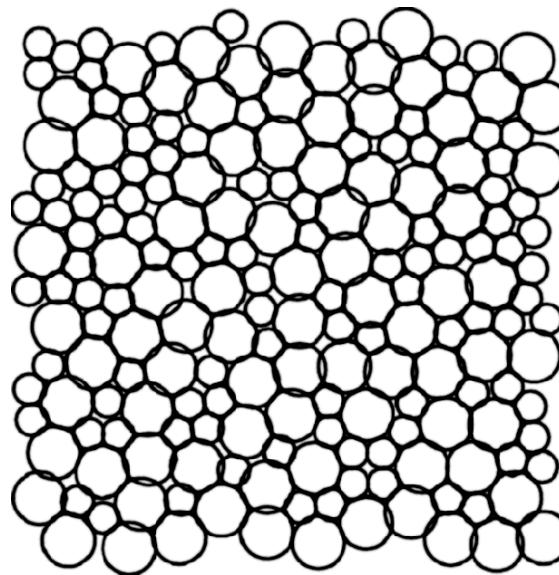


Amorphous Materials in Quasistatic Shear

Craig Maloney

UCSB Physics

LLNL Chemistry and Materials Science



Acknowledgements: A. Lemaître, J.S. Langer, V.V. Bulatov

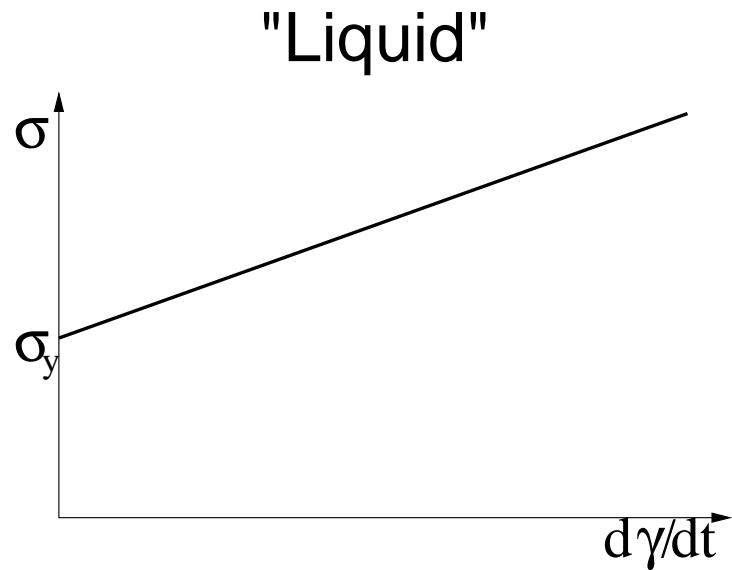
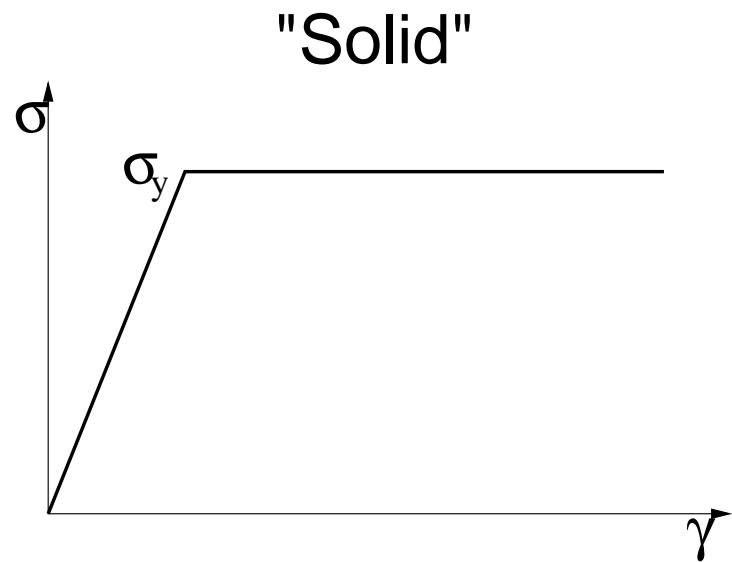
UCSB-MRL: NSF-DMR00-80034

LLNL-CMS: DOE-W-7405-Eng-48



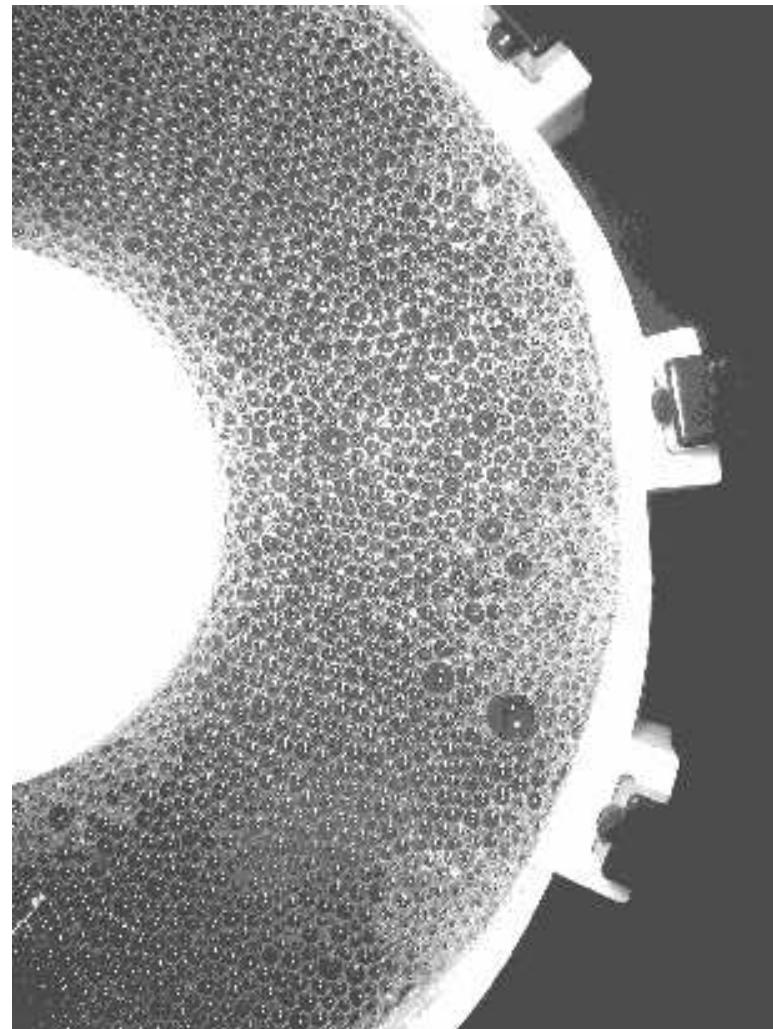
Solid or Liquid?

- Many materials behave like **solids** at low loads but **liquids** at higher loads.



Solid or Liquid?

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- Examples:
 - "Bubbles"



(from Michael Dennin's Group)

Solid or Liquid?

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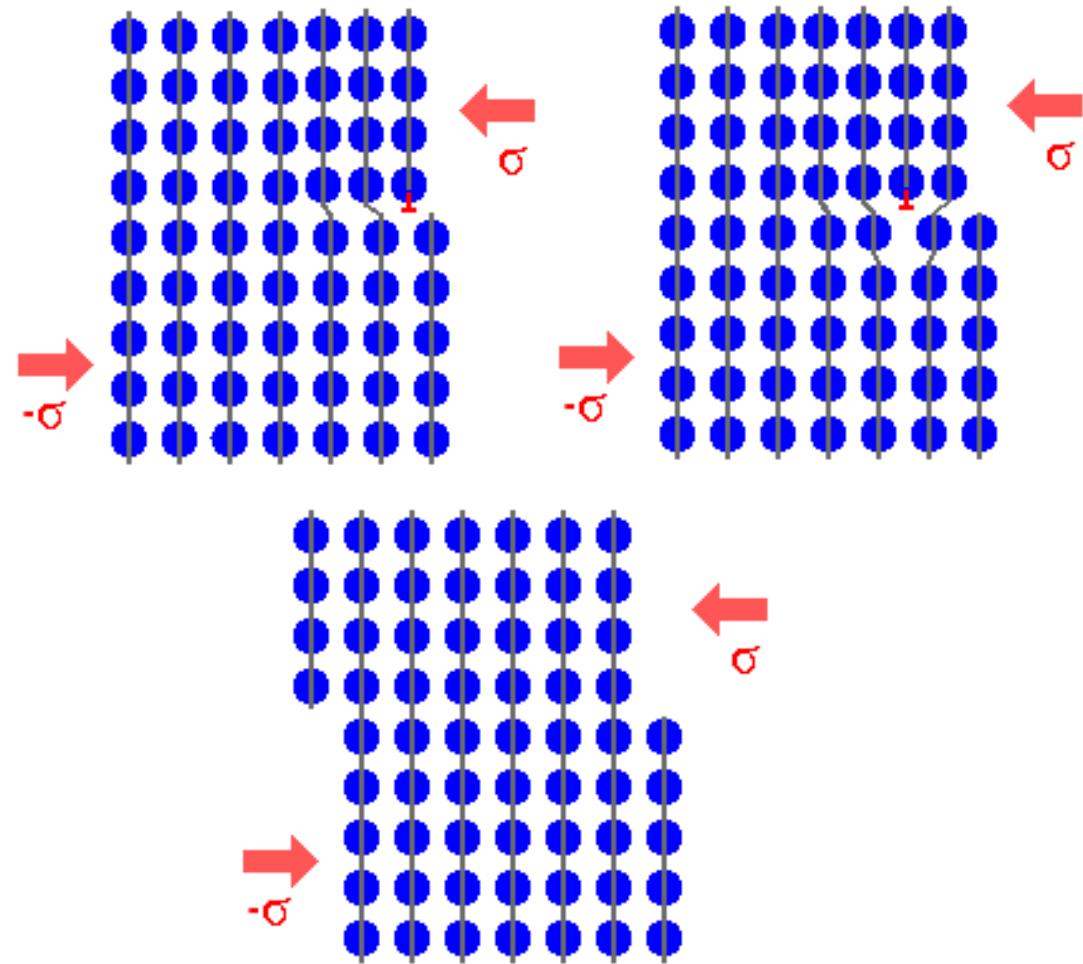
(from Bob Behringer's Group)

Solid or Liquid?

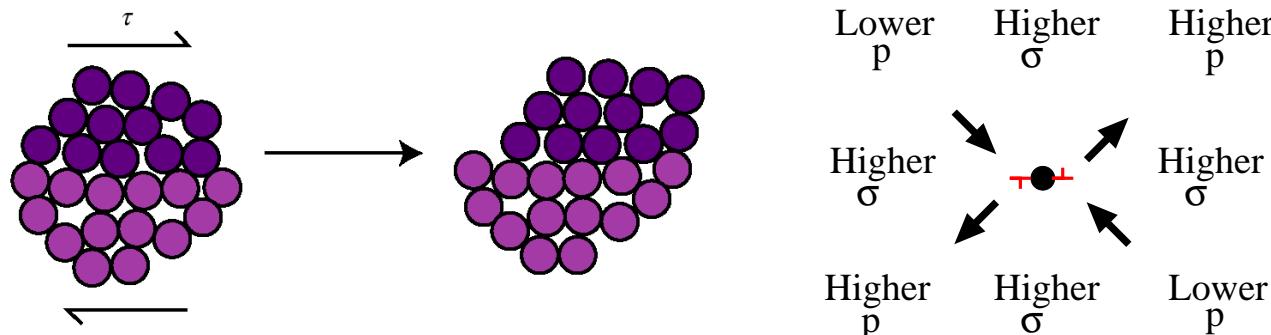
- Many materials behave like **solids** at low loads but **liquids** at higher loads.
 - Examples:
 - "Bubbles"
 - "Grains"
 - "Atoms"
- Atoms ???

Dislocations?

- “Glide”: Mechanism for flow!
- Well defined topological defect.
- Production at boundaries or in pairs.
- Source of stress.



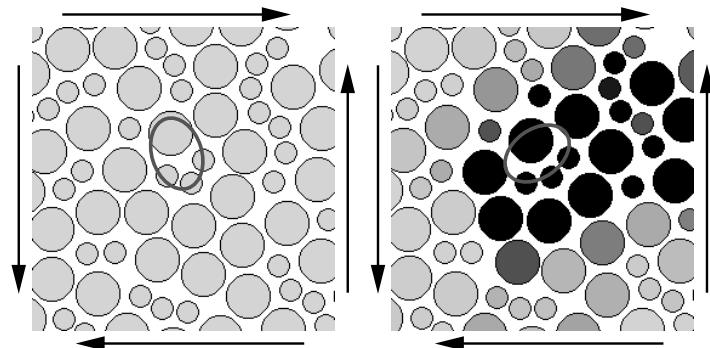
Shear Transformation Zones (STZs)



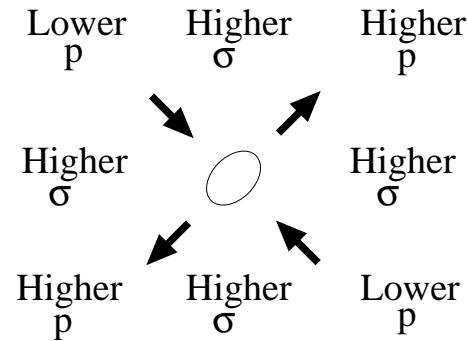
(from C. Schuh; after Argon 1979)

- Shear Transformations (Argon 79, Maeda and Takeuchi 81)
 - Small cluster of particles
 - Looks like pair nucleation (back stresses)

Shear Transformation Zones (STZs)

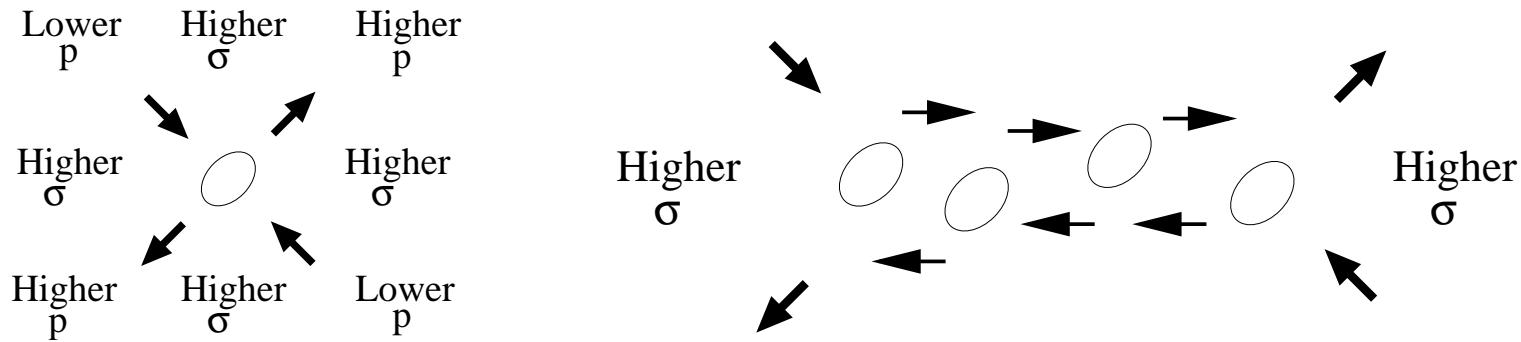


(from Falk and Langer 1998)



- STZ theory (Falk and Langer 1998)
 - Two-state picture
 - Captures memory effects.

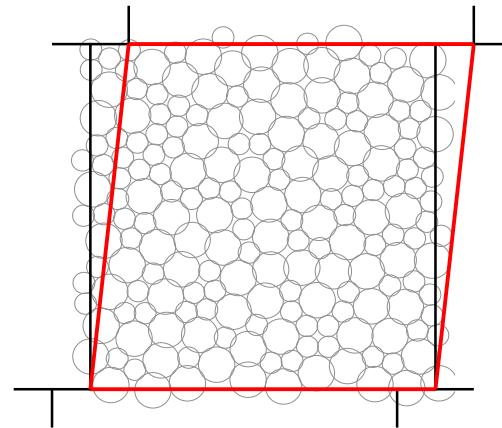
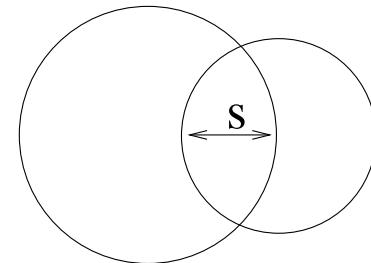
Shear Transformation Zones (STZs)



- "Local Inelastic Transformation" model (Bulatov and Argon 1994)
 - Transformations can organize
 - Resembles dislocation nucleation + glide
 - Constructed mesoscale model.
 - Related models constructed: Langer (2001), Baret et. al. (2002), Onuki (2003), Picard et. al. (2004)

Atomistic Model and Algorithm

- Potentials:
 - Harmonic: $U = \frac{1}{2}ks^2$
 - Hertzian: $U = \frac{1}{2}ks^{5/2}$
 - Lennard-Jones: $U = k(r^{-12} - 2r^{-6})$
- Binary mixture.
- “Lees-Edwards” boundaries.
- Quasistatic Shearing:
 - Apply uniform shear.
 - Minimize energy at fixed box.
 - Repeat.



Energy Landscape Perspective

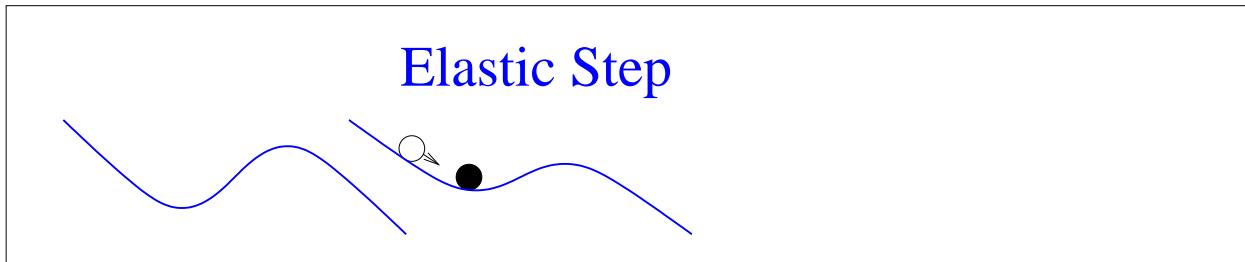
- Strain biases landscape. (Malandro and Lacks 98)



Elastic segment: system follows energy minimum. Reversible.

Energy Landscape Perspective

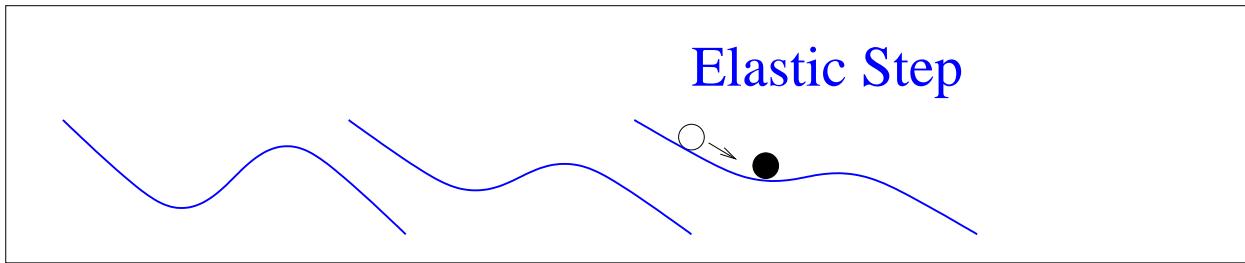
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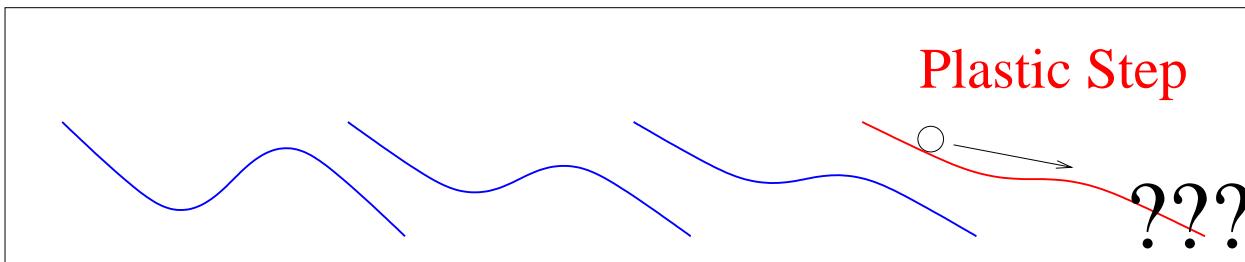
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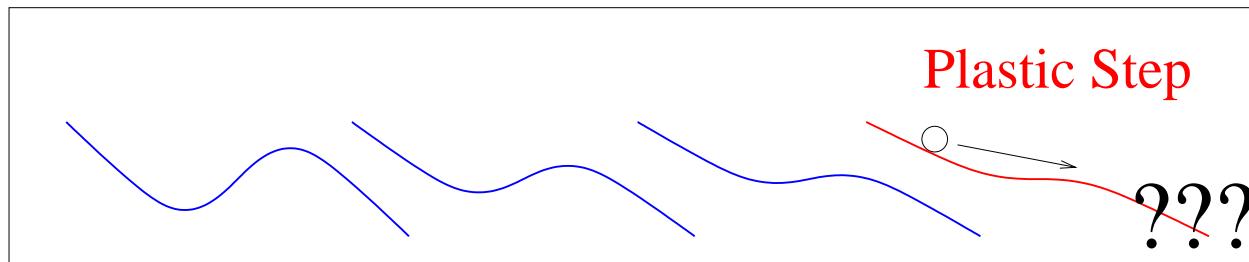


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Plastic event: local energy minimum vanishes. Irreversible.

Energy Landscape Perspective

- Strain biases landscape. (Malandro and Lacks 98)



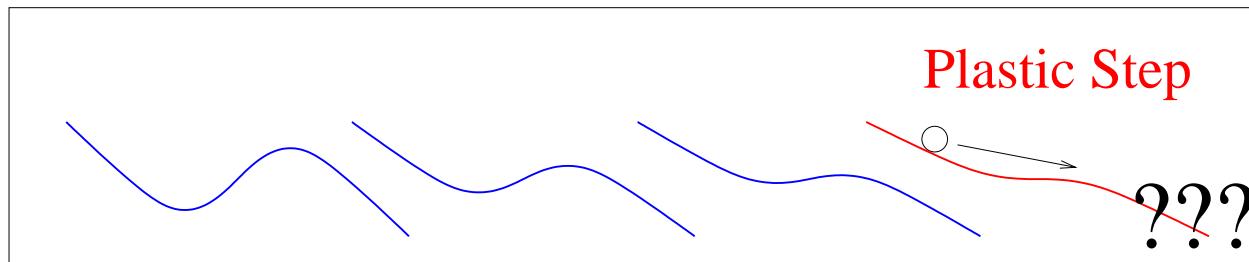
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Energy Landscape Perspective

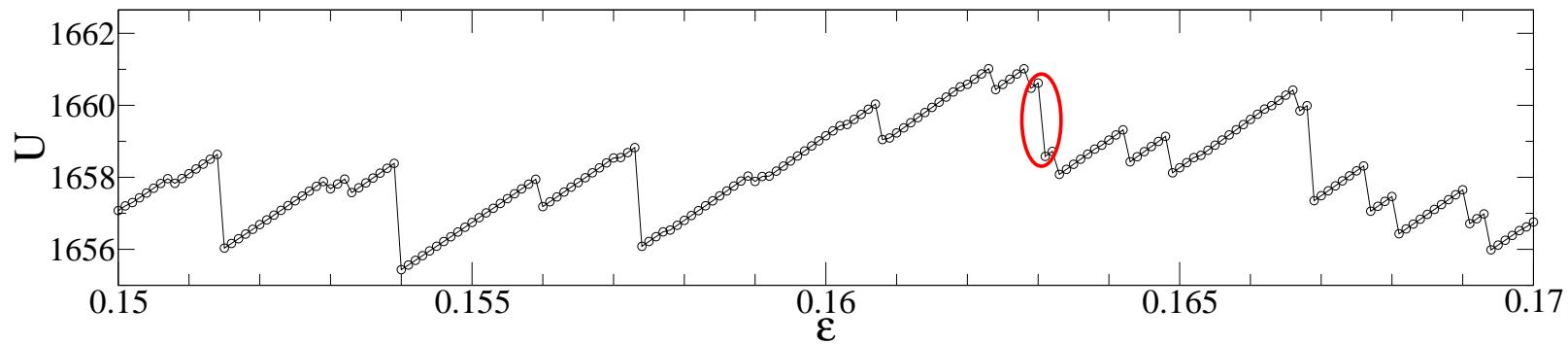
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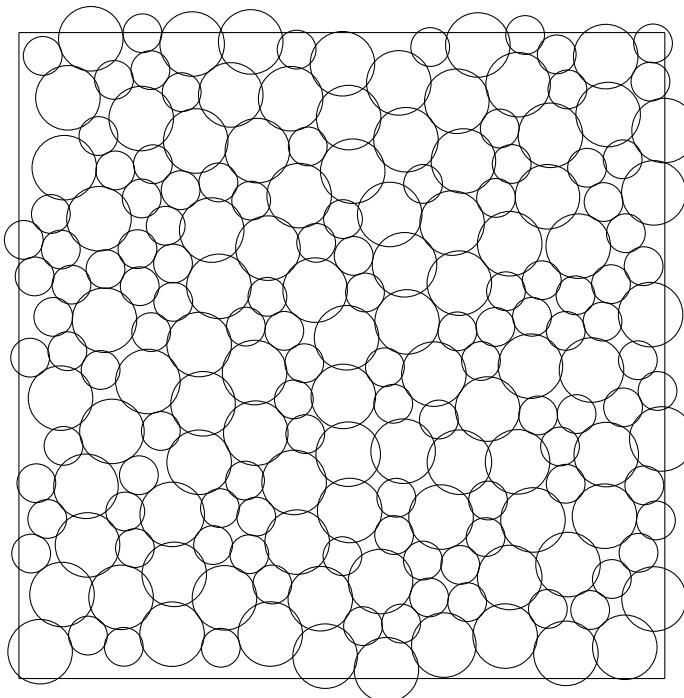
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Part I

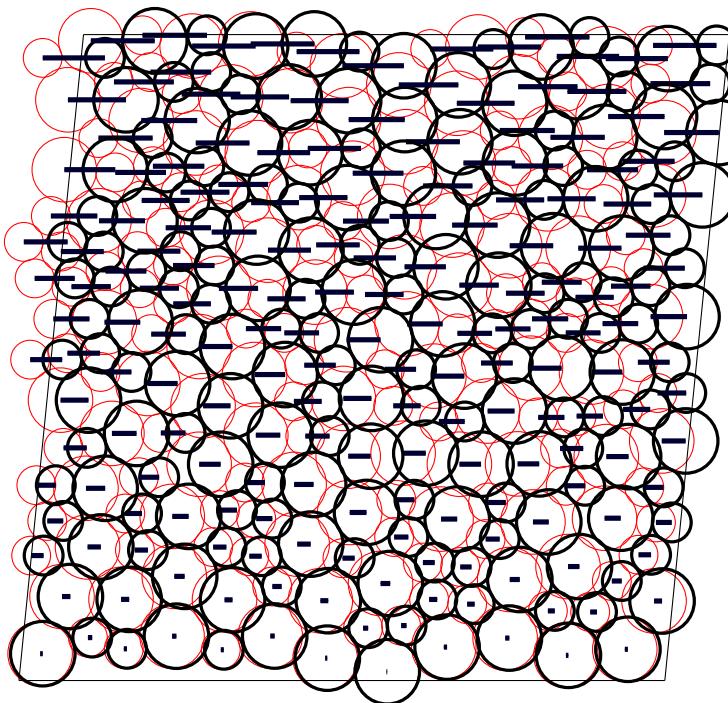
Elastic Segments

Non-affine Elasticity: Transformations



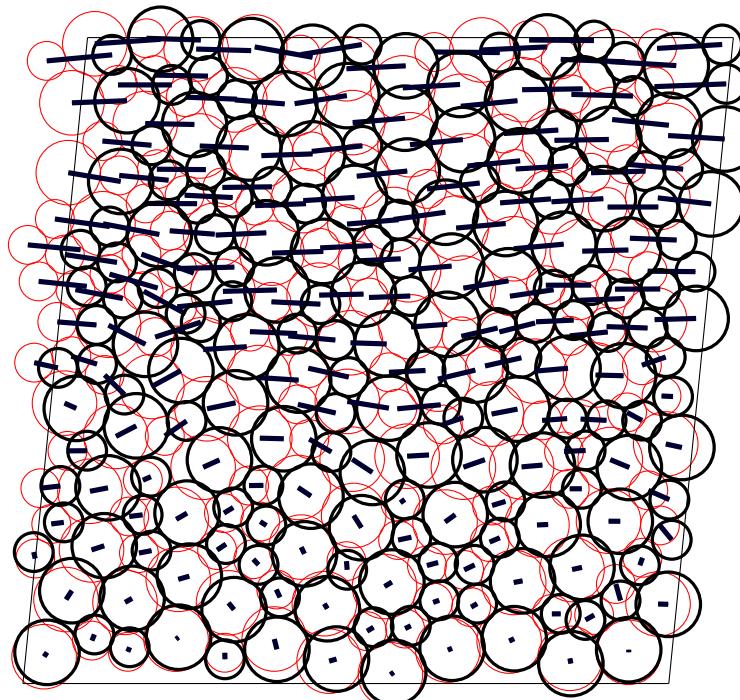
- Initial packing. Forces = 0.

Non-affine Elasticity: Transformations



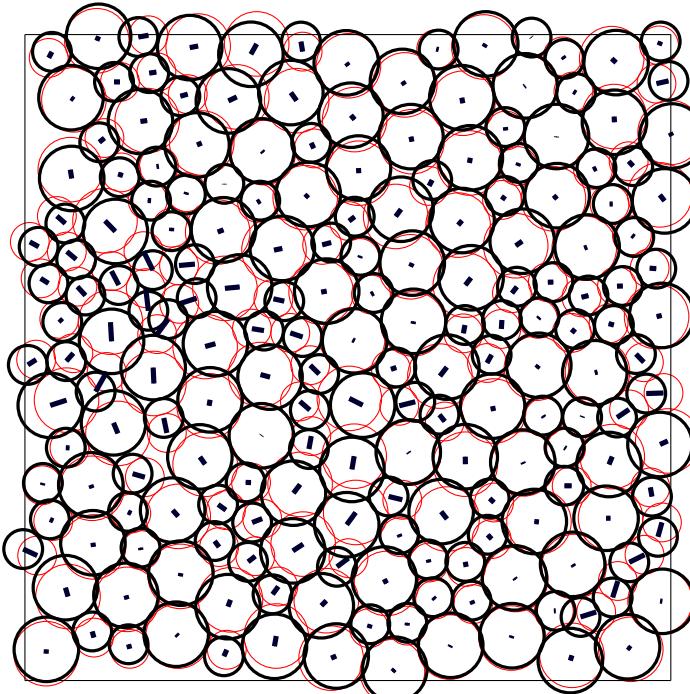
- Uniform strain. Forces $\neq 0$.

Non-affine Elasticity: Transformations



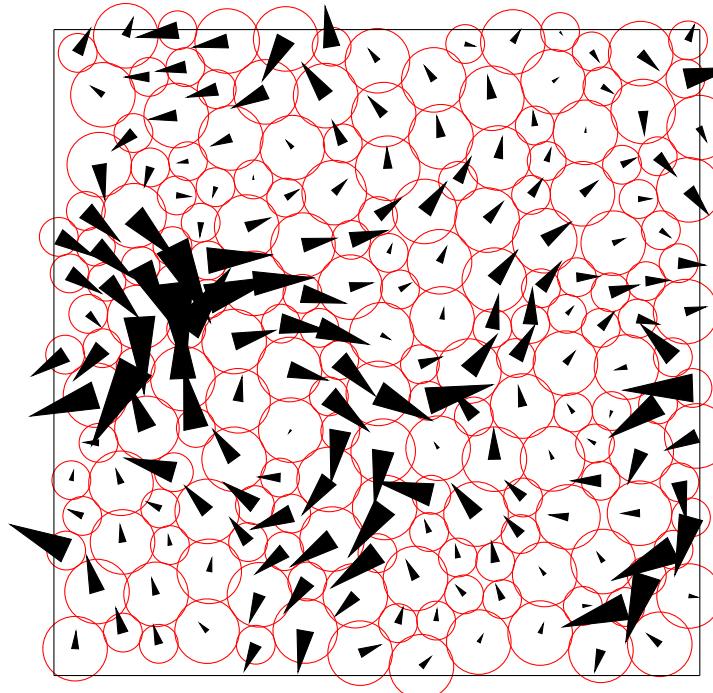
- Apply correction. $\text{Forces} = 0.$

Non-affine Elasticity: Transformations



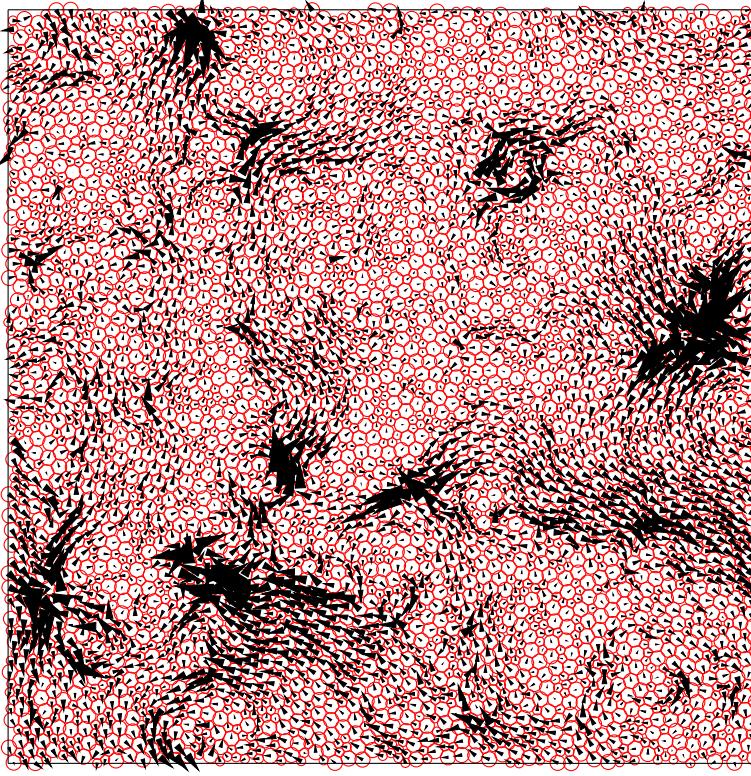
- Subtract uniform strain.

Non-affine Elasticity: Transformations



- “Arrows” more illustrative.

Non-affine Elasticity: Transformations



- Same procedure. Larger system.

Analytical Expressions

$$U(\{s_{i\alpha}\}, h_{ij}(\gamma))$$

- Control parameter, γ , controls shape of box.
- Particle co-ordinates, $s_{i\alpha}$, determine energy for fixed γ .

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

- Forces, $F_{i\alpha}$. Energy derivative with respect to particle motion at fixed box shape.

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

$$\frac{\partial U}{\partial \gamma} \doteq \sigma$$

- Stress, σ . Energy derivative with respect to box shape with particle positions fixed *in the reference box*. That is... an *affine* derivative.

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

- Hessian matrix, $\mathcal{H}_{i\alpha j\beta}$. Change in force on particle i with respect to move of particle j .

$$\frac{\partial U}{\partial \gamma} \doteq \sigma$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial s_{j\beta}} \doteq \mathcal{H}_{i\alpha j\beta}$$

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

$$\frac{\partial U}{\partial \gamma} \doteq \sigma$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial s_{j\beta}} \doteq \mathcal{H}_{i\alpha j\beta}$$

$$\frac{\partial^2 U}{\partial \gamma \partial \gamma} \doteq \mu_a$$

- Affine modulus, μ_a . Derivative of stress with respect to box shape which *presupposes* affine particle motion.

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

$$\frac{\partial U}{\partial \gamma} \doteq \sigma$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial s_{j\beta}} \doteq \mathcal{H}_{i\alpha j\beta}$$

$$\frac{\partial^2 U}{\partial \gamma \partial \gamma} \doteq \mu_a$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial \gamma} \doteq \Xi_{i\alpha}$$

- Local disorder field, $\Xi_{i\alpha}$. Change in force on particle i with respect to an affine motion. The non-affine motion must end up cancelling this extra force after an affine displacement to maintain $F_{i\alpha} = 0$.

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

- Can solve analytically for elastic response!

$$\frac{\partial U}{\partial \gamma} \doteq \sigma$$

- Track energy minimum.
- Require forces remain zero.
(Wallace).

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial s_{j\beta}} \doteq \mathcal{H}_{i\alpha j\beta}$$

$$\frac{\partial^2 U}{\partial \gamma \partial \gamma} \doteq \mu_a$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial \gamma} \doteq \Xi_{i\alpha}$$

$$\frac{d}{d\gamma} \left(\frac{\partial U}{\partial s_{i\alpha}} \right) = \mathcal{H}_{i\alpha j\beta} \frac{ds_{j\beta}}{d\gamma} + \Xi_{i\alpha}$$

$$\Rightarrow \frac{ds_{i\alpha}}{d\gamma} = -\mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta}$$

Analytical Expressions

$$-\frac{\partial U}{\partial s_{i\alpha}} \doteq F_{i\alpha}$$

$$\frac{\partial U}{\partial \gamma} \doteq \sigma$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial s_{j\beta}} \doteq \mathcal{H}_{i\alpha j\beta}$$

$$\frac{\partial^2 U}{\partial \gamma \partial \gamma} \doteq \mu_a$$

$$\frac{\partial^2 U}{\partial s_{i\alpha} \partial \gamma} \doteq \Xi_{i\alpha}$$

- Consequence: Modulus, $\left. \frac{d^2 U}{d \gamma^2} \right|_{F=0}$, will always be **smaller** than the naive expectation.

$$\left. \frac{dU}{d\gamma} \right|_{F=0} = \sigma - F_{i\alpha} \frac{ds_{i\alpha}}{d\gamma} = \sigma$$

$$\left. \frac{d\sigma}{d\gamma} \right|_{F=0} = \mu_a + \Xi_{i\alpha} \frac{ds_{i\alpha}}{d\gamma}$$

$$= \mu_a - \Xi_{i\alpha} \mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta}$$

Applications?

- Normal mode decomposition

Applications?

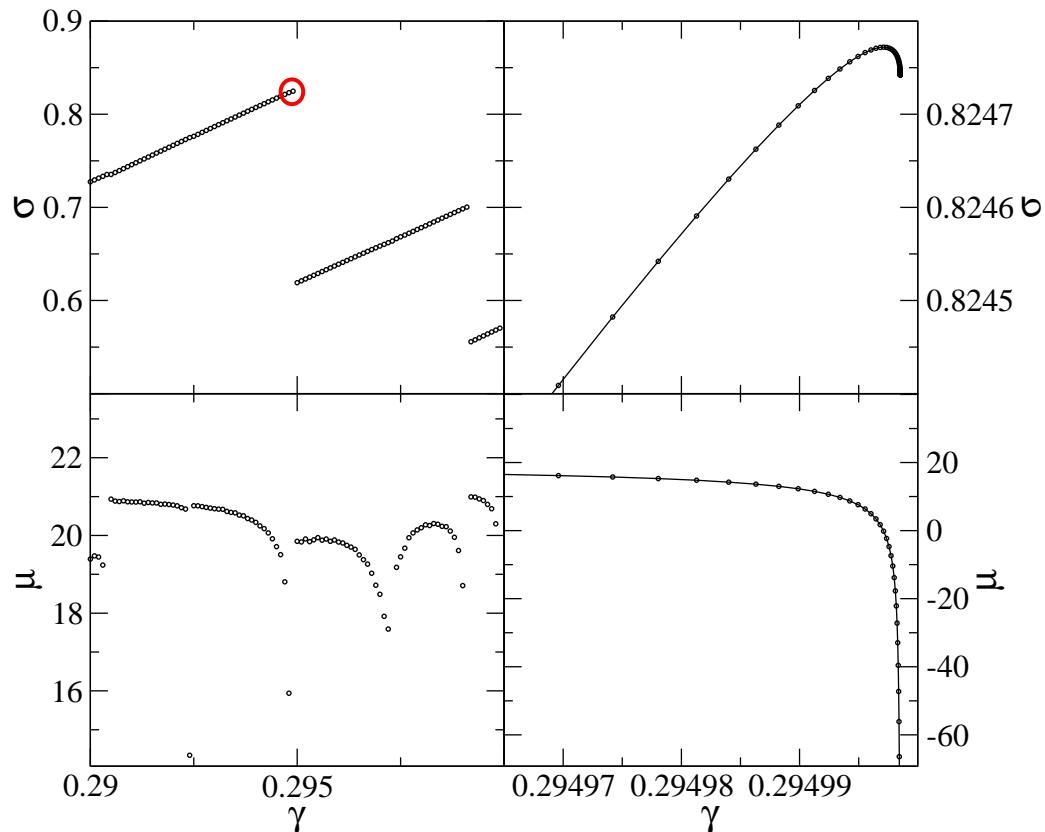
- Normal mode decomposition
- Extension to viscoelastic response

Applications?

- Normal mode decomposition
- Extension to viscoelastic response
- Analysis of nucleation of plastic events

Catastrophes

- What happens when $\mathcal{H}_{i\alpha j\beta}$ becomes singular?
- $\frac{ds_{i\alpha}}{d\gamma} \rightarrow \infty, \frac{d\sigma}{d\gamma} \rightarrow -\infty.$



Scaling Argument

- Recall:

$$\frac{ds_{i\alpha}}{d\gamma} = -\mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta}$$

- Approx: $\frac{ds_0}{d\gamma} \sim -\frac{1}{\lambda_0}$

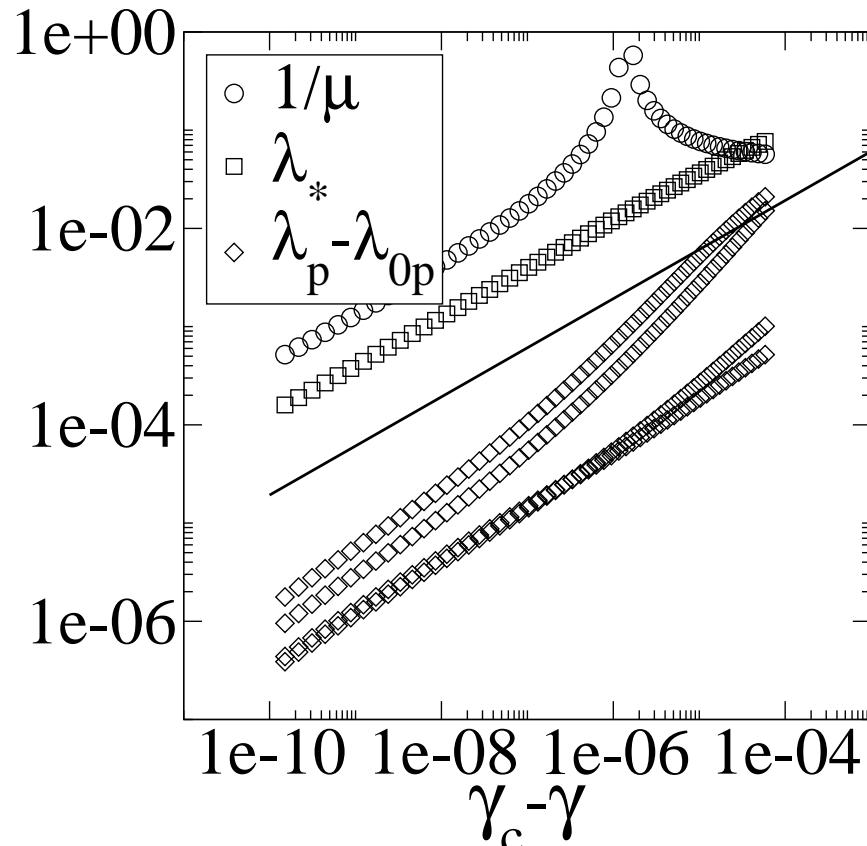
- Suppose: $\lambda_0 \sim s_0$

- $\Rightarrow s_0 \sim \sqrt{\gamma}$

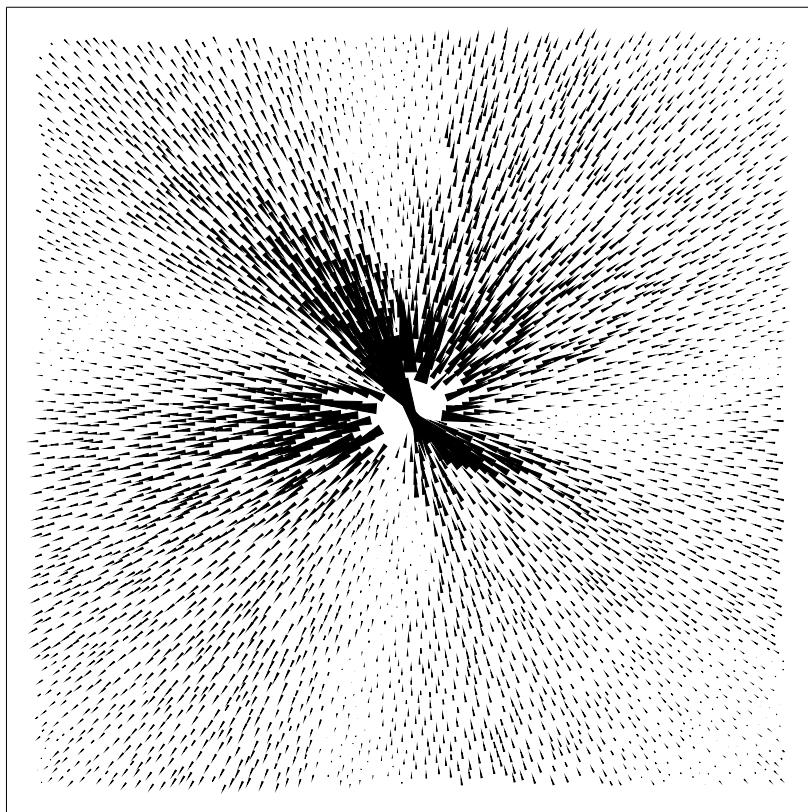
- Recall:

$$\mu = \mu_a - \Xi_{i\alpha} \mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta}$$

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

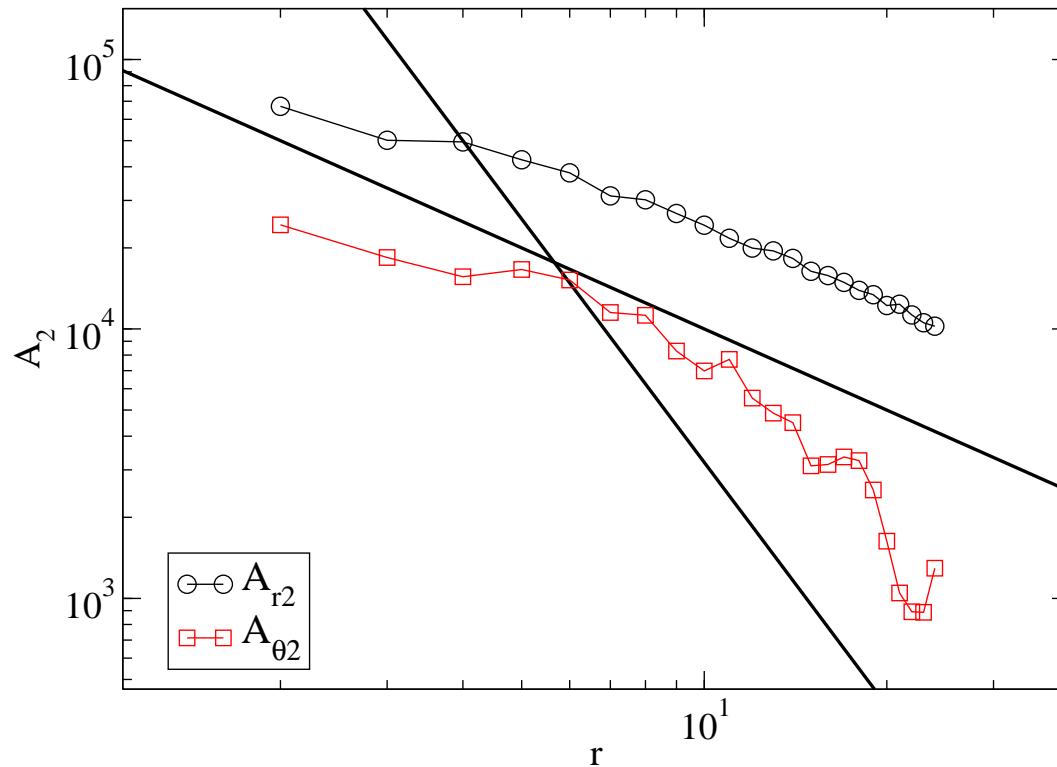


Critical Mode in Real Space



- Displacement Analysis:
 - Center on max displacement
 - Group into annuli
 - Take radial part
- Note that:
 - Quadrupole dominates.
 - Resembles nucleation of dislocation pair or small crack.
 - Consistent with picture of an incipient STZ.

Critical Mode in Real Space (II)



Quadrupolar projection of \vec{u}
Elasticity theory $\Rightarrow Ar^{-1} + Br^{-3}$

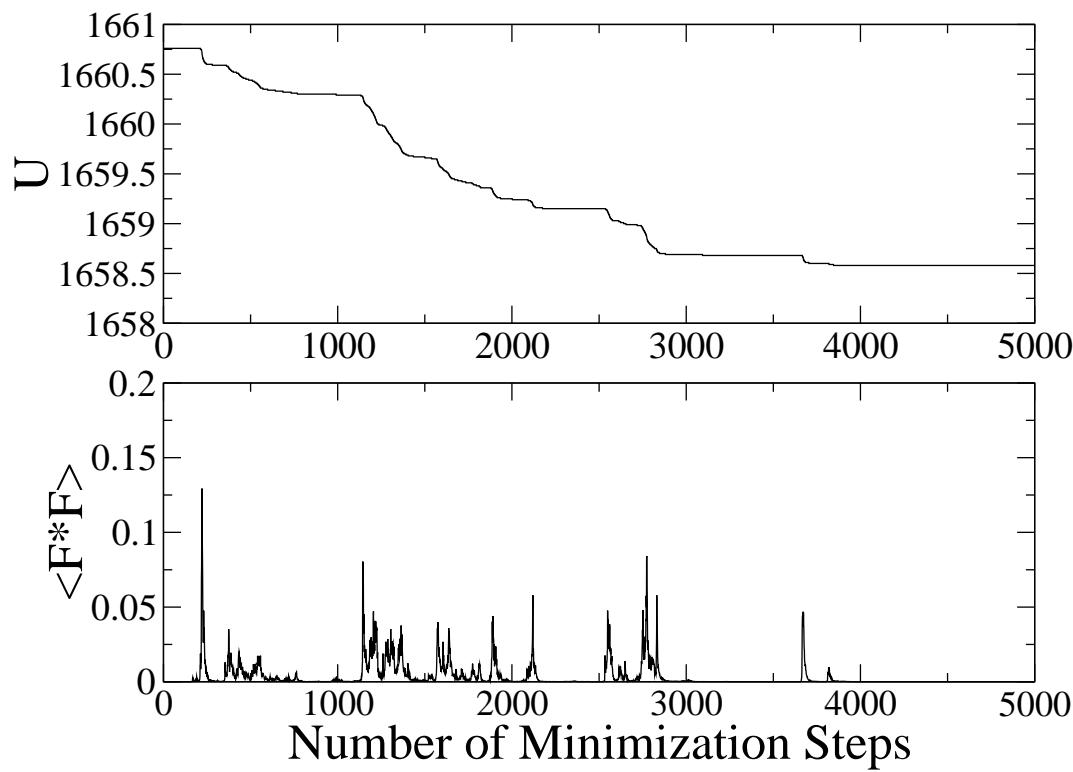
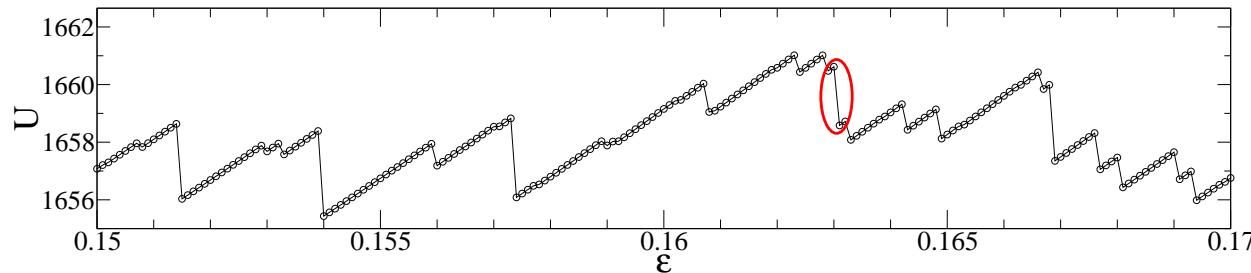
Conclusions: Elastic Segments

- Analytical expressions exist for elastic response
- Single eigenmode responsible for breakdown of smoothness
- Spatial structure of eigenmode consistent with nucleating pair of dislocations
- Instability intrinsically long-ranged

Part II

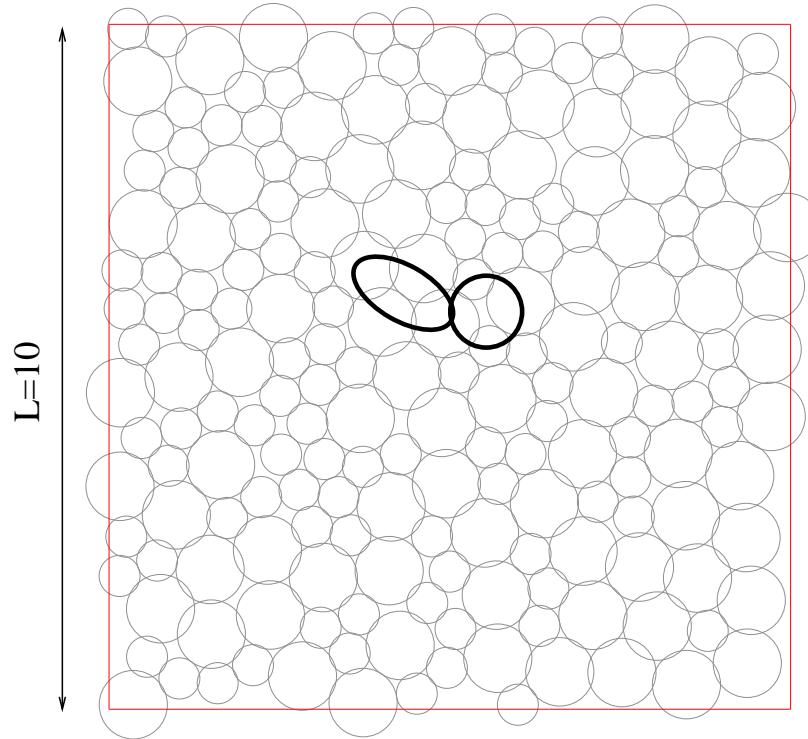
A Typical Plastic Event

Plasticity: One Typical Event

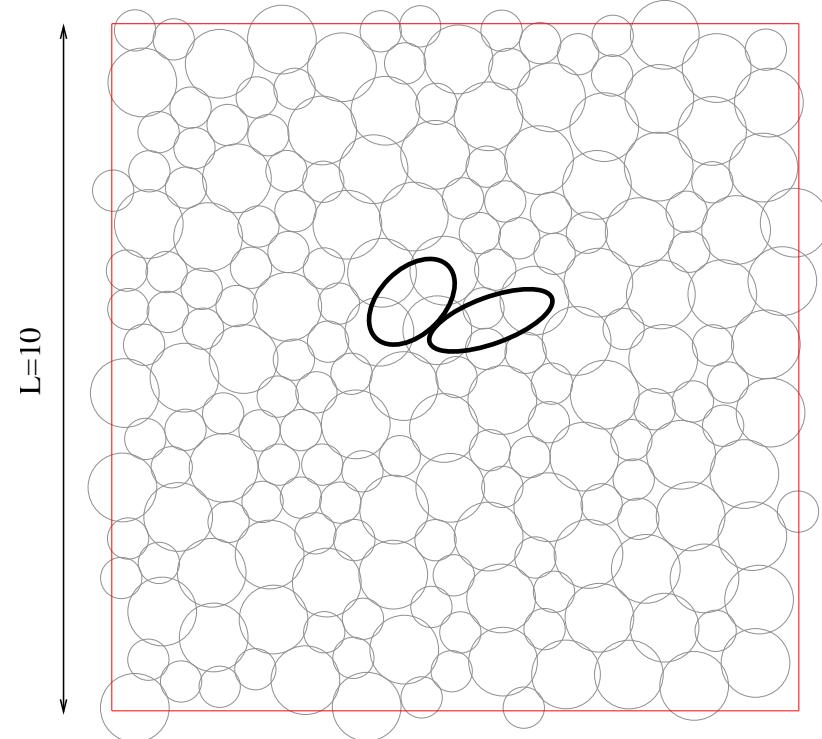


- Relaxation at *single* strain
- "Number of steps" \sim time.
- $\langle F^* F \rangle \sim \frac{dU}{dt}$

Same Typical Event: First Peak

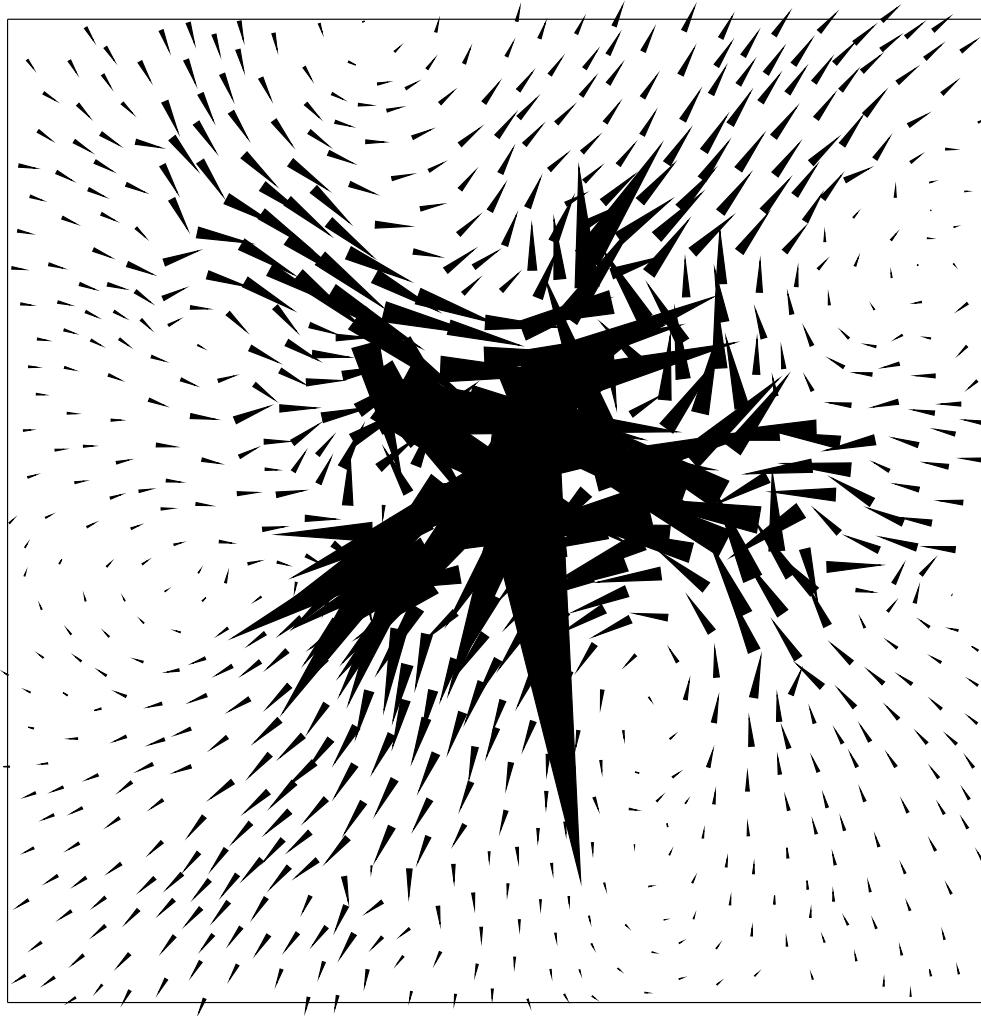


Pre-peak



Post-peak

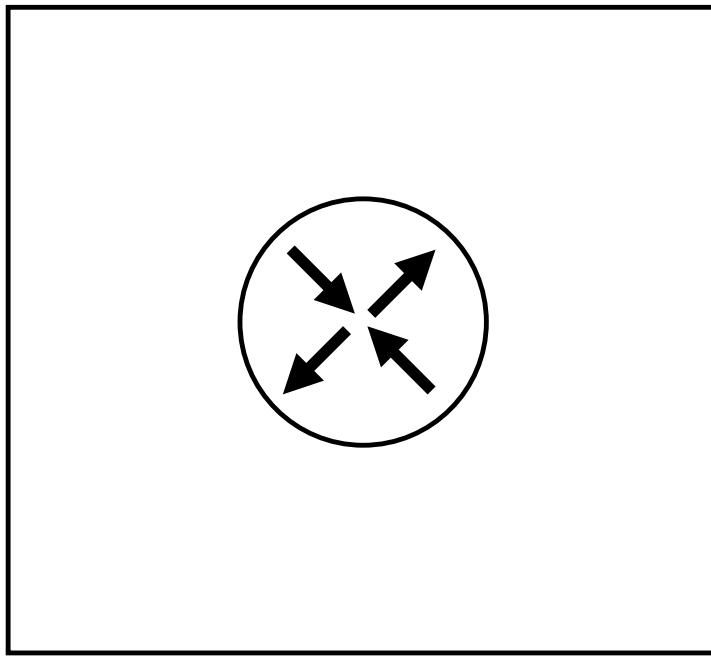
Same Typical Event: First Peak



Real Space Analysis

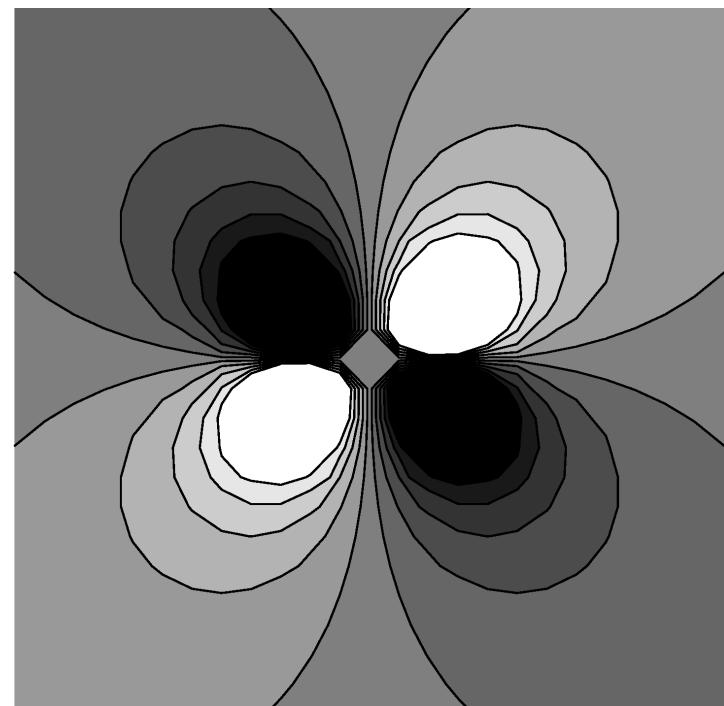
- Local "slip"

- Take $\vec{v} - \langle \vec{v} \rangle$ locally.
 - Expect:

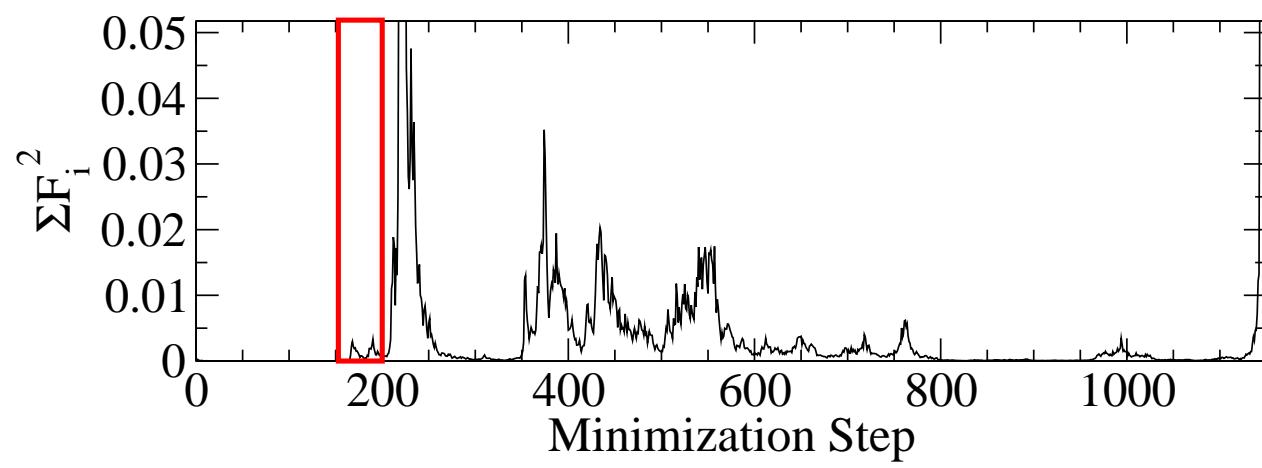
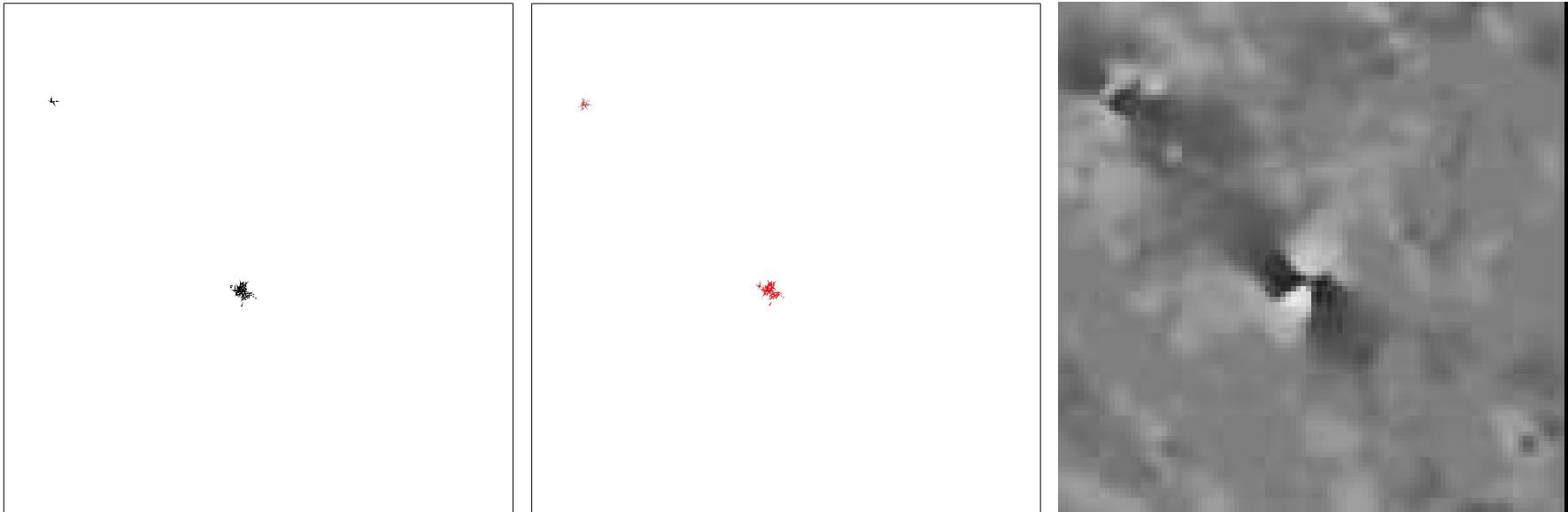


- Local dissipation

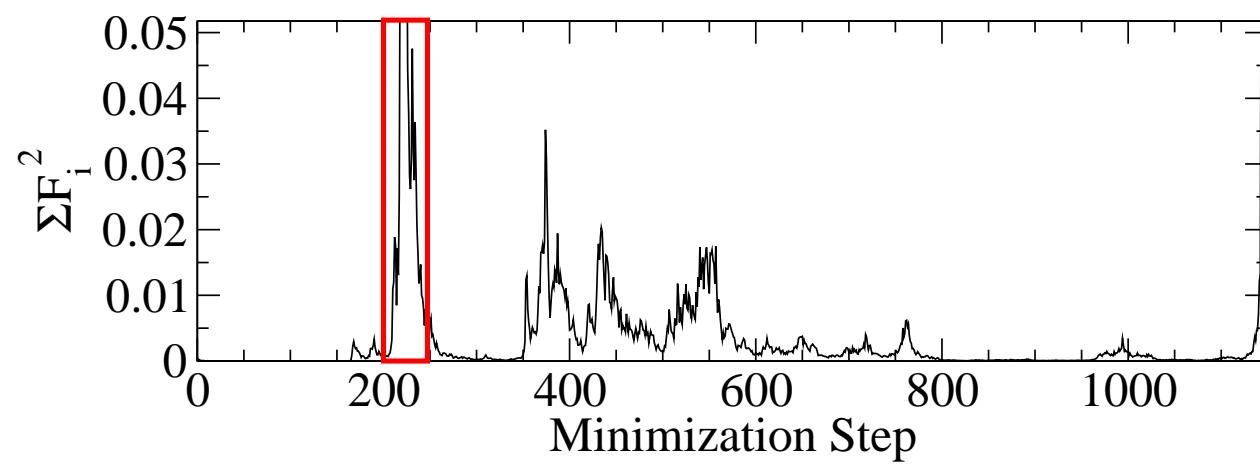
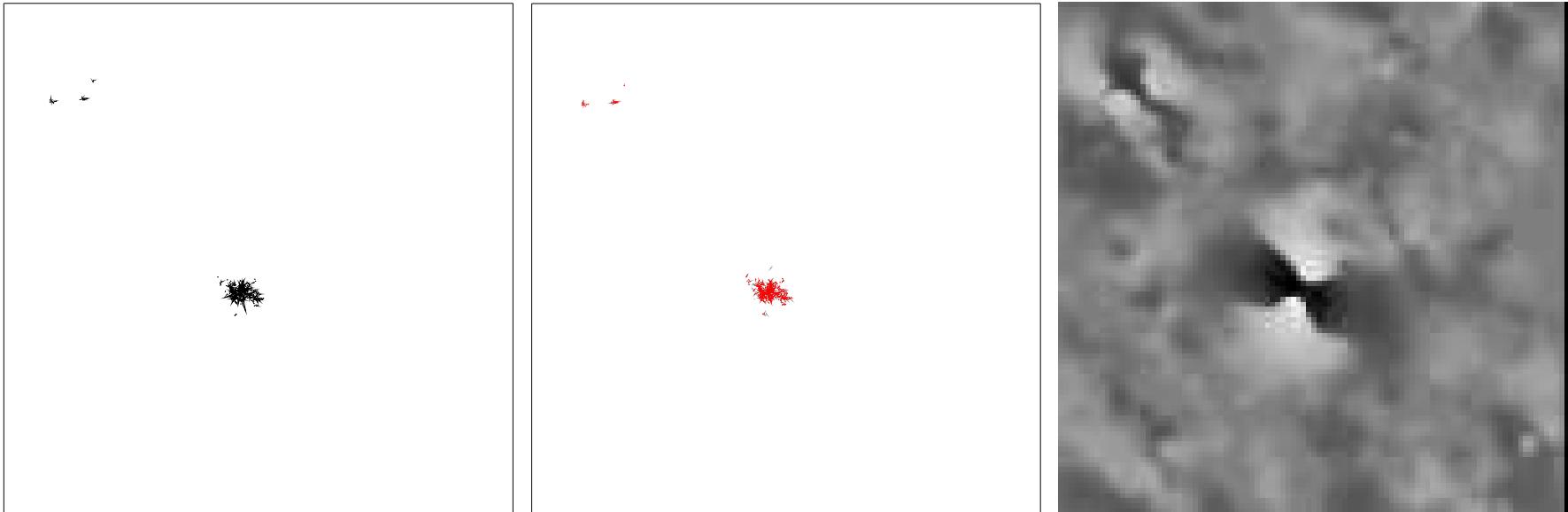
- Take ΔU locally
 - Expect:



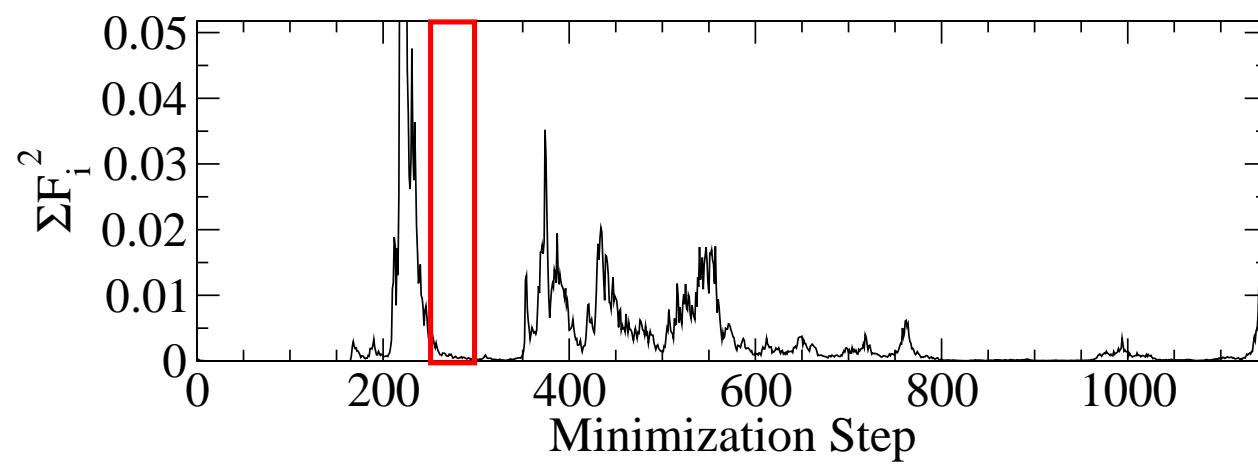
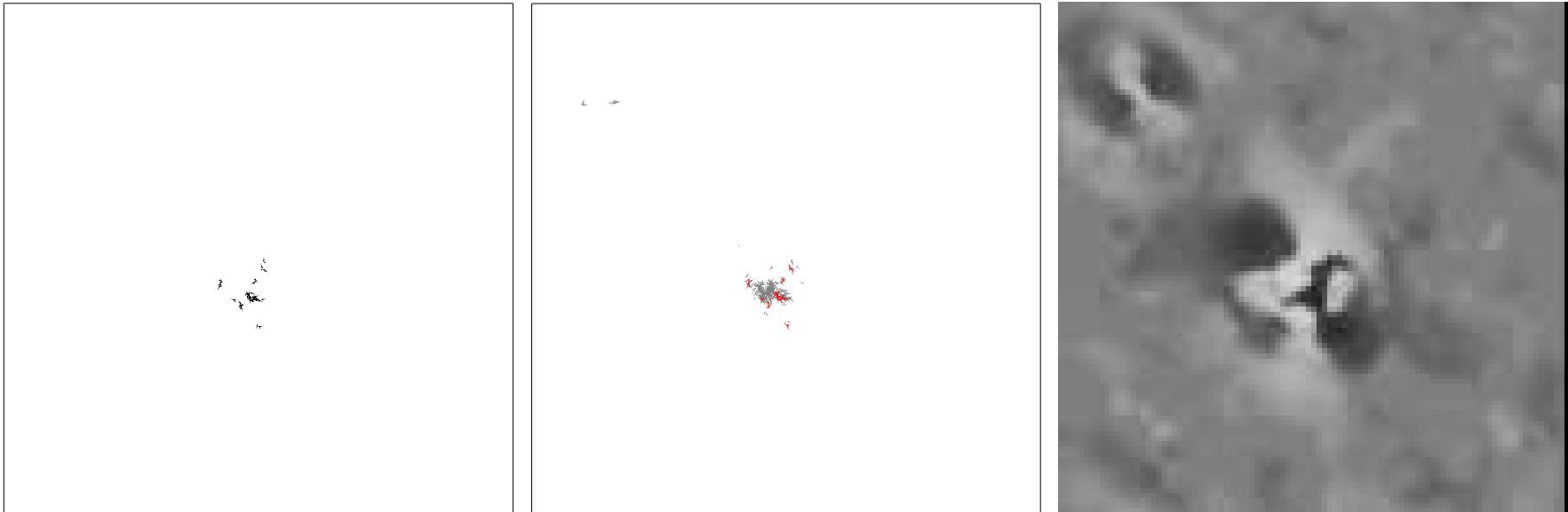
Cascade



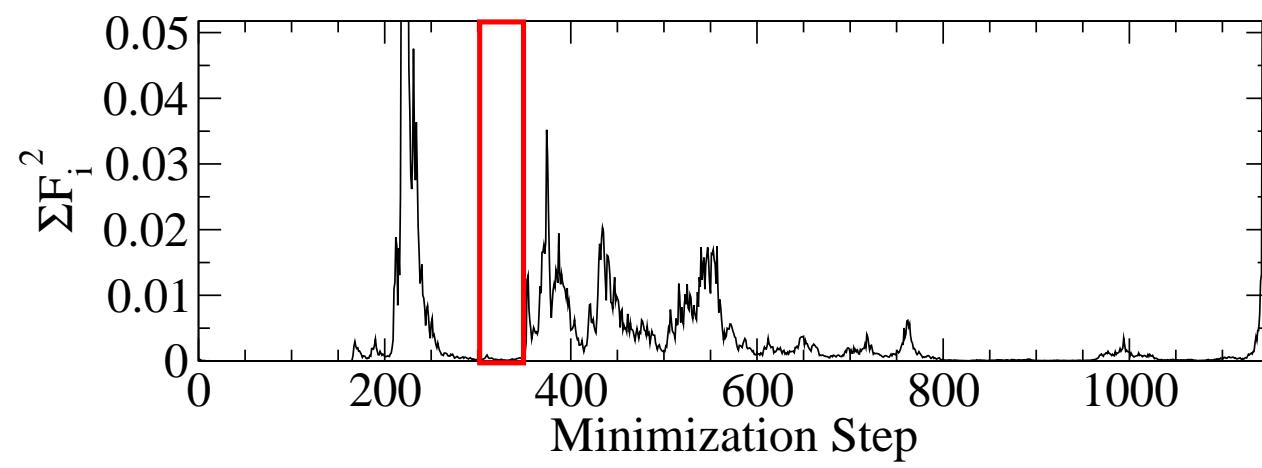
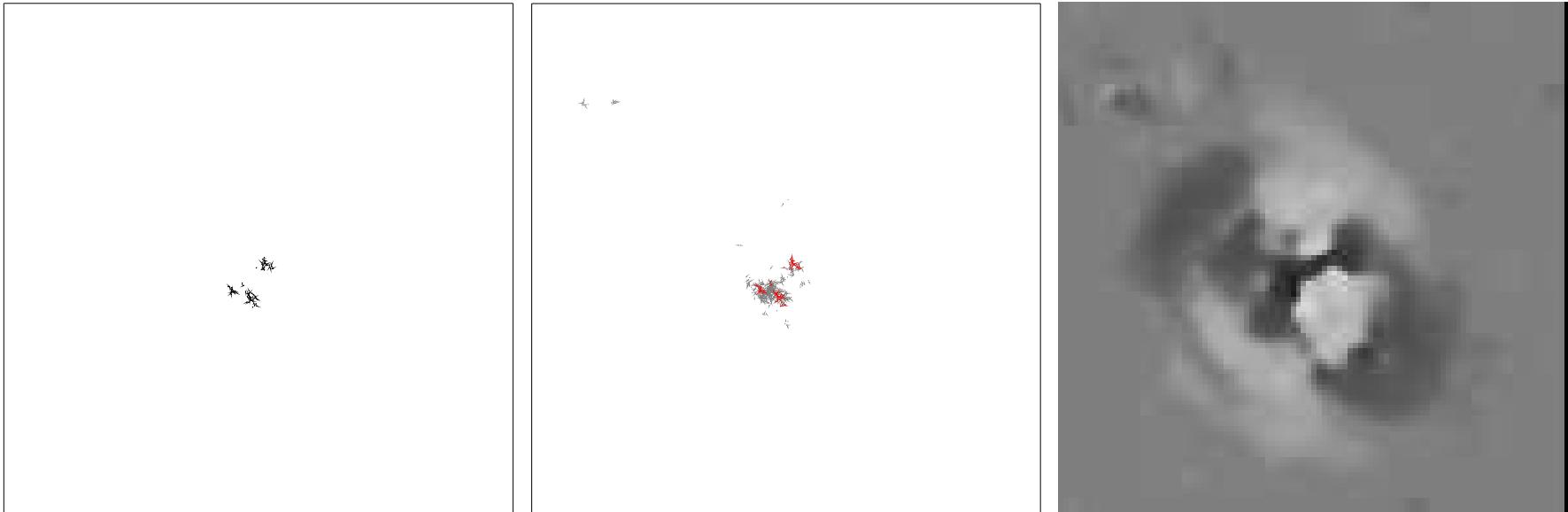
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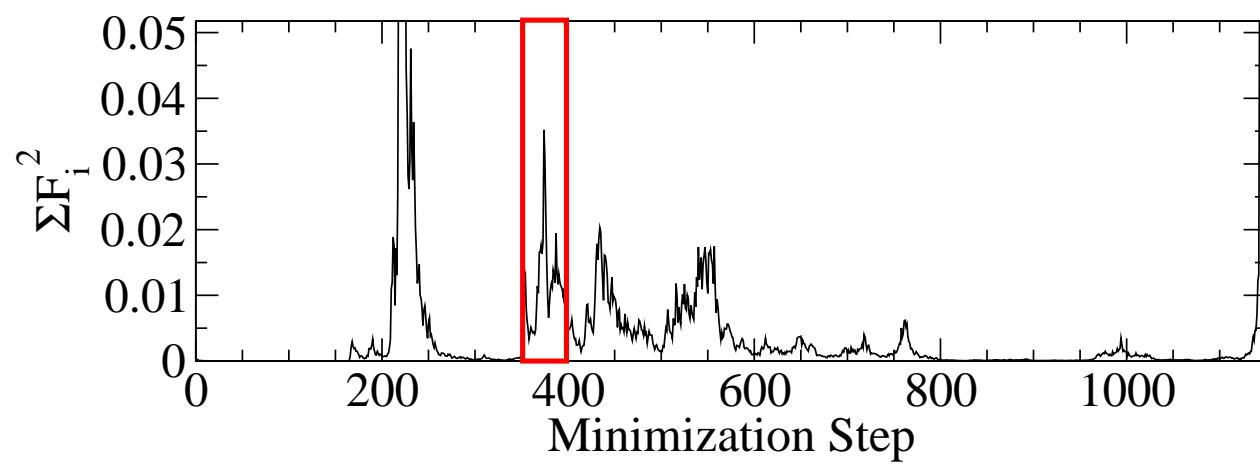
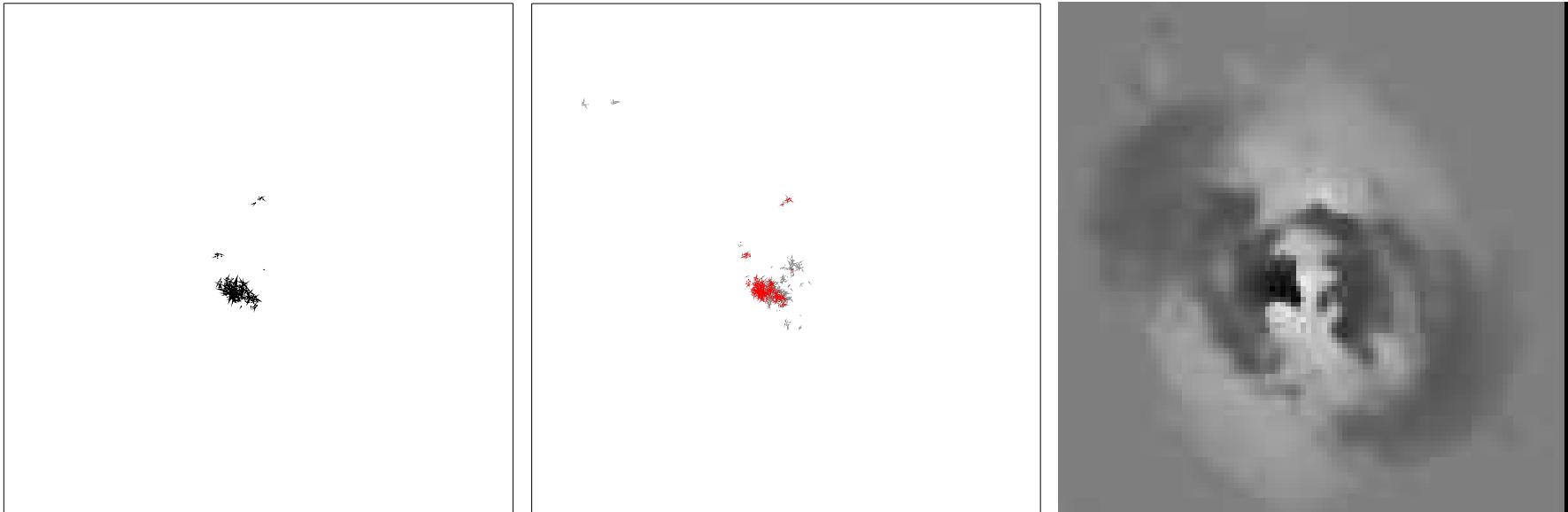
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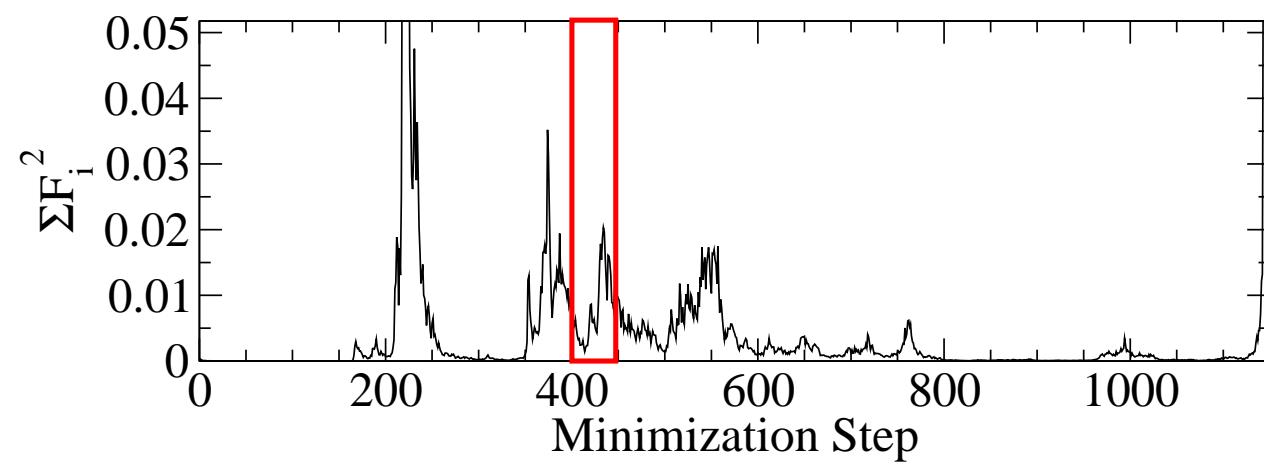
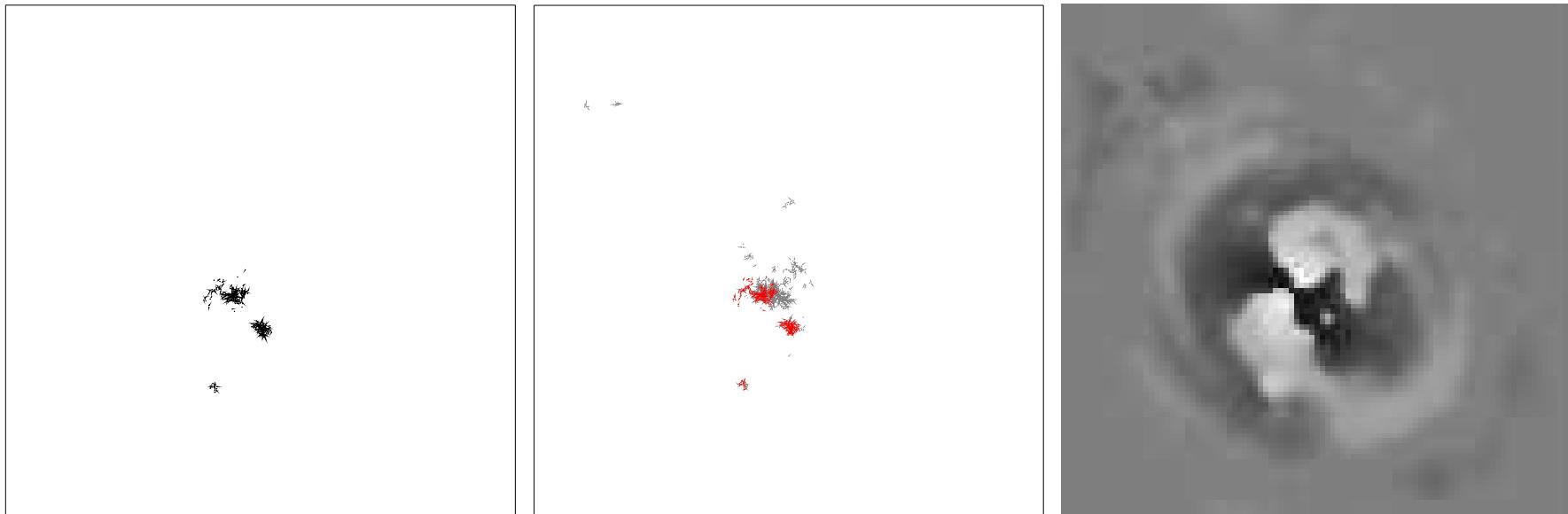
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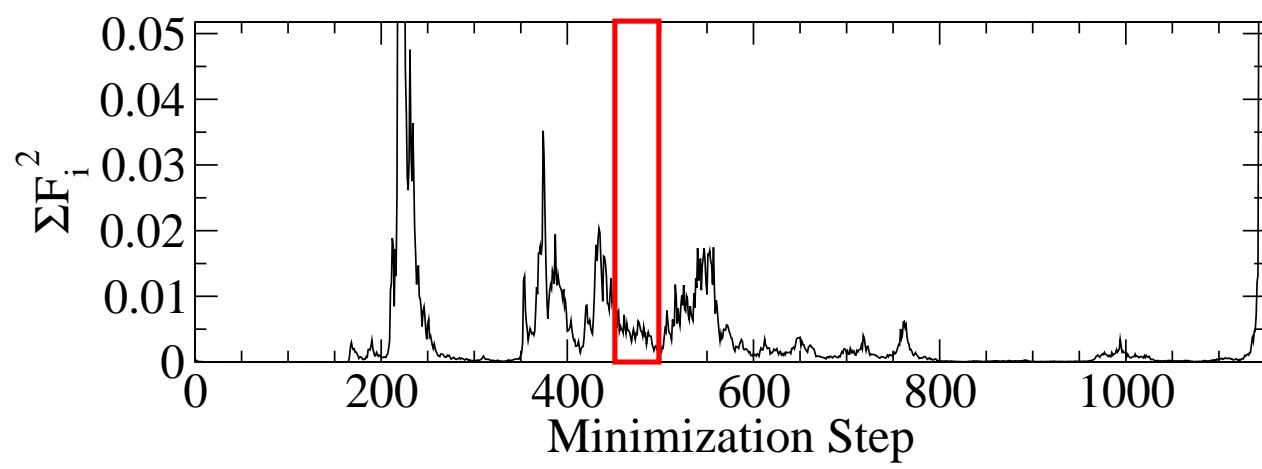
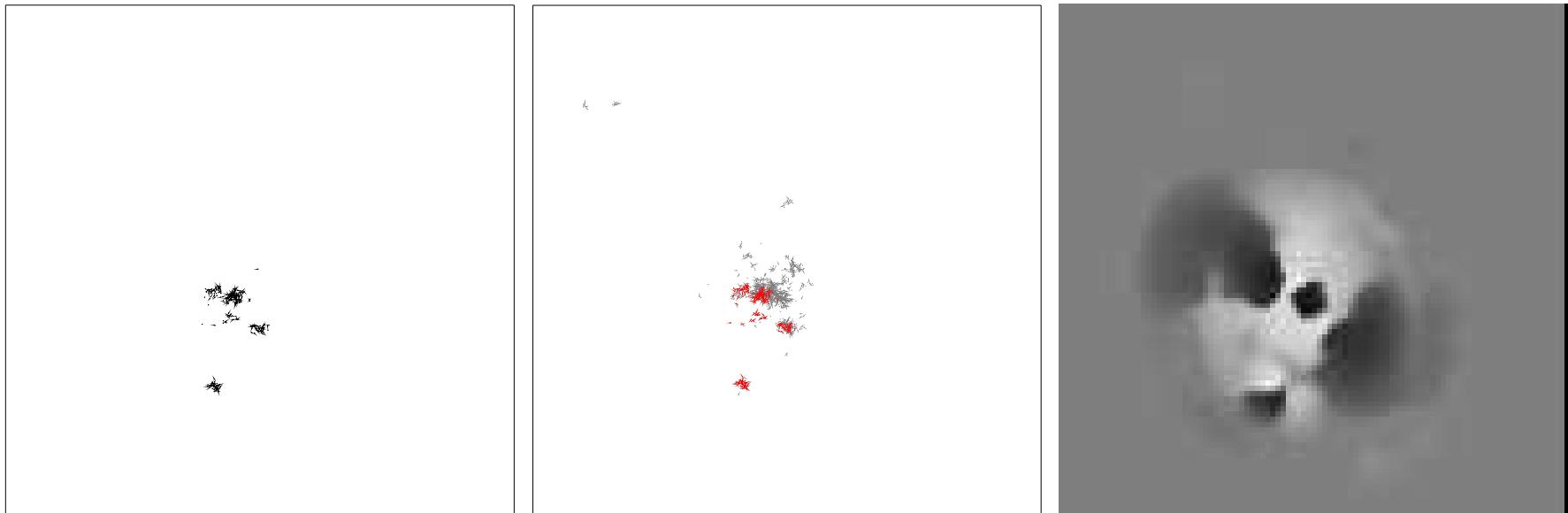
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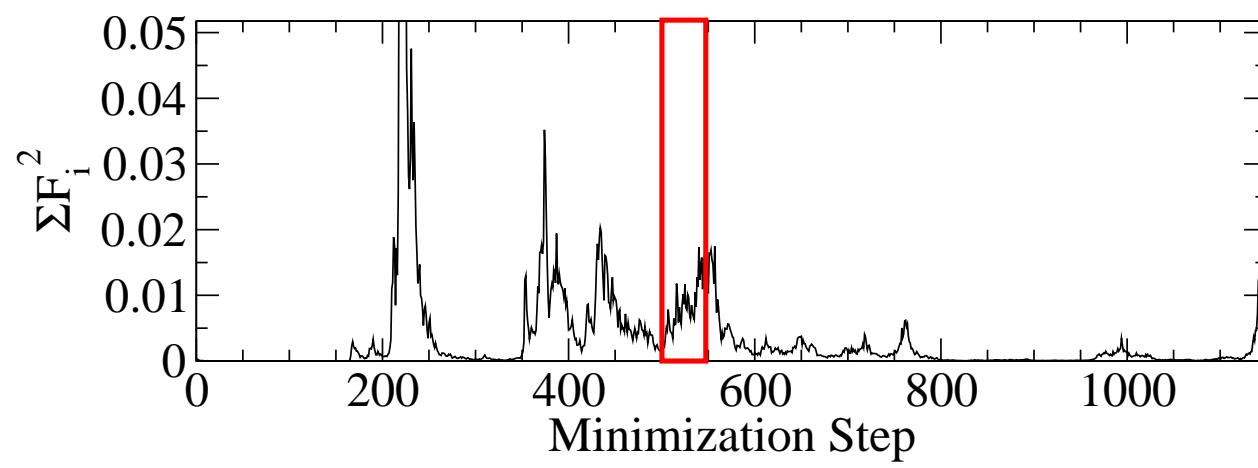
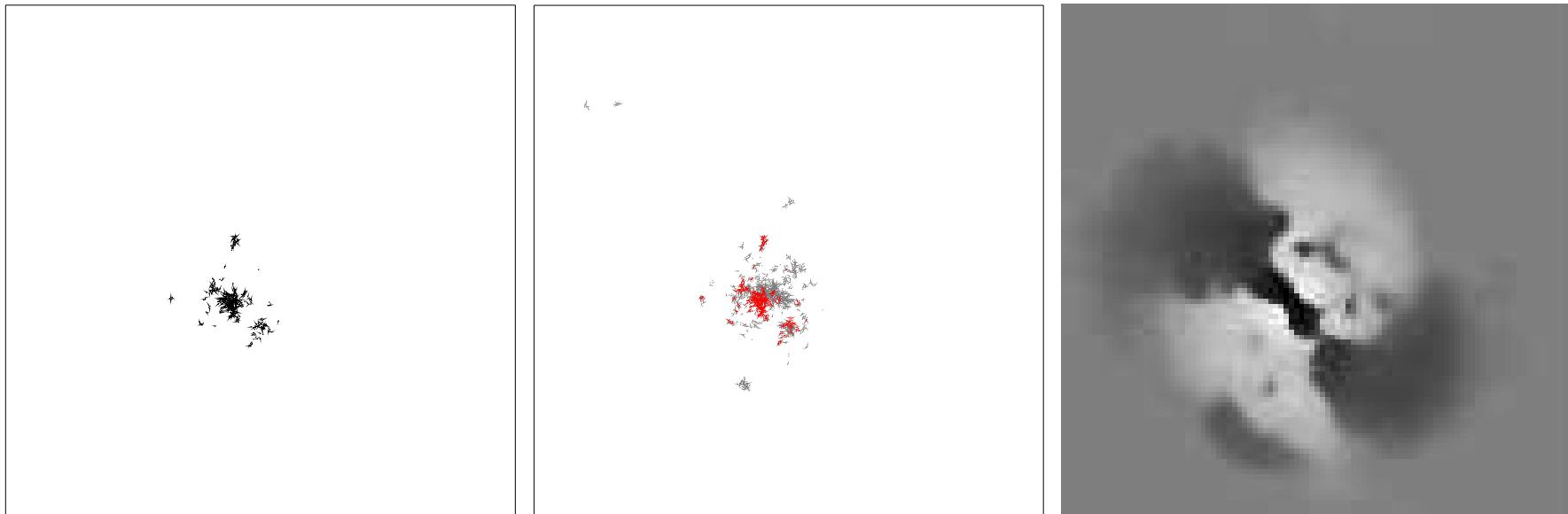
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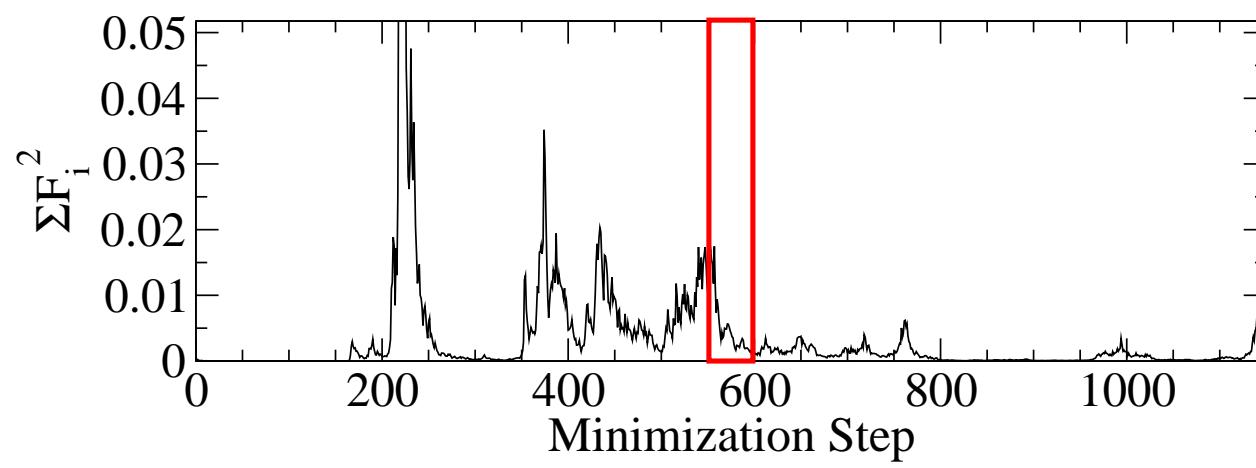
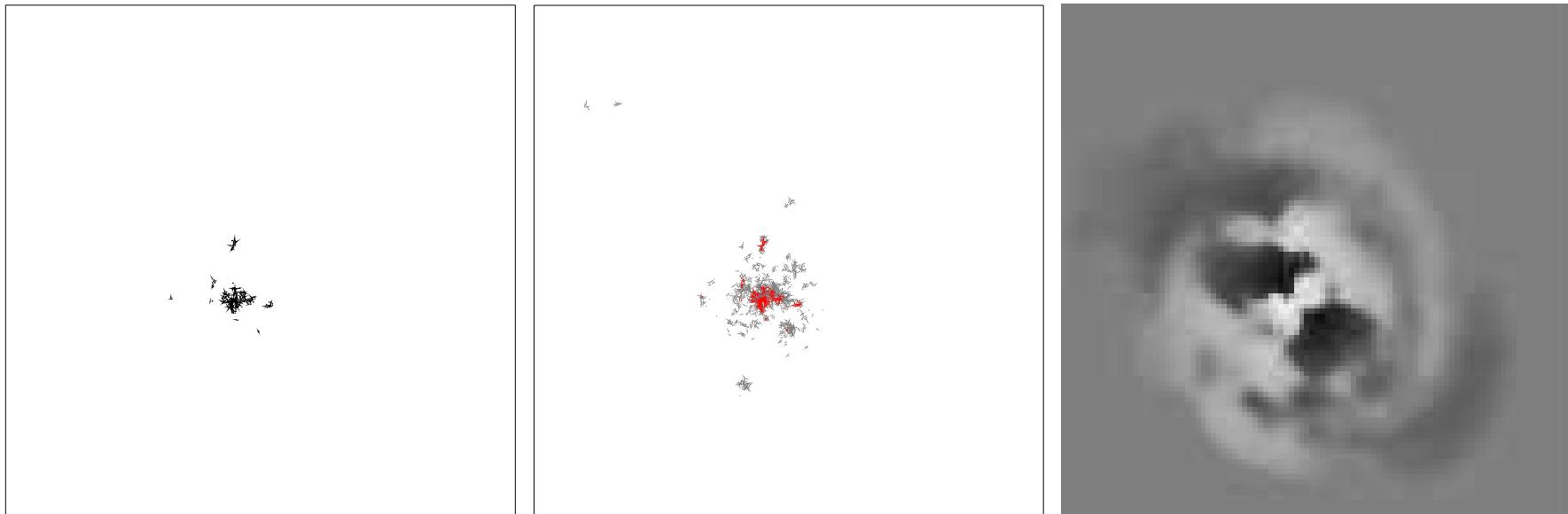
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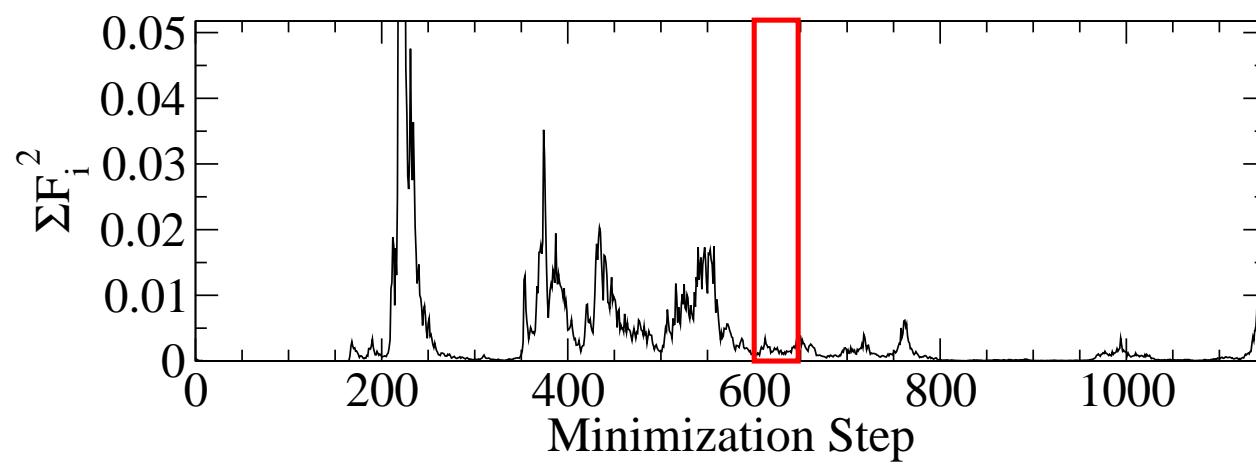
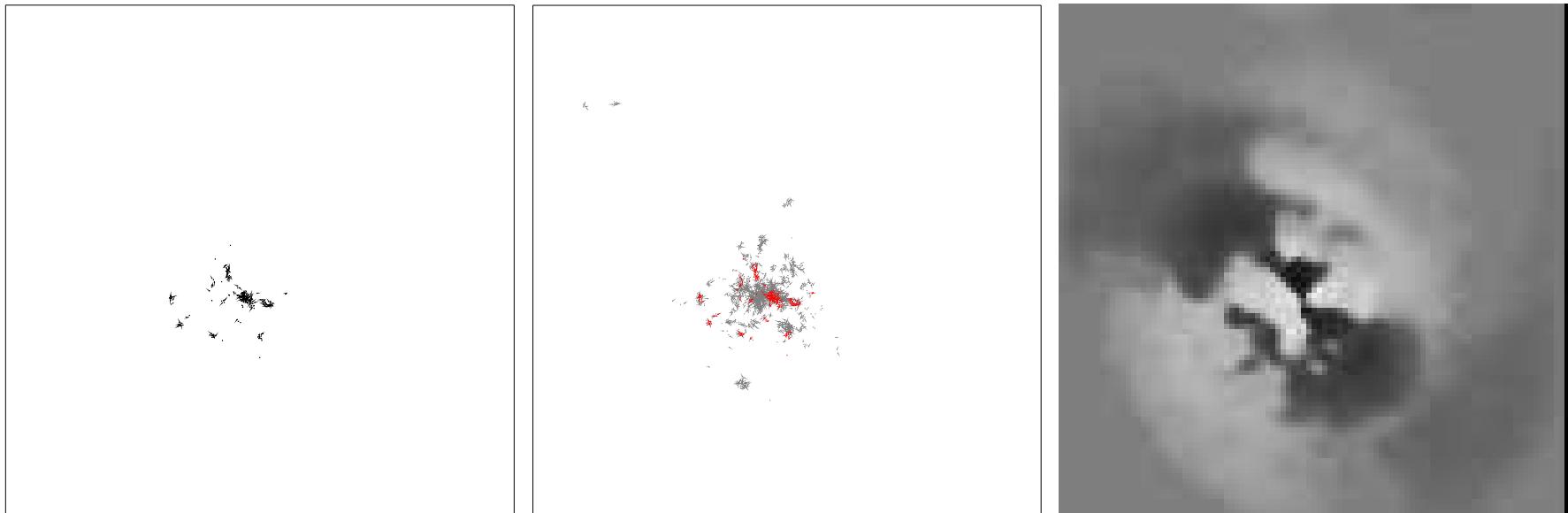
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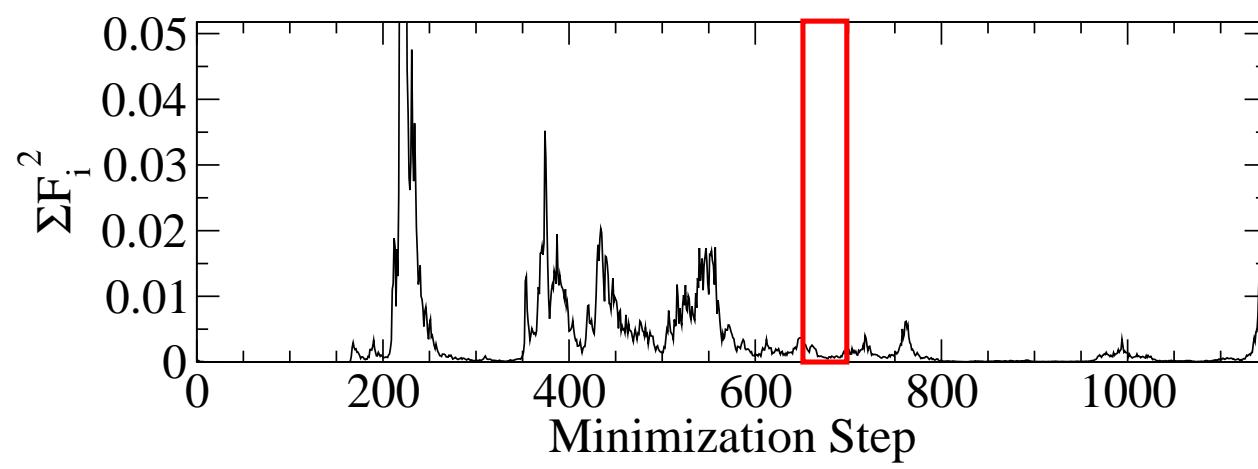
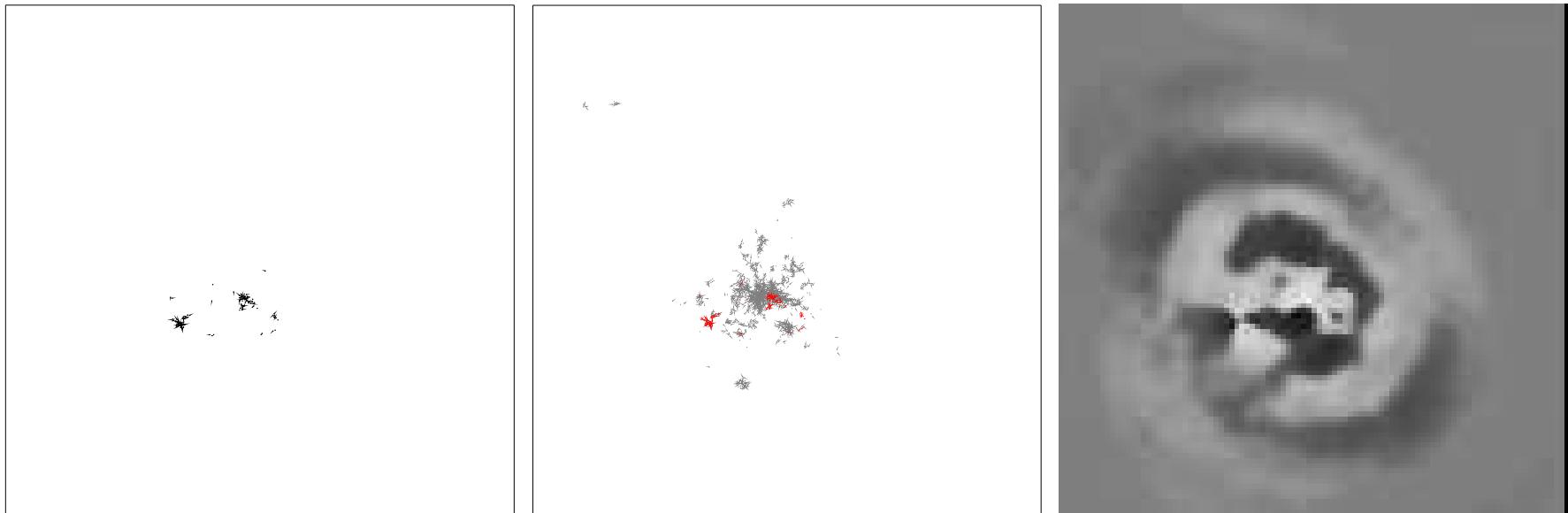
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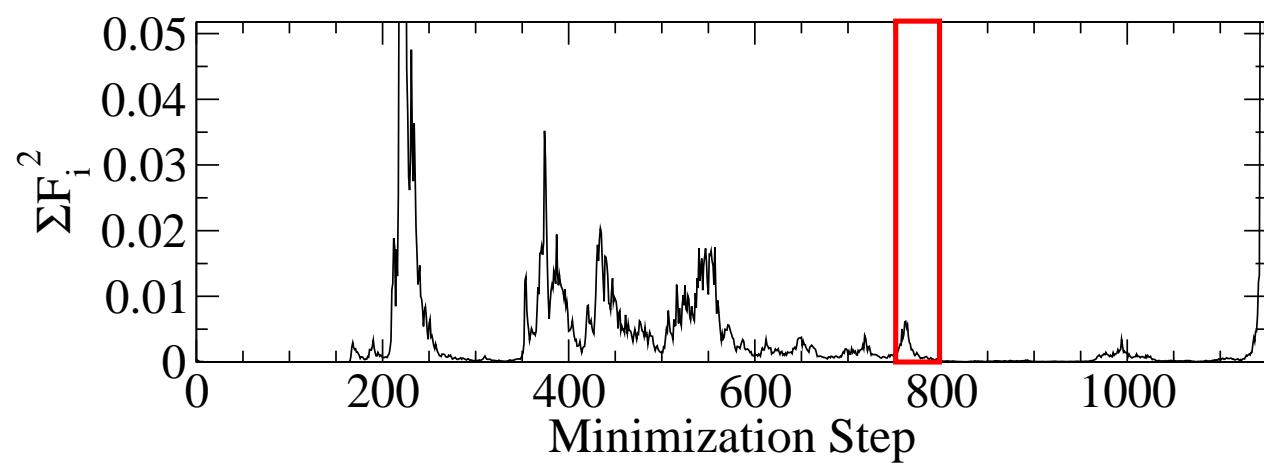
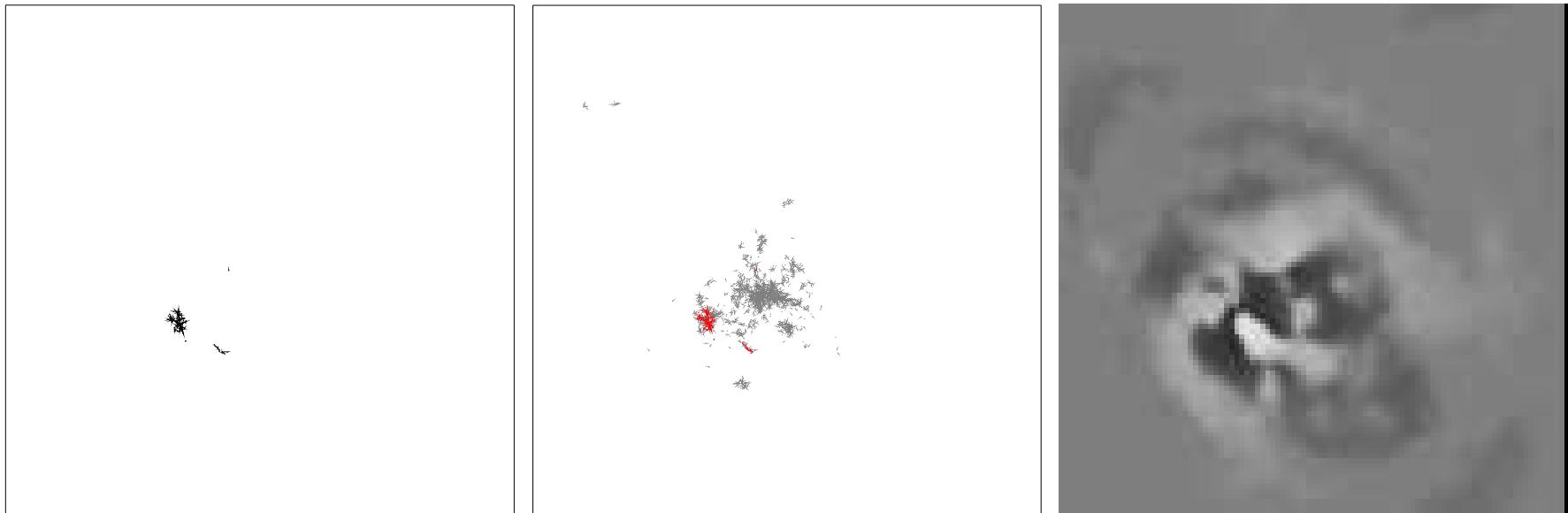
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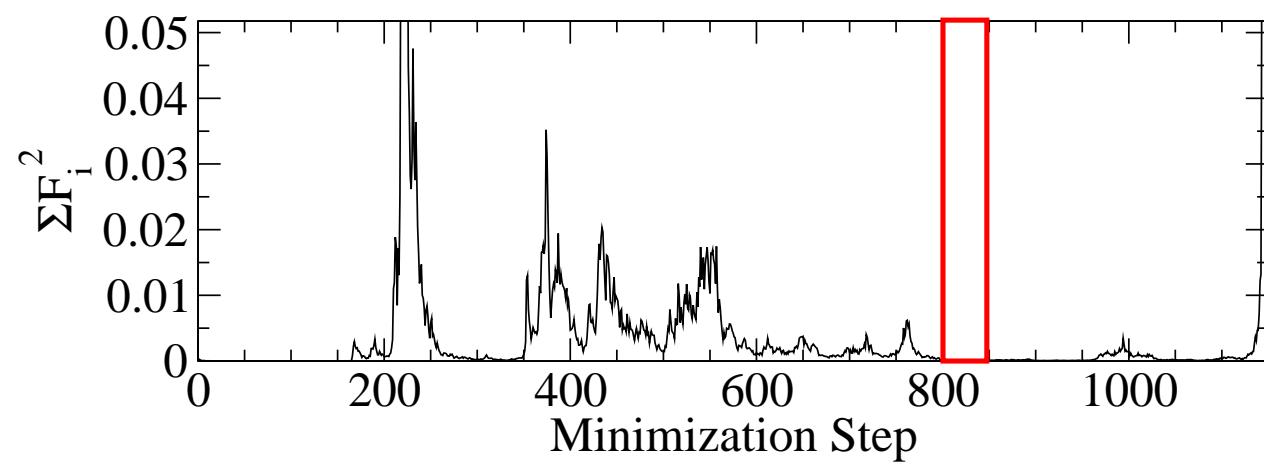
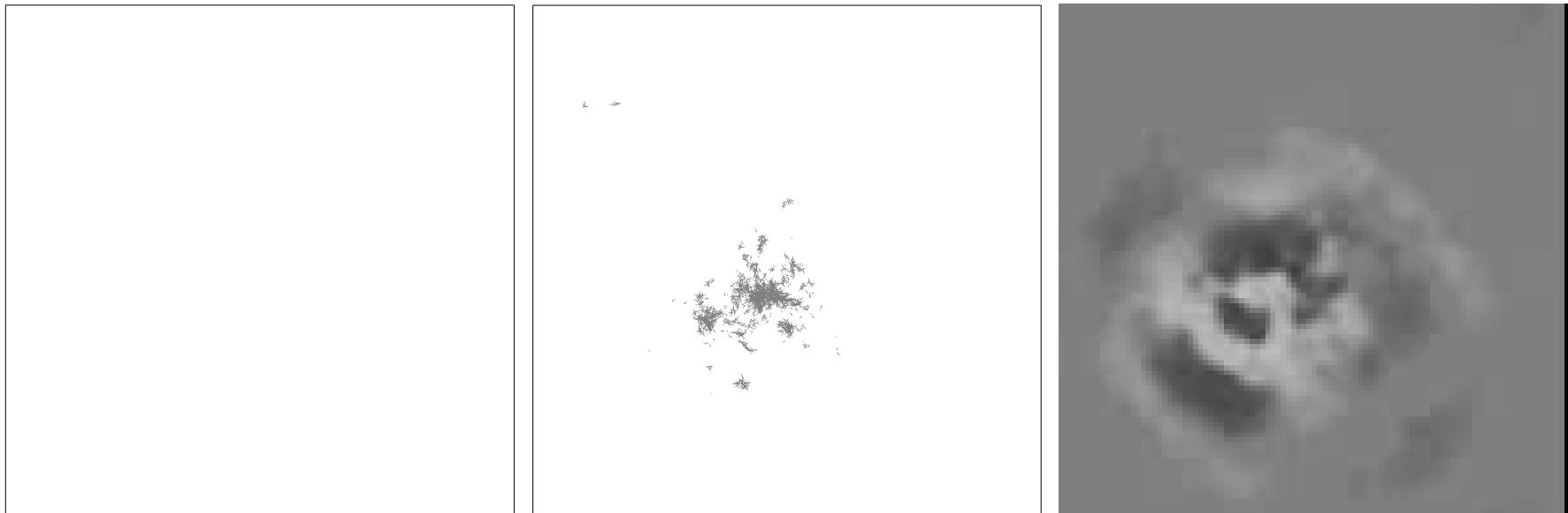
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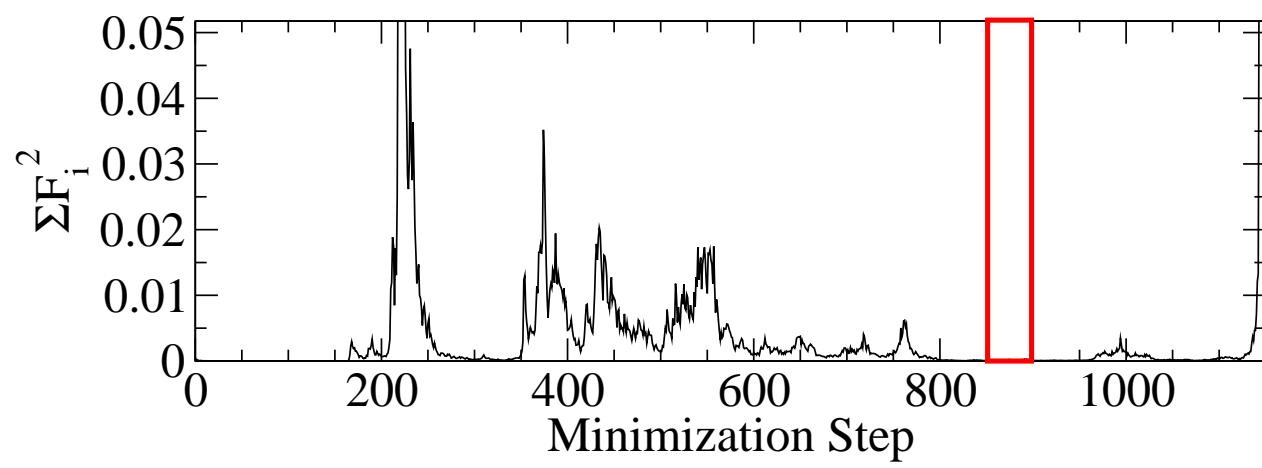
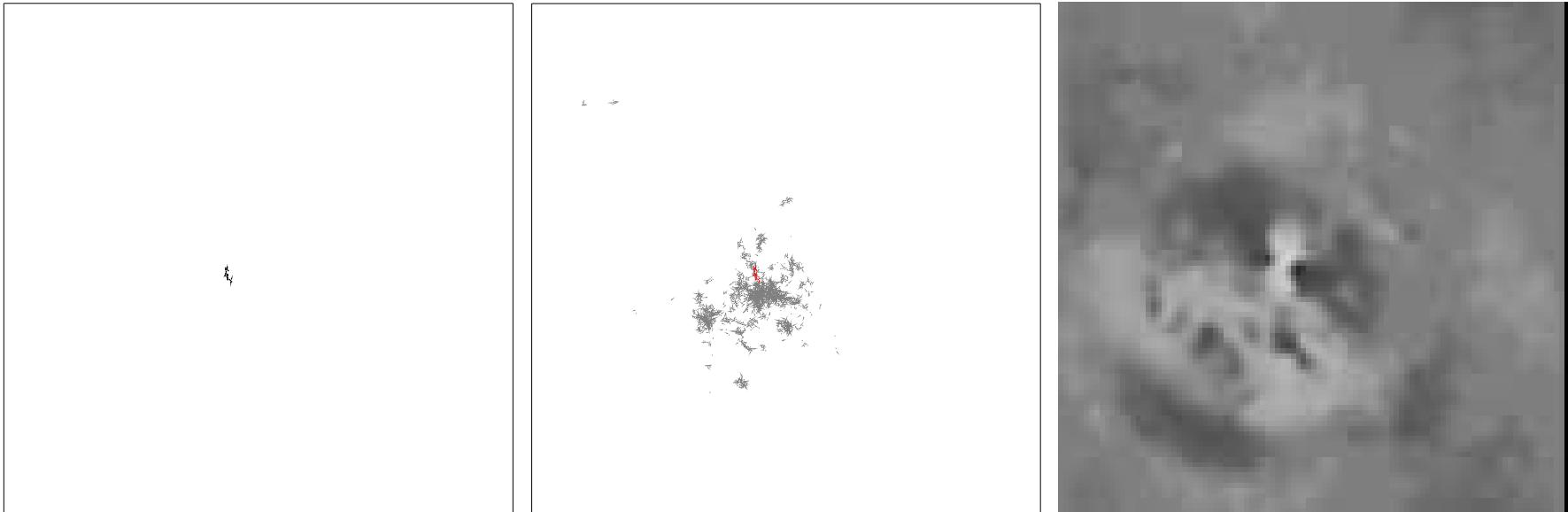
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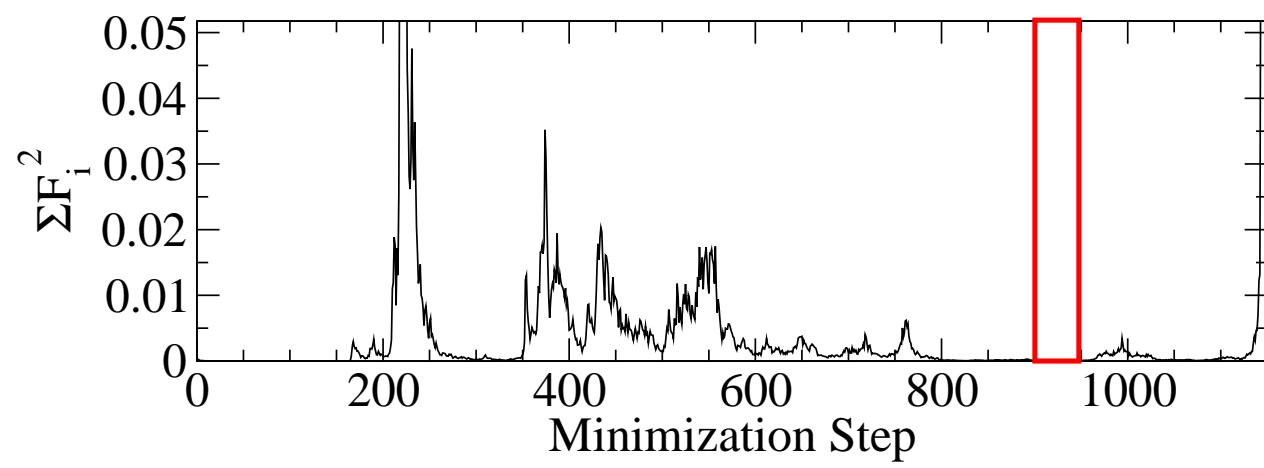
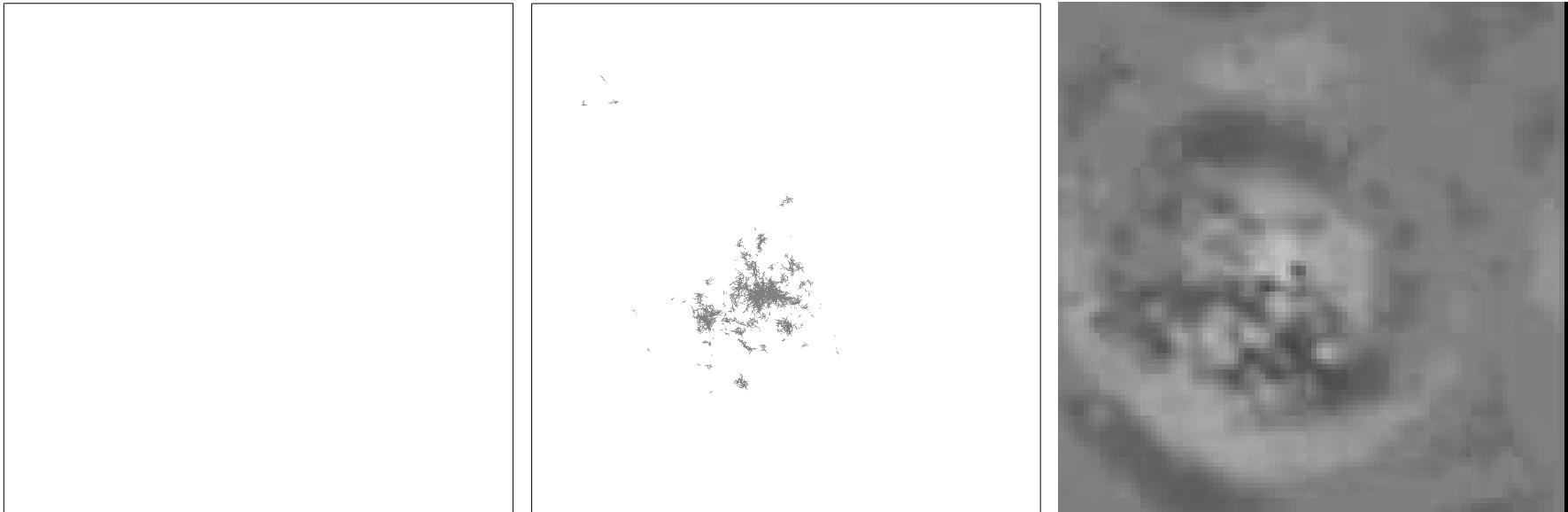
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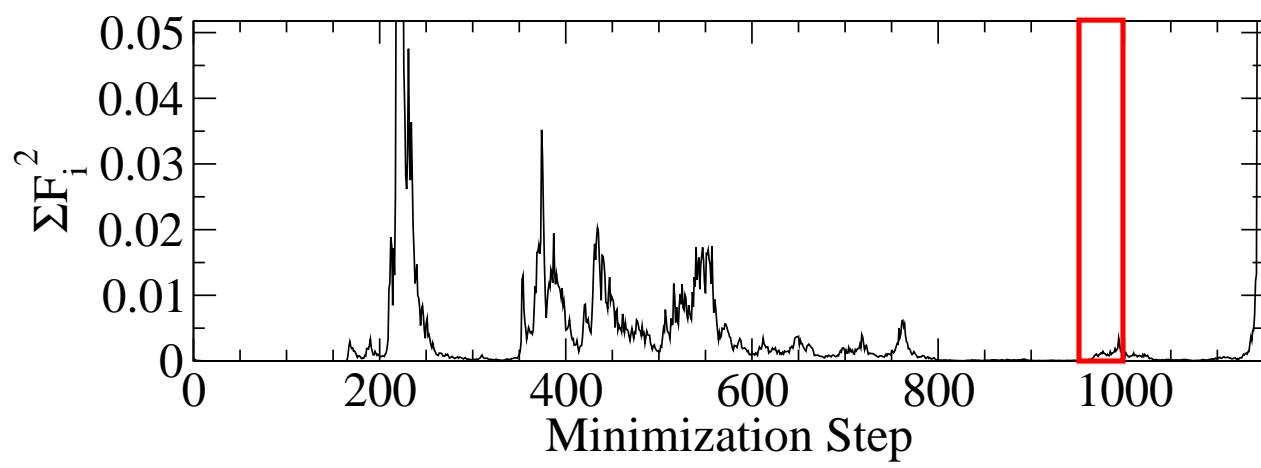
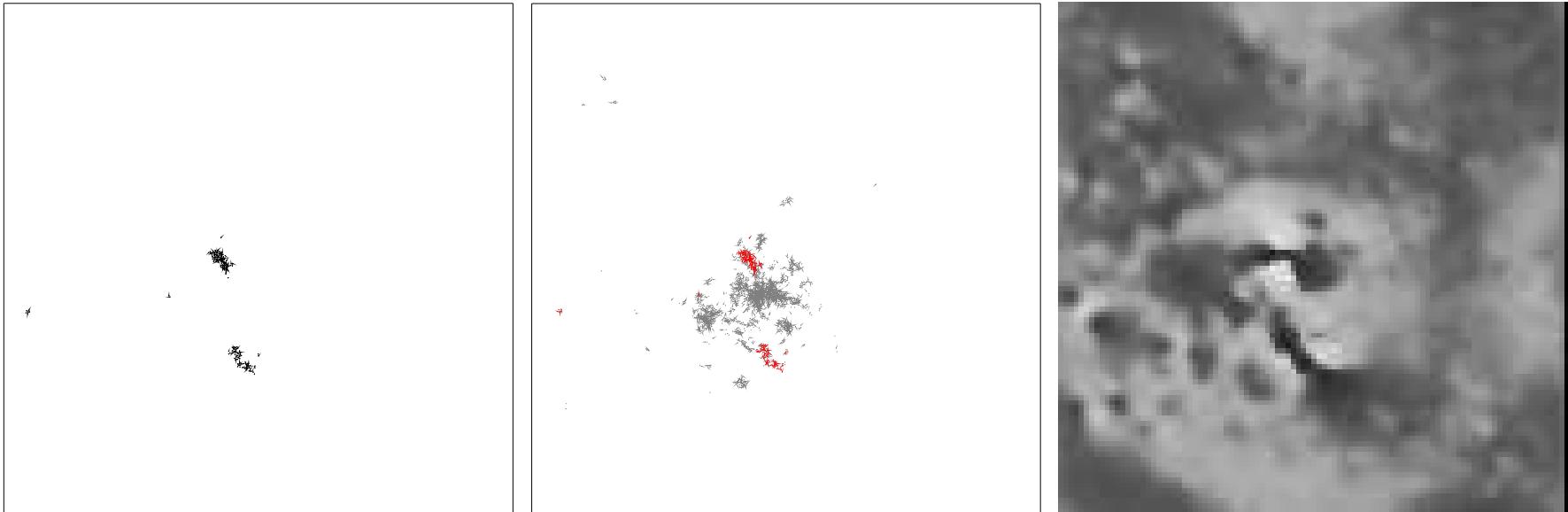
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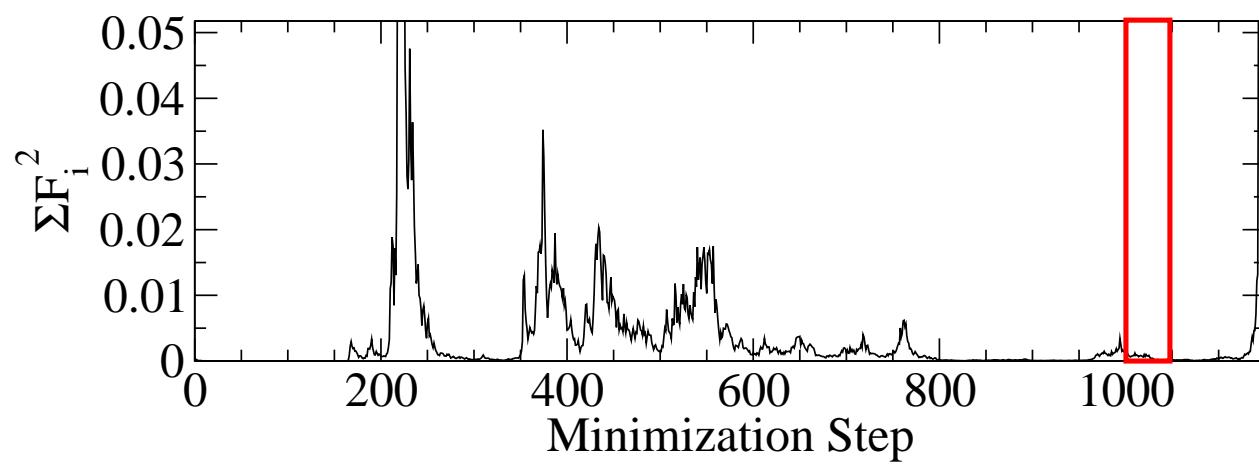
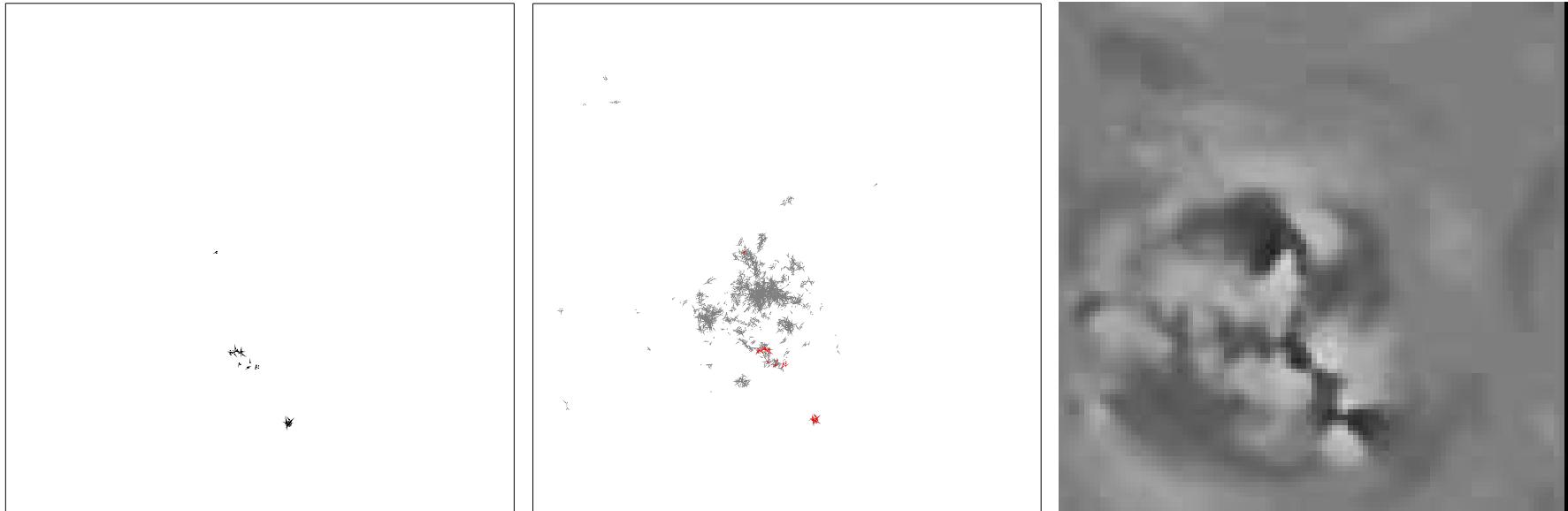
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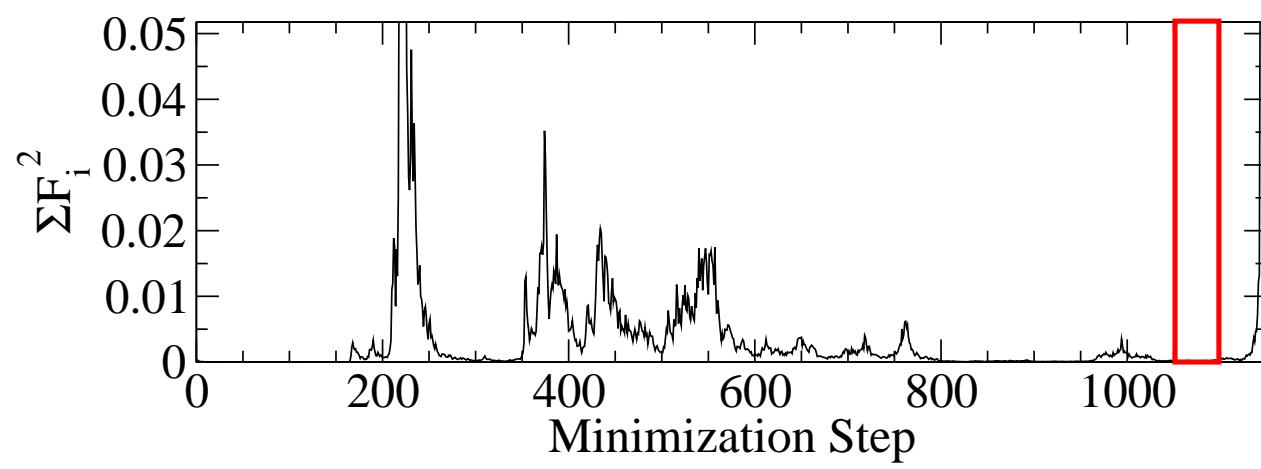
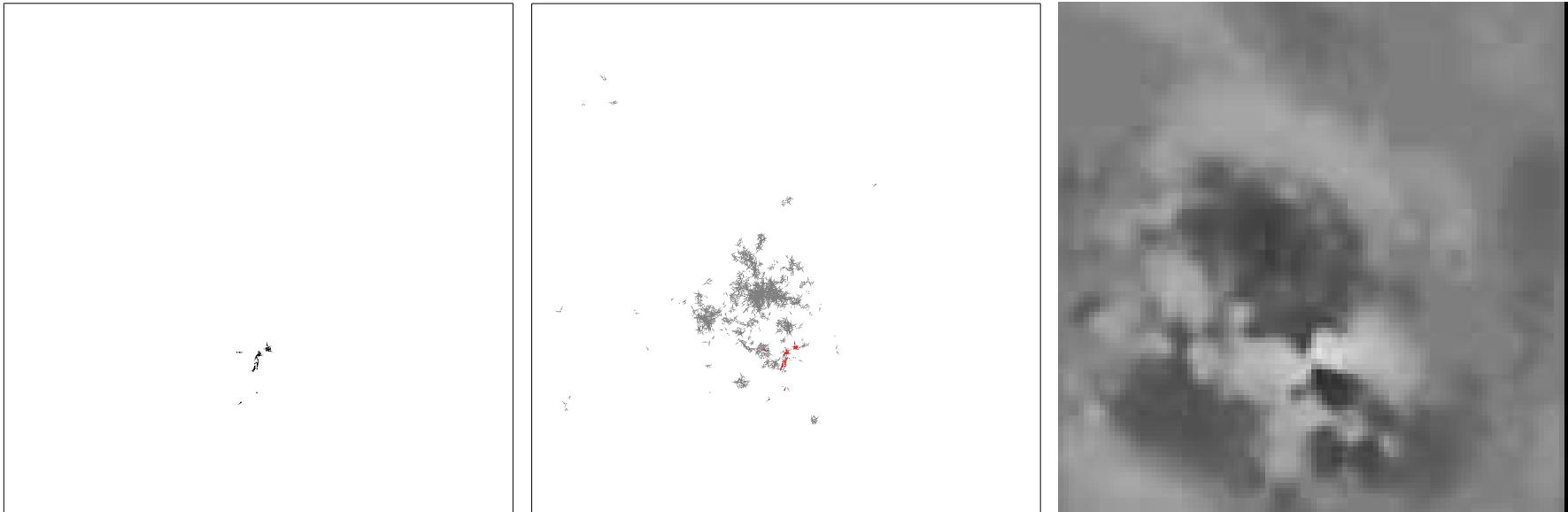
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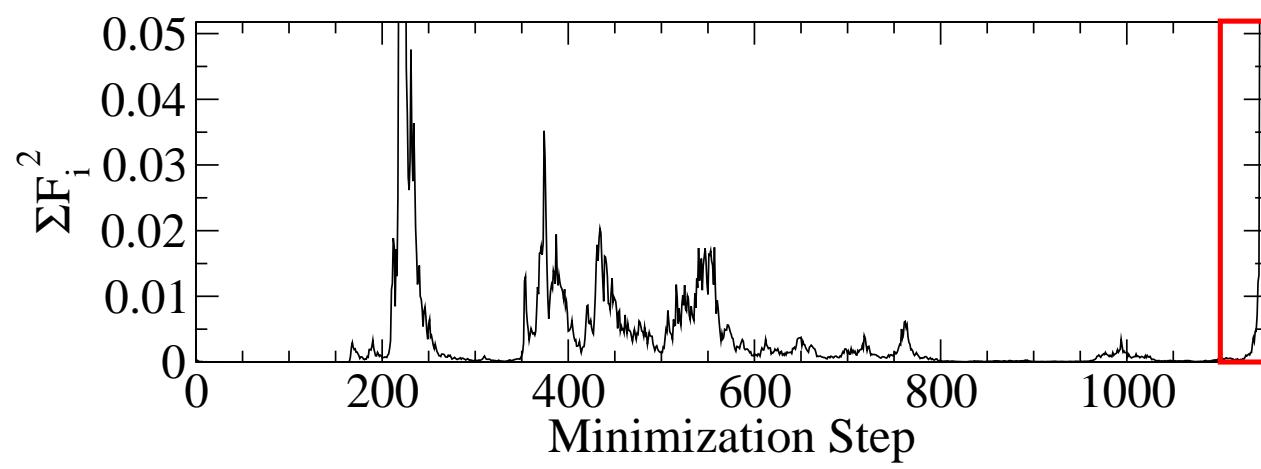
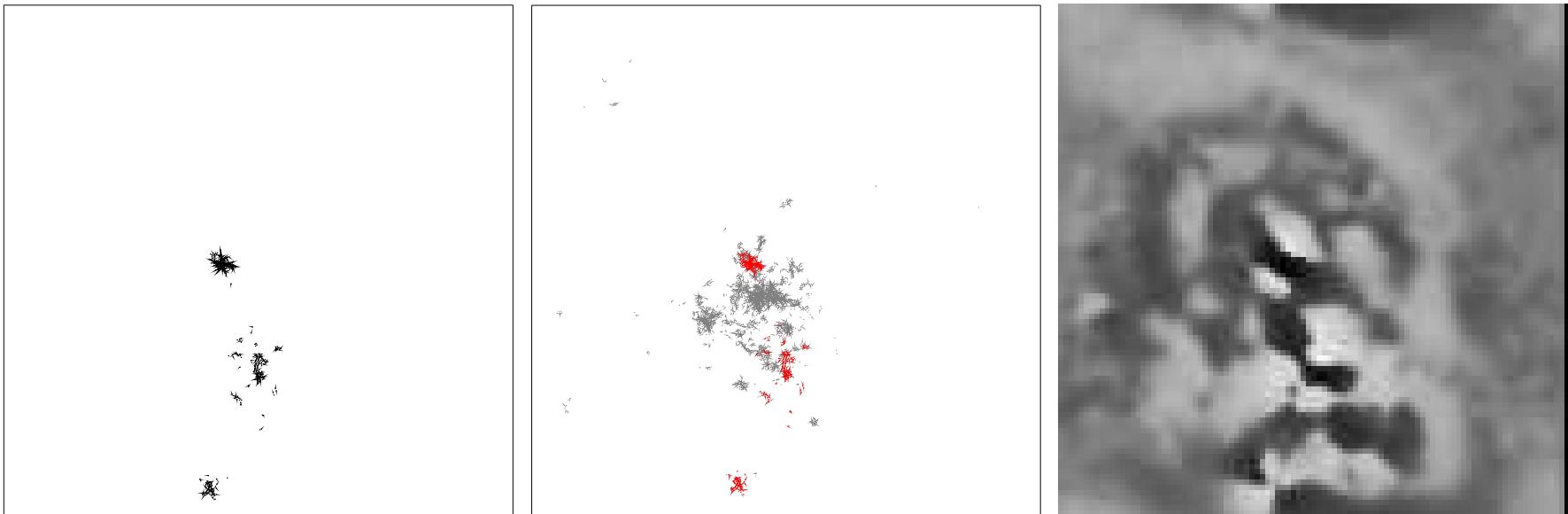
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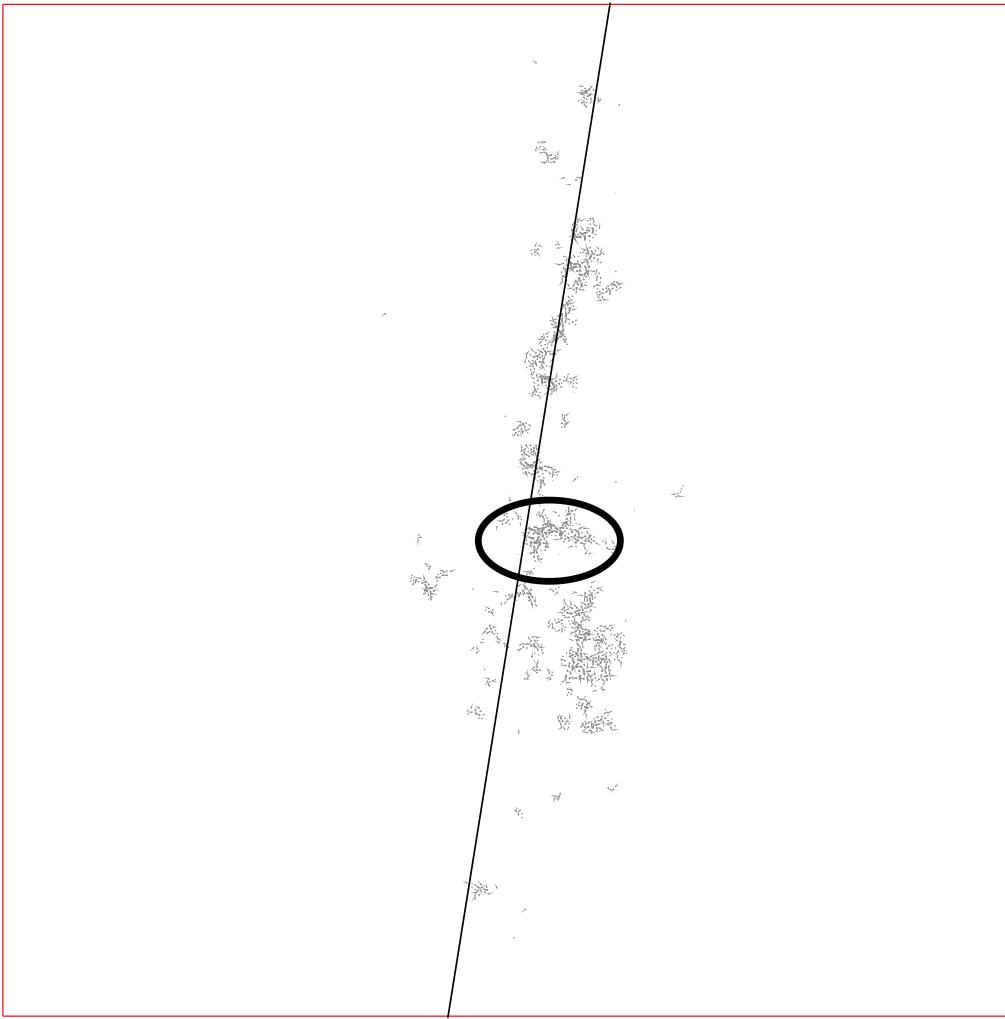
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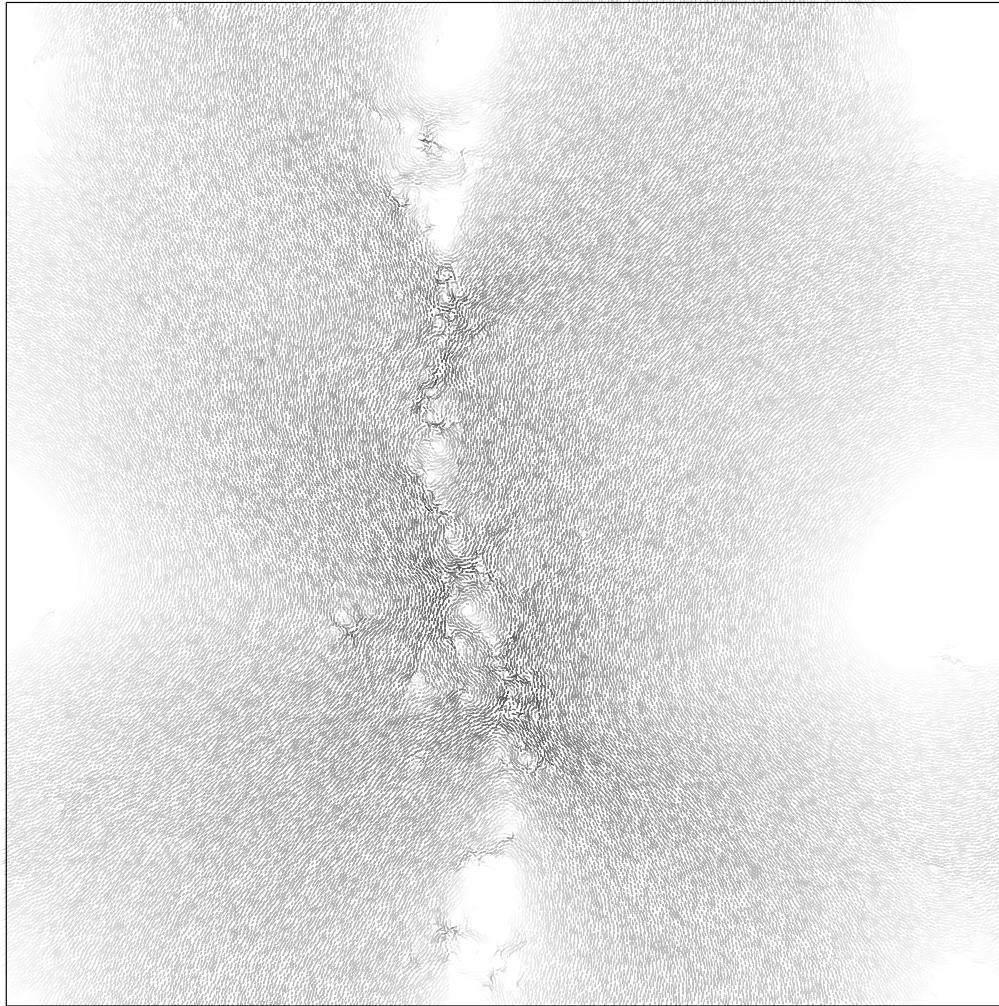
Cascade



Entire Event (Slip)



Entire Event (Displacement)



Conclusion: Single Cascade

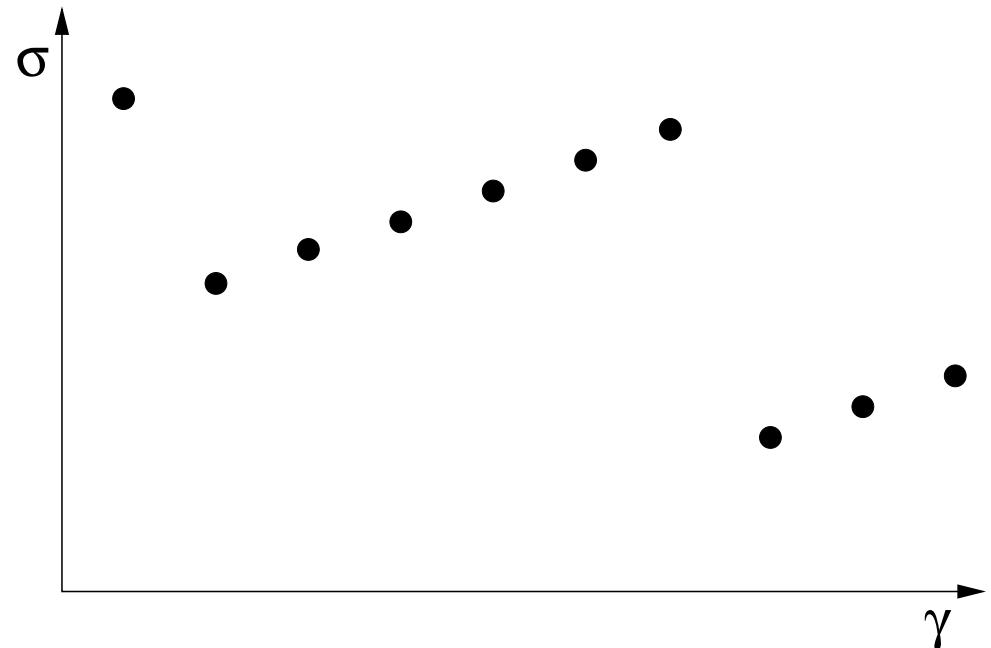
- Elementary plastic events are themselves composite
- Energy descent is intermittent
- Energy drops can be roughly identified with cluster of rearranging particles
- Quadrupolar elastic response can be identified with each cluster
- Resulting displacement field reminiscent of a partially unbroken line of slip, resembling dislocation glide.

Part III

Statistics and Scalings

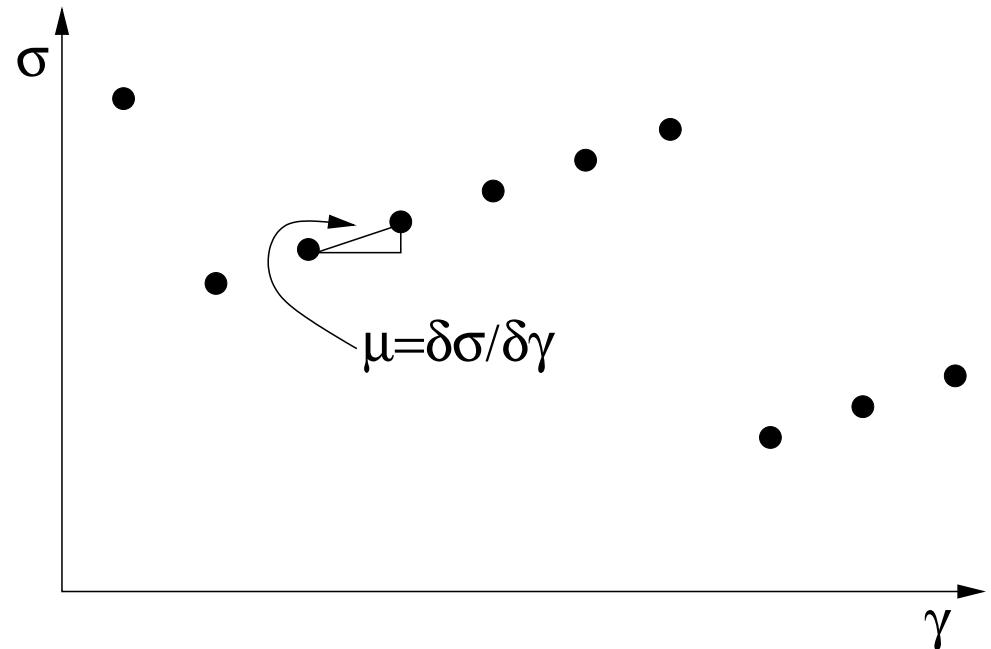
Event Statistics

- Collect stats on:



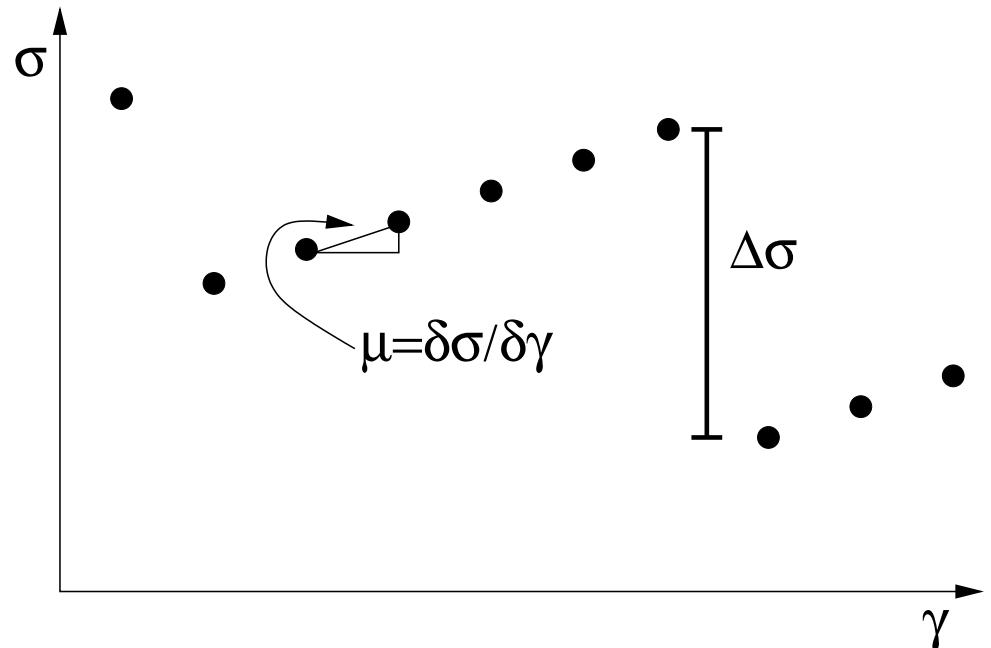
Event Statistics

- Collect stats on:
 - "Instantaneous" modulus



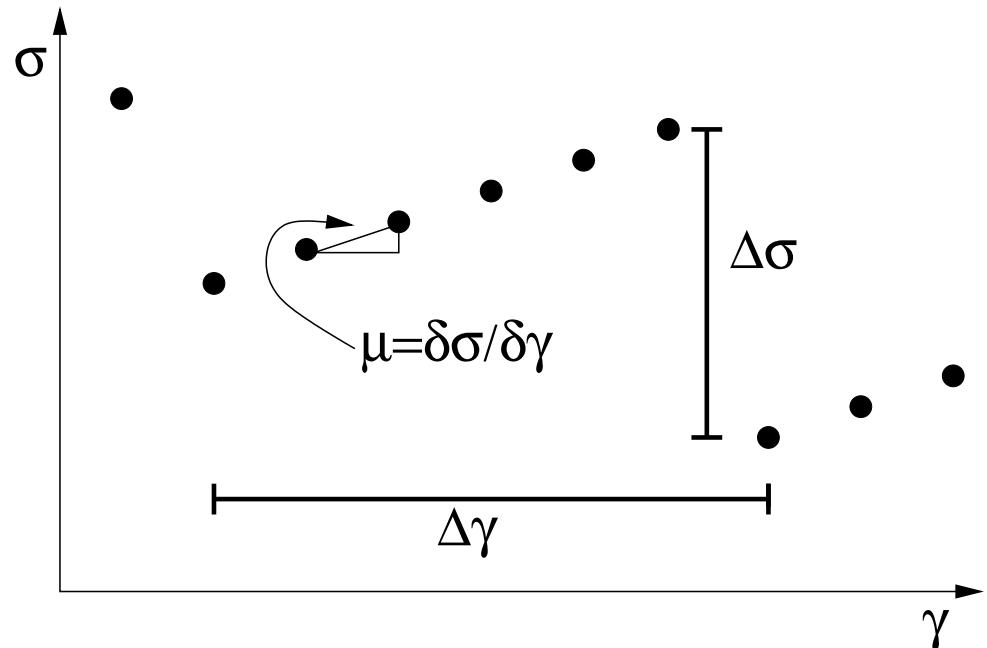
Event Statistics

- Collect stats on:
 - "Instantaneous" modulus
 - Stress drops, $\Delta\sigma$



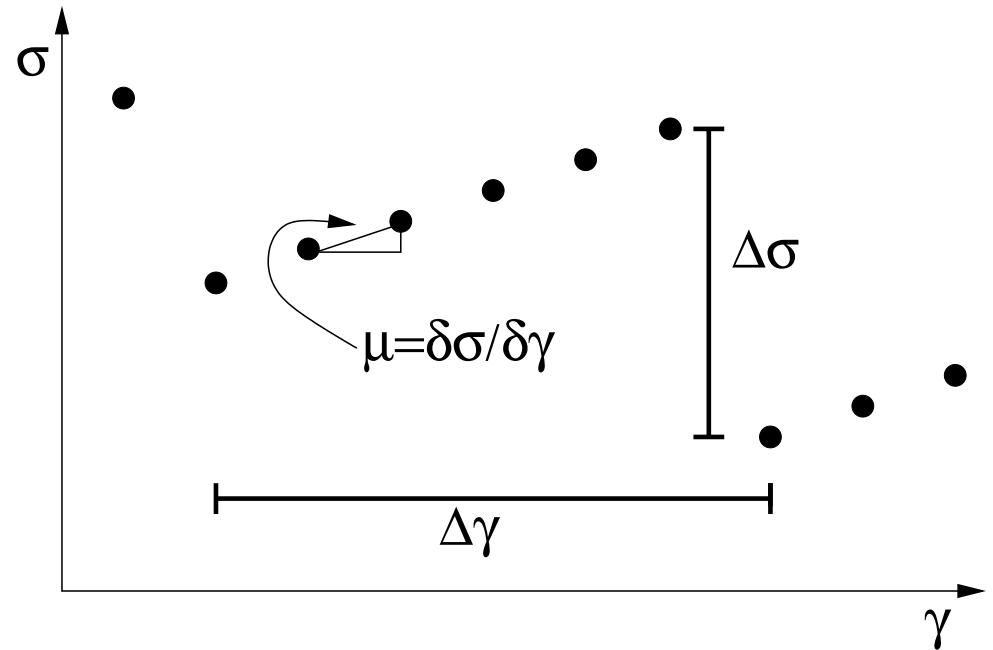
Event Statistics

- Collect stats on:
 - "Instantaneous" modulus
 - Stress drops, $\Delta\sigma$
 - Segment length, $\Delta\gamma$



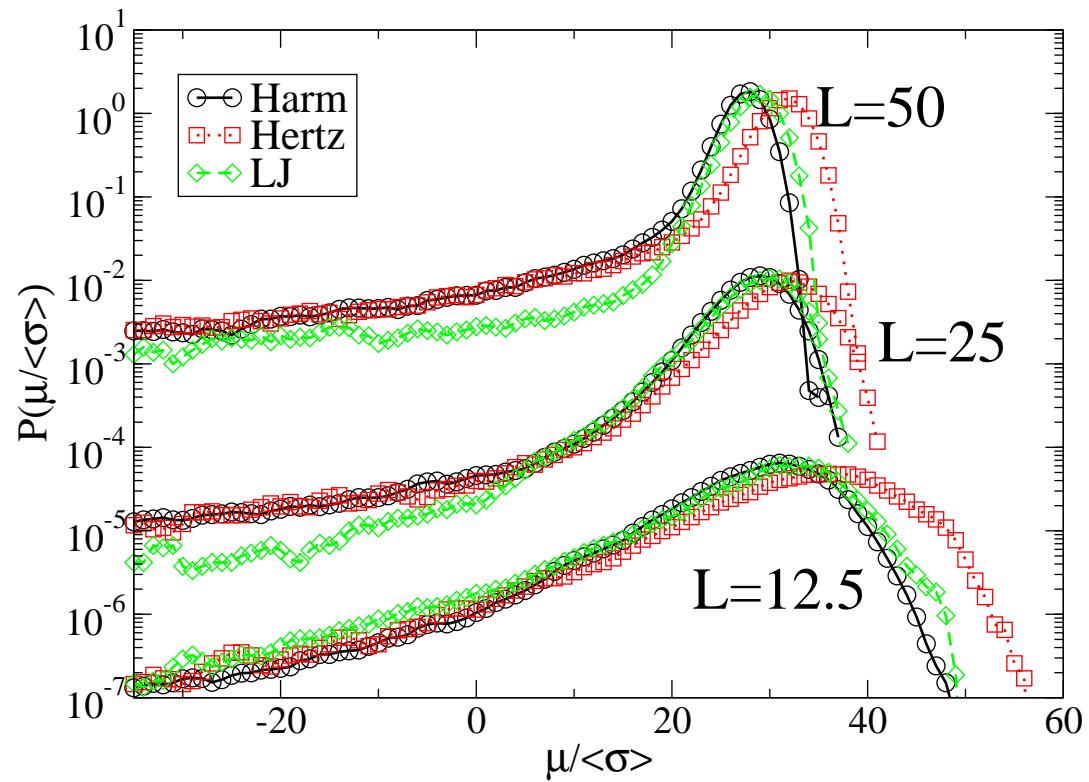
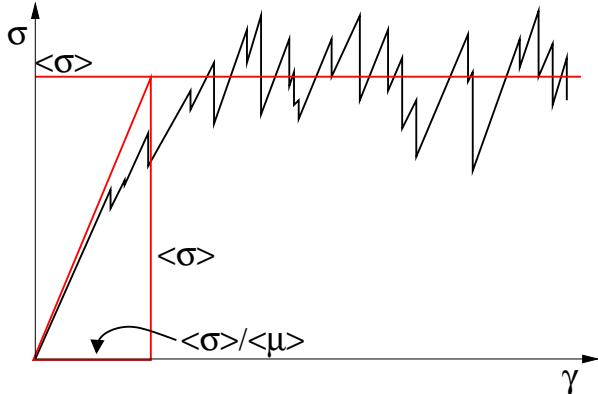
Event Statistics

- Collect stats on:
 - "Instantaneous" modulus
 - Stress drops, $\Delta\sigma$
 - Segment length, $\Delta\gamma$
 - Energy drops, ΔU



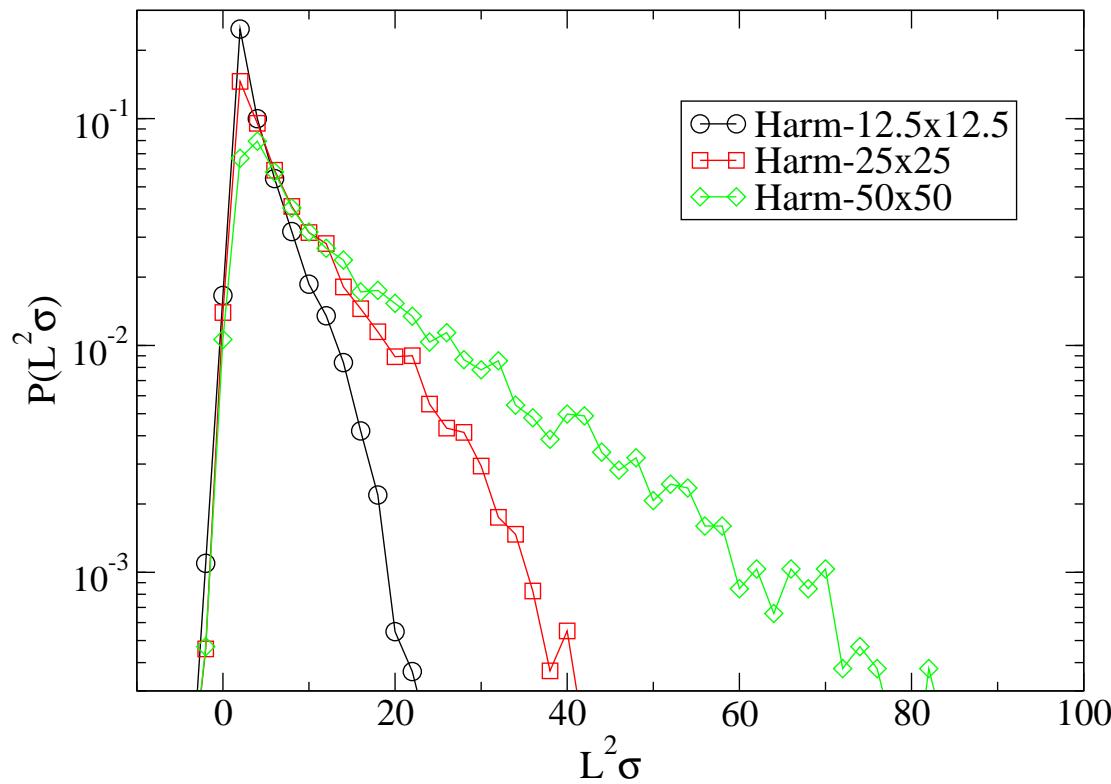
Average Modulus and Yield Strain

- Finite size study
- Well defined μ
- Universal yield strain $\sim 3\%$.



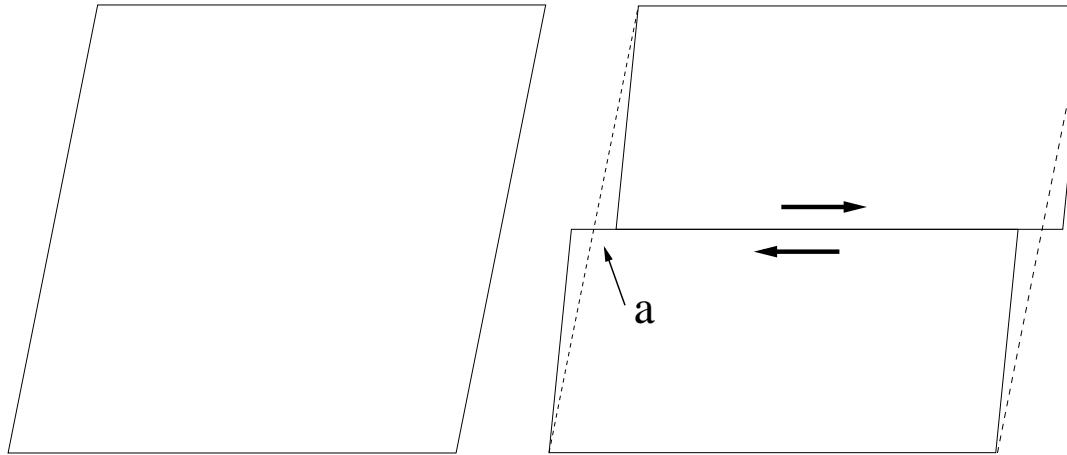
Finite Size Scalings

Naive stress distribution



Finite Size Scalings

- Simple scaling argument:

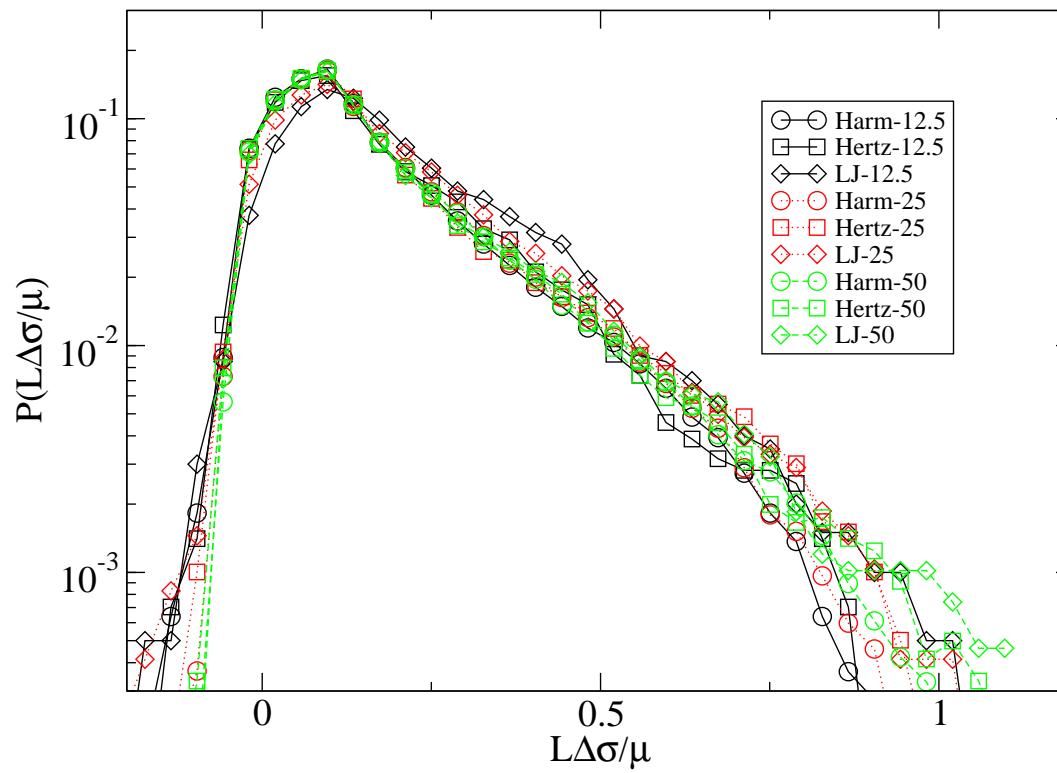


- $\Delta\sigma \sim \mu a/L$
- $\Delta U \sim \frac{\langle\sigma\rangle\Delta\sigma}{\mu} \sim a\langle\sigma\rangle L$
- $\Delta\gamma \sim a/L$

Finite Size Scalings

- Expect: $\Delta\sigma \sim \mu a/L$

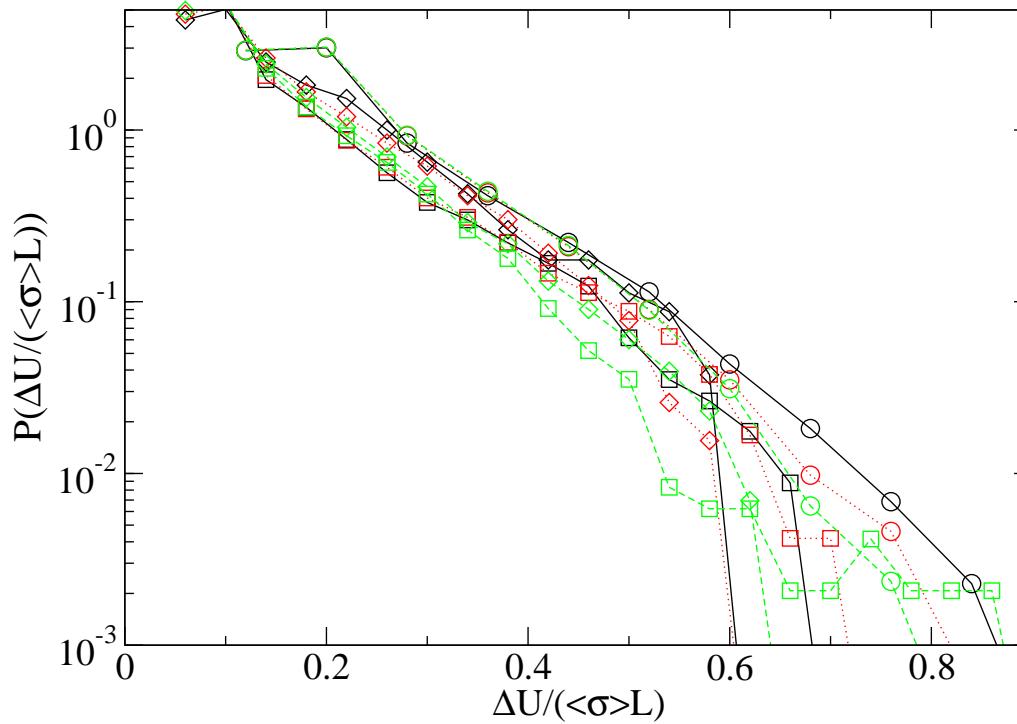
Scaled stress drop distribution



Finite Size Scalings

- Expect: $\Delta U \sim \frac{\langle \sigma \rangle \Delta \sigma}{\mu} \sim a \langle \sigma \rangle L$

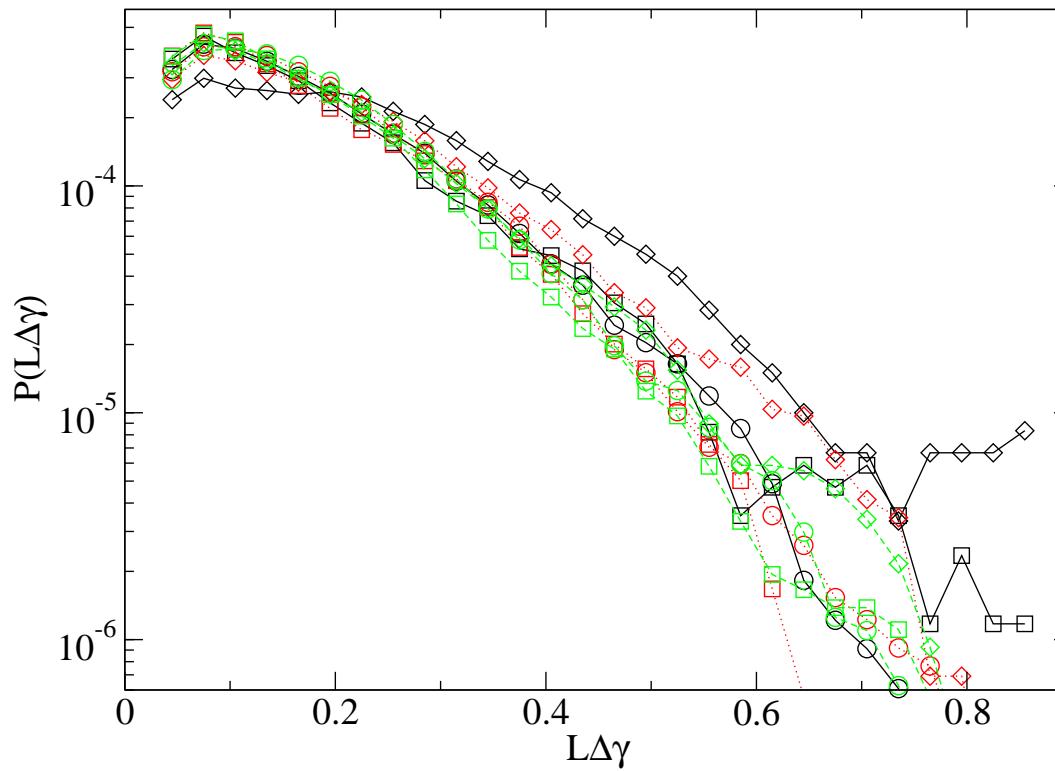
Scaled energy drop distribution



Finite Size Scalings

- Expect: $\Delta\gamma \sim a/L$

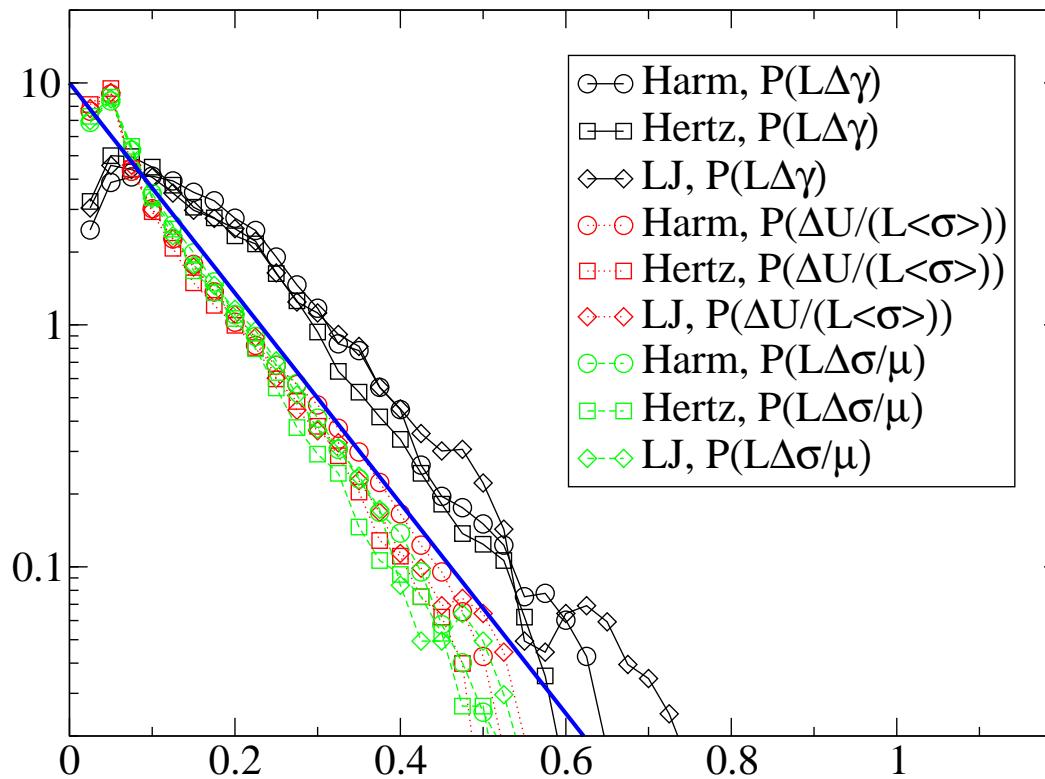
Scaled elastic interval length distribution



Finite Size Scalings

- Expect: $P(L\Delta\gamma) \sim P(\Delta U/L\langle\sigma\rangle) \sim P(L\Delta\sigma/\mu) \sim a$

$P(\Delta\sigma), P(\Delta U), P(\Delta\gamma)$ all resecaled



Conclusion: Statistics and Scalings

- All results independent of interaction potential
- Universal yield strain $\sim 3\%$
- Average event size scales like **length** of cell.
- \Rightarrow Universal exponential drop distribution.

Future Directions

- Finite rates (and temperature)
- Vary pressure: (Mohr-Coulomb relation?)
- Zero pressure (hard sphere limit)
- Particle mixture
- Mesoscale models

Inter-event Correlations

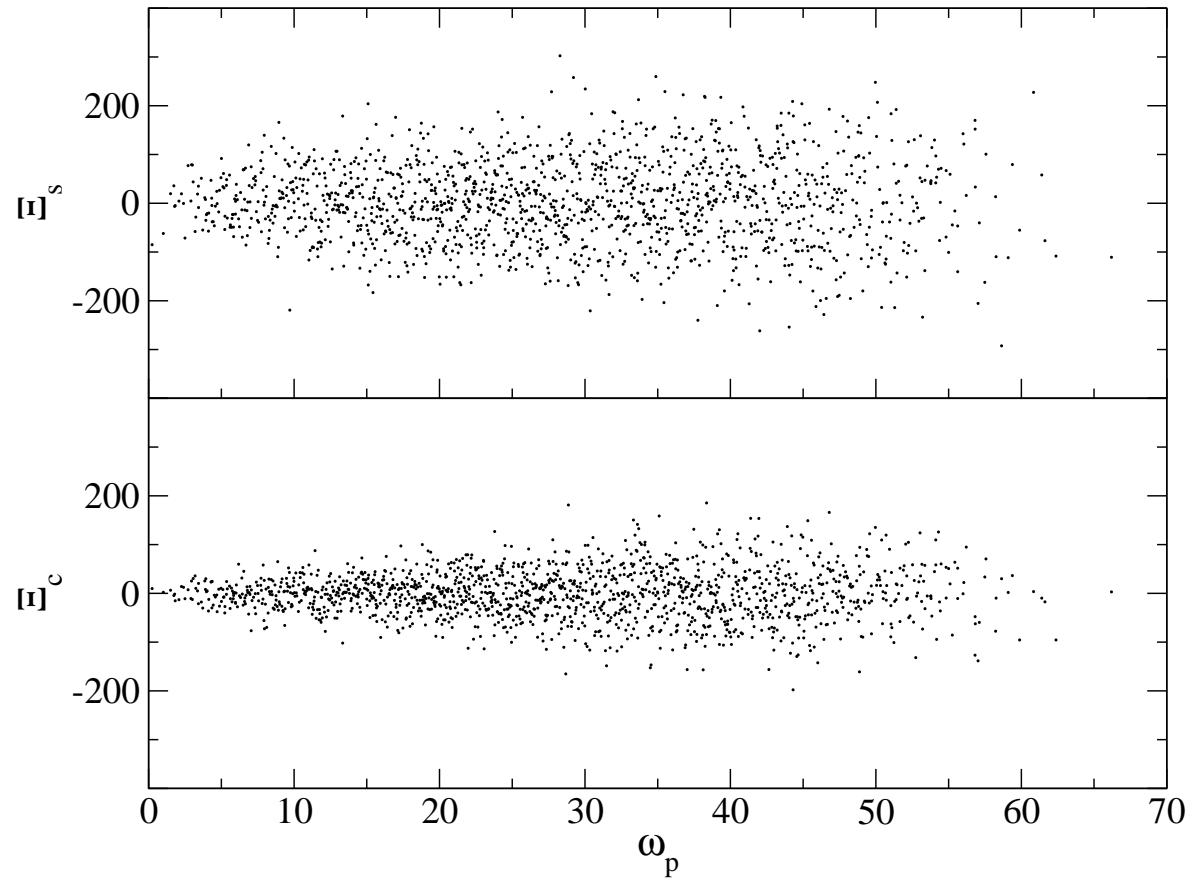
Play Movie

- Spatial correlations at short times.
- Weak at long times.
- No pronounced persistent localization.

Normal Mode Decomposition

Recall: $\mu = \mu_a - \Xi_{i\alpha} \mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta} \rightarrow \mu_a - \sum_p \left(\frac{\Xi_p^2}{\omega_p^2} \right)$

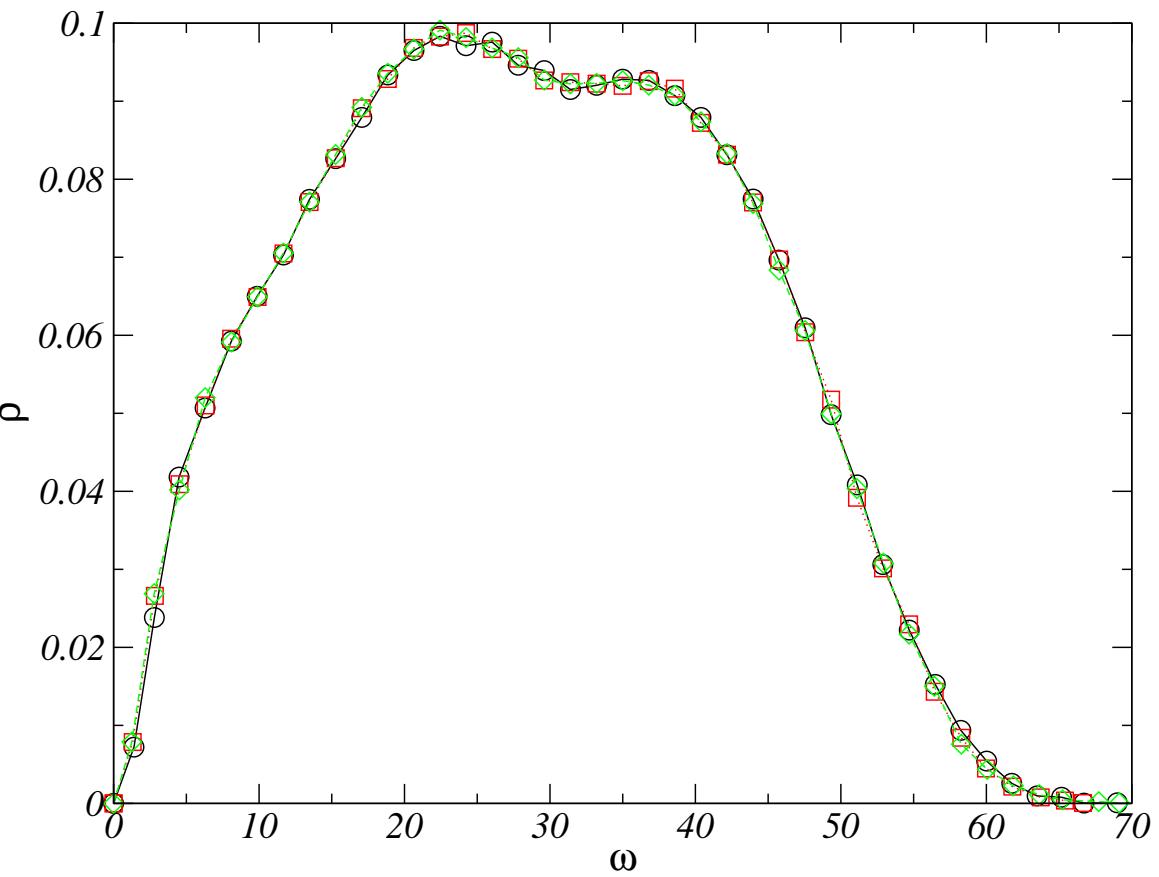
- Scatter plot of Ξ_p



Normal Mode Decomposition

Recall: $\mu = \mu_a - \Xi_{i\alpha} \mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta} \rightarrow \mu_a - \sum_p \left(\frac{\Xi_p^2}{\omega_p^2} \right)$

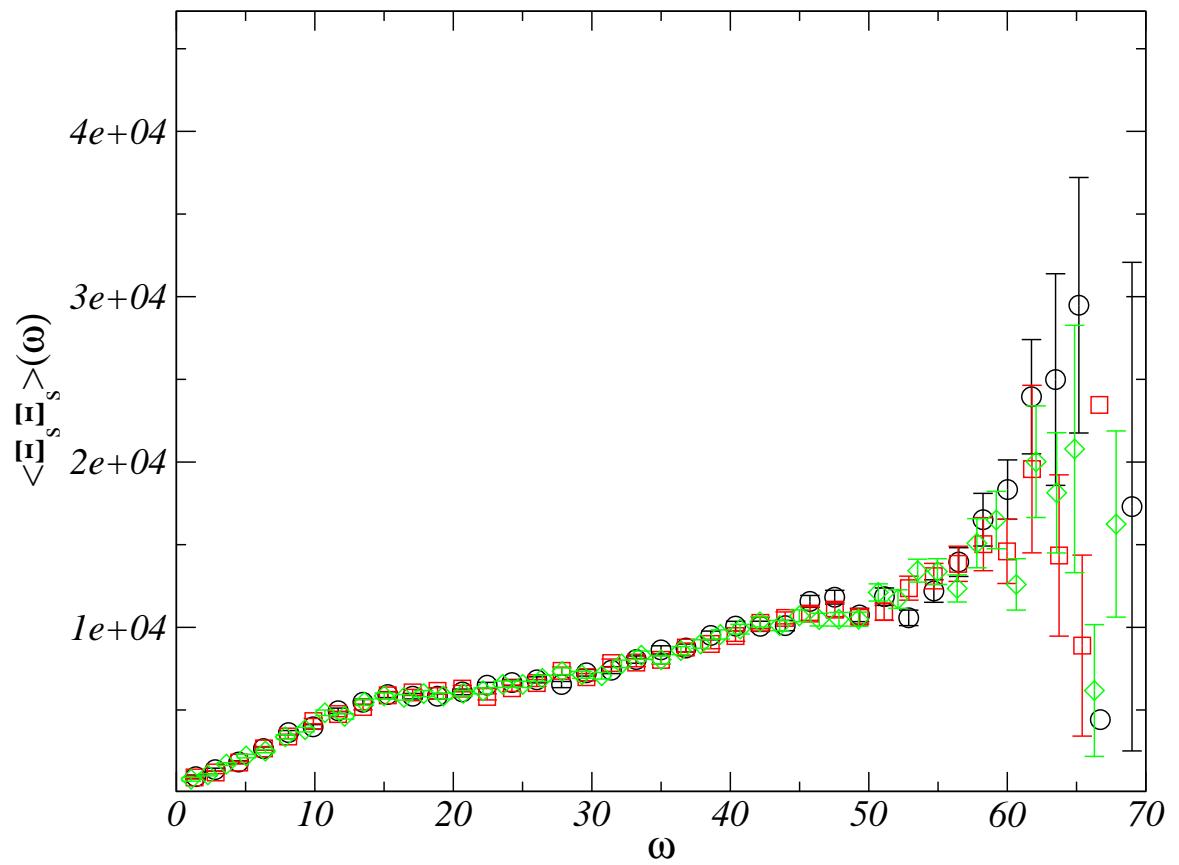
- Density of states, $\rho(\omega)$



Normal Mode Decomposition

Recall: $\mu = \mu_a - \Xi_{i\alpha} \mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta} \rightarrow \mu_a - \sum_p \left(\frac{\Xi_p^2}{\omega_p^2} \right)$

- $\langle \Xi^2(\omega) \rangle$



Normal Mode Decomposition

Recall: $\mu = \mu_a - \Xi_{i\alpha} \mathcal{H}_{i\alpha j\beta}^{-1} \Xi_{j\beta} \rightarrow \mu_a - \sum_p \left(\frac{\Xi_p^2}{\omega_p^2} \right)$

● $\frac{\rho(\omega) \langle \Xi^2 \rangle(\omega)}{\omega^2}$

