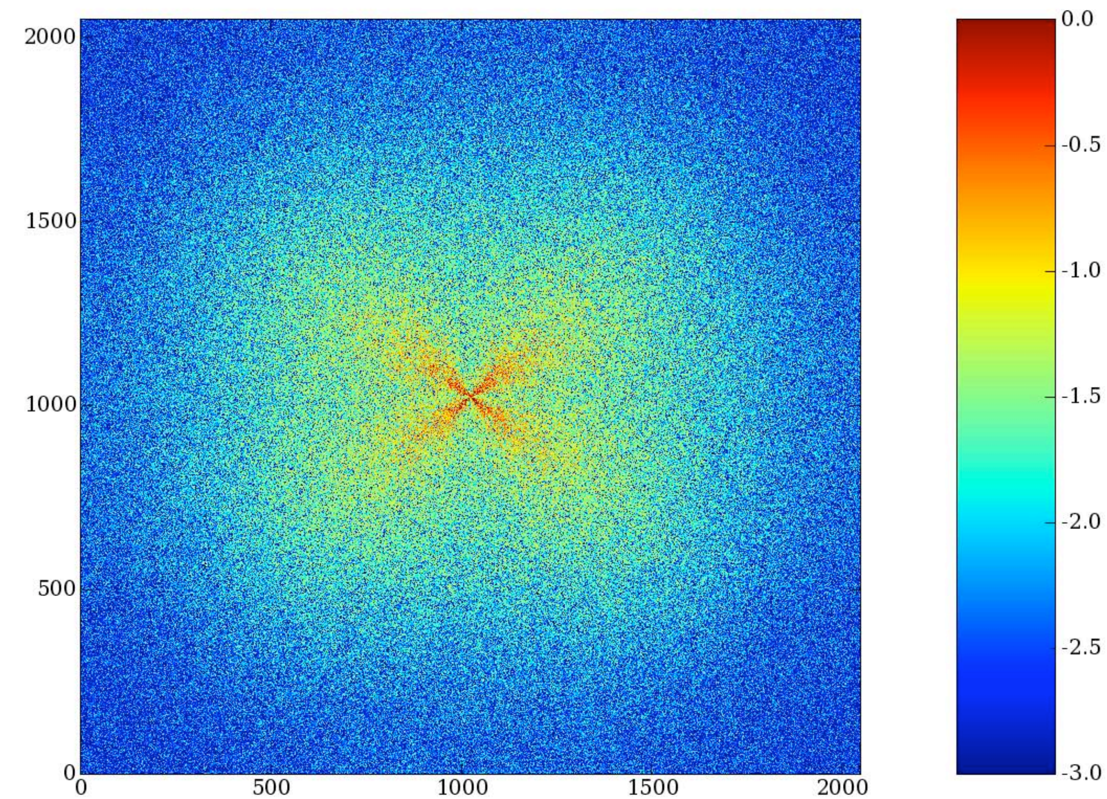
Local Strain (ω)

5% Strain

ω



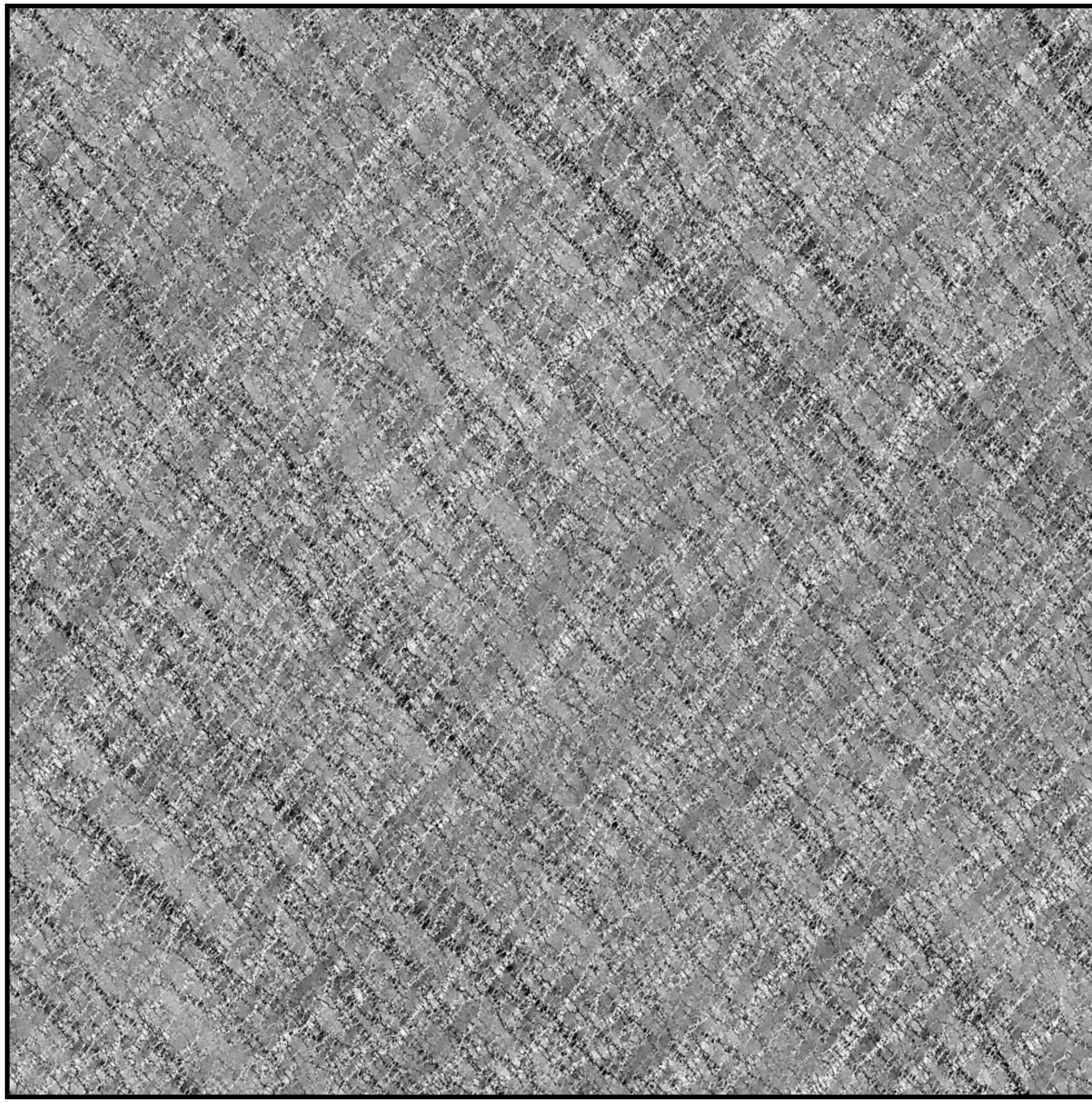
$\log_{10}[S(q_x,q_y)]$



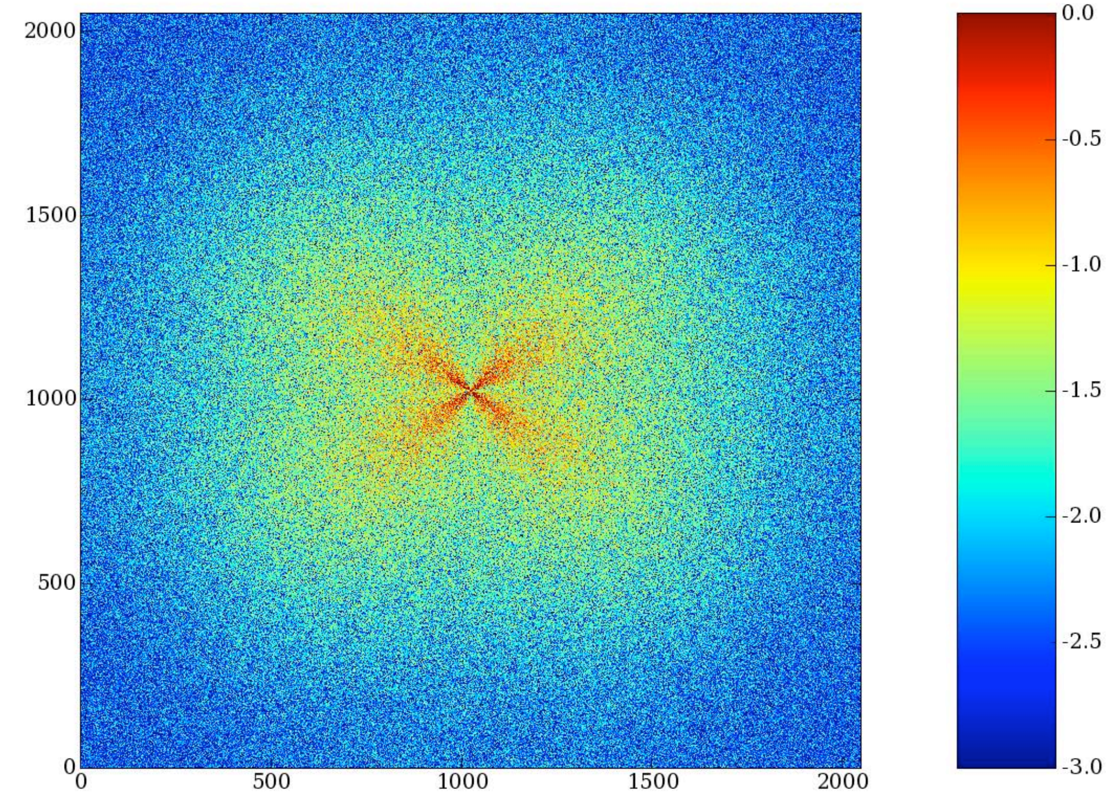
Local Strain (ω)

6% Strain

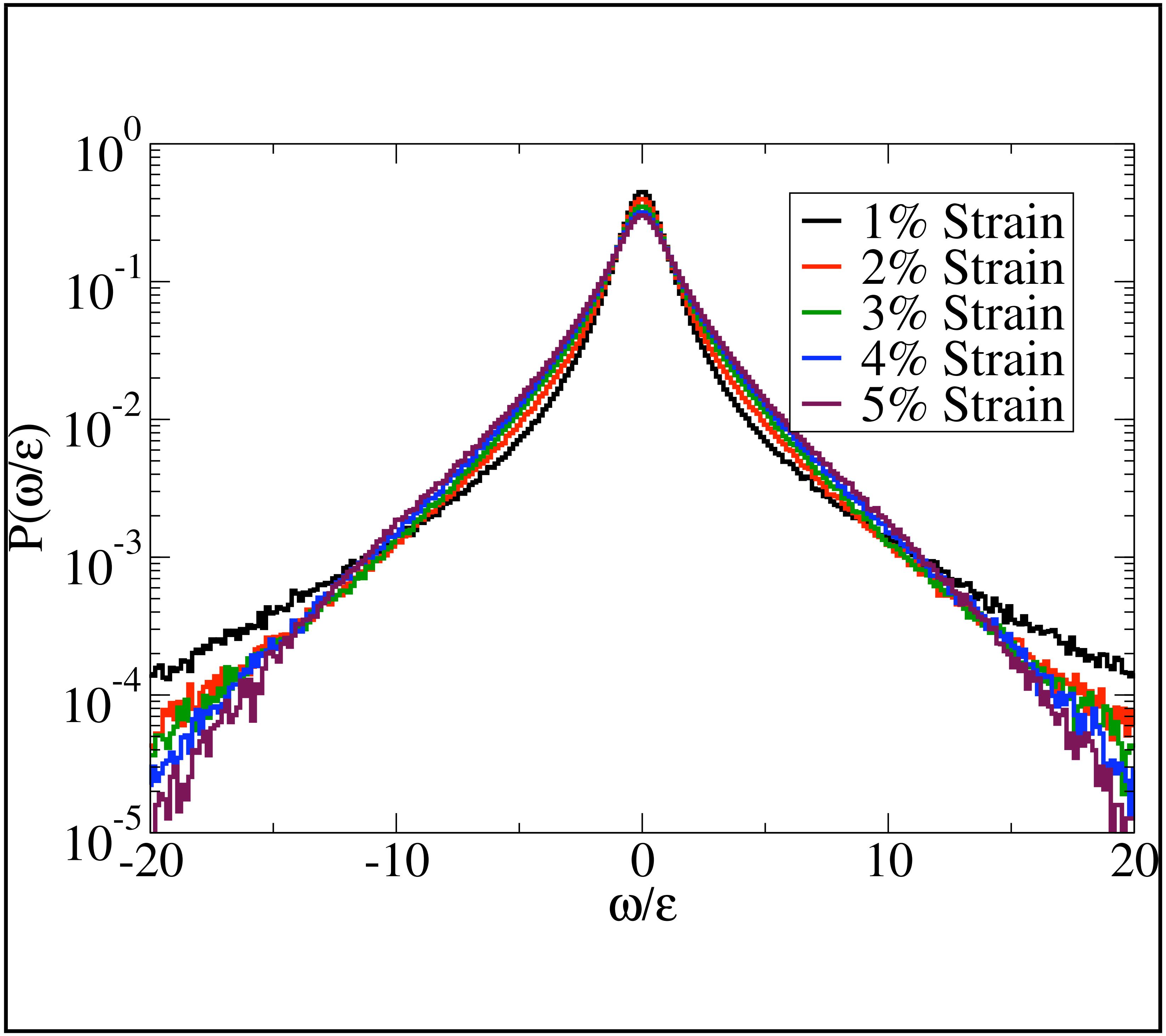
ω



$\log_{10}[S(q_x,q_y)]$



Distribution of Local ω



Distribution of ω has exponential tail and scales roughly with applied strain!

$P(\omega) \sim e^{-\omega/\omega^*}$

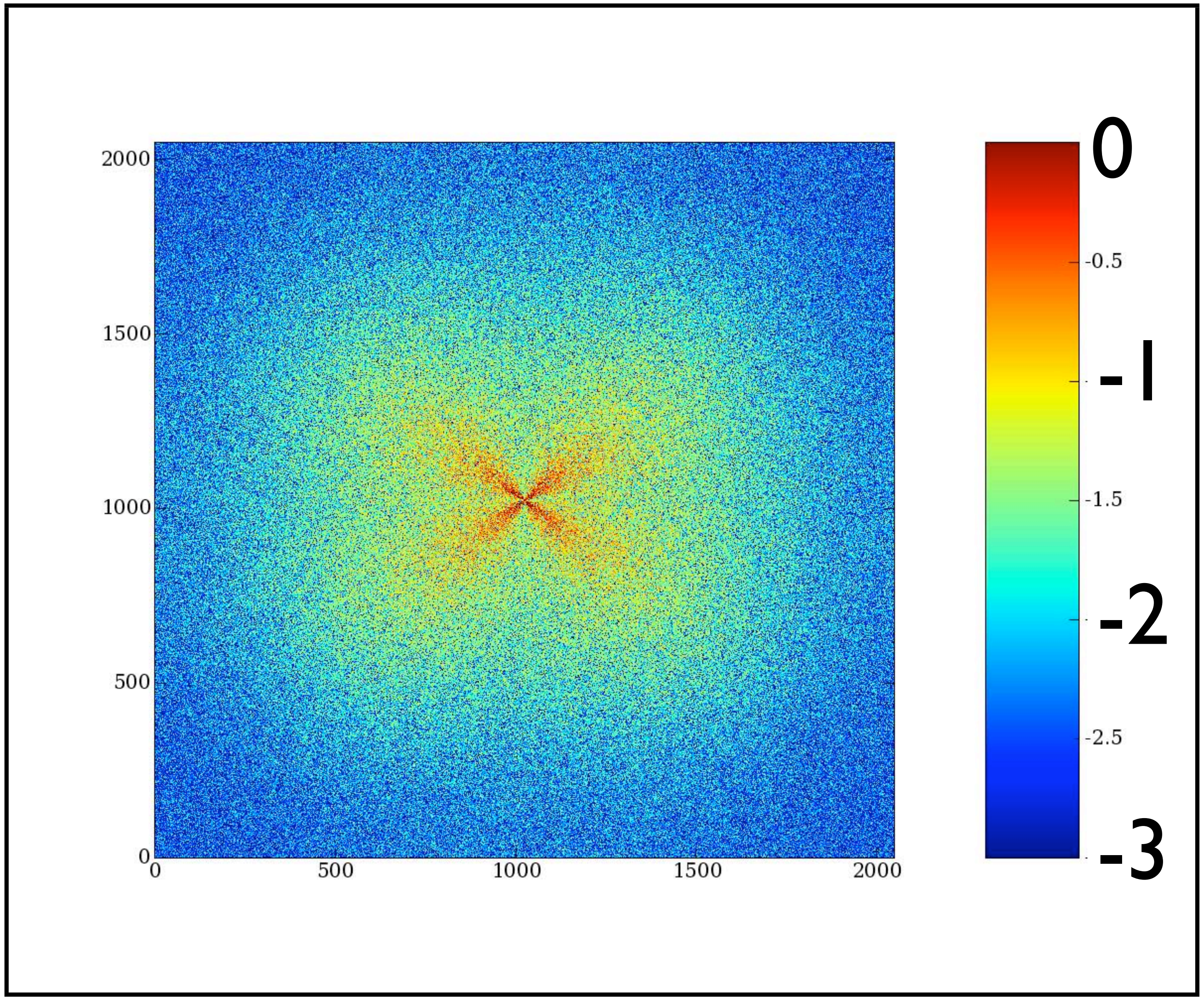
$\omega^* \sim A\epsilon_{applied}$

$A \sim 2.2$

A seems size and rate independent.

Scenarios for S(q)

$\log_{10}[S(q_x,q_y)]$



Two power-law scenarios for S(q)

Scenario A: $S \sim q^{\alpha} \sin^2(2\theta)$

$$\ln(S) \sim \alpha \ln(q) + \ln(\sin^2(2\theta))$$

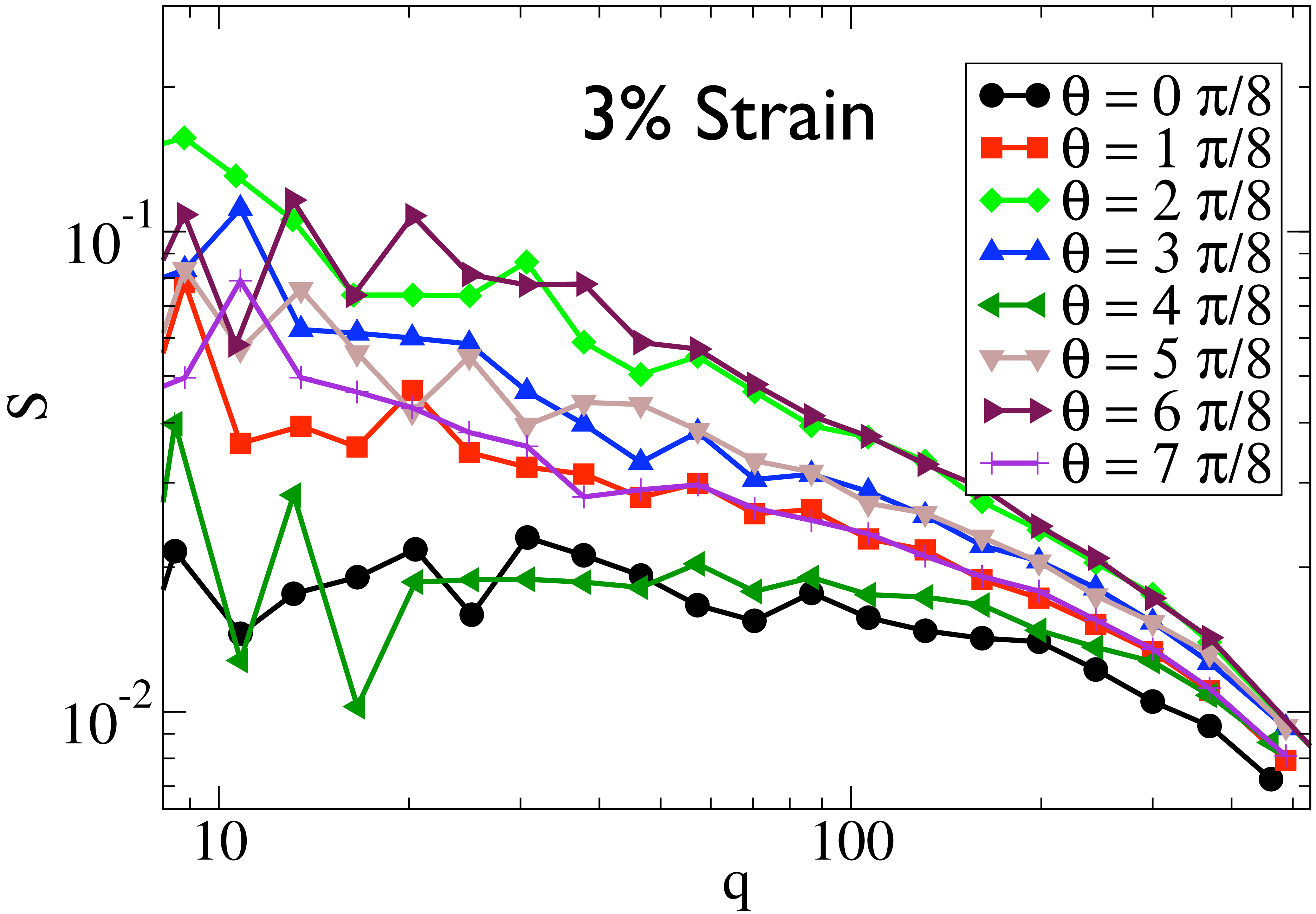
$$\ln(\langle S \rangle_\theta) \sim \alpha \ln(q)$$

Scenario B: $S \sim q^{\alpha \sin^2(2\theta)}$

$$\ln(S) \sim \alpha \sin^2(2\theta) \ln(q)$$

$$\langle \ln(S) \rangle_\theta \sim \frac{\alpha}{2} \ln q$$

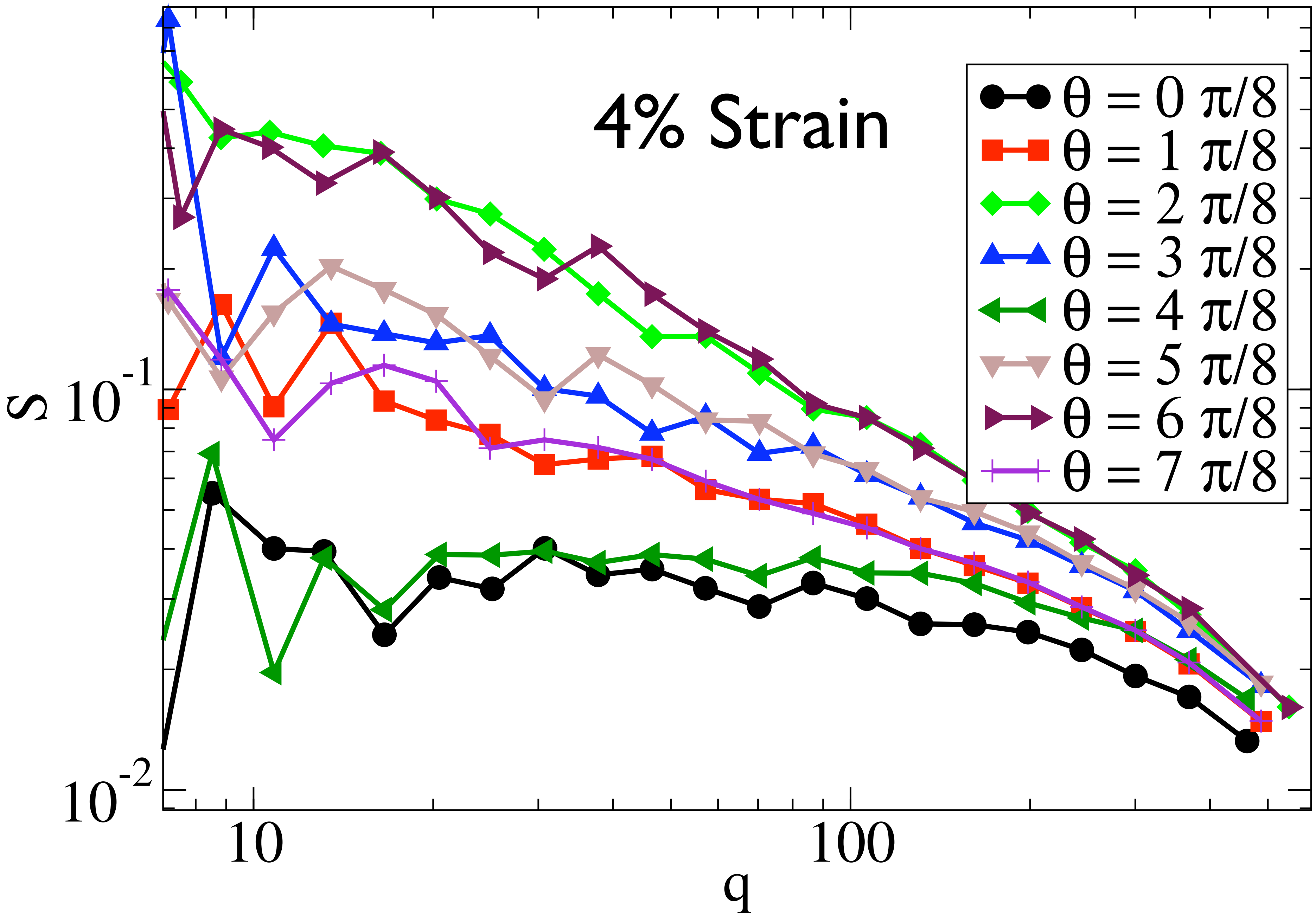
S(q;θ)



Note:

- Signal is strong along diagonals and flat along θ~0 and π/2
- Increasing strain revelas an apparent power law.
- Either exponent or low-q cutoff (or both) depends strongly on angle.

S(q;θ)



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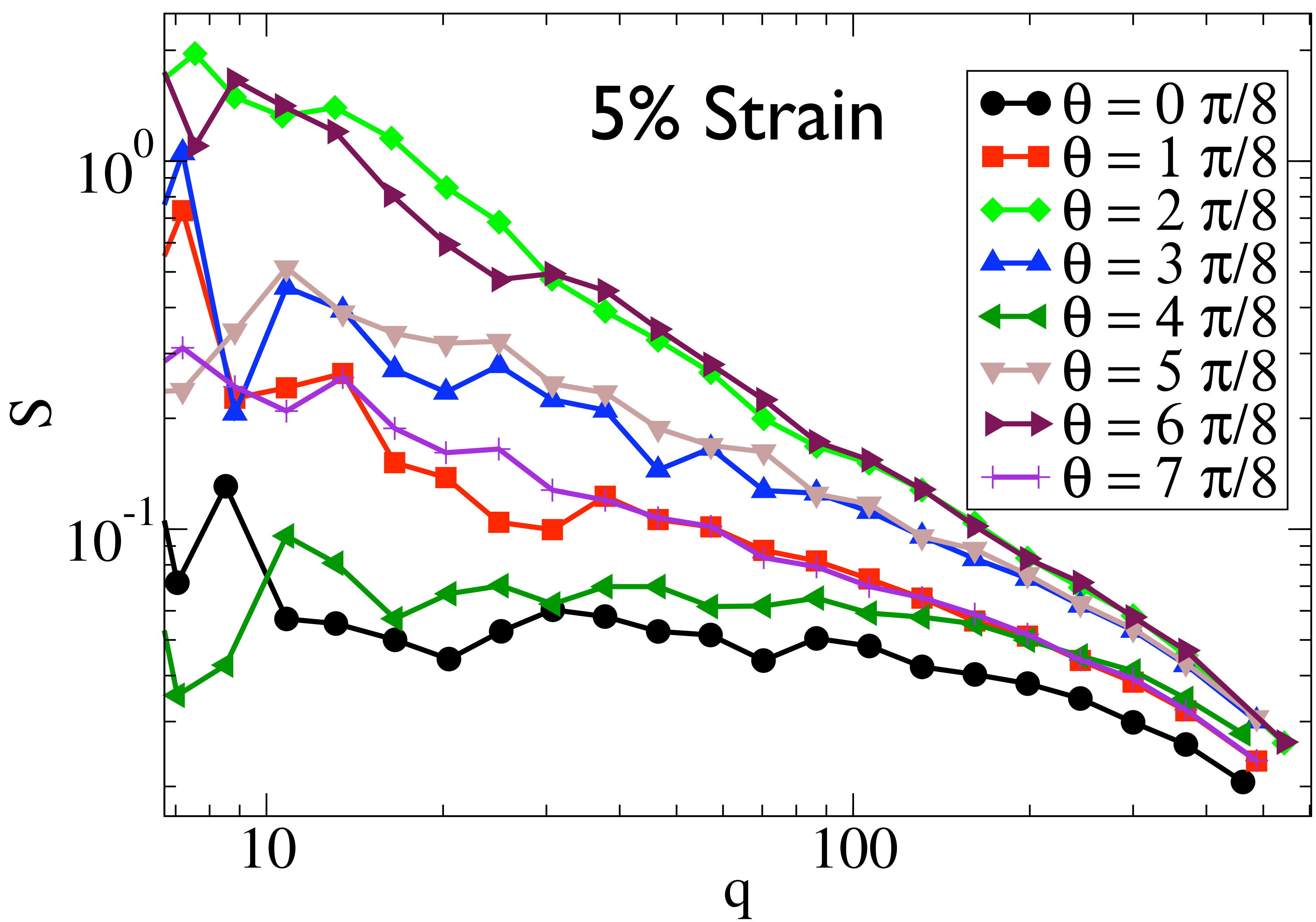
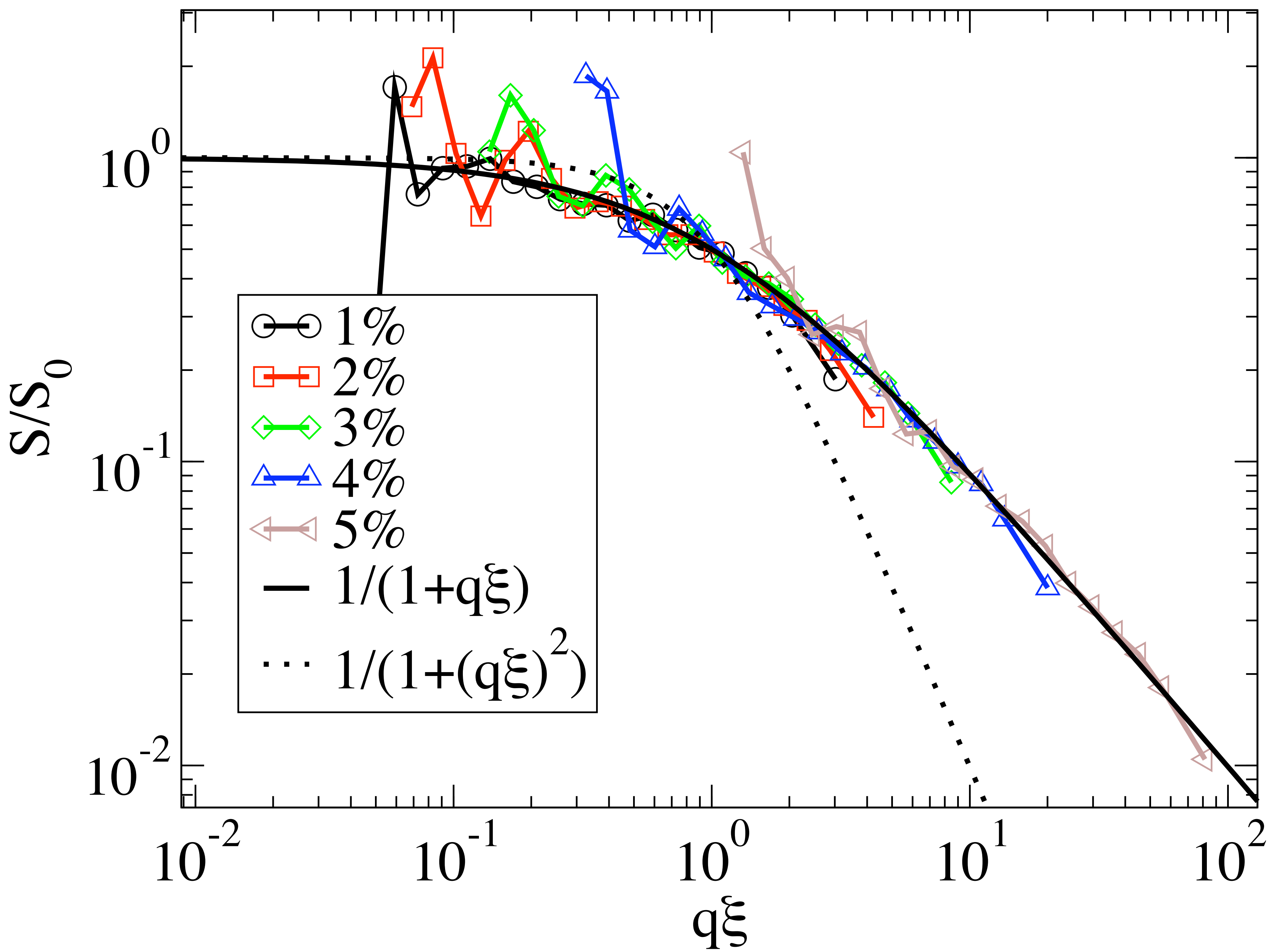


Note:

- Signal is strong along diagonals and flat along θ~0 and π/2
- Increasing strain revelas an apparent power law.
- Either exponent or low-q cutoff (or both) depends strongly on angle.

S(q) collapse for particular θ (=π/4)



Note:

- S(q) along diagonal at various applied strain.

Relation to Thermal Relaxation

PHYSICAL REVIEW E VOLUME 58, NUMBER 3 SEPTEMBER 1998

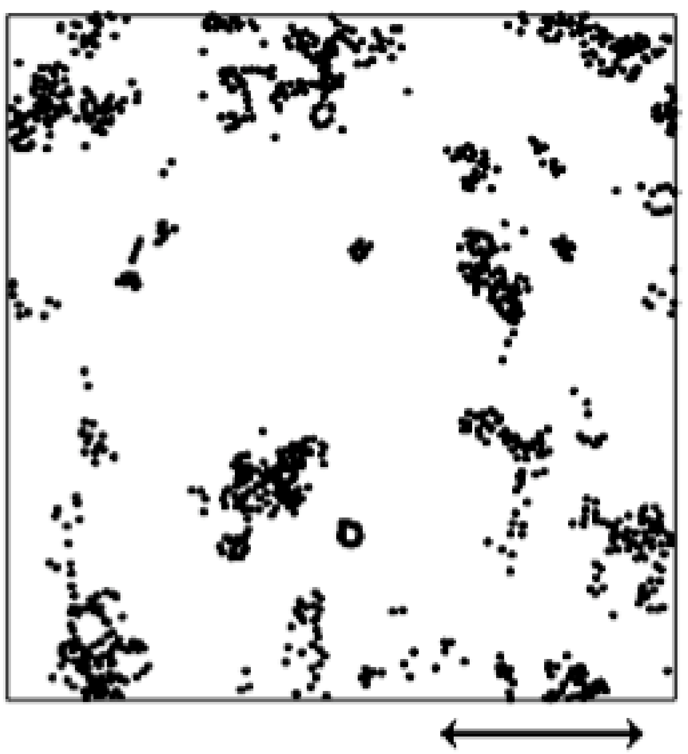
Dynamics of highly supercooled liquids: Heterogeneity, rheology, and diffusion

Ryoichi Yamamoto and Akira Onuki
Department of Physics, Kyoto University, Kyoto 606-8502, Japan
(Received 20 March 1998)

Method: locate neighboring pairs of particles which become separated after some time.

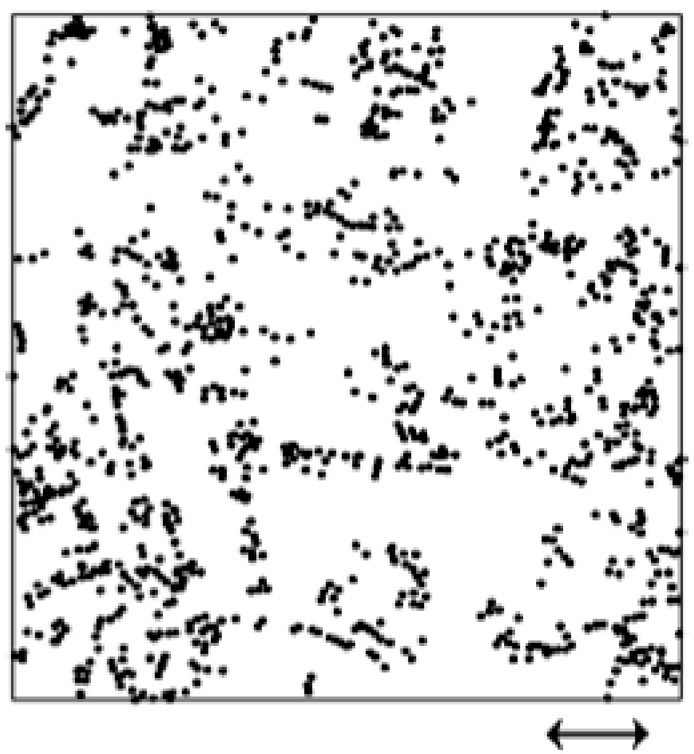
For large enough strain rate, lowering T doesn't change dynamics

$\tau_\alpha \sim 10^5$ No Shear



(b) $\Gamma_{eff} = 1.4$, $\dot{\gamma} = 0$

Shear ⟶



(c) $\Gamma_{eff} = 1.4$, $\dot{\gamma} = 0.25 \times 10^{-2}$

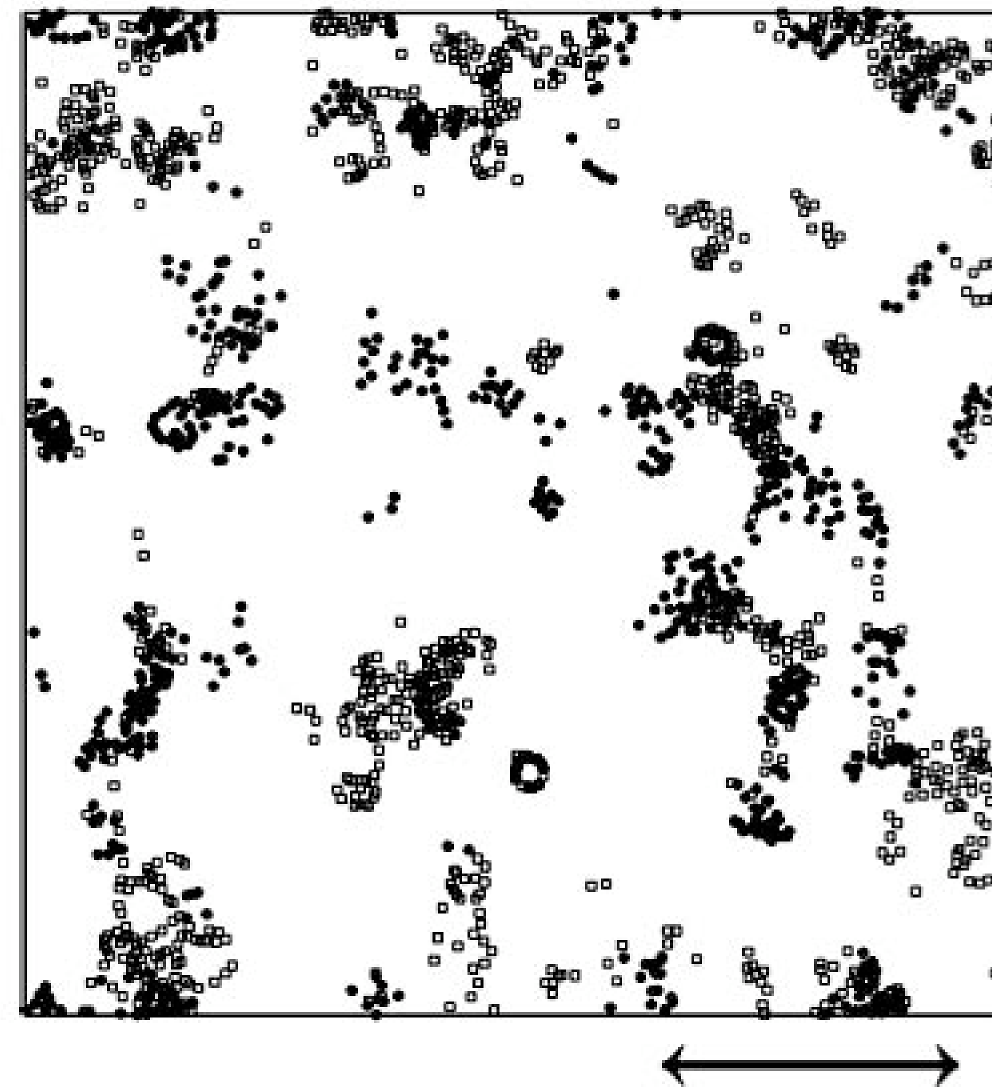


FIG. 7. Broken bond distributions in two consecutive time intervals, $[t_0, t_0+0.05\tau_b]$ (□) and $[t_0+0.05\tau_b, t_0+0.1\tau_b]$ (●), at $\Gamma_{eff}=1.4$ in 2D. The arrow indicates ξ.

Relation to Thermal Relaxation

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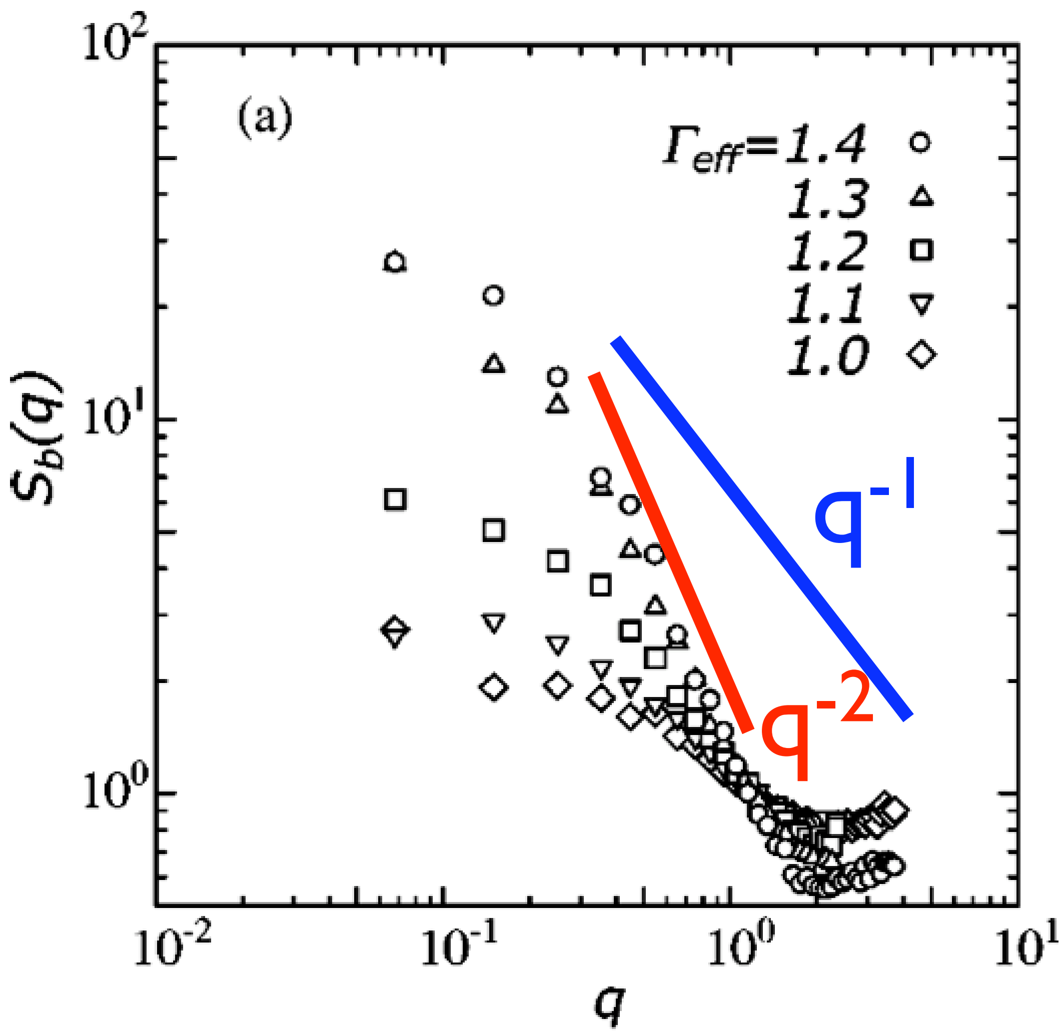
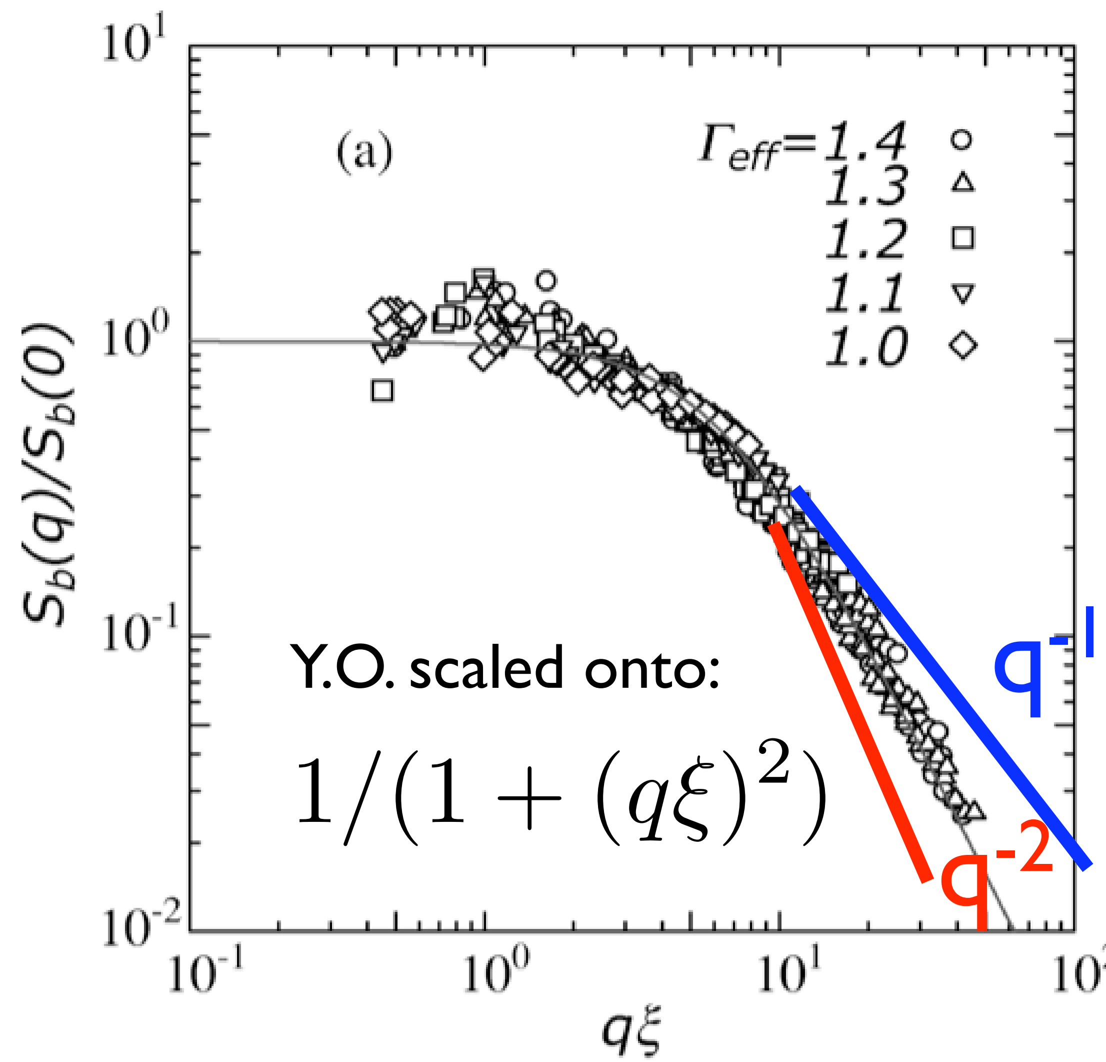
(iii) It is of great interest how the kinetic heterogeneities, which satisfy the dynamic scaling (4.4), evolve in space and time and why they look so similar to the critical fluctuations in Ising systems in the mean field level. In our steady-state problem T and $\dot{\gamma}$ are two relevant scaling fields, the *critical point* being located at $T=\dot{\gamma}=0$. No divergence has been detected at a nonzero temperature in our simulations.

Raw S(q) for no shear



Scaled S(q) for all data



Summary

- Athermal, quasistatic dynamics characterized by intermittent avalanche events with long range spatial correlations.

- Yield stress is about 3% times the shear modulus regardless of interactions!

- Data for event size based on i) strain interval, ii) stress drop, iii) energy drop collapse onto single master curve for all interactions and system sizes. Gives characteristic length of a few tenths of a particle diameter.

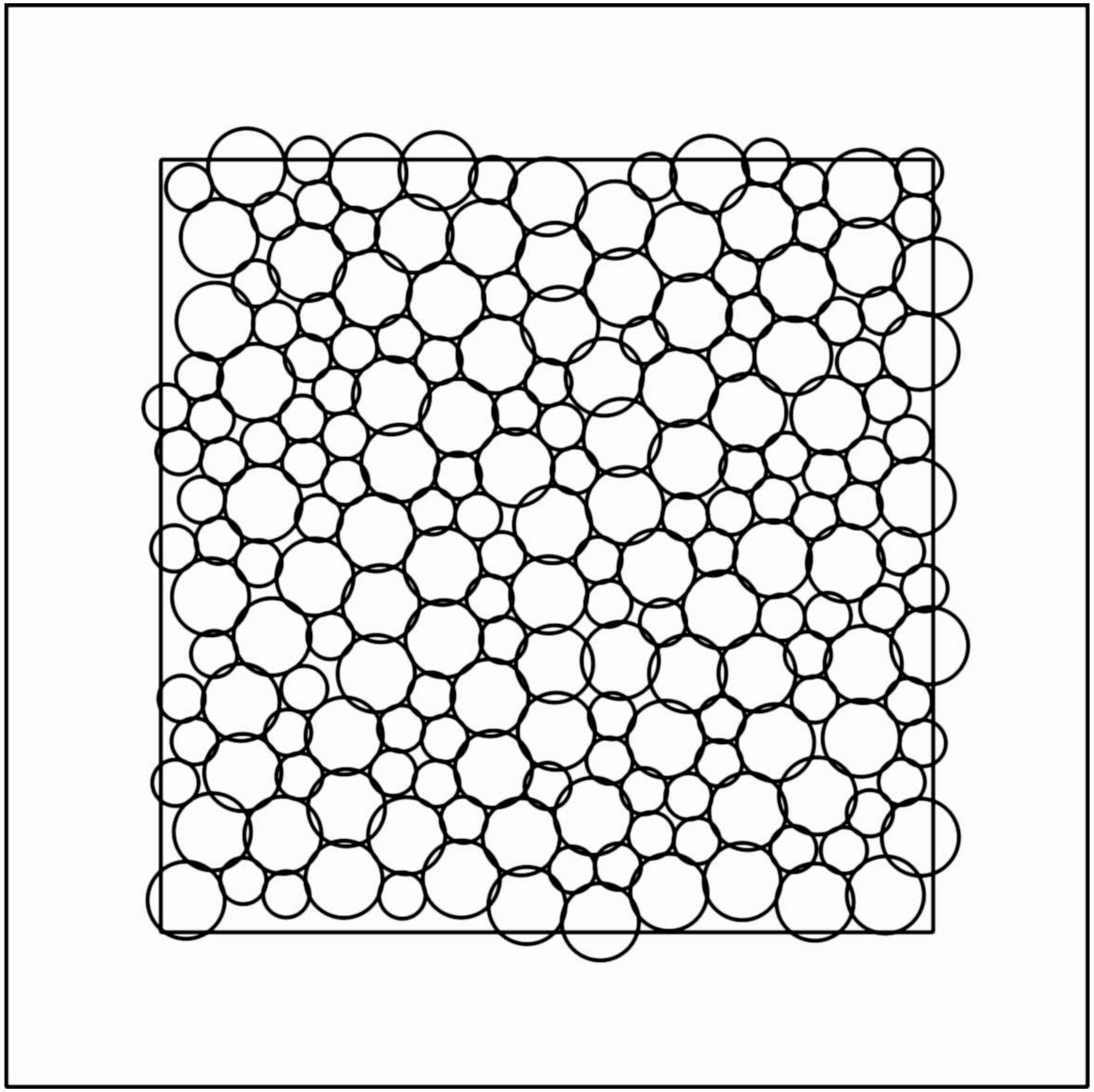
- Long-range spatial correlations and avalanche events remain in "plain old MD" at finite strain rate.

- Distribution of local slip is exponential.

- S(q) consistent with power-law (exponent~one) cut off by a lengthscale which grows with applied strain.

Non-affine Elastic Response

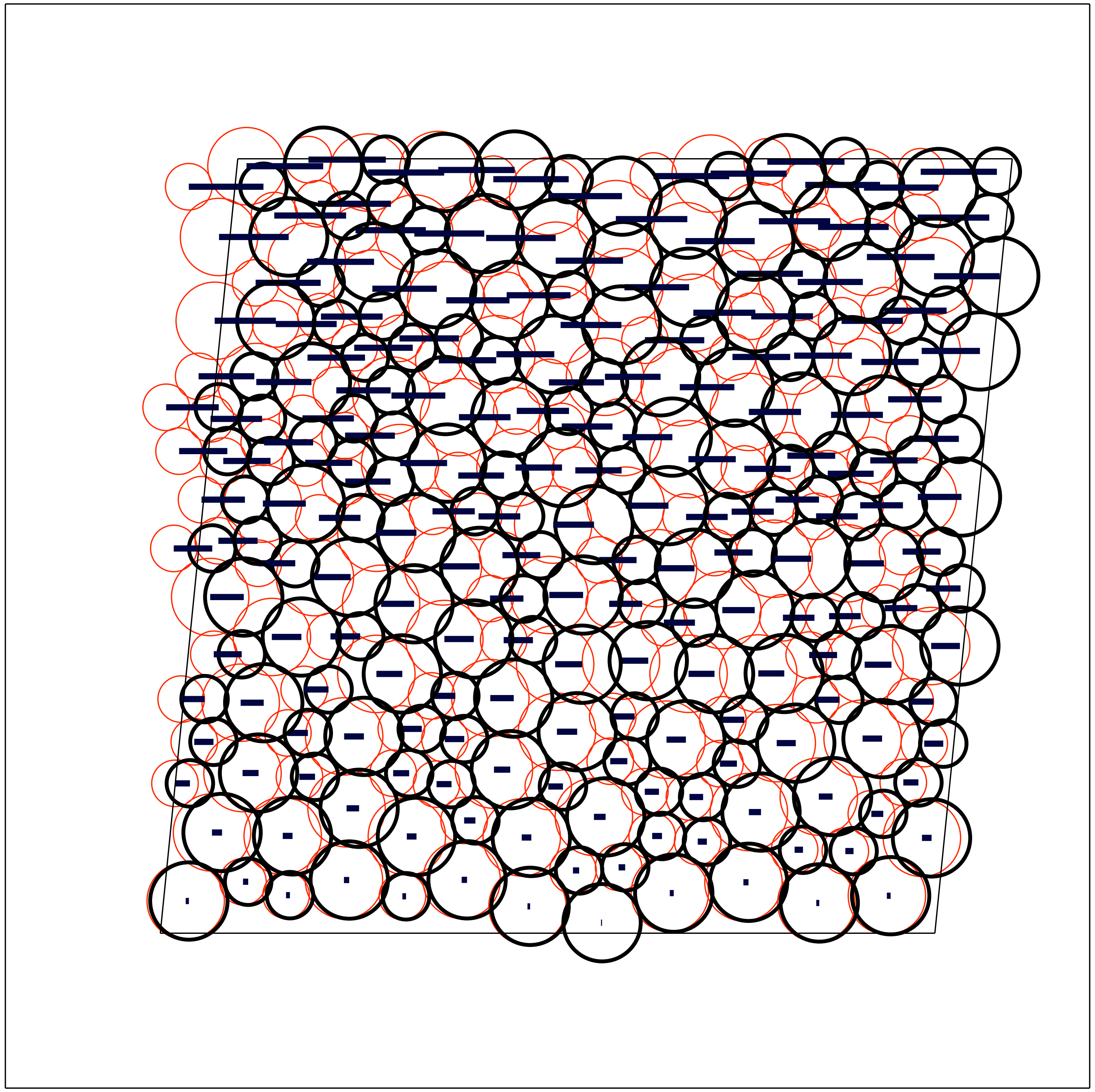
- Sequence:
  - Initial packing, F=0



- What is this stuff?
  - Bubbles or
  - Grains or
  - Atoms

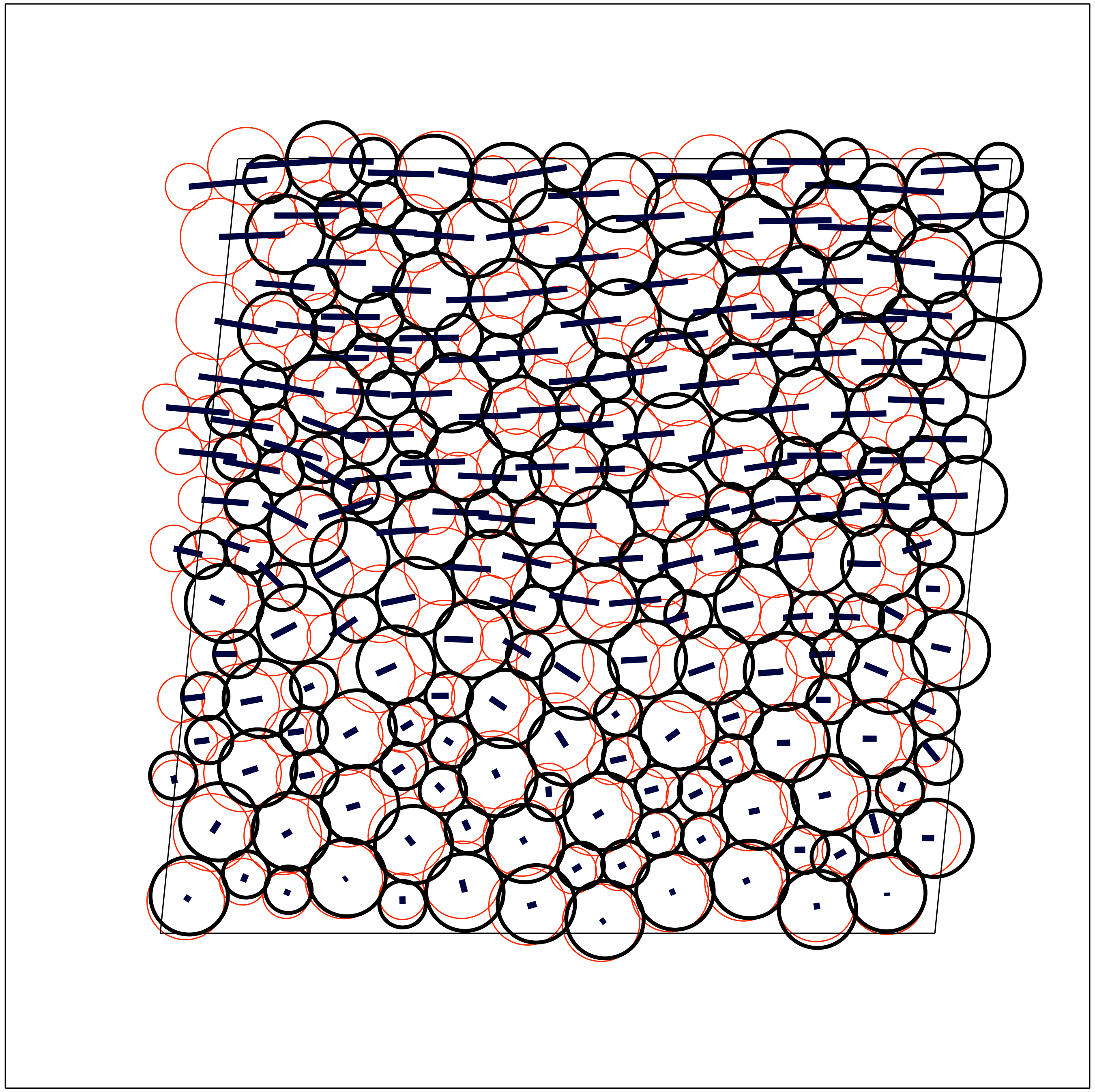
Non-affine Elastic Response

- Sequence:
  - Initial packing, F=0
  - Sheared state, F!=0



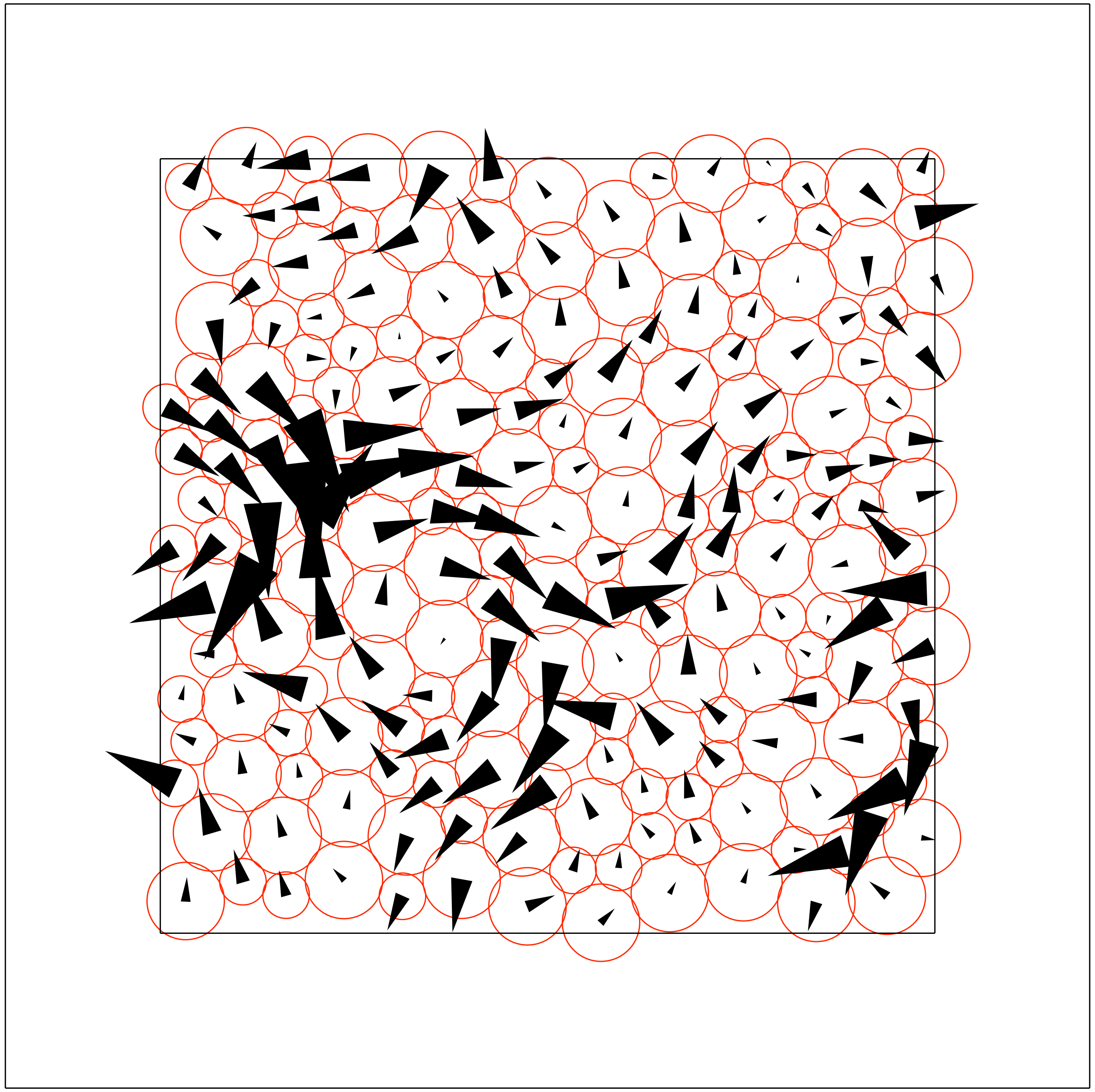
Non-affine Elastic Response

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



Non-affine Elastic Response

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



Motivation:

Q) How to characterize the local disorder?

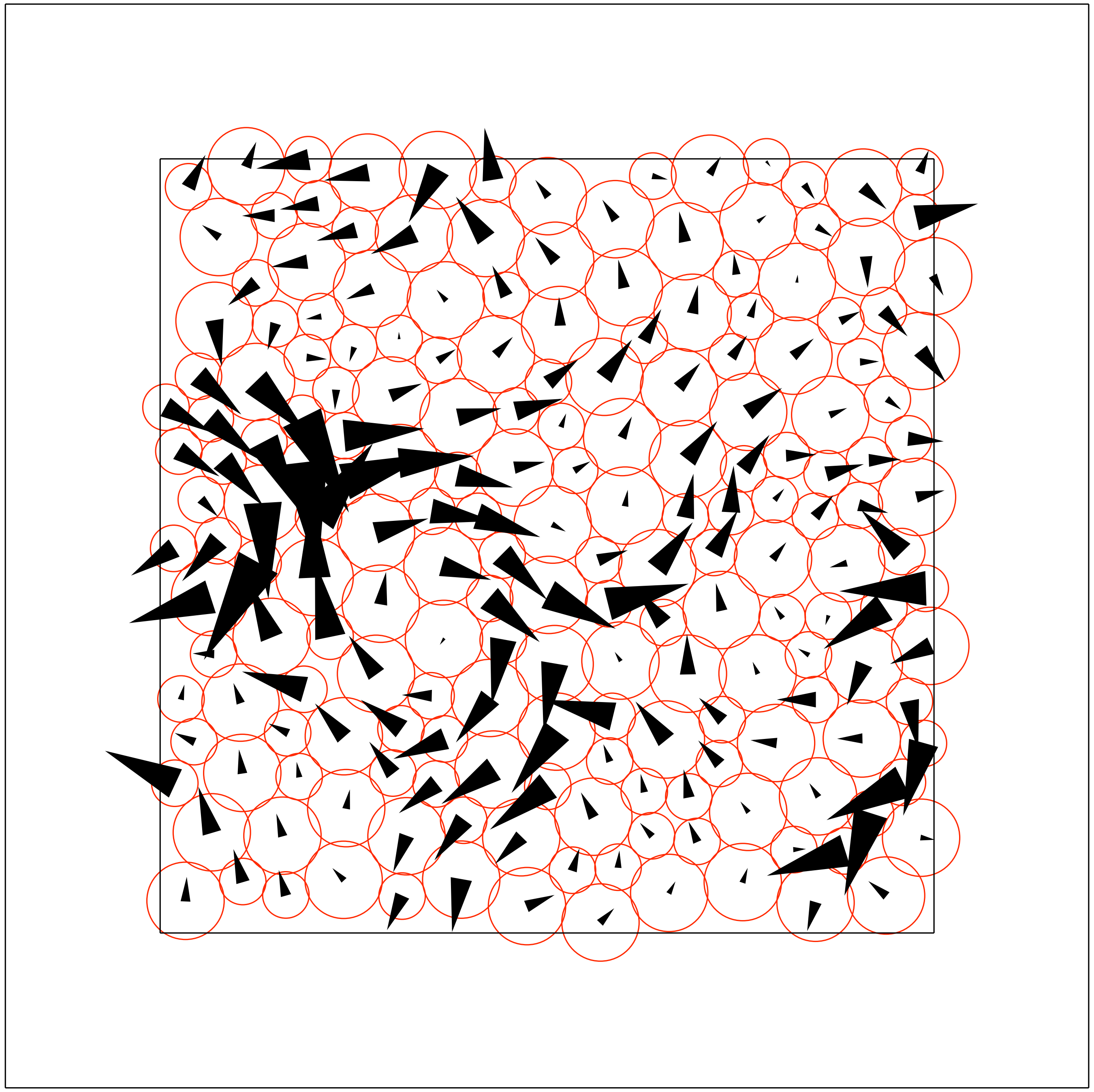
A) The "affine forces", Ξ

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?
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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.

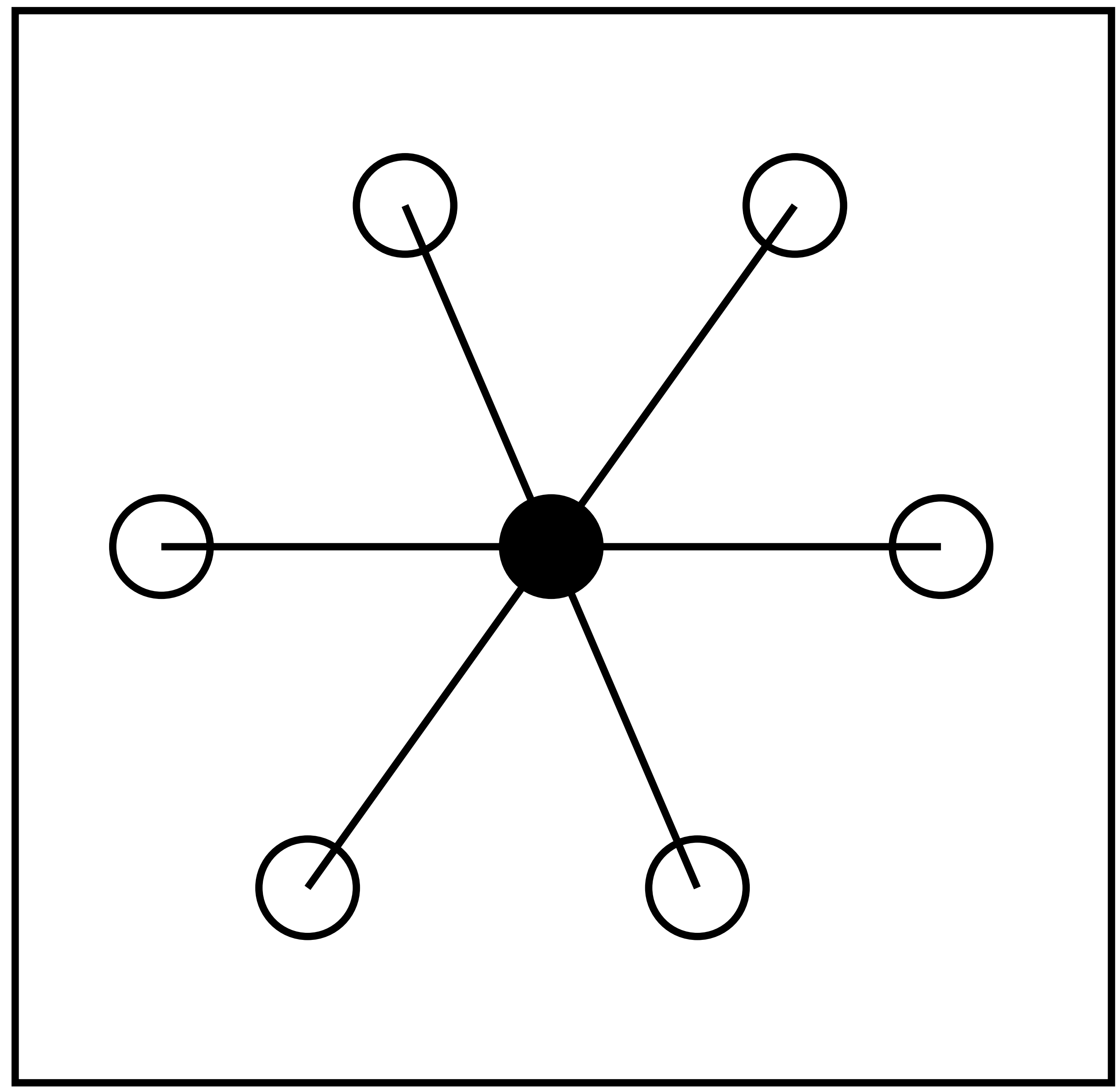
Q) How do heterogeneities in the elasticity initiate plasticity?
A) Elastic response localizes into a shear zone

- 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

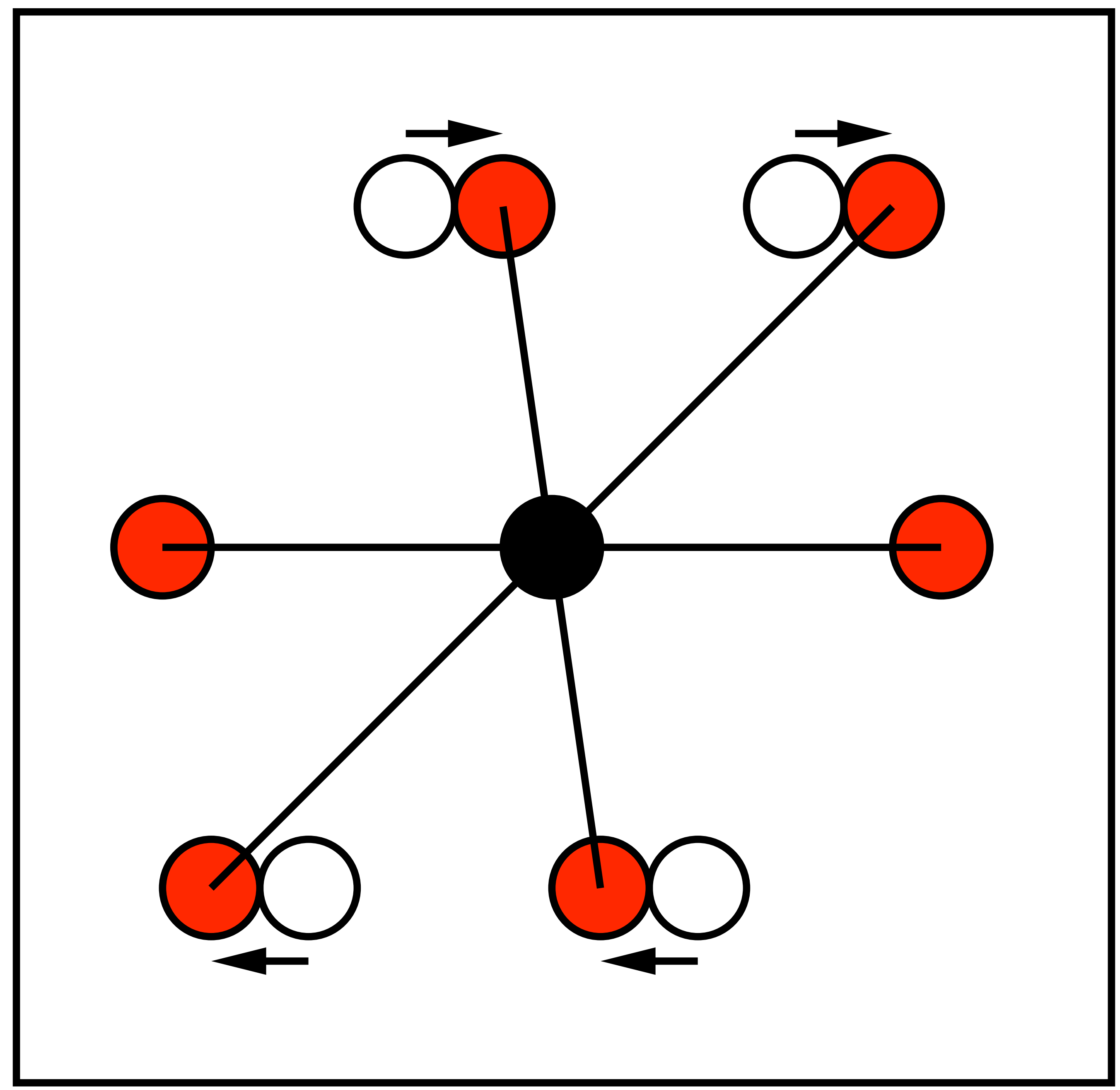
Ordered Case



Computing the response

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

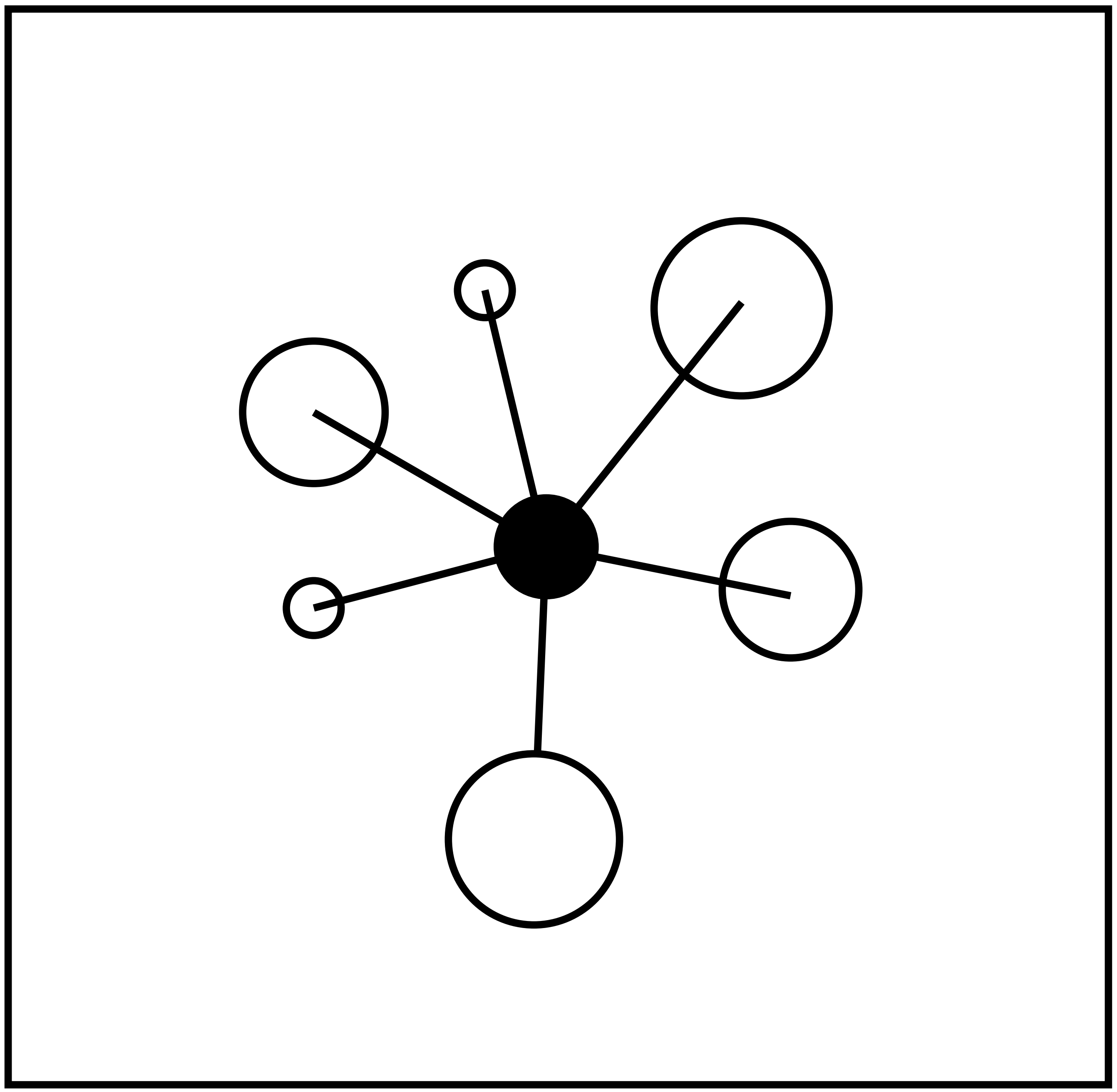
Ordered Case



Computing the response

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

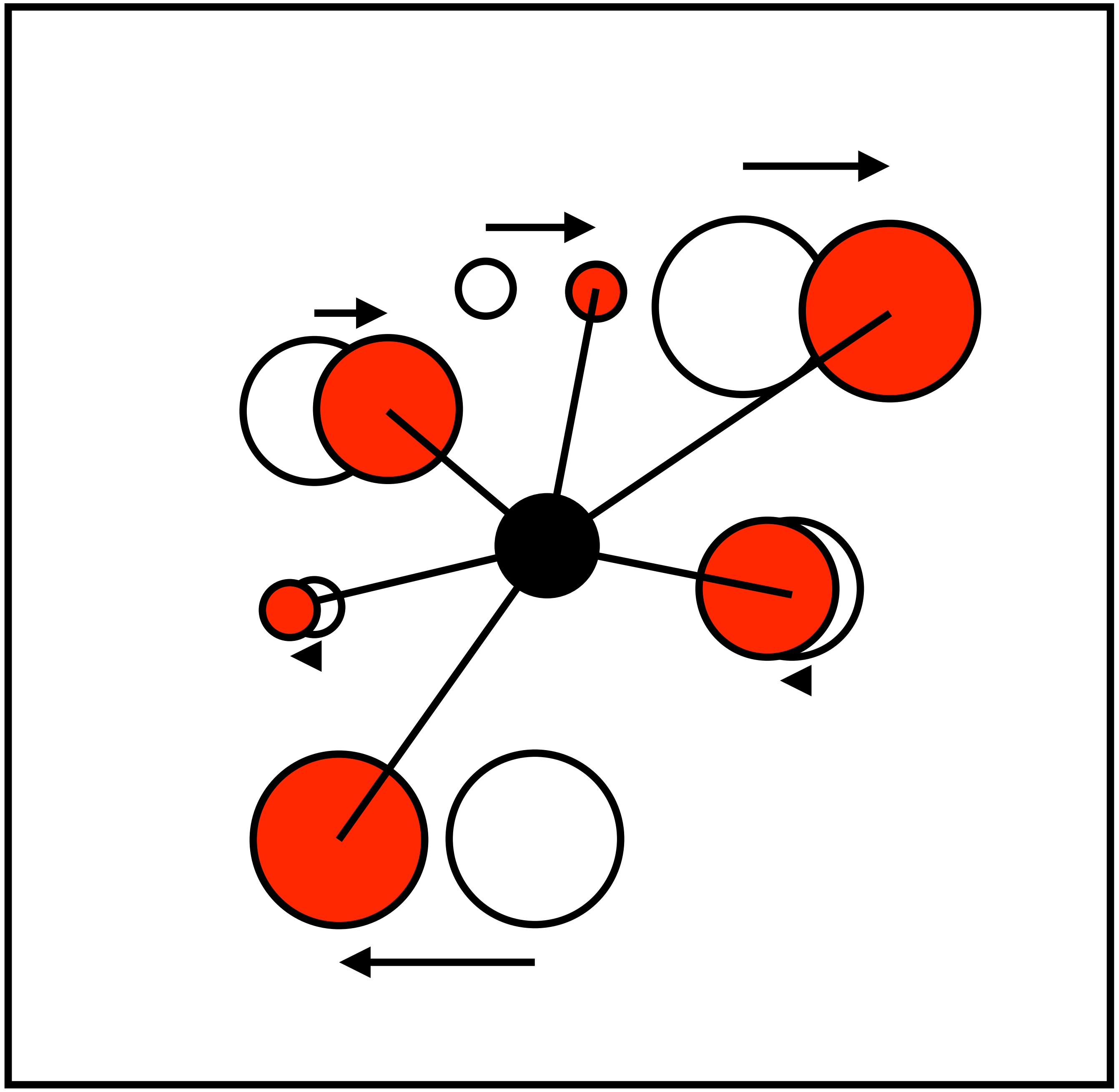
Disordered Case



Computing the response

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

Disordered Case



Computing the response

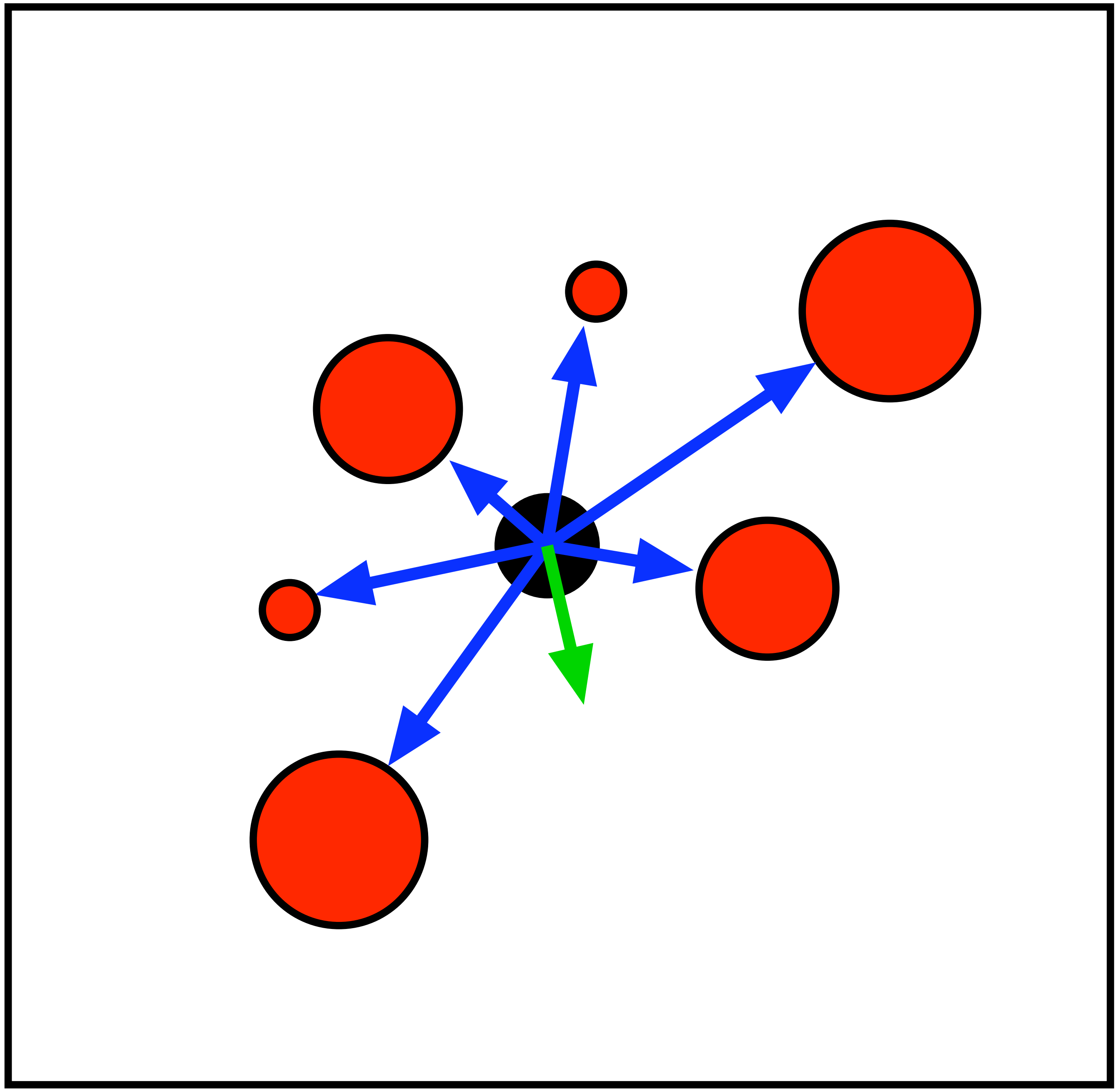
- Single particle toy problem:
  - Start at F=0
  - Apply strain

Use Hessian to compute "Affine force"

$$\vec{\Xi}_i = \sum_j \mathbf{H}_{ij} \vec{dr}_j$$

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

Disordered Case



Computing the response

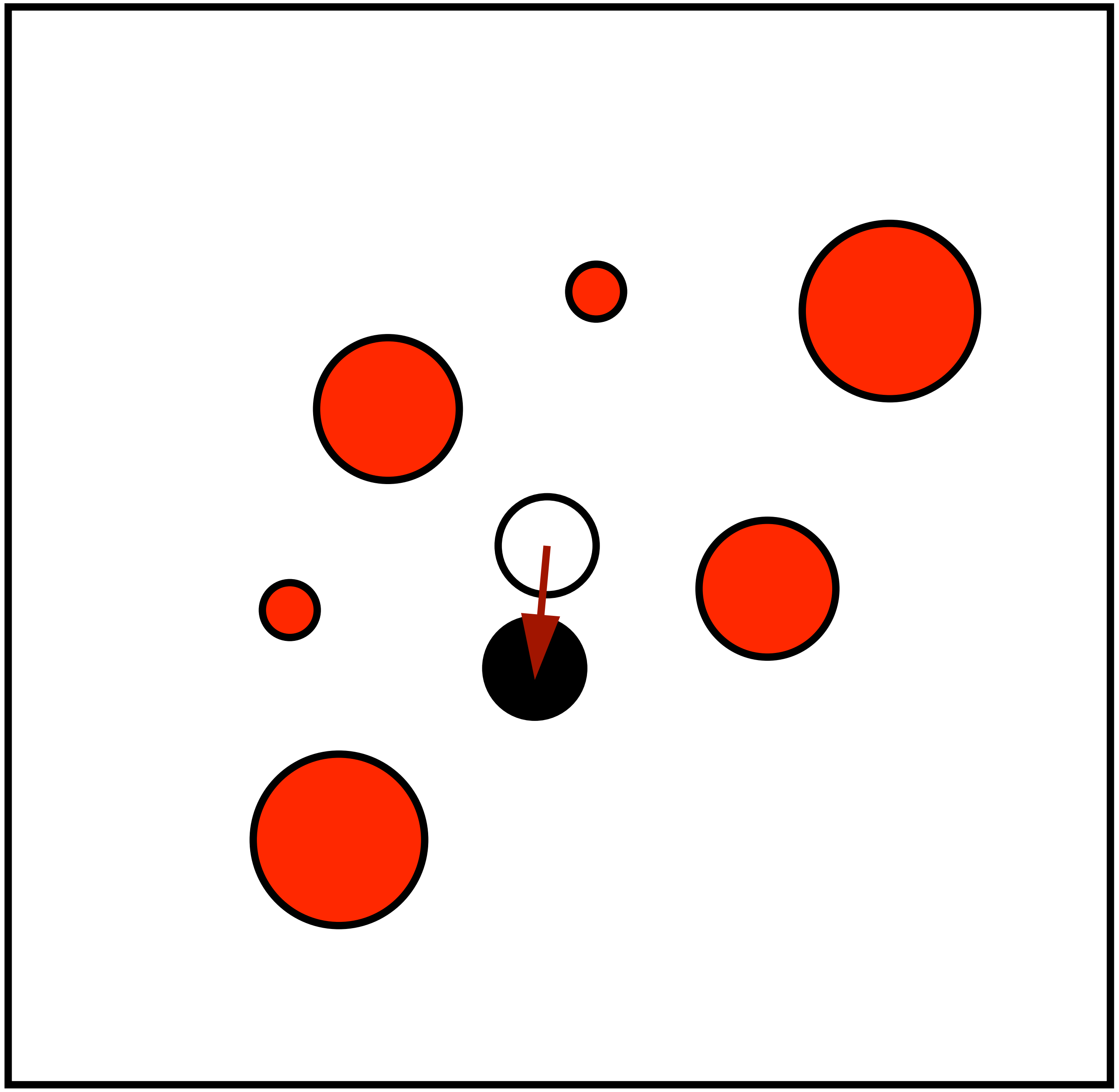
- Single particle toy problem:
  - Start at F=0
  - Apply strain

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

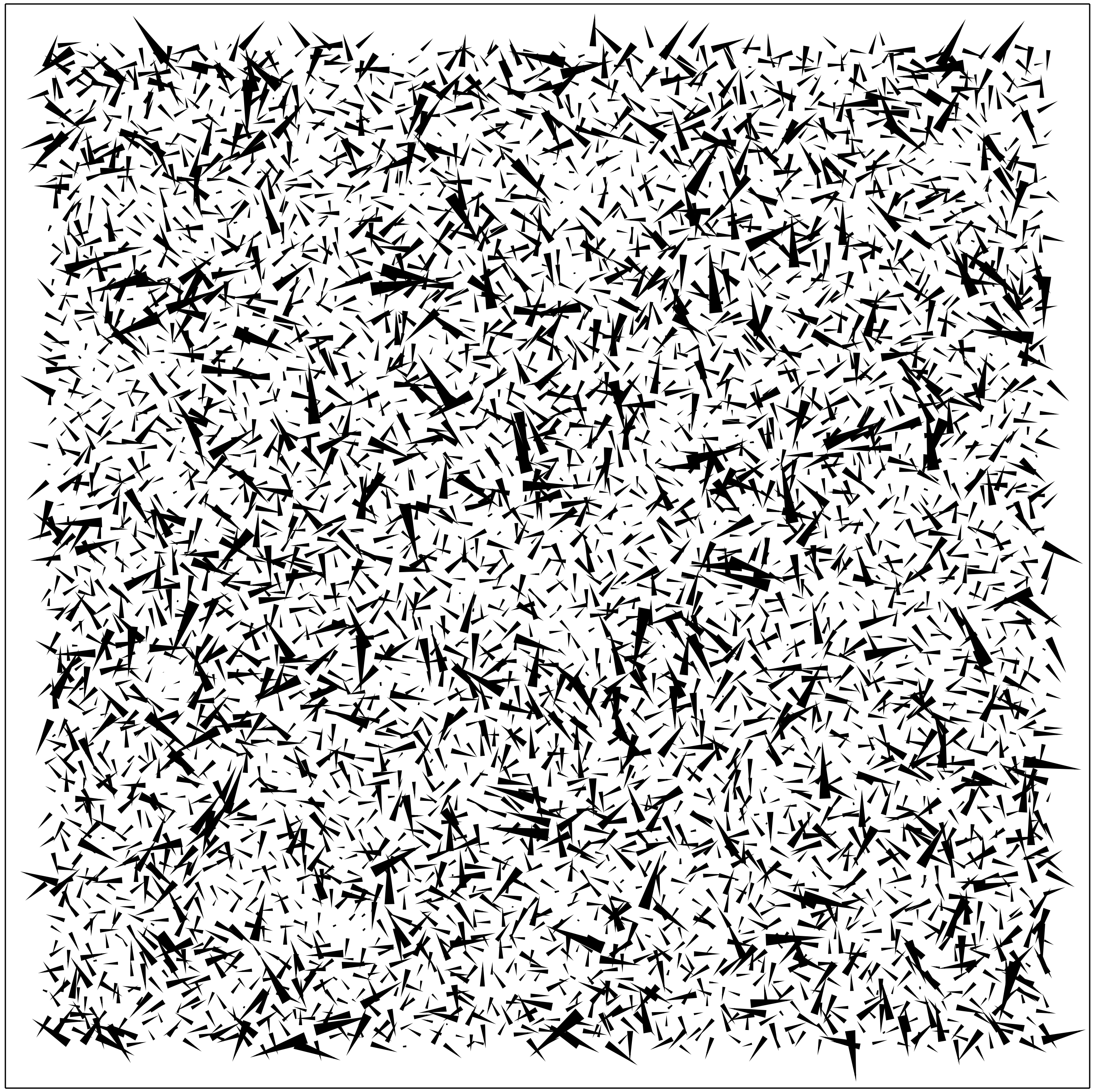


Computing the response

- Back to full assembly:

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

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

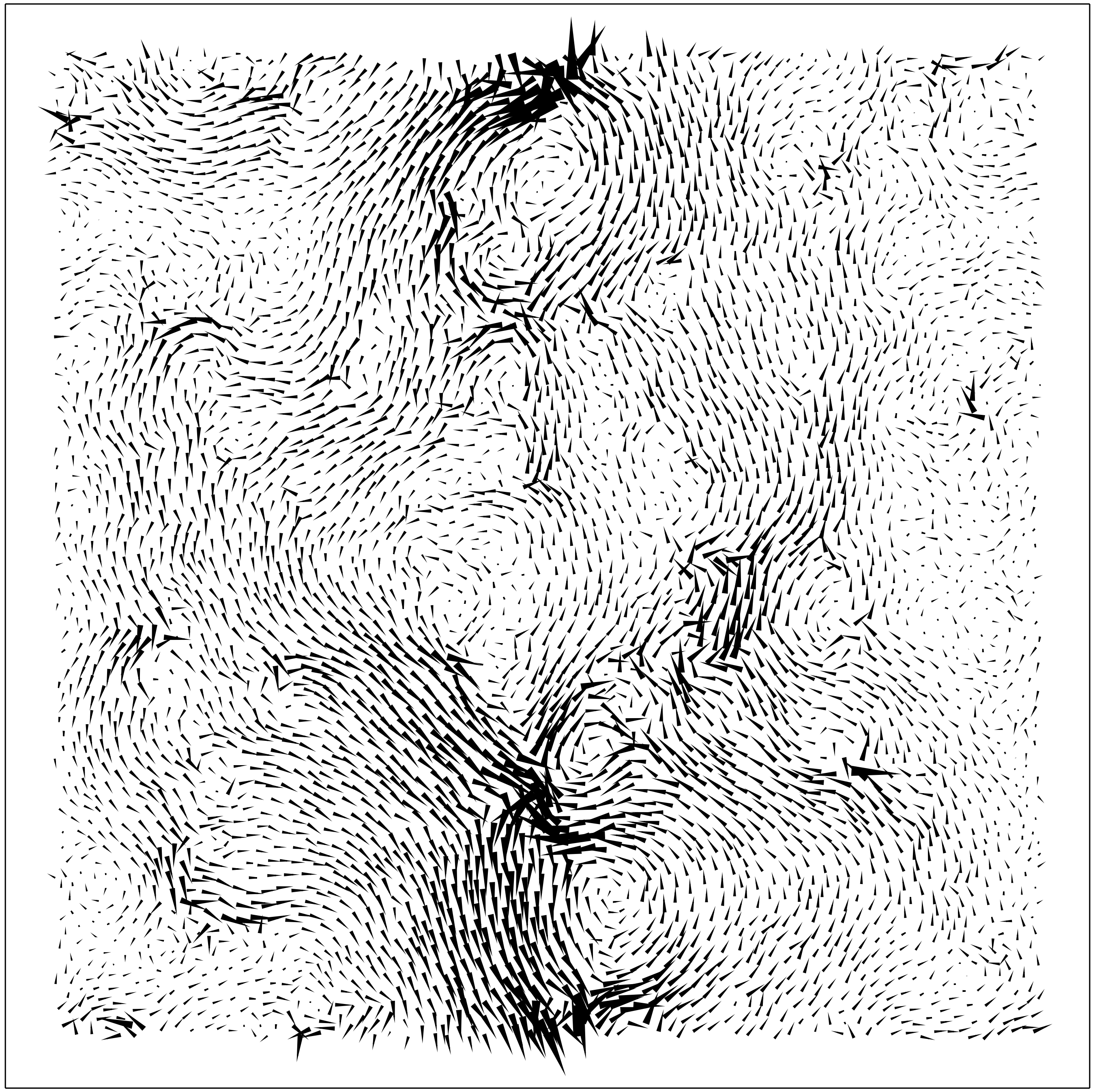


Computing the response

- Back to full assembly:

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

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



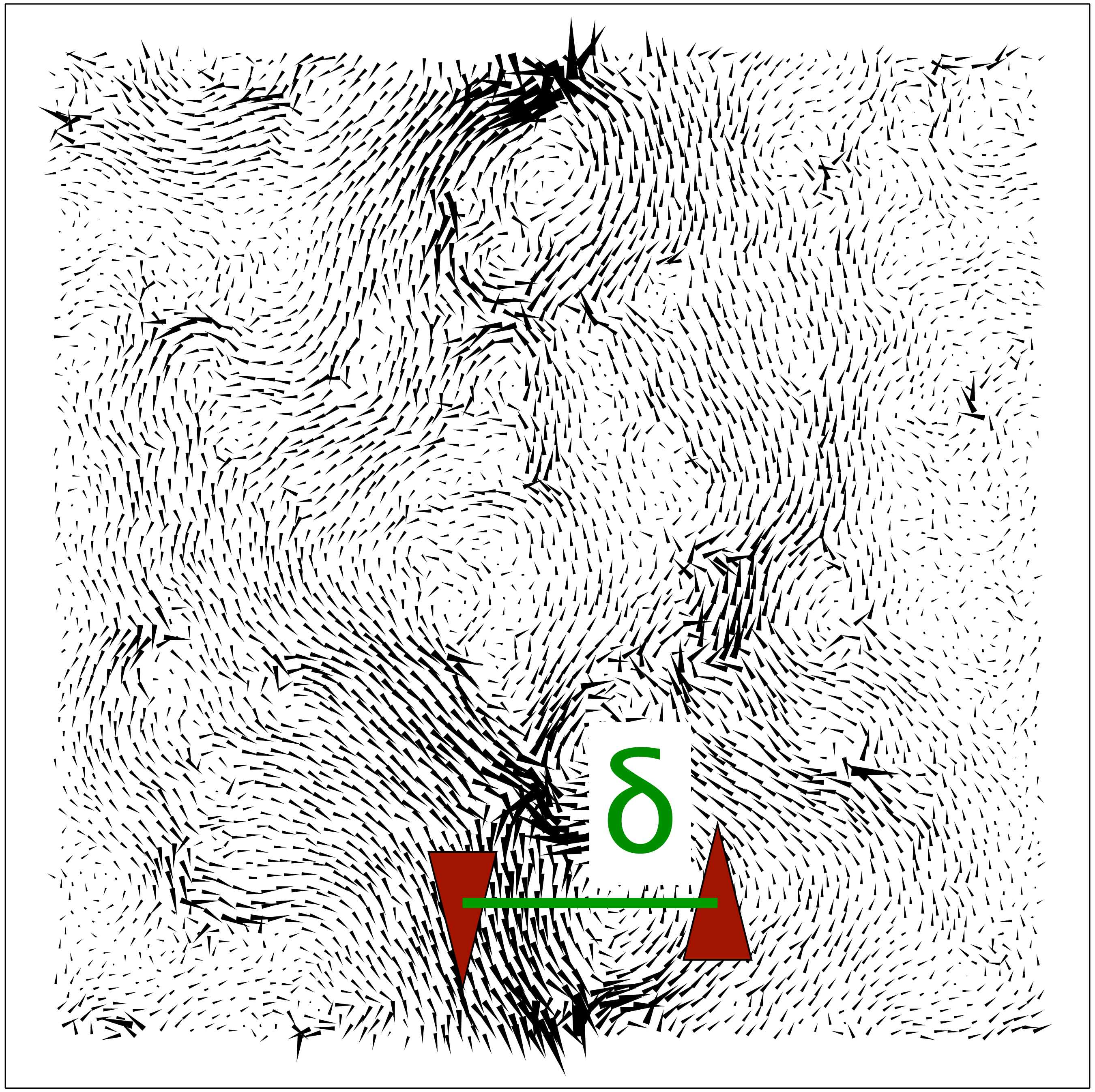
Outline

- Overview
- Scale free vortices: (CEM [PRL 2006])
  - Autocorrelation g(r)
  - Normal-mode decomposition
- Plastic nucleation
- Outlook

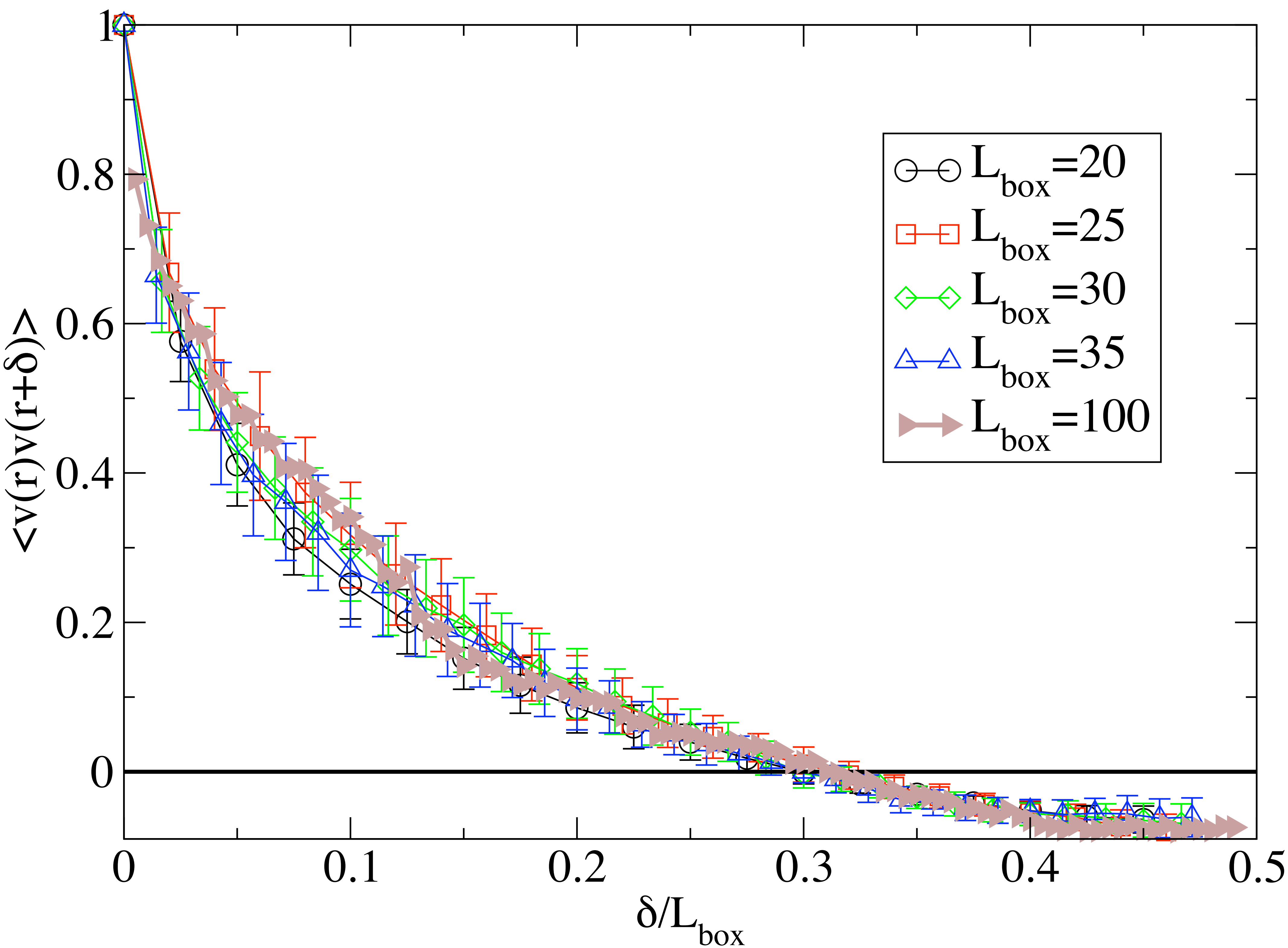
Autocorrelation, g(δ)

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

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



Autocorrelation, g(δ)



g(δ): Theoretical form

Recall:

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

Then:

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

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

g(δ): Theoretical form

Recall:

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

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

Approximate dr_i as random sum of plane waves:

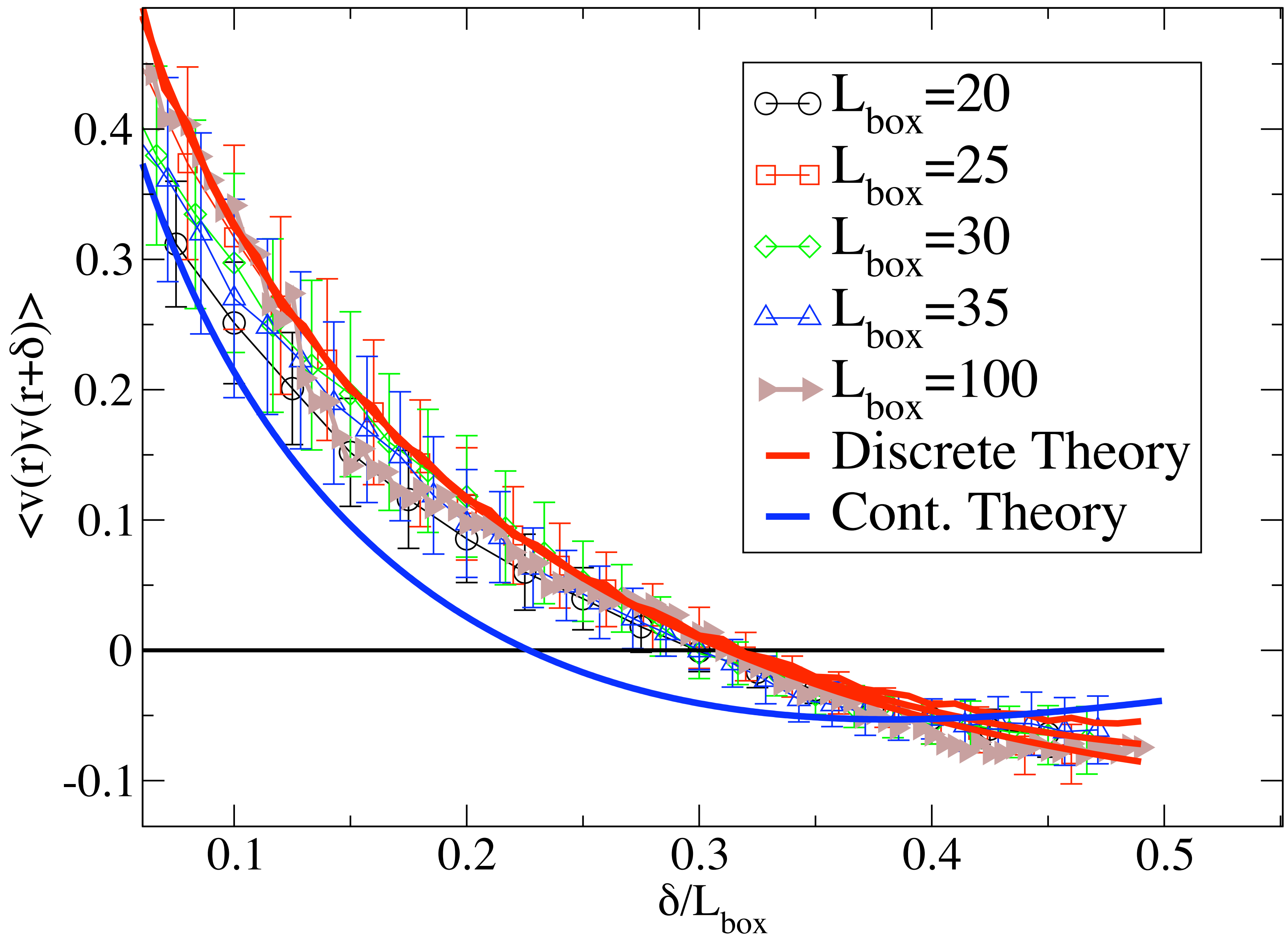
$$\vec{dr}_i \sim \sum_{k=(m,n)} \phi_{mn} \frac{e^{2\pi i \vec{k} \cdot \vec{x}_i / L}}{|\vec{k}|}$$

Then g(δ) 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" ~ .32 L_{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?

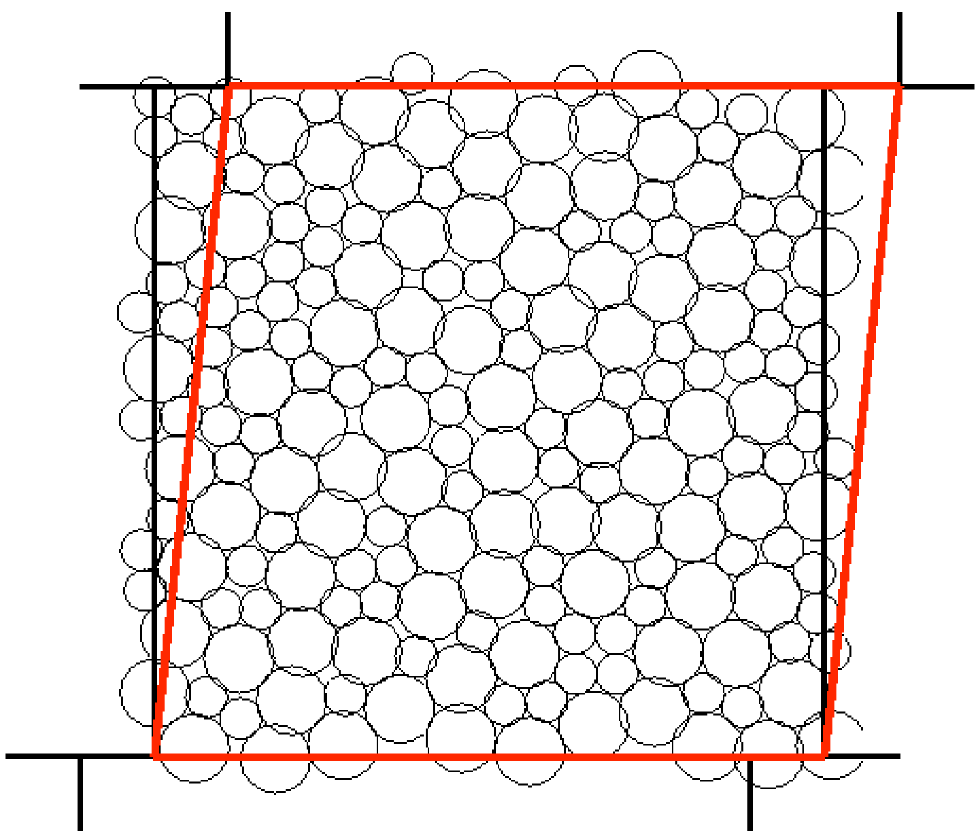
Only if I have time.

Large Strains

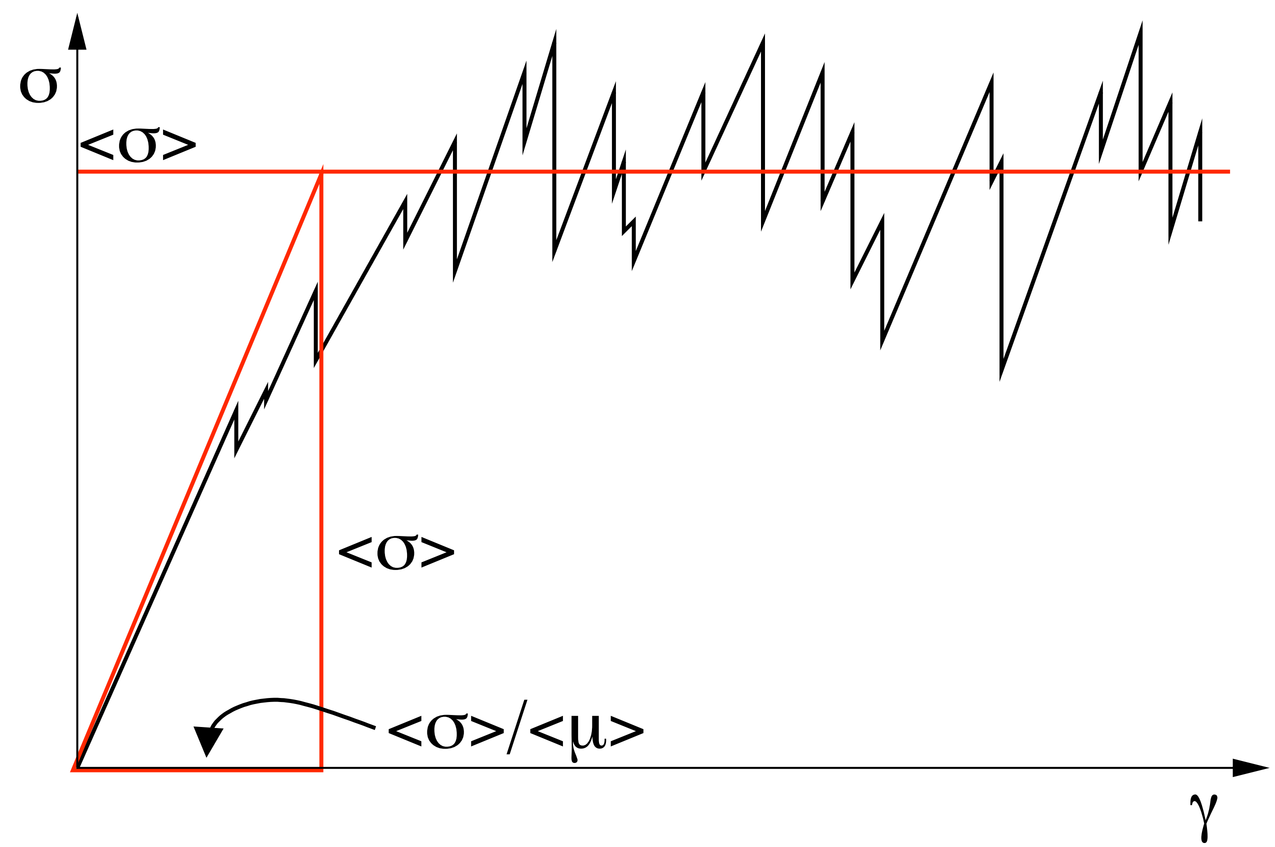
ol:

- Minimize energy
- Shear system
- Repeat

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



“Lees-Edwards” Cell

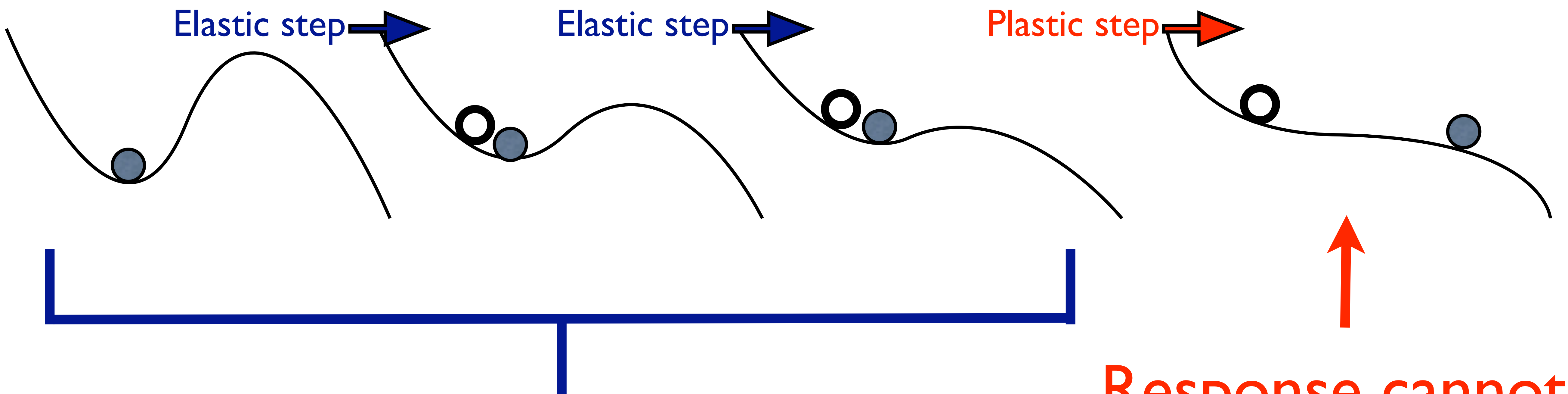


Typical Stress-Strain Curve

Landscape Perspective

Increasing strain ⇨

After Malandro and Lacks

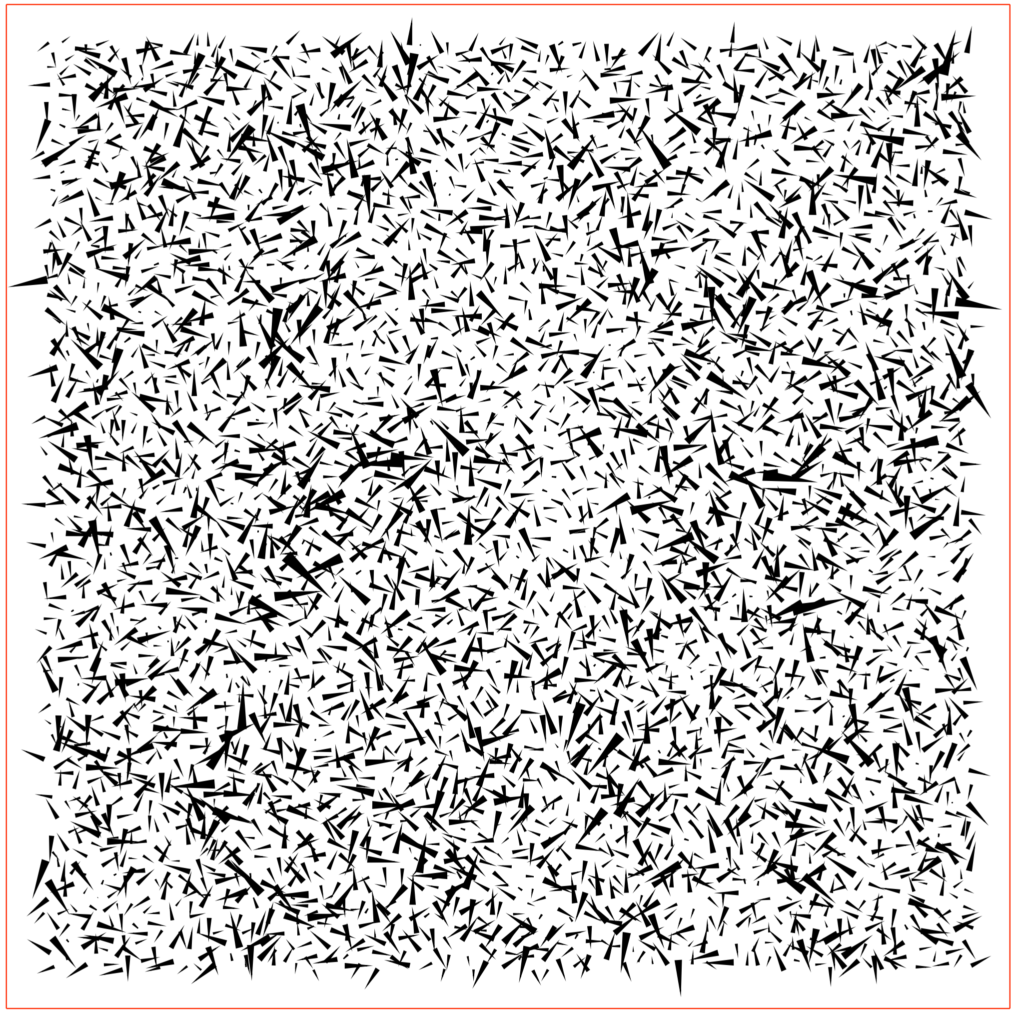


Response can be linearized.
Deformation is reversible (elastic).

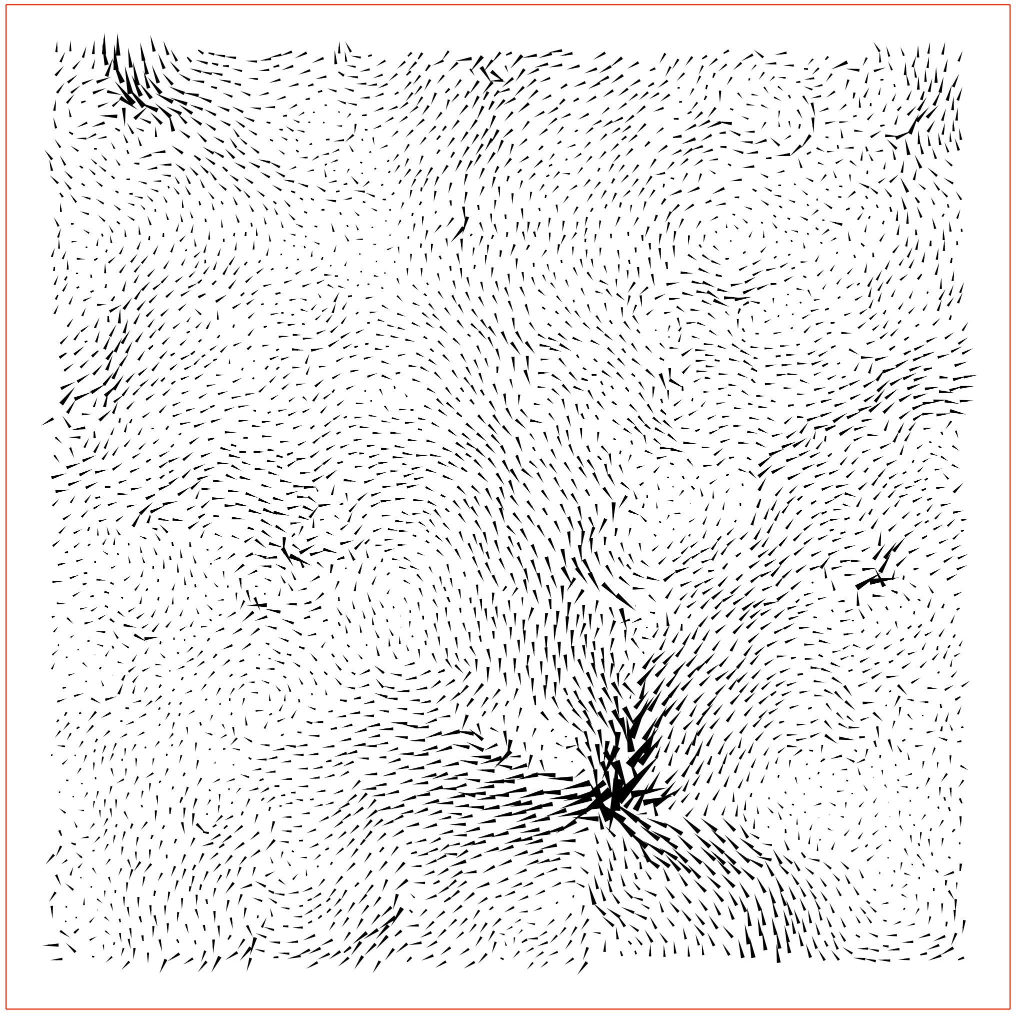
Response cannot be linearized.
Deformation is irreversible (plastic).

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

Singular Mode



Ξ



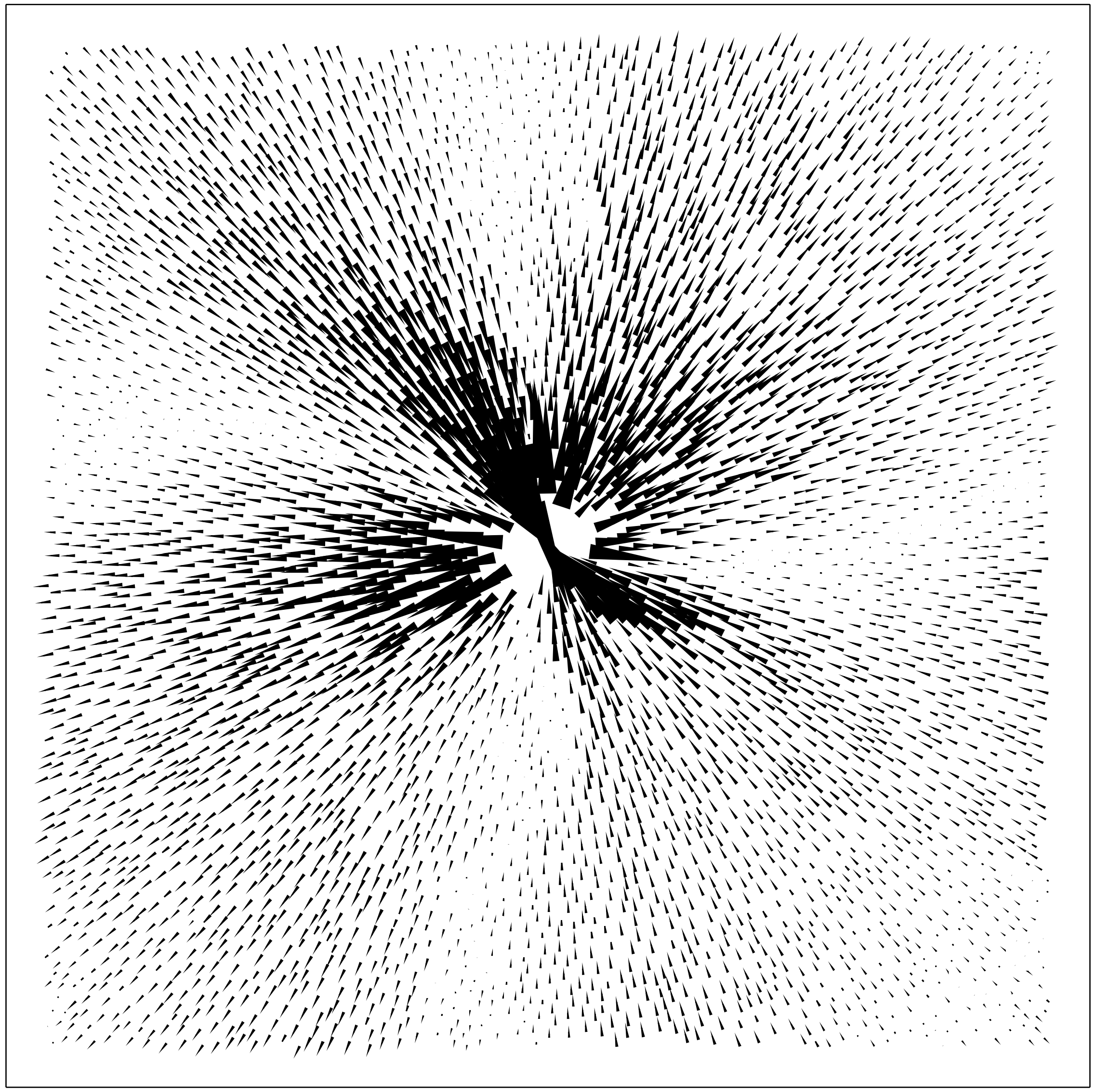
dr

Plastic nucleation is intrinsically non-local!

Cannot be detected via Ξ!

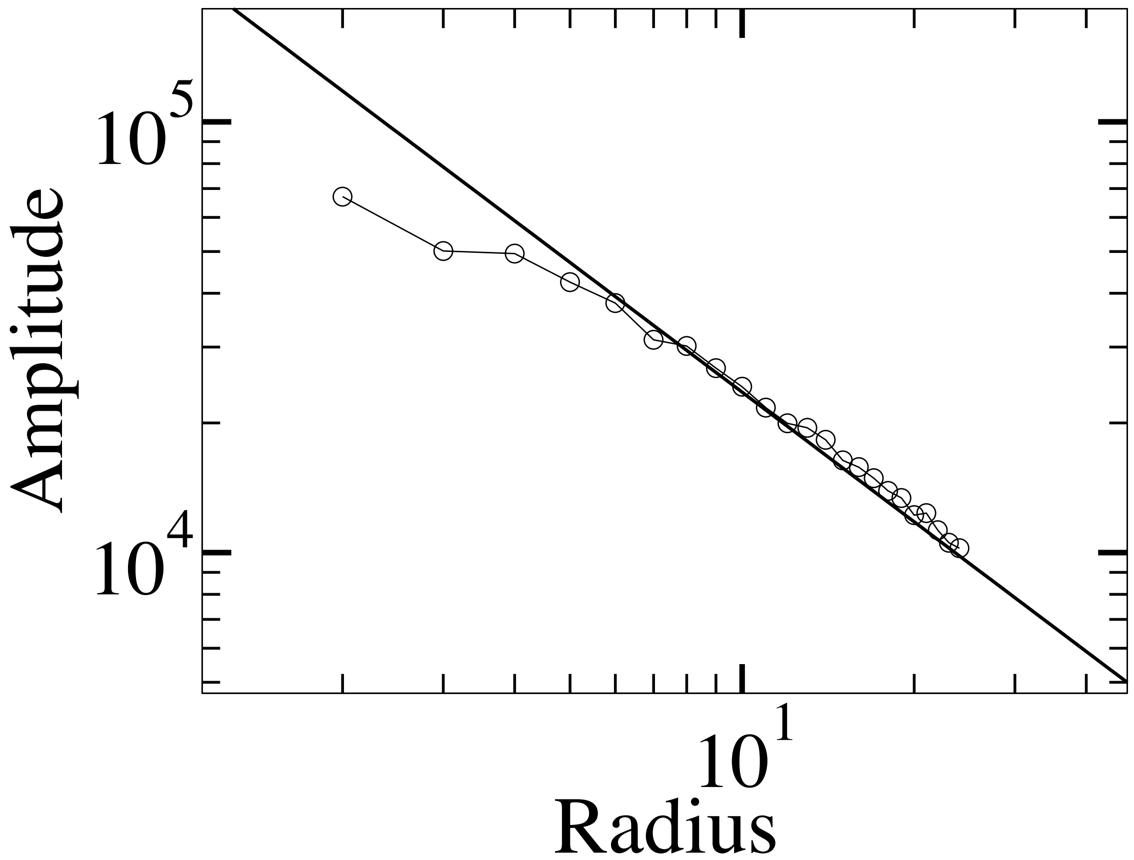
Singular Mode

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:

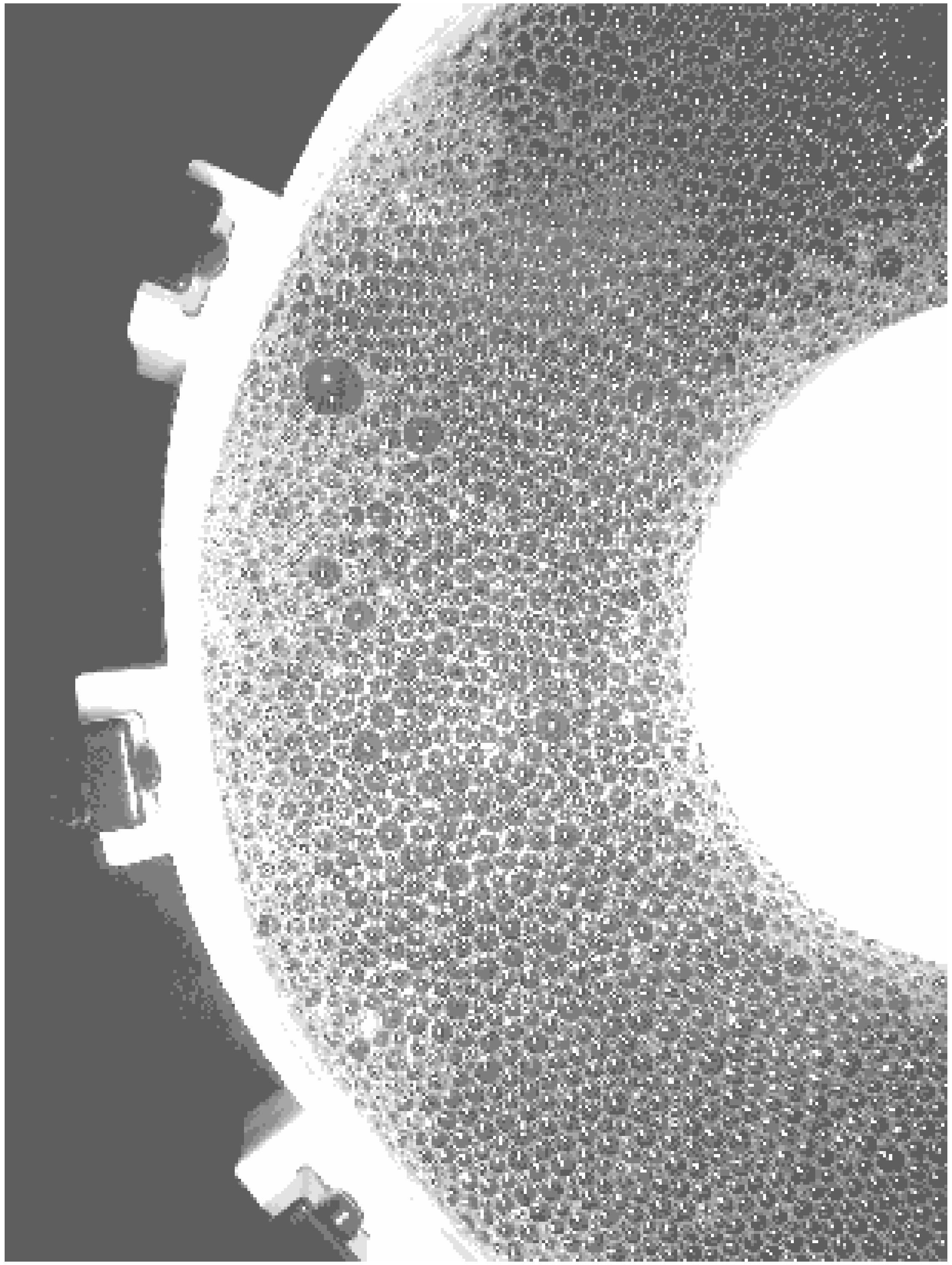
- Diverging elastic displacement triggers plastic nucleation
- Onset of plasticity is NOT detectable via the local quantities (σ,Ξ,μ_{Born}, etc)

Future Direction:

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

Jammed Systems

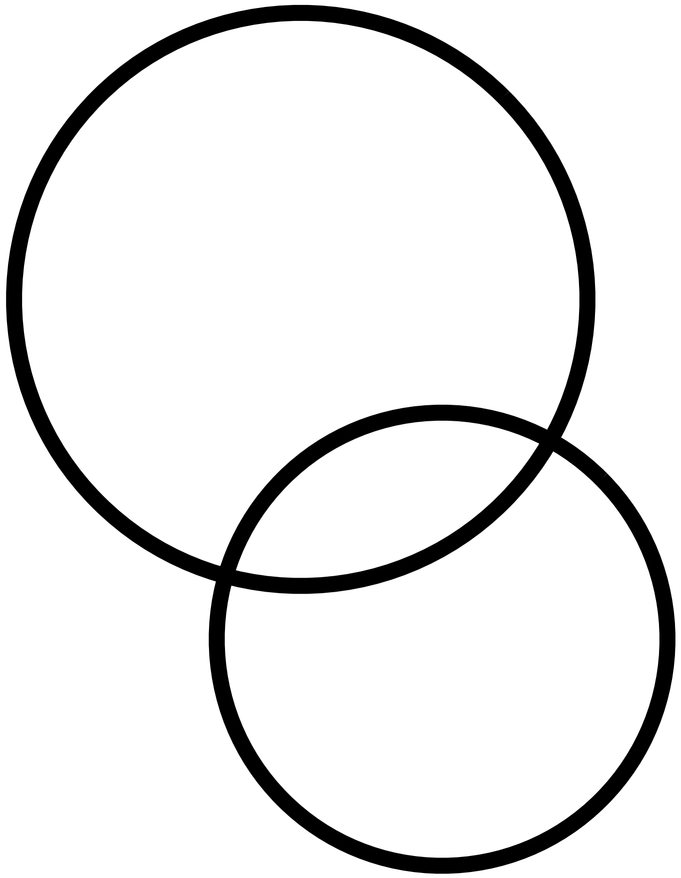
- Examples:
  - Bubbles/Emulsions
  - Grains
  - Glasses
- Non examples:
  - Suspensions / Rigid Grains
- Differences:
  - Inertia/Temp/Dissipation
- Similarity:
  - Geometry!
- Issues:
  - Characterizing disorder
  - Elasticity / Vibrations
  - Plasticity / Yielding



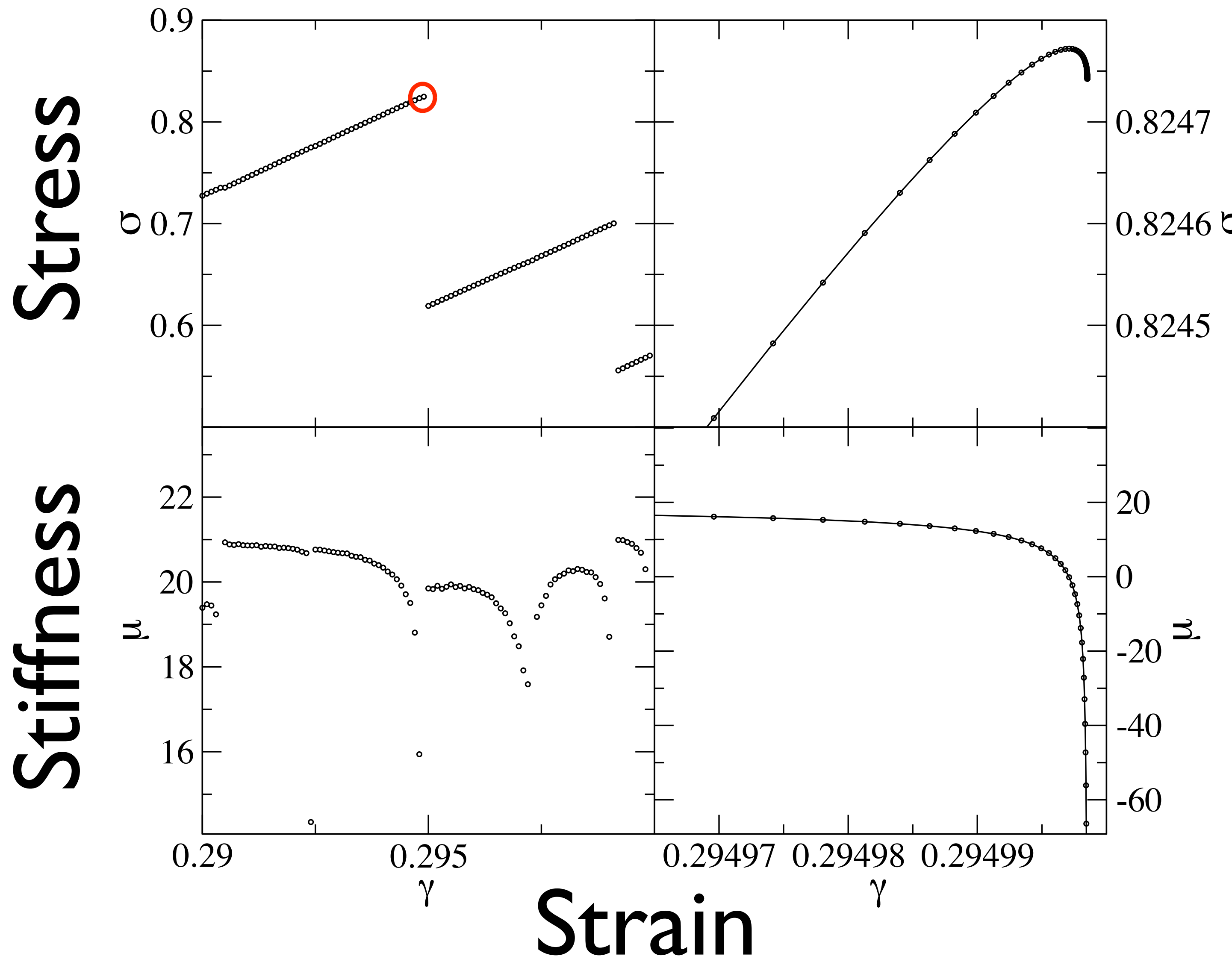
From (M Dennin)

Numerical protocol

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



Approach to Singularity



Initiation of single plastic event

$$\frac{d\sigma}{d\gamma} = \frac{\partial\sigma}{\partial\gamma} + \sum_i \frac{\partial\sigma}{\partial r_{i\alpha}} \frac{dr_{i\alpha}}{d\gamma}$$

$$= \frac{\partial\sigma}{\partial\gamma} - \sum_{ij} \Xi_{i\alpha} H^{-1}_{i\alpha j\beta} \Xi_{j\beta}$$

$$= \frac{\partial\sigma}{\partial\gamma} - \sum_p \frac{\Xi_p^2}{\lambda_p}$$

Catastrophe Theory:

$$\lambda_0 \sim \sqrt{\delta\gamma}$$

$$\mu \sim -(\delta\gamma)^{-1/2}$$