Mesoscale lattice models for amorphous solids: Diffusion, rheology, and memory

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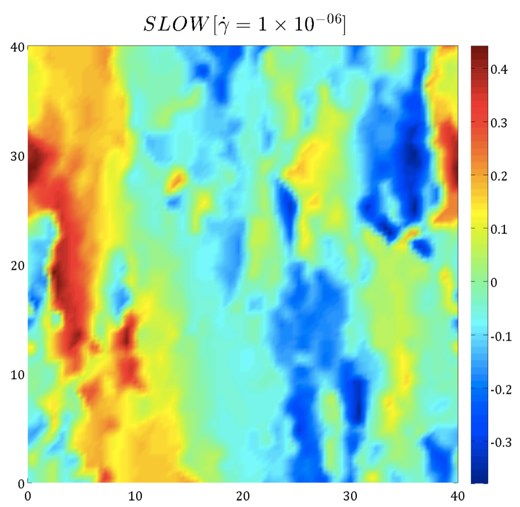

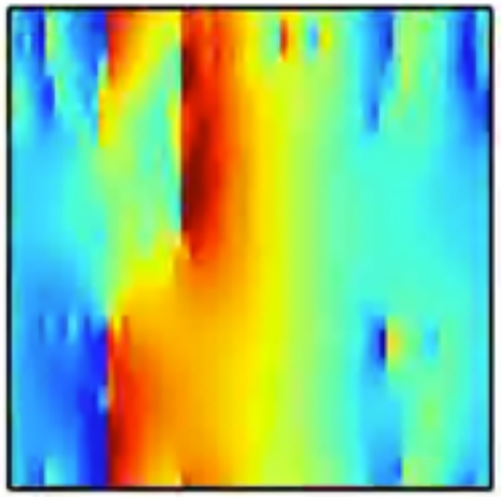

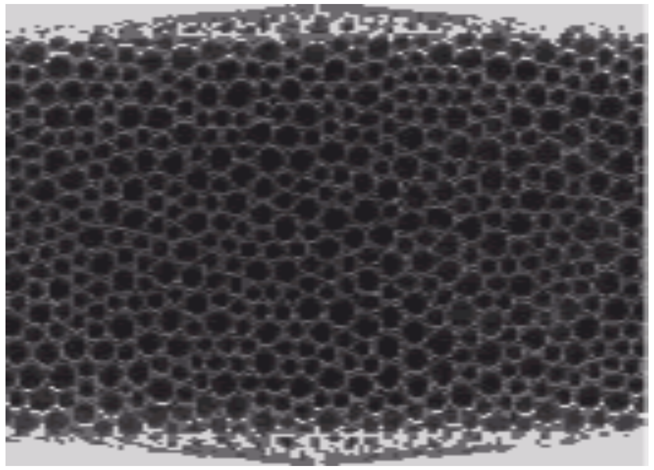

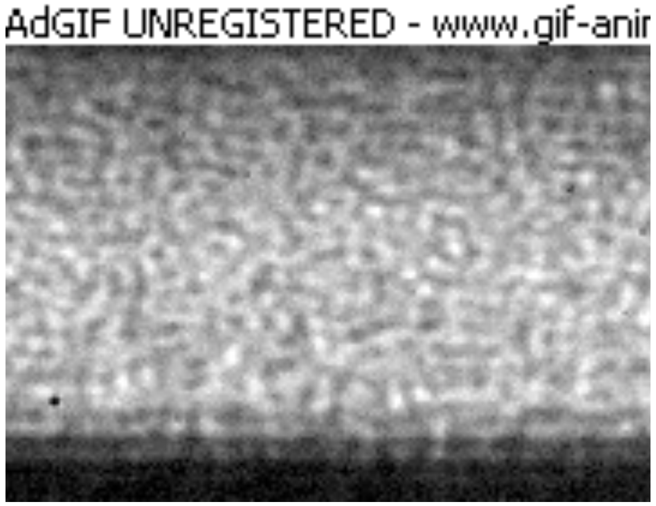

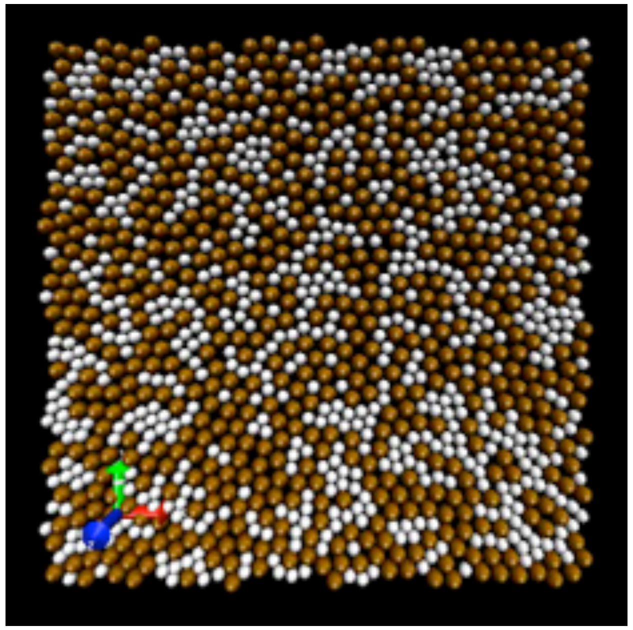

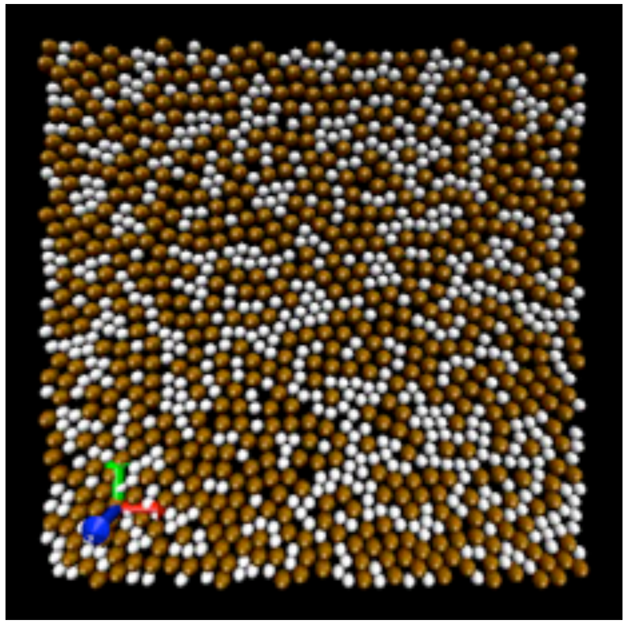

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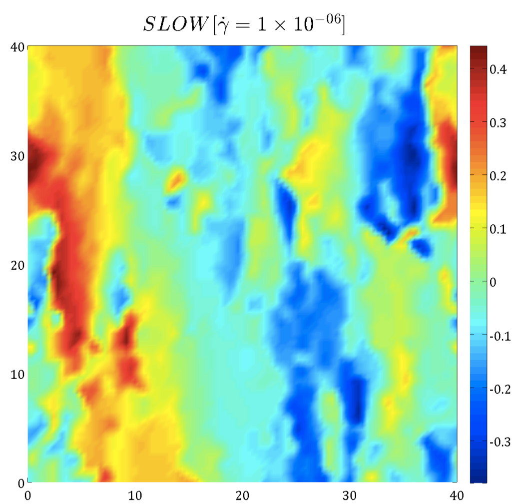

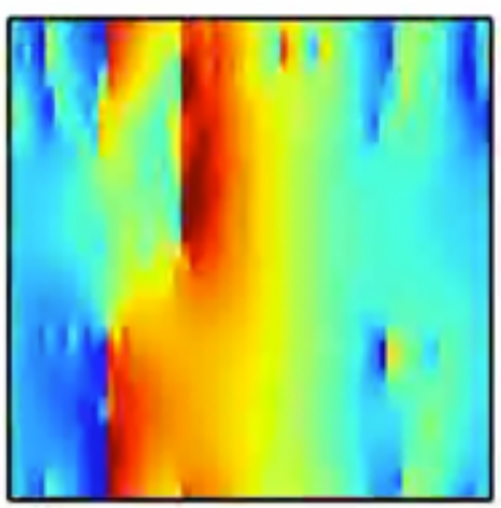

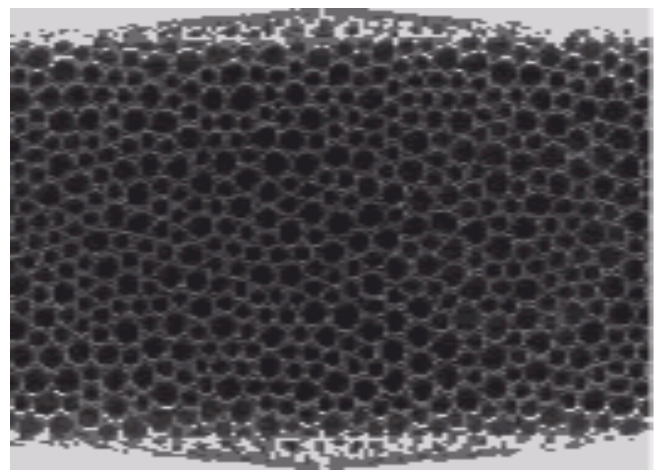

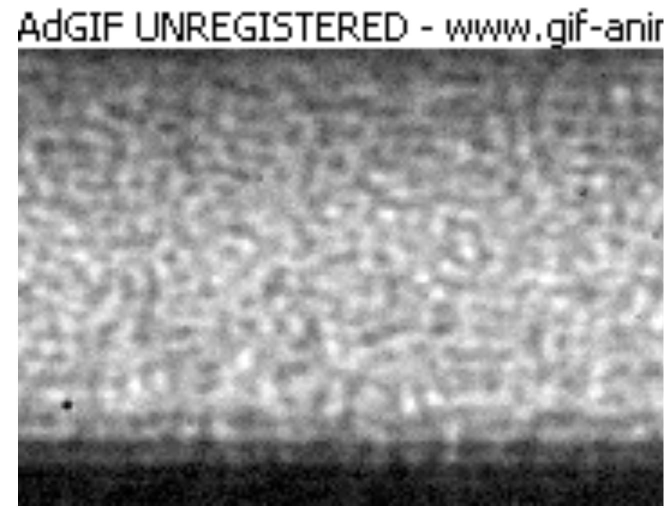

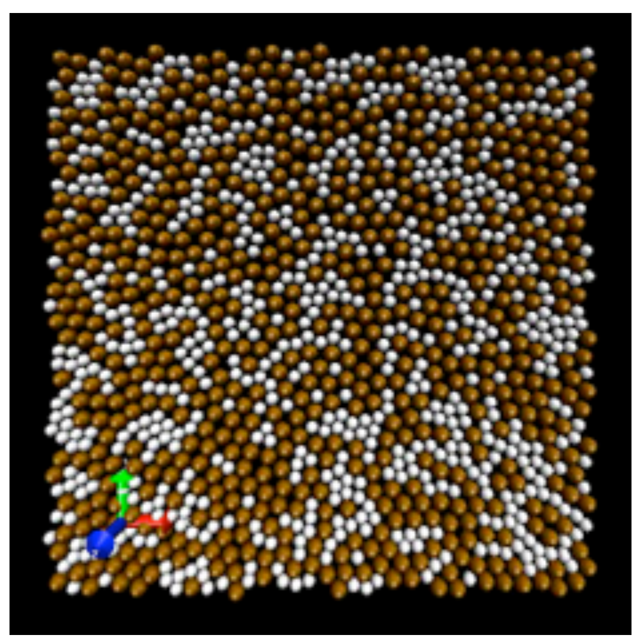

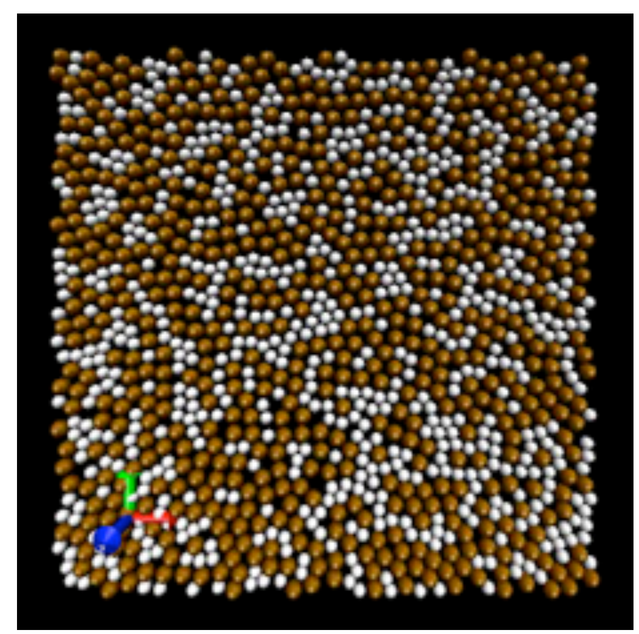

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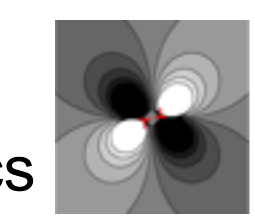

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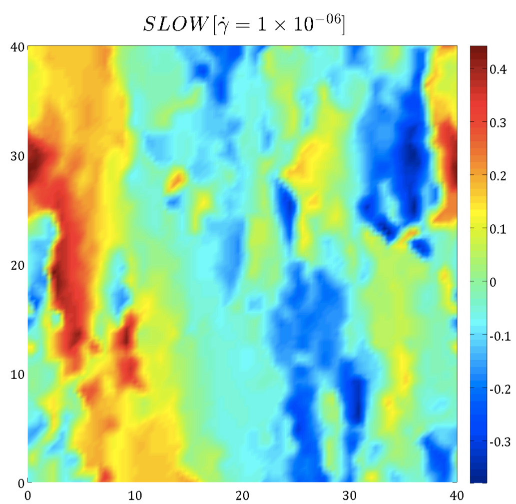

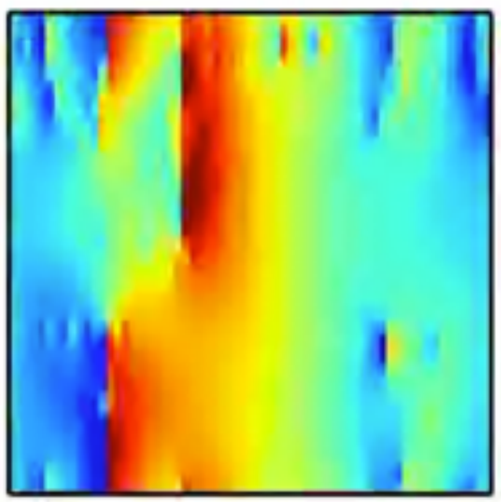

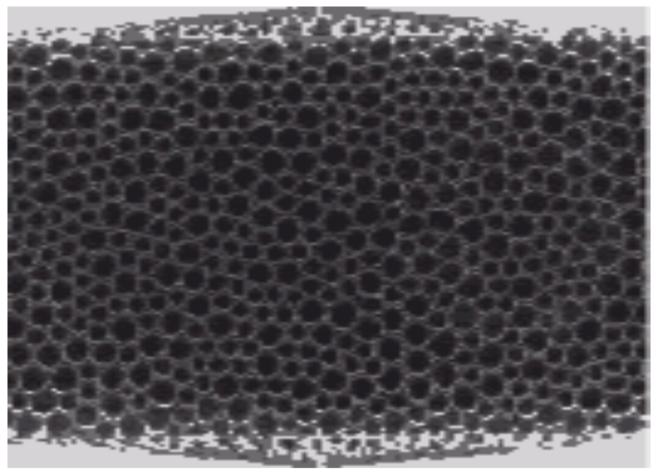

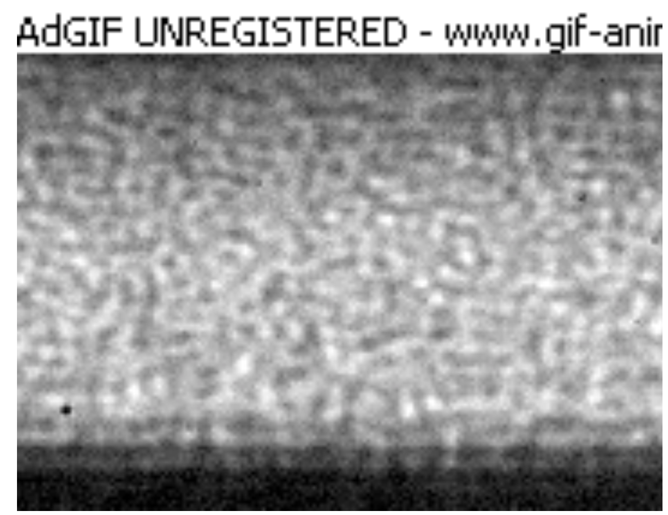

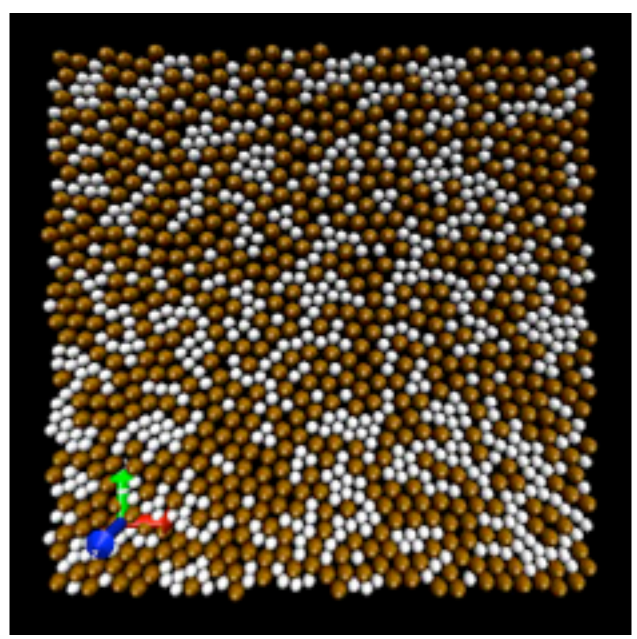

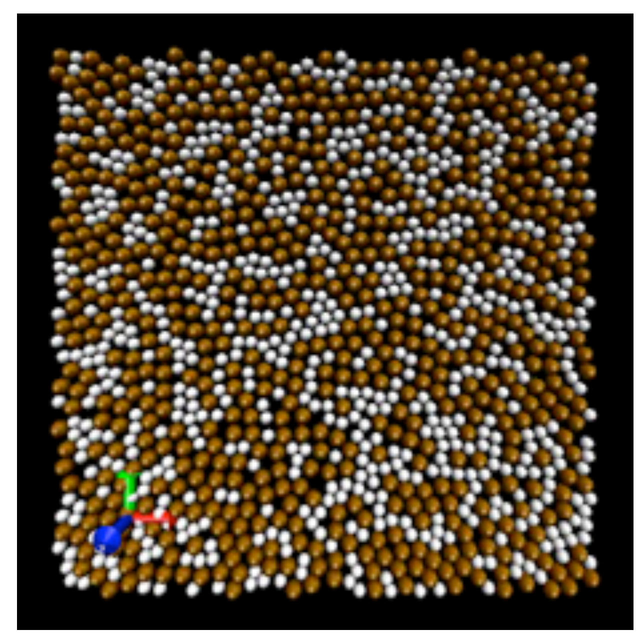

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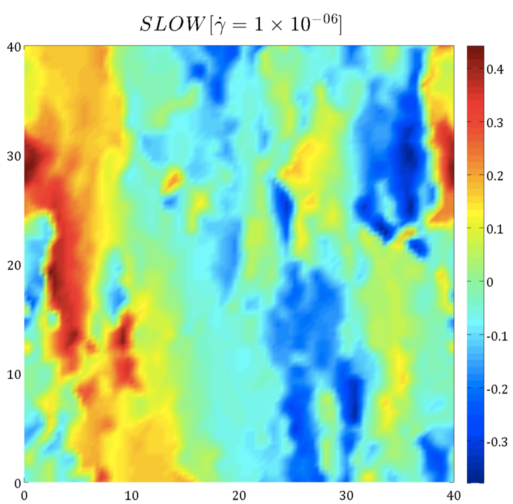

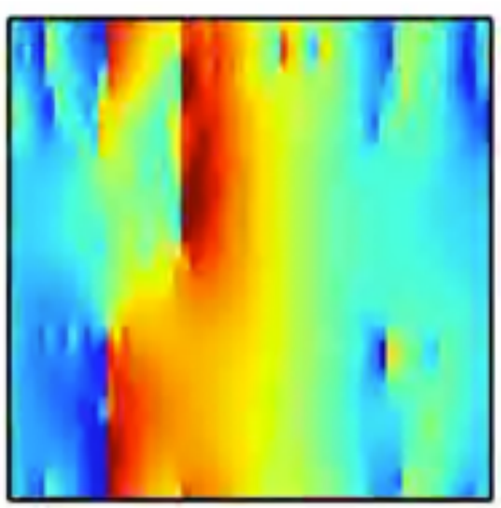

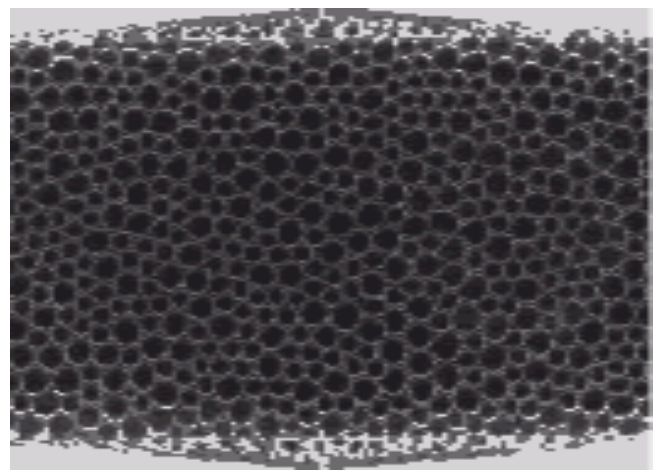

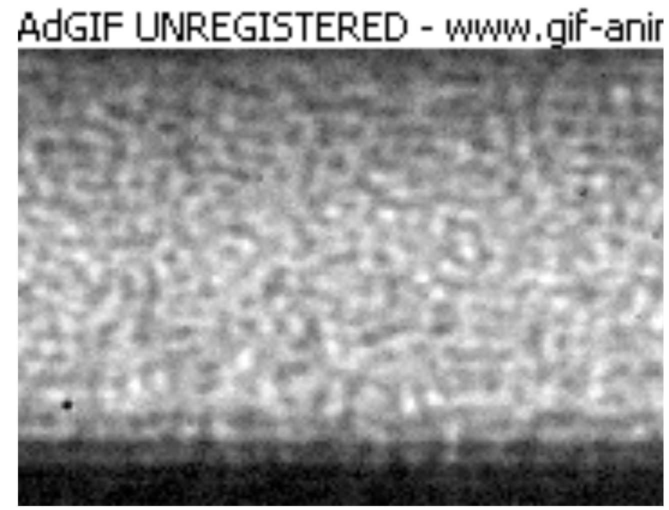

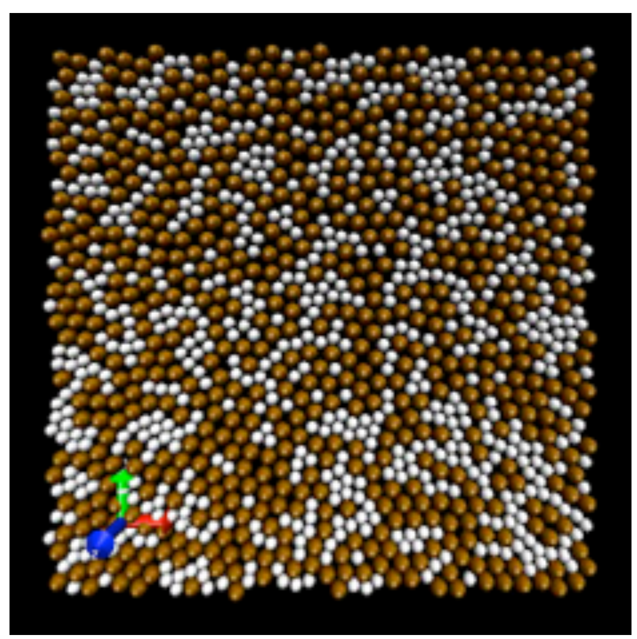

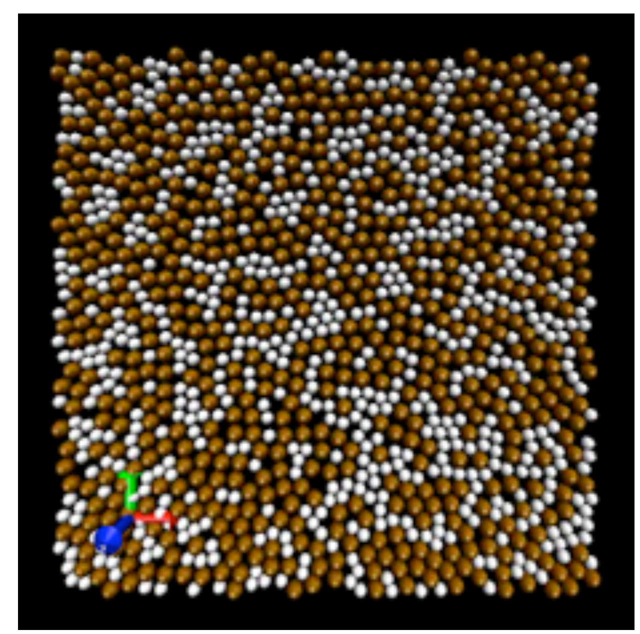

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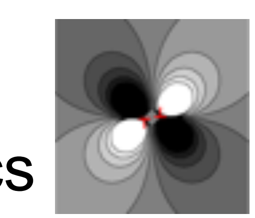

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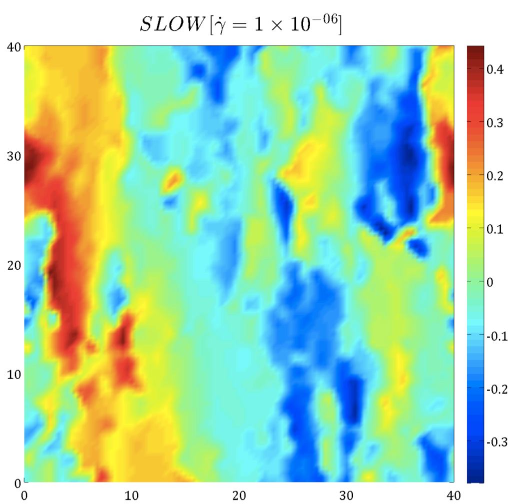

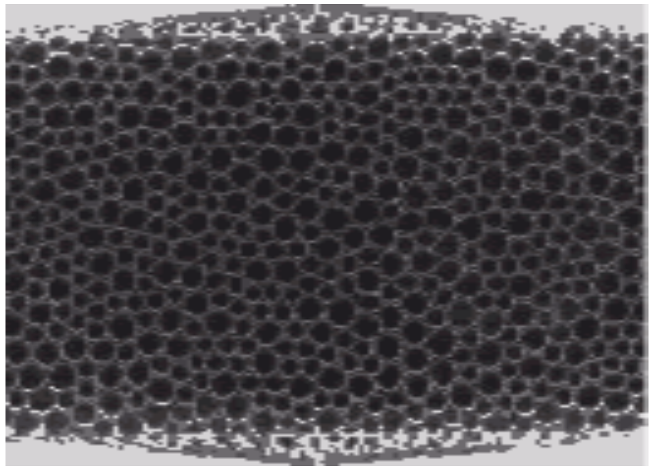

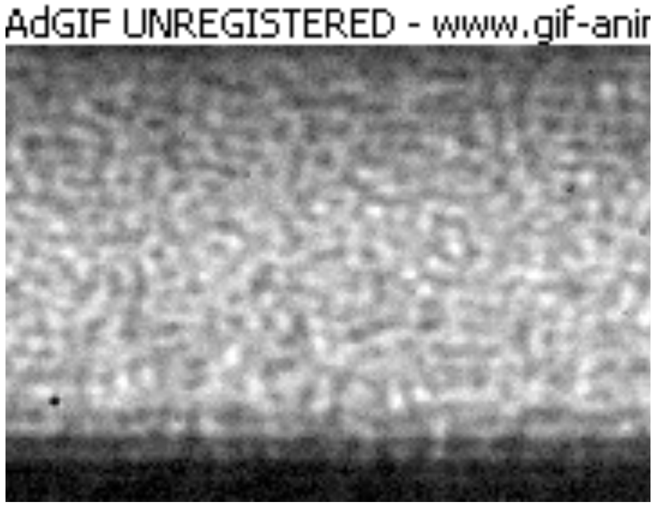

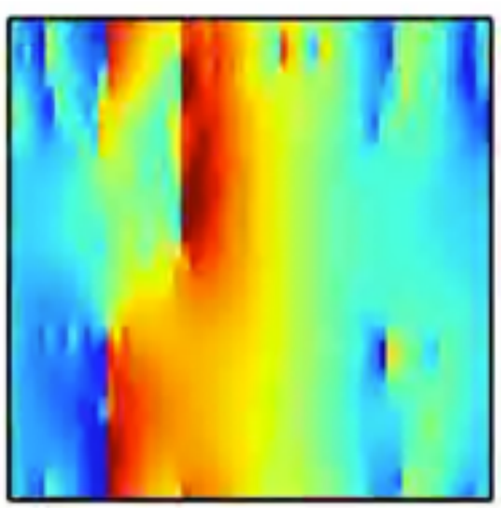

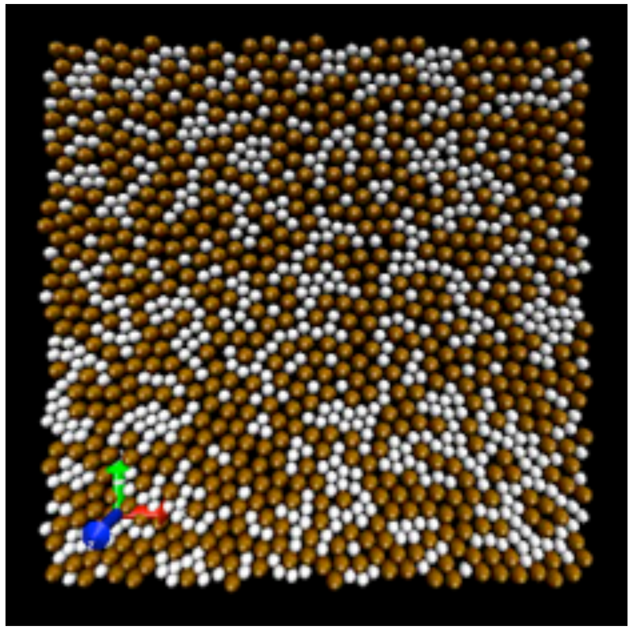

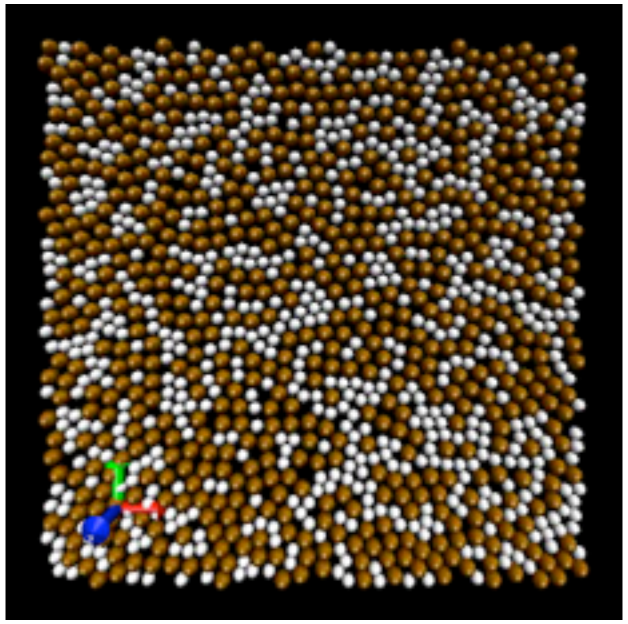

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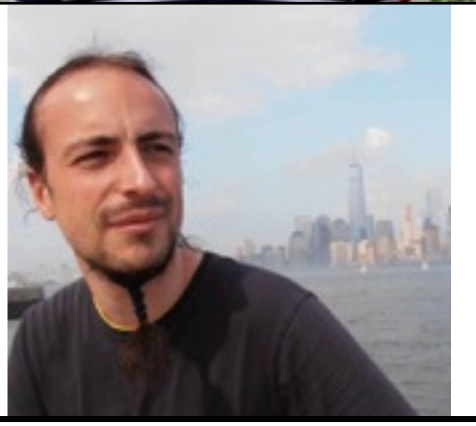
Acknowledgements

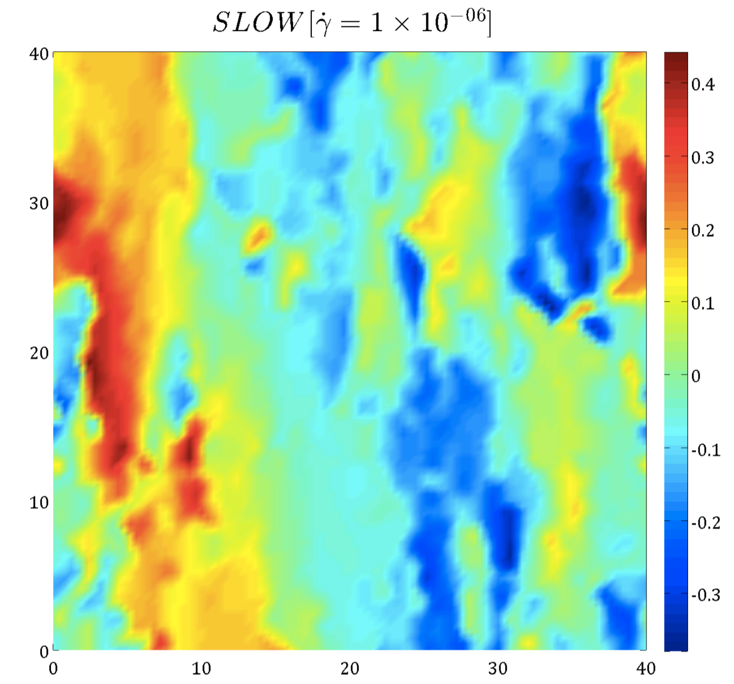
- Arka Roy (Bubble model simulations)
- Botond Tyukodi (NEU/ESPCI) (Elasto-plastic model)
- Damien Vandembroucq, ESPCI

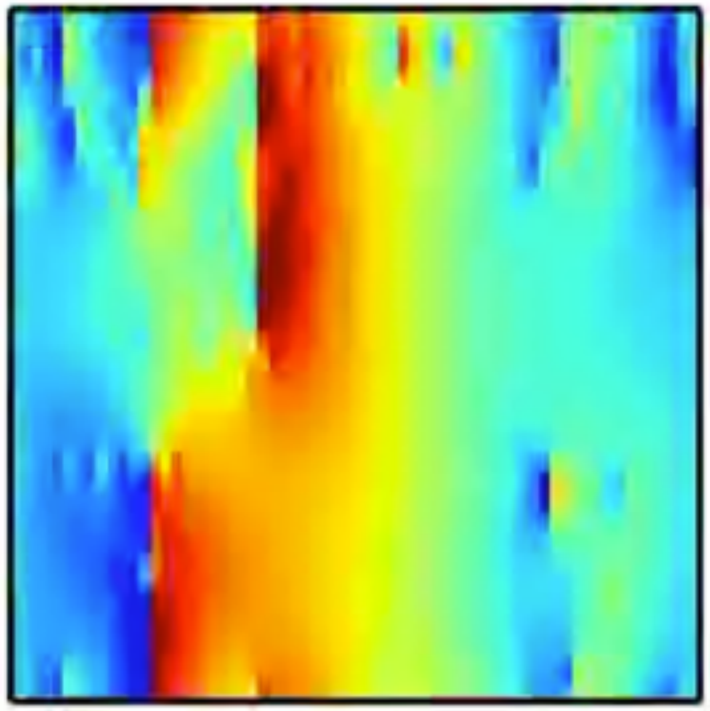


- DMR-1056564

Outline

- Background:
  - Phenomenology: rheology, localization
  - Particle-scale models and results
  - Scaling of diffusion and rheology for particle models
- Rationale for coarse-grained description
- Quasi-static finite size scaling: Avalanches and diffusion
- Finite rate: Rheology
- Hysteresis near the yield point: erasing memory?





Soft glassy solids

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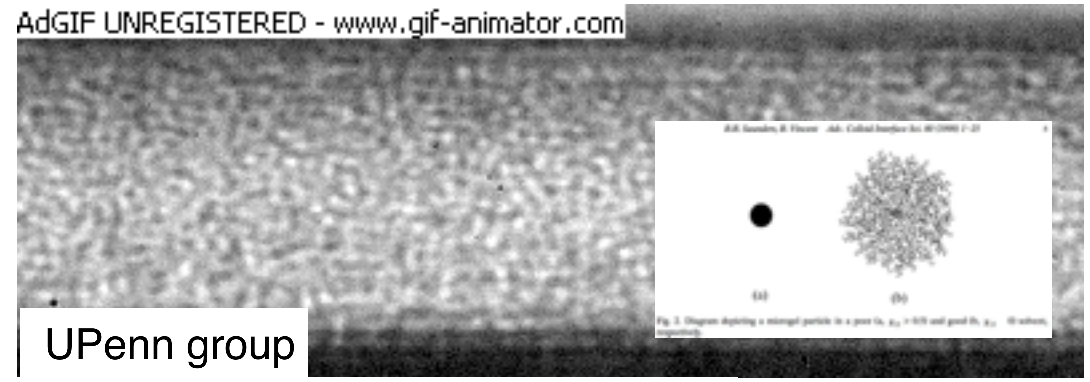

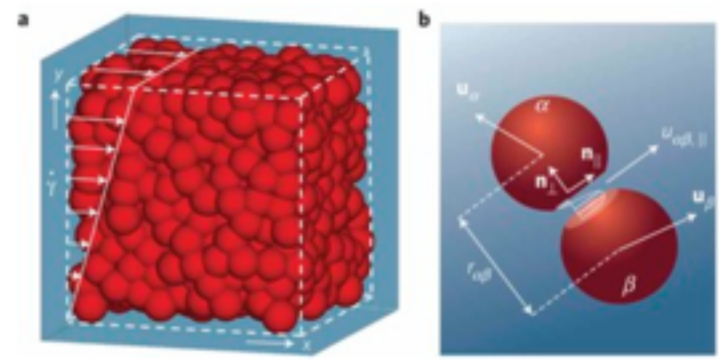

Seth et. al. (Cloitre, Bonnecaze)

- Many other examples!
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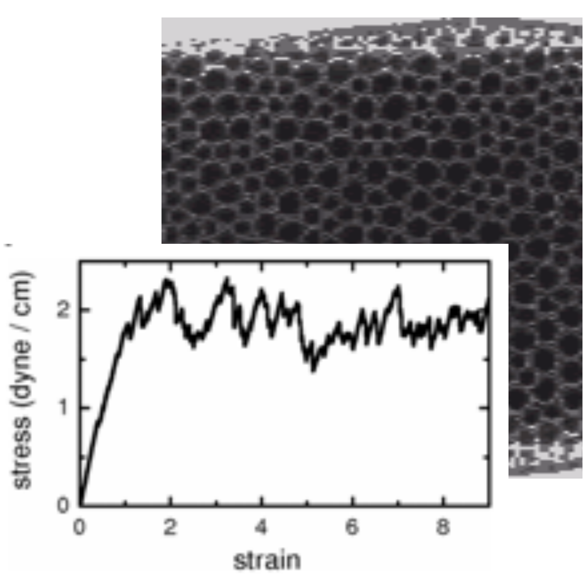
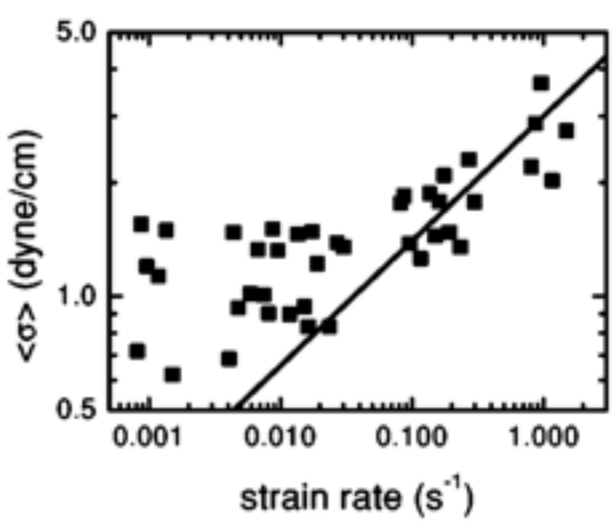
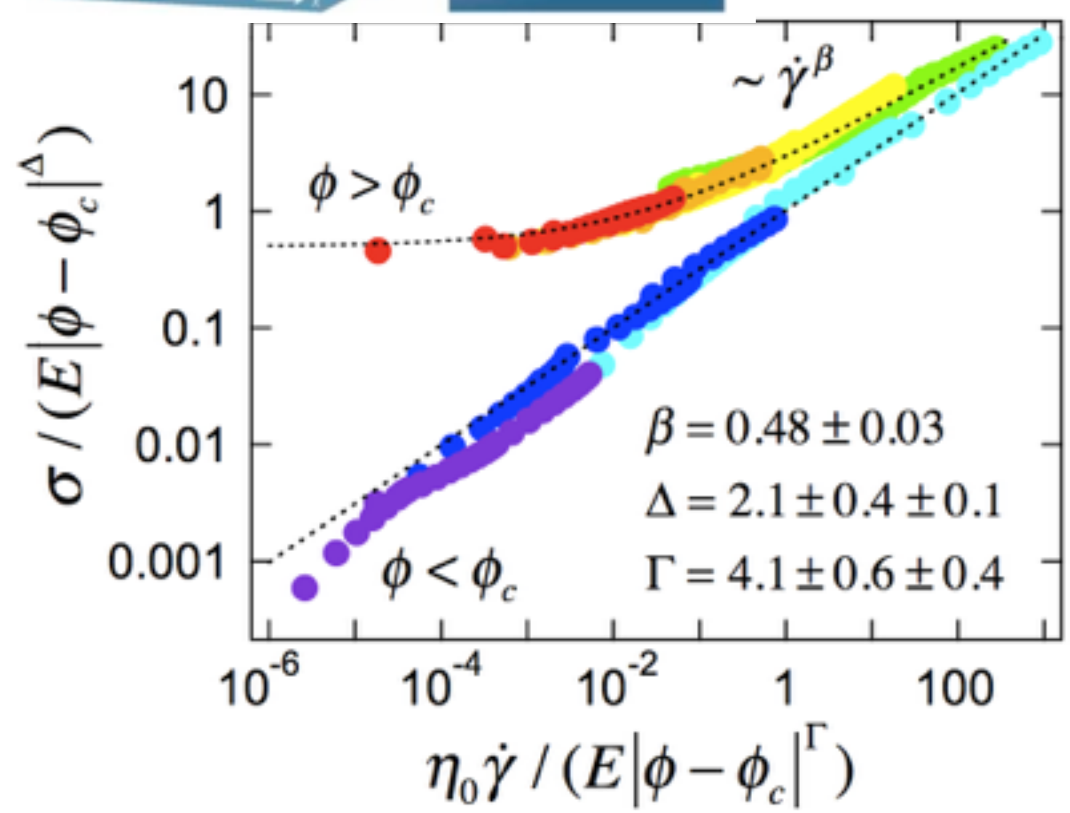
- β around 0.5 for NIPAM particles and emulsions, 0.3-0.4 for bubbles







Today's talk: Jammed branch only!

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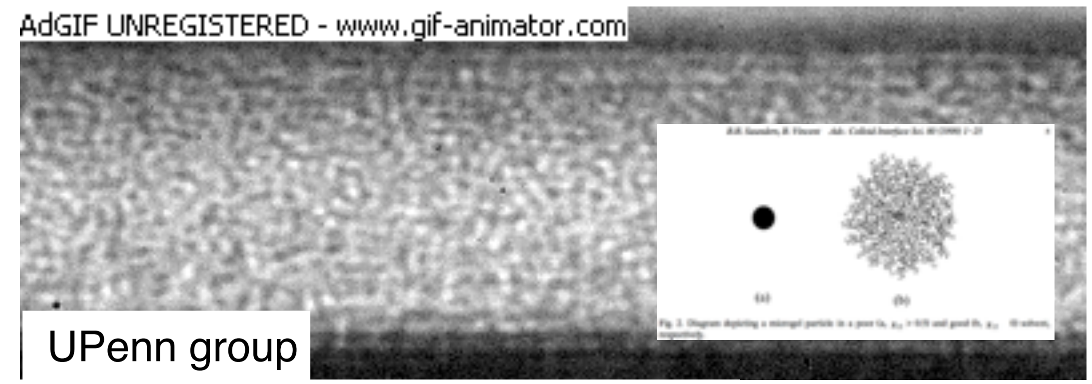

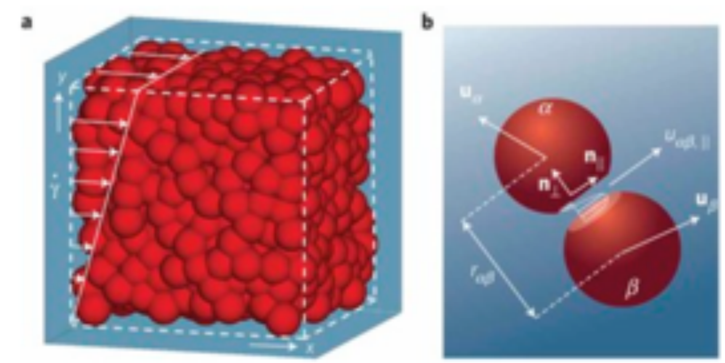

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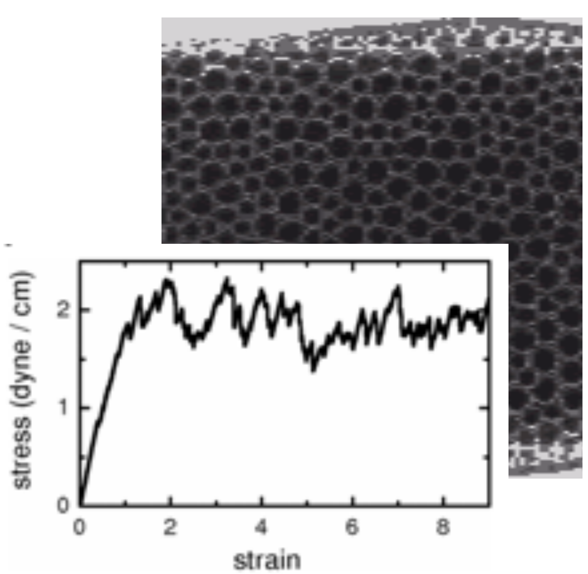

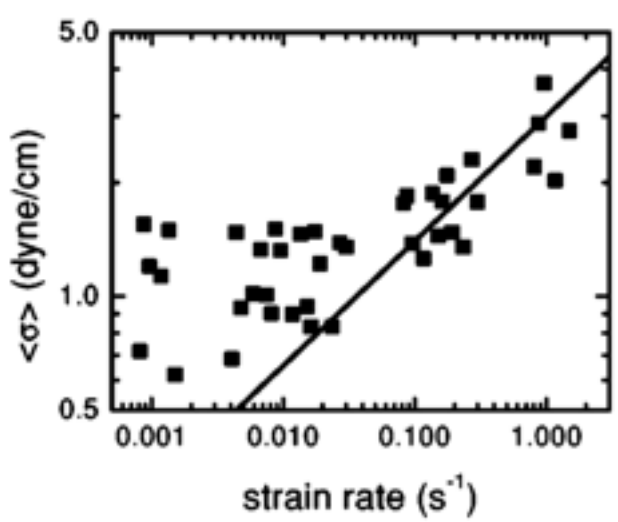

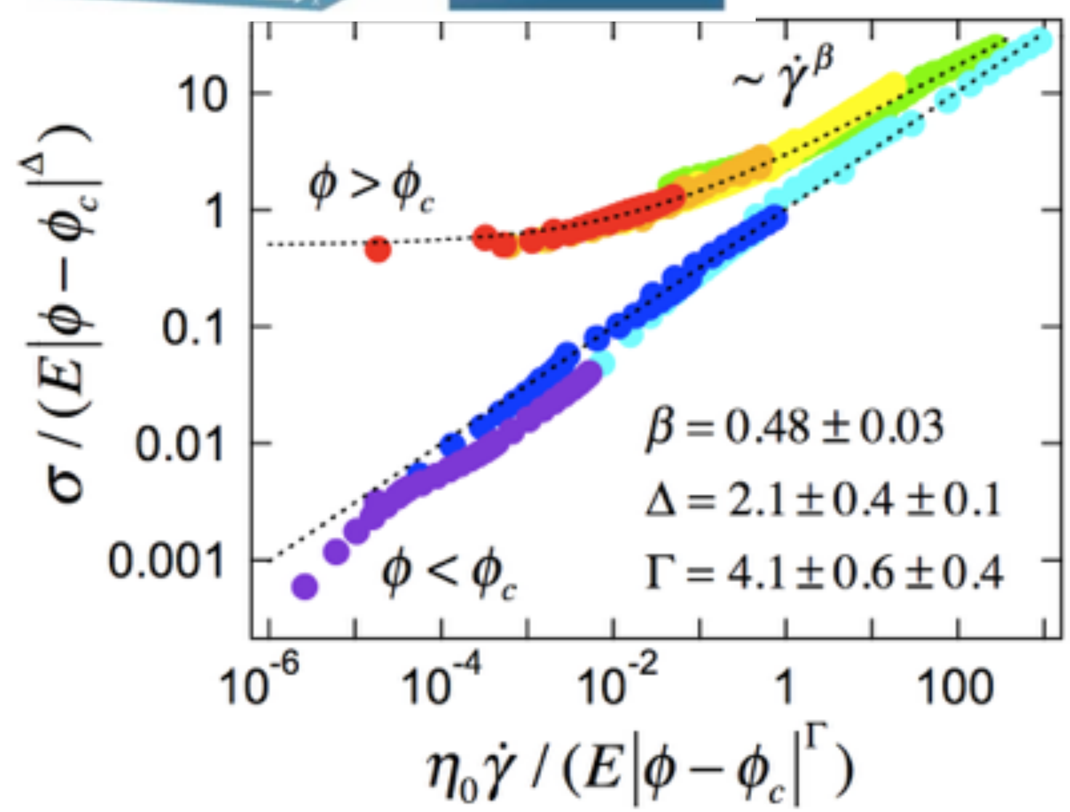

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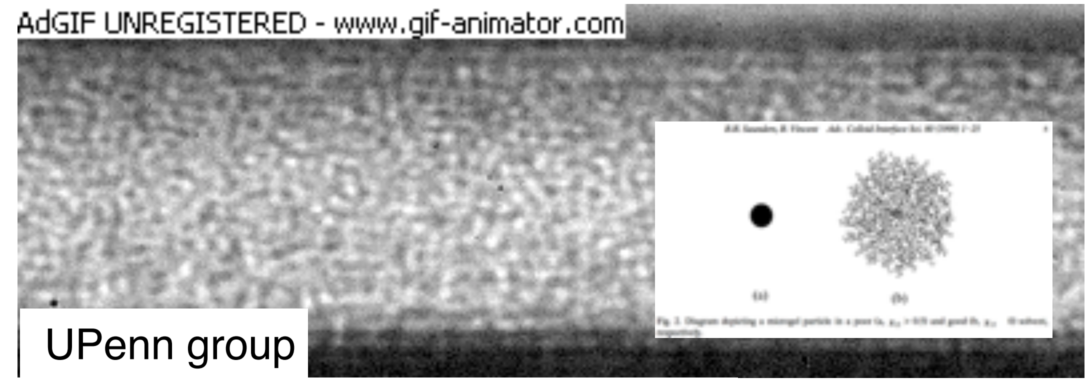

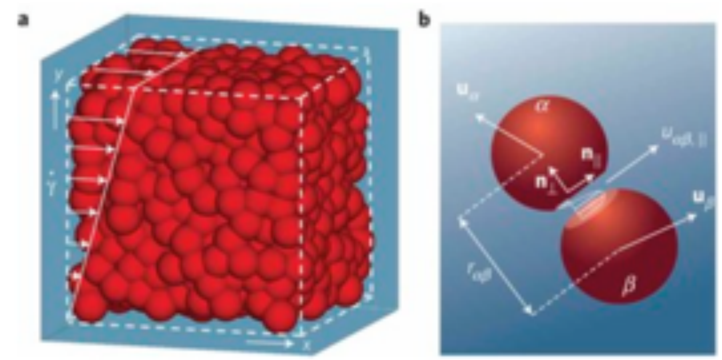

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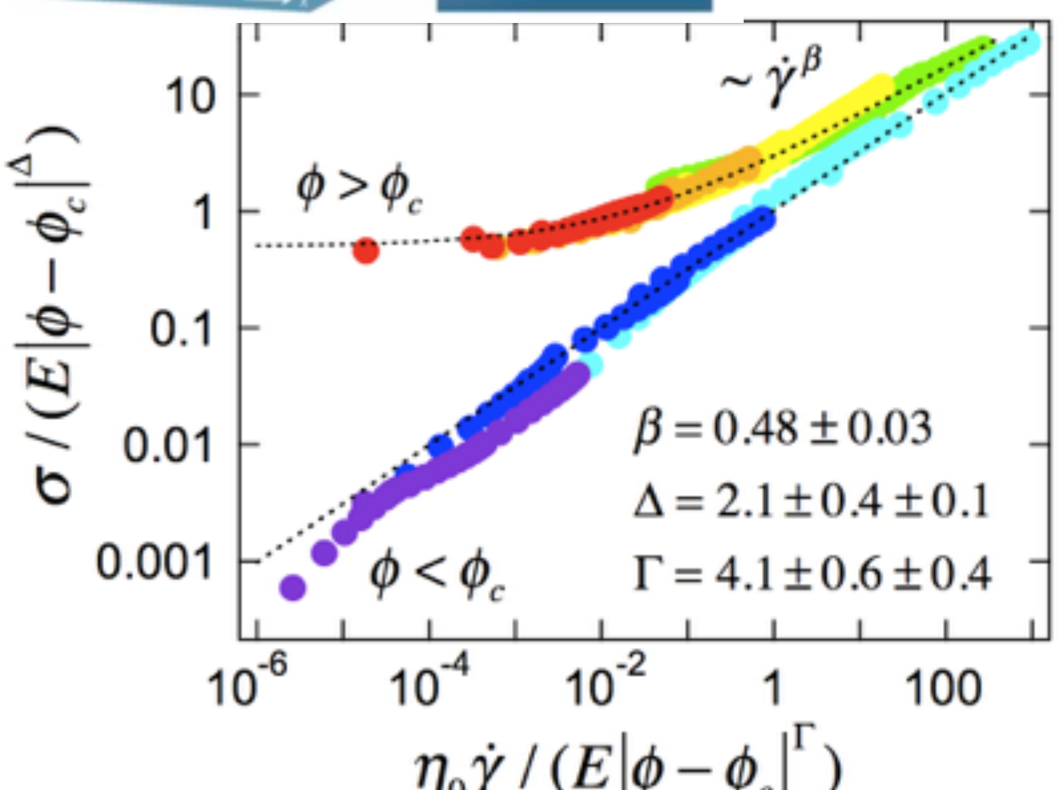
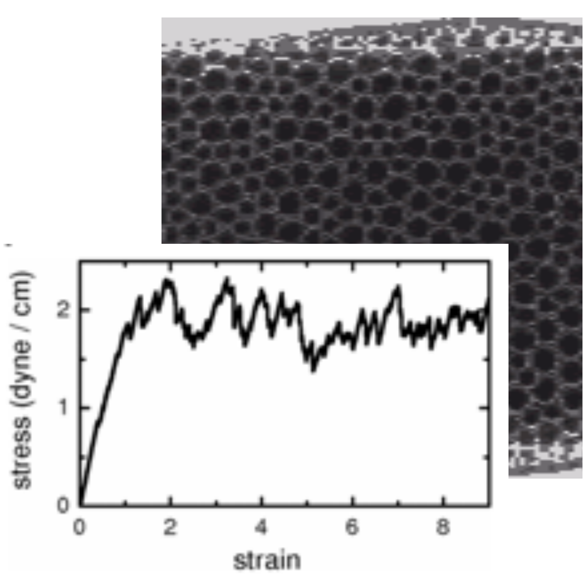
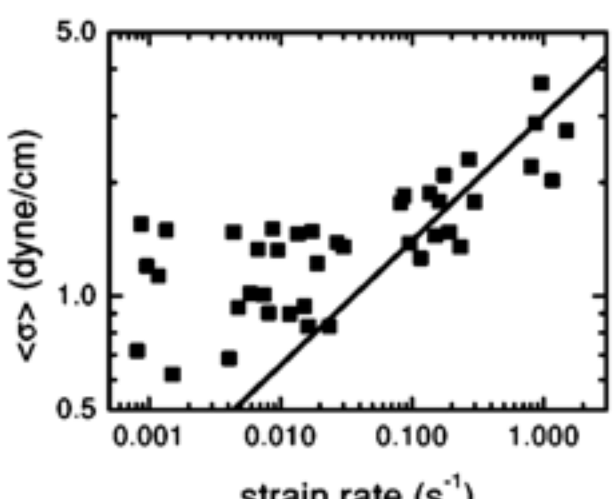


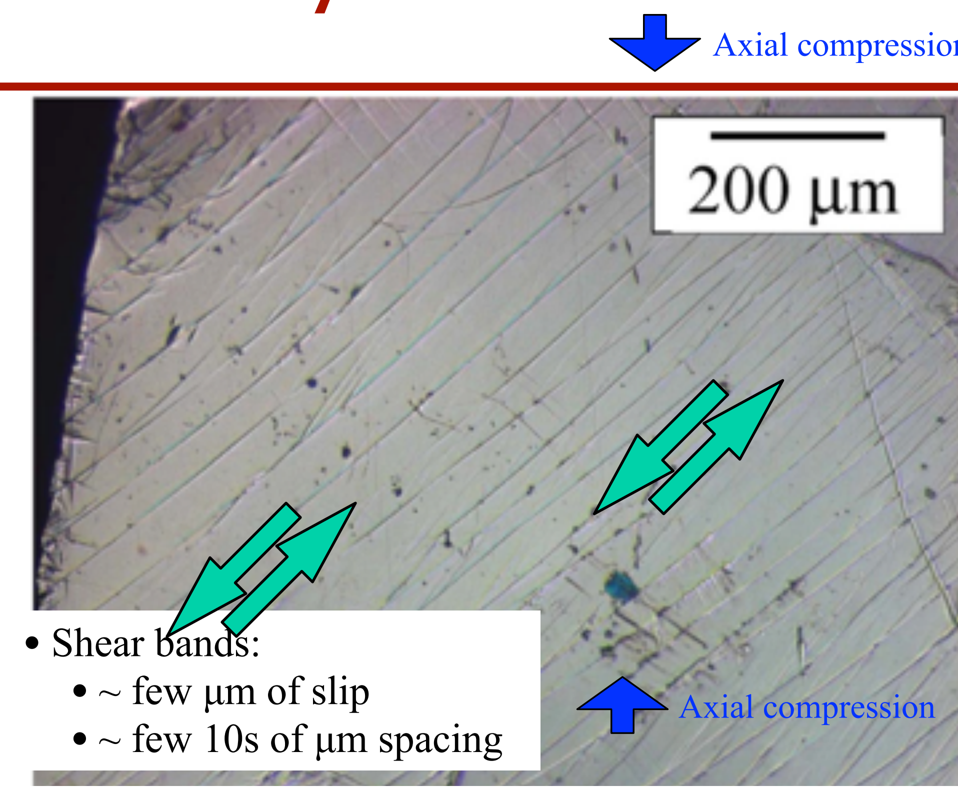




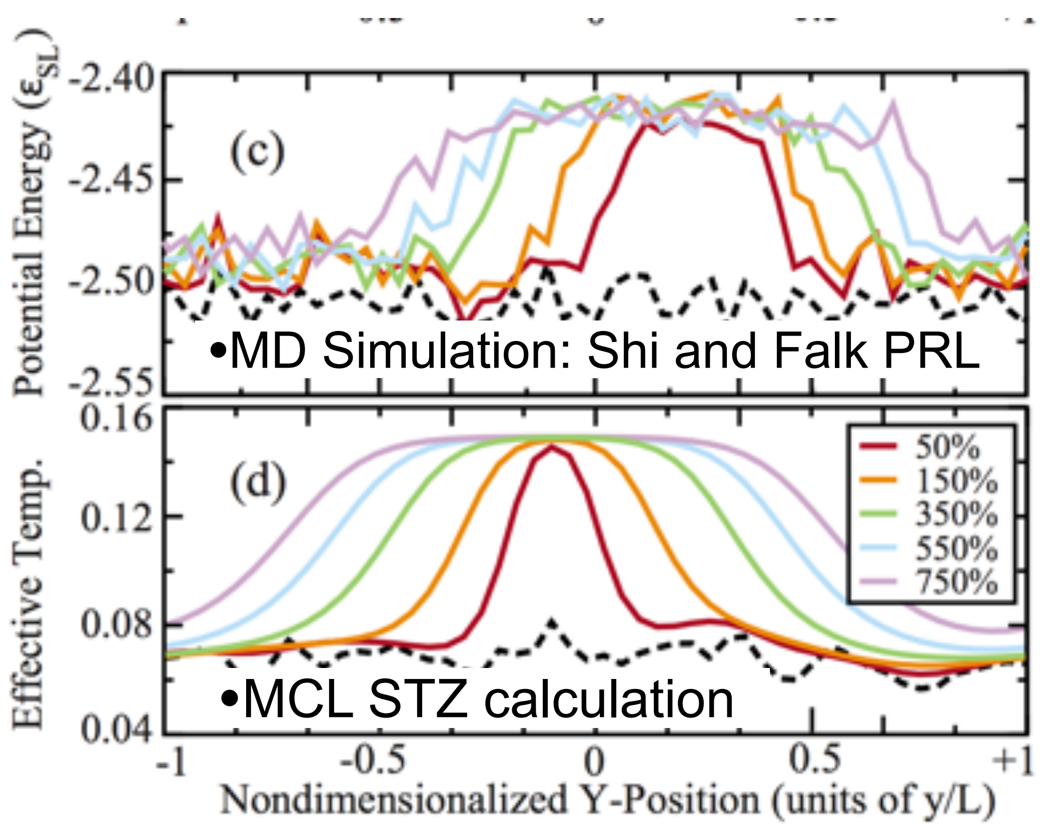
Today's talk: Jammed branch only!

Persistent shear localization and hysteresis

- Shear can spontaneously localize onto bands.
- Observed in all materials (metallic glass, colloids, foams).
- Dependence on initial state important but not perfectly understood.



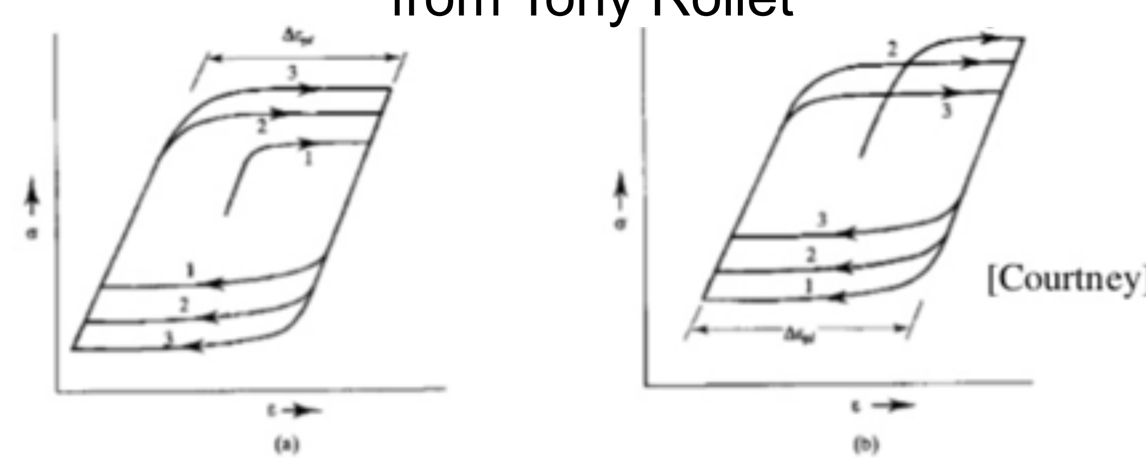
• From Schroers and Johnson: $Pt_{57.5}Cu_{14.7}Ni_{5.3}P_{22.5}$



•Manning, Carlson, and Langer PRE 2007

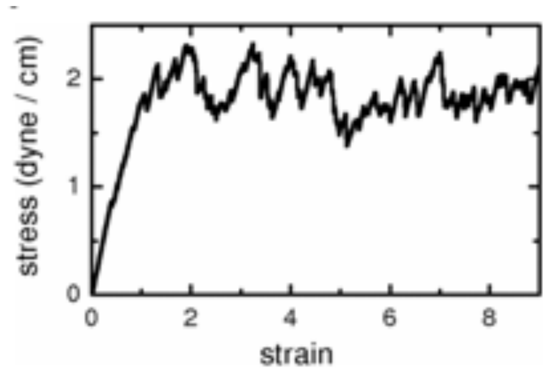
•Memory questions:
- What structurally encodes propensity for localization?
- Can it be erased?

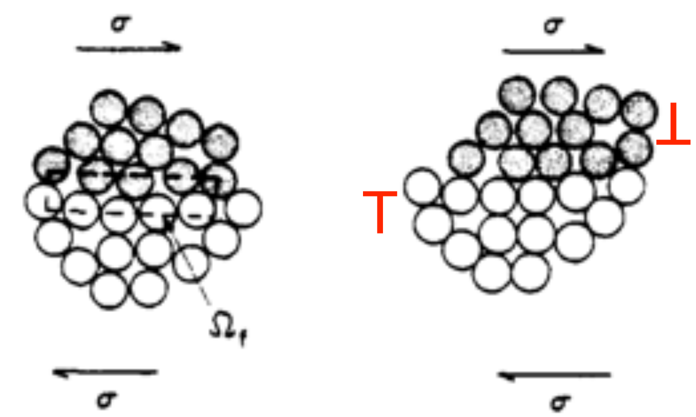
from Tony Rollet



Amorphous solids and shear transformation zones

- Examples:
  - Metallic glasses
  - Colloidal glasses
  - Emulsions/foams
  - Granular packings



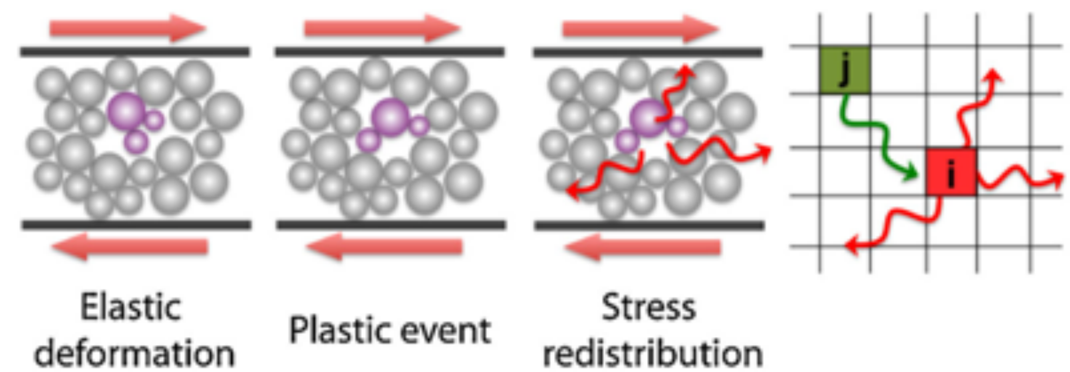


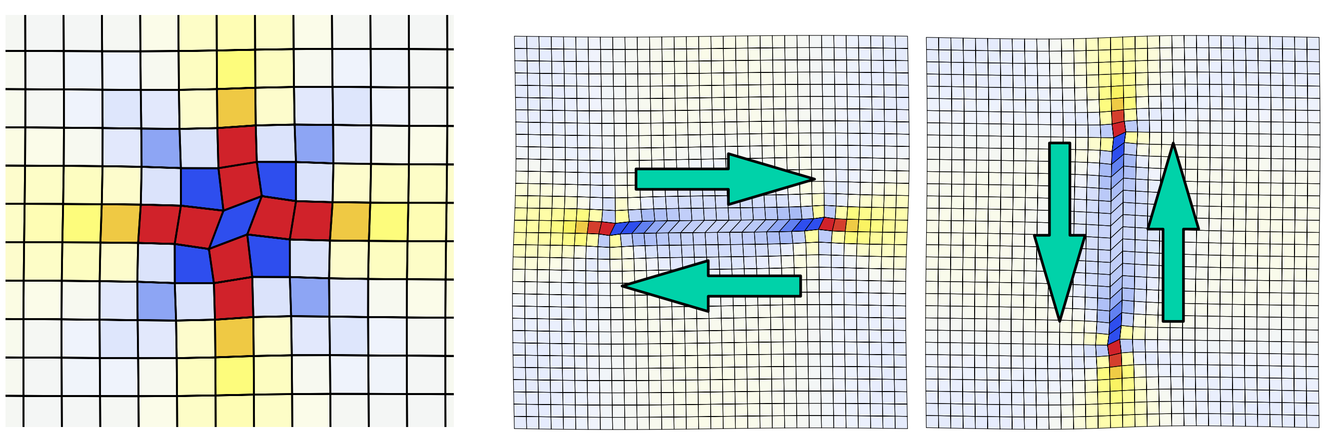
Strain order unity

Like creating a dislocation loop (dipole)

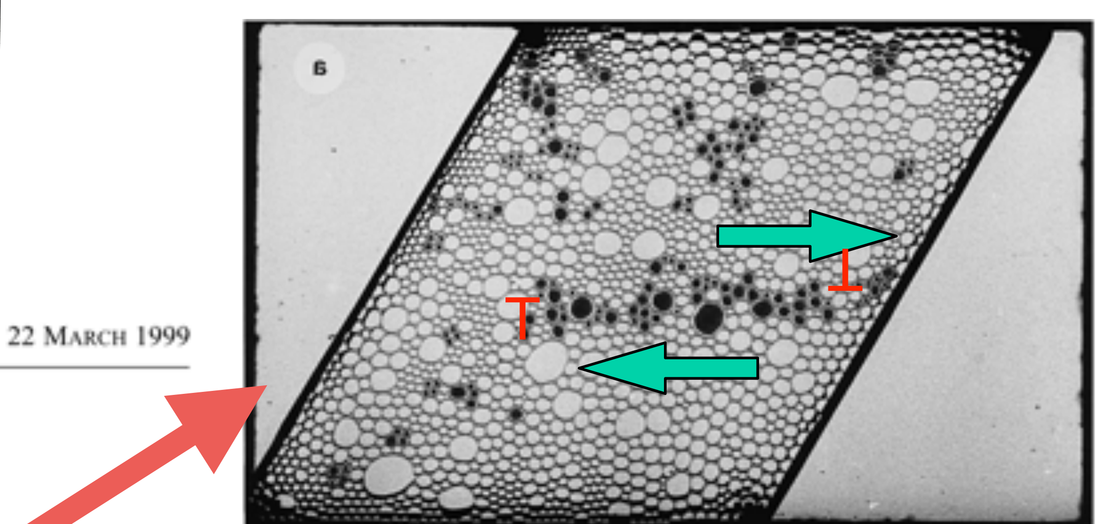
- no crystal ==> no dislocations

- Elastic stress transfer after local yield
- (Transient) localization in avalanches





- Colin, Bocquet, Ajdari, Barrat, Picard, Martens, Nicolas, et. al.



VOLUME 82, NUMBER 12 PHYSICAL REVIEW LETTERS 22 MARCH 1999

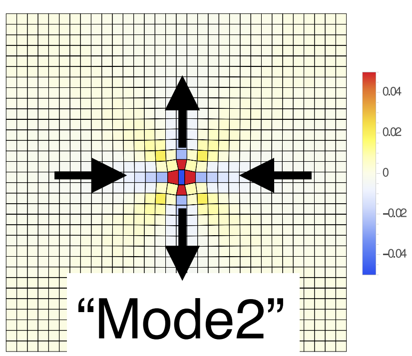
Shear-Induced Changes in Two-Dimensional Foam

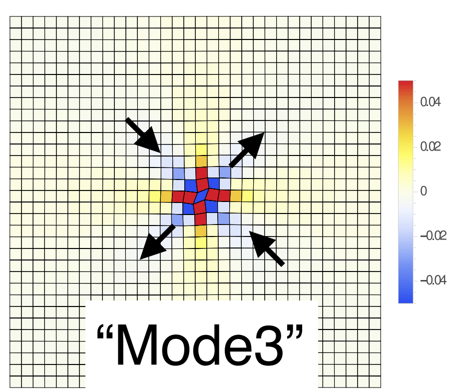
A. Abd el Kader and J. C. Earnshaw
Irish Centre for Colloid Science and Biomaterials, The Department of Pure and Applied Physics, The Queen's University of Belfast, Belfast BT7 1NN, United Kingdom
(Received 5 August 1998)

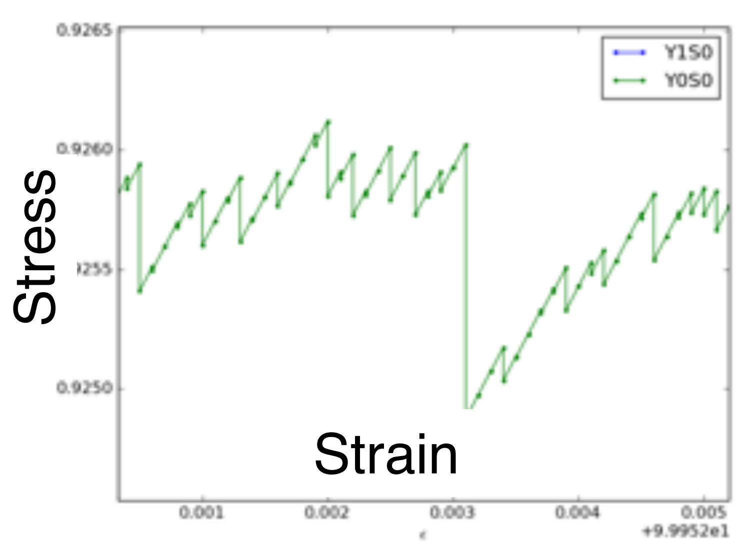
- Abd el Kader and Earnshaw

Coarse-grained model

- Tile space into squares
- For each square, J, assign energy ϕ_J:
  - $\Phi_J=(K/2)\varepsilon_{1J}^2+(G/2)(\varepsilon_{2J}-\varepsilon_{pJ})^2 + (G/2)\varepsilon_{3J}^2$
  - K: compression modulus
  - G: shear modulus
  - ε_{1J}: volumetric strain at site J
  - ε_{2J}: axial shear strain at site J
  - ε_{3J}: diagonal shear strain at site J
  - ε_{pJ}: plastic strain at site J







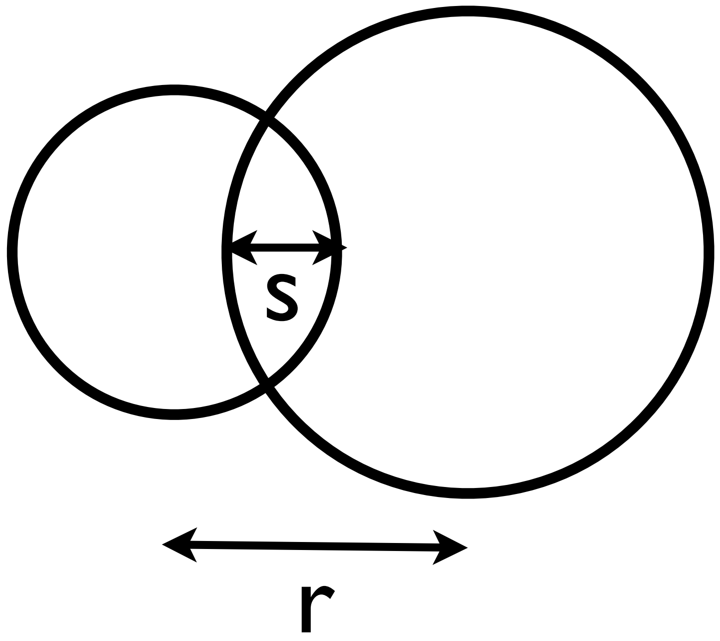
- Strains derived from displacements
- Compatibility is automatic
- Quadratic energy… all elasticity is linear
- Loading:
  - Increment global strain
  - Check for stability ($\sigma_J<\sigma_{yJ}$)
  - Recursively transform sites until stable
  - Repeat

- Two "flavors" for injecting disorder:
  - Stochastic plastic strain
  - Stochastic yield stress

- Two loading modes:
  - "Mode2" diagonal
  - "Mode3" axial:
  - $\Phi_J=(K/2)\varepsilon_{1J}^2+(G/2)\varepsilon_{2J}^2 + (G/2)(\varepsilon_{3J}-\varepsilon_{pJ})^2$

- How are we different than others?
  - Realistic near-field kernel
  - Quasi-static dynamics
  - Disorder prescribed explicitly

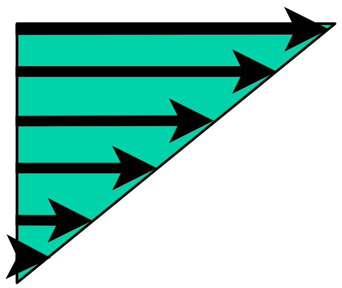
Bubble model (Durian): Two different drag models



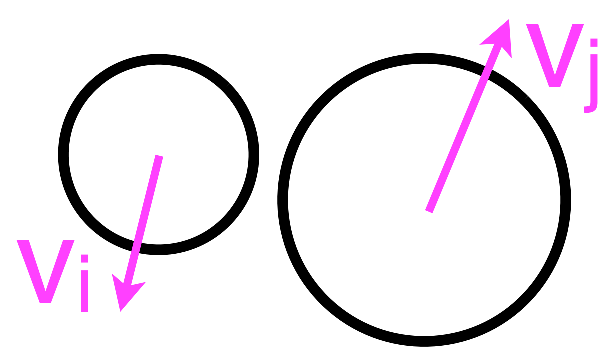
- 50:50 bidisperse
- R_{Small} = 1.4 R_{Big}

- Repulsion, F_{rep}, linear in overlap, s:
  - $F_{rep}=ks$
  - (could be arbitrary power of s)
- Drag, F_{drag}, w/r/t "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)

"Mean" drag: v_{flow} is affine

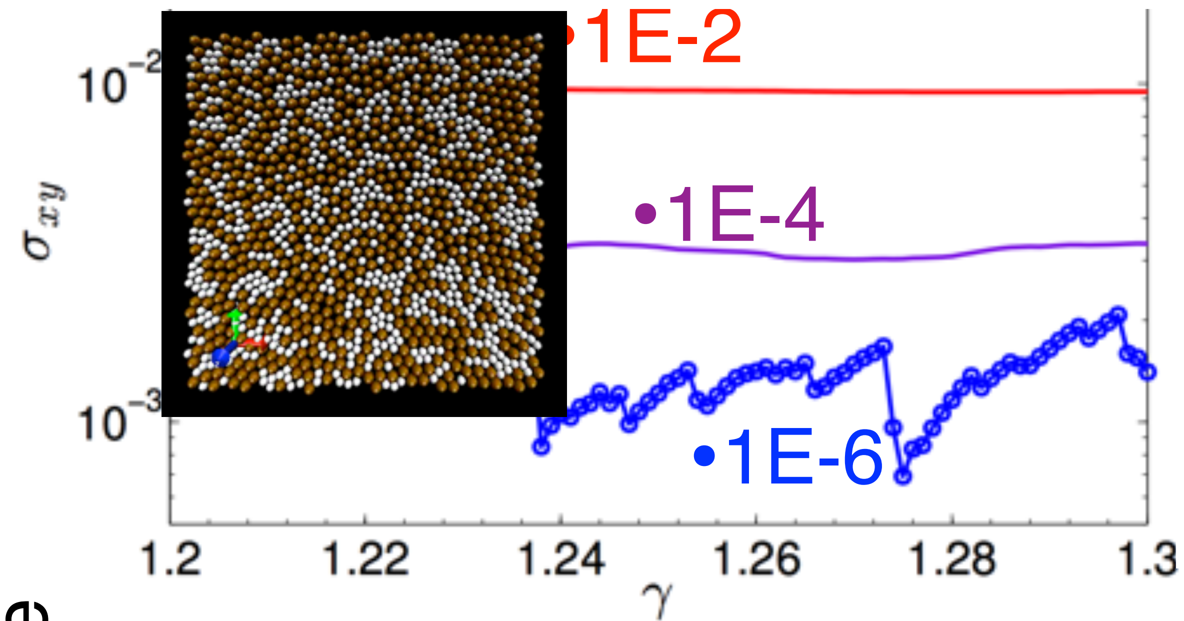


"Pair" drag: v_{flow} is local average



Diffusion and rheology (both: "Pair" and "Mean").

- Loading curves various rate

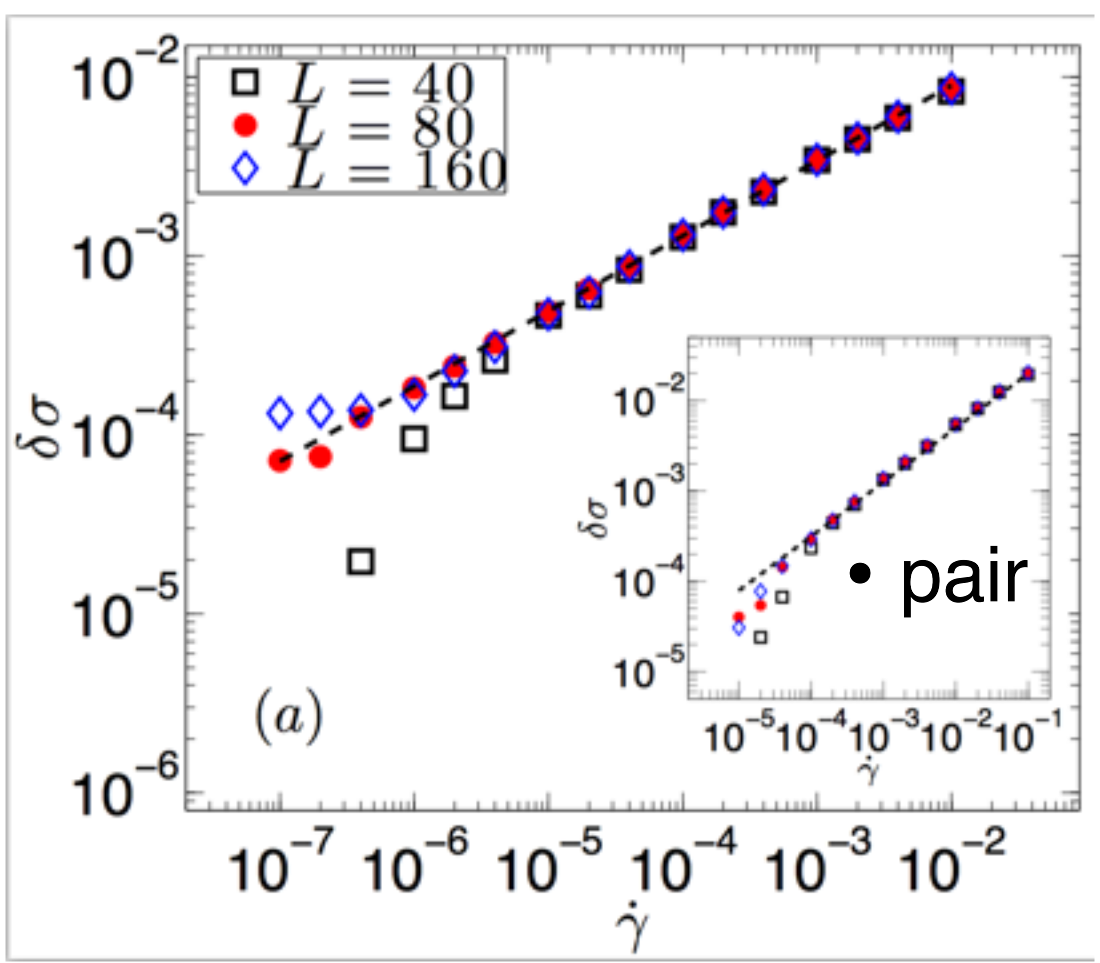


- Roy, Karimi and CEM (PRL Submitted)

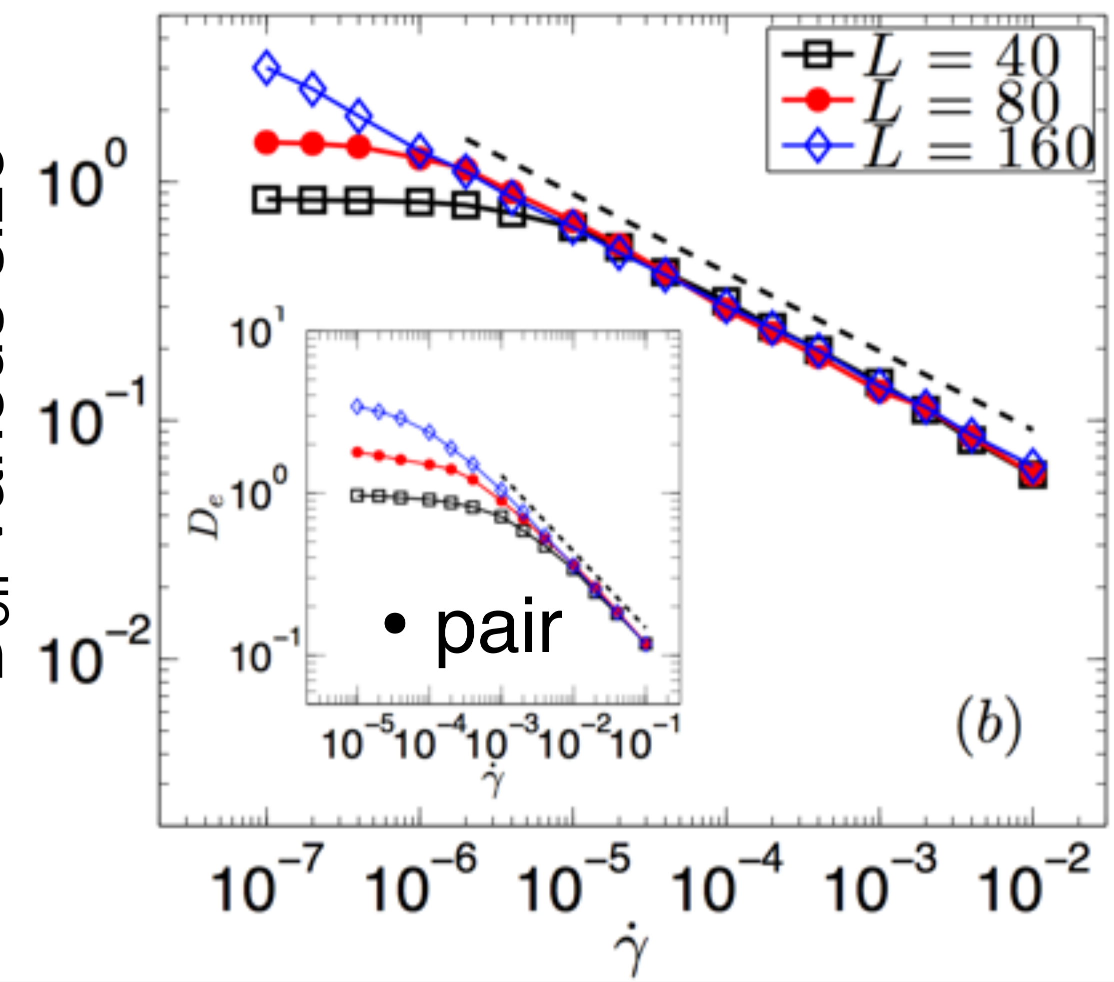
- "Effective diffusion" D_{eff}: mean squared displacement per unit strain

- mean: $\delta\sigma \sim (d\gamma/dt)^{0.33}$, $D_{eff} \sim (d\gamma/dt)^{-0.42}$.
- pair: $\delta\sigma \sim (d\gamma/dt)^{0.47}$, $D_{eff} \sim (d\gamma/dt)^{-0.60}$

- Flow curves at various size



- D_{eff} various size



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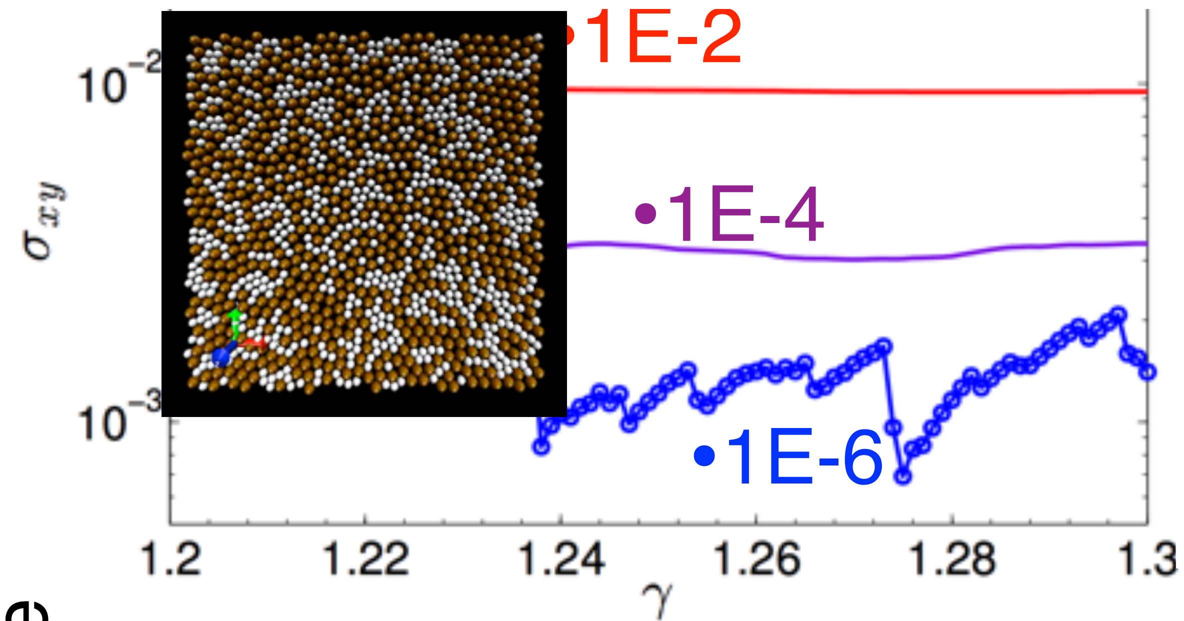

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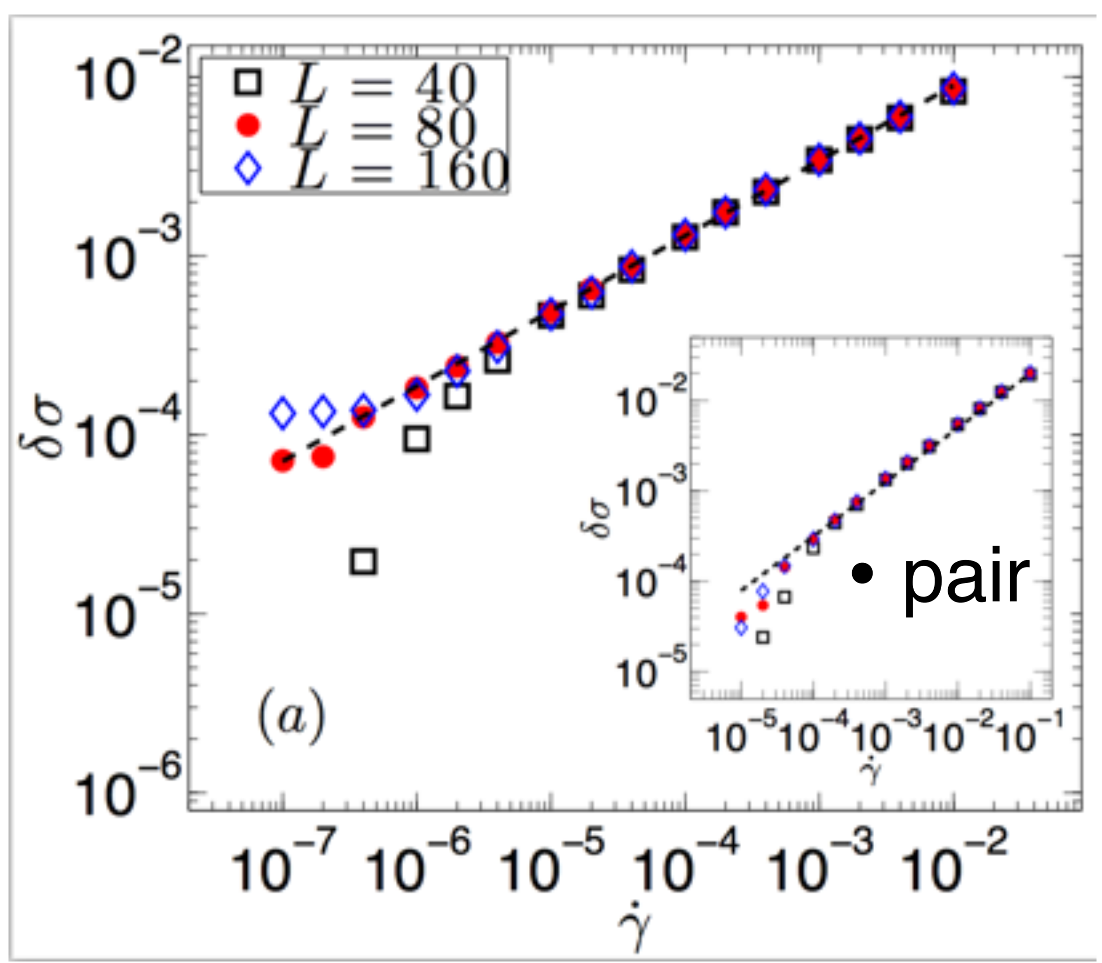
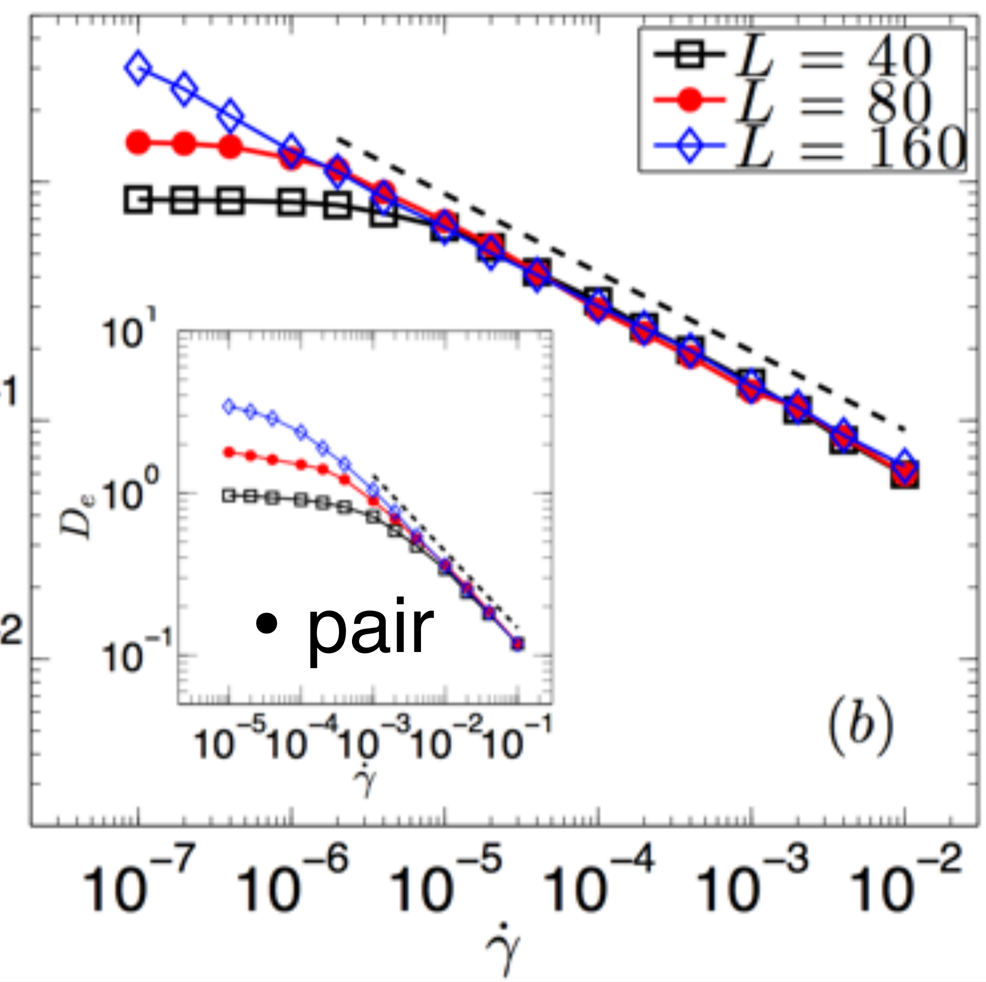
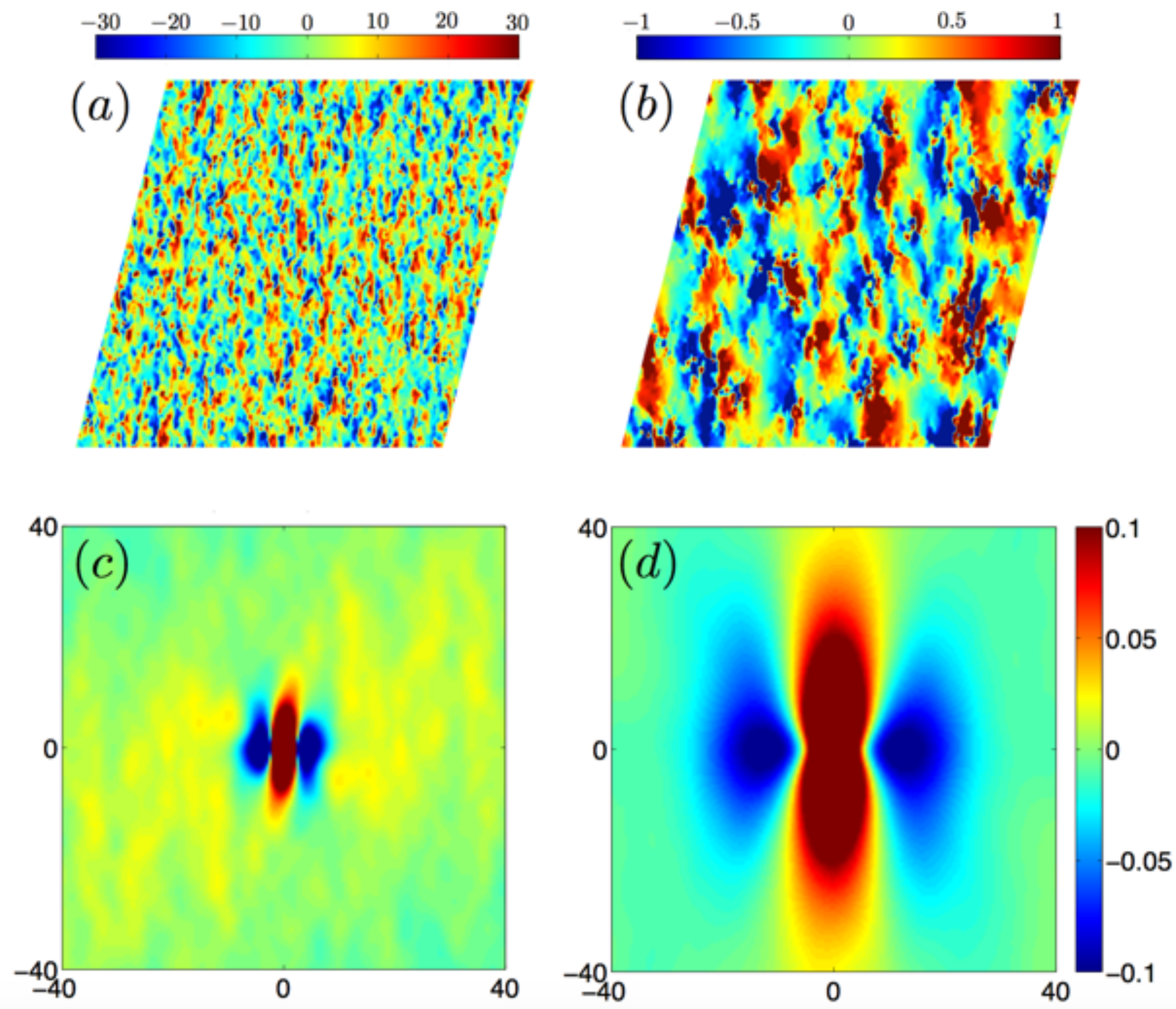


•D_{eff} various size



Velocity field, L=160

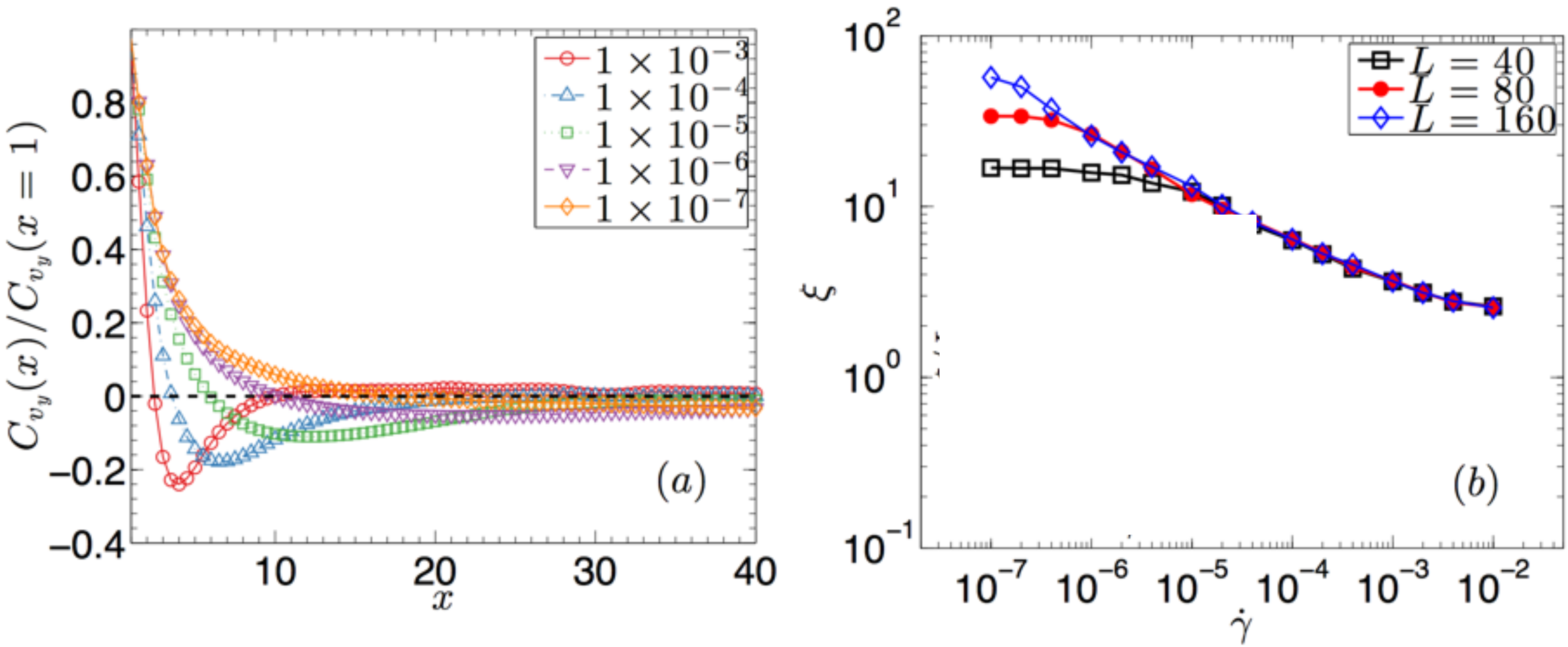
- Typical velocity (gradient direction)
- Velocity correlation



•Rate = 1E-2

•Rate = 1E-6

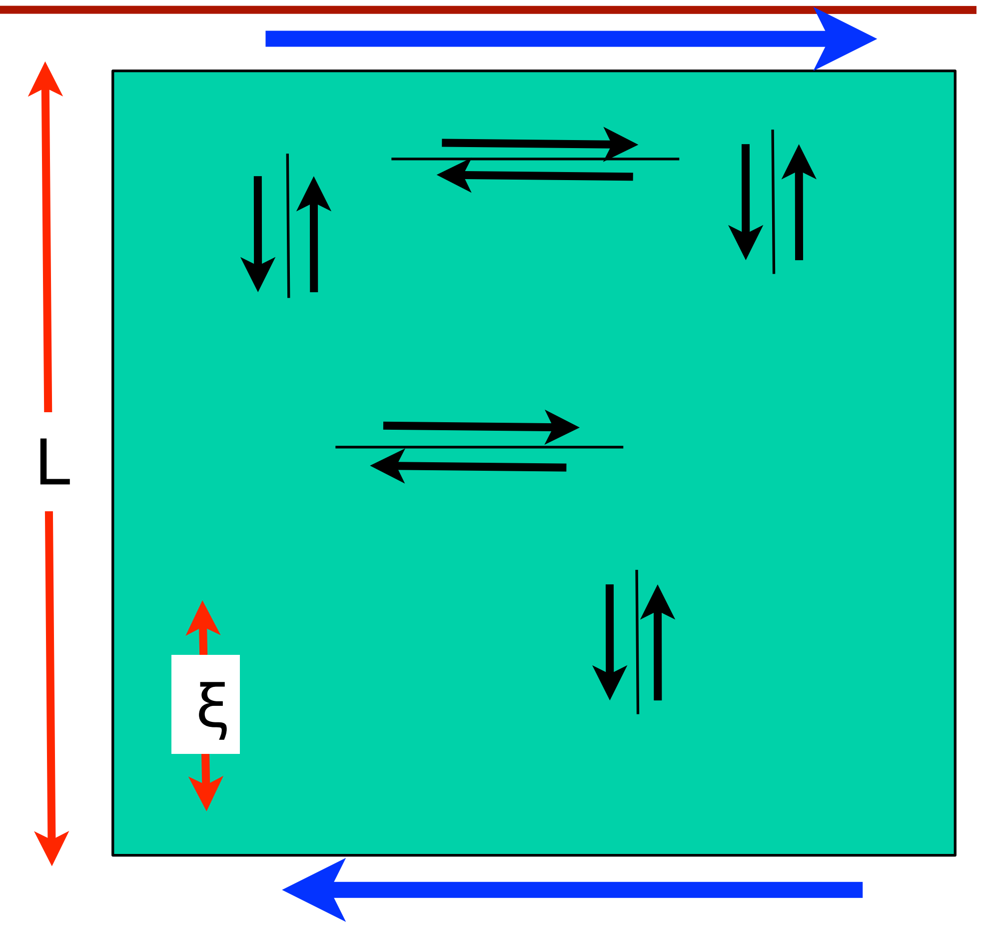
Length scale, ξ, from velocity field (“mean drag”)

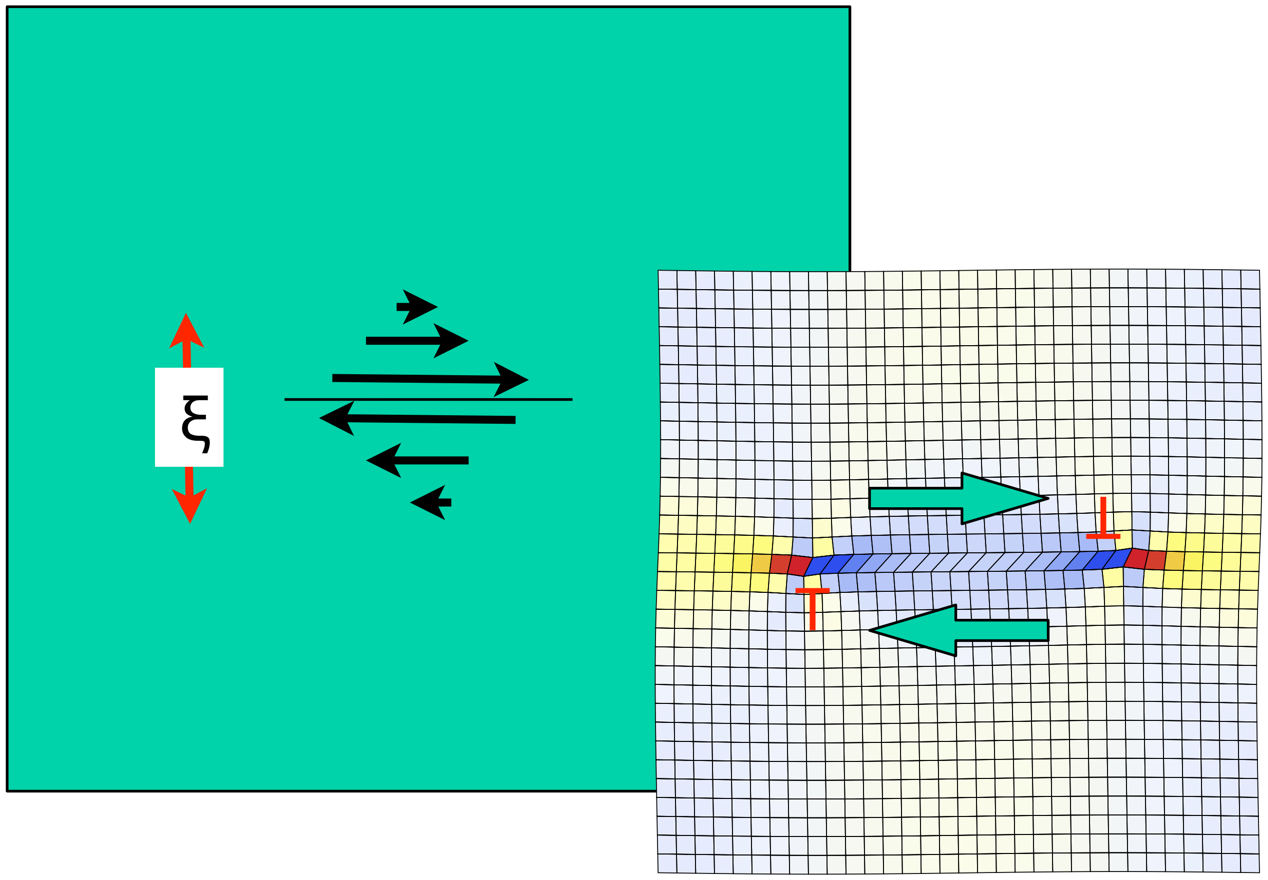


- Correlation length, $\xi \sim (d\gamma/dt)^{-0.42}$. (for mean drag)
- Same as the effective diffusion coefficient!
- Why?
- (For “pair drag” ξ and Deff **both** go like $(d\gamma/dt)^{-0.47}$)

Argument for ξ <—> D_{eff} relation

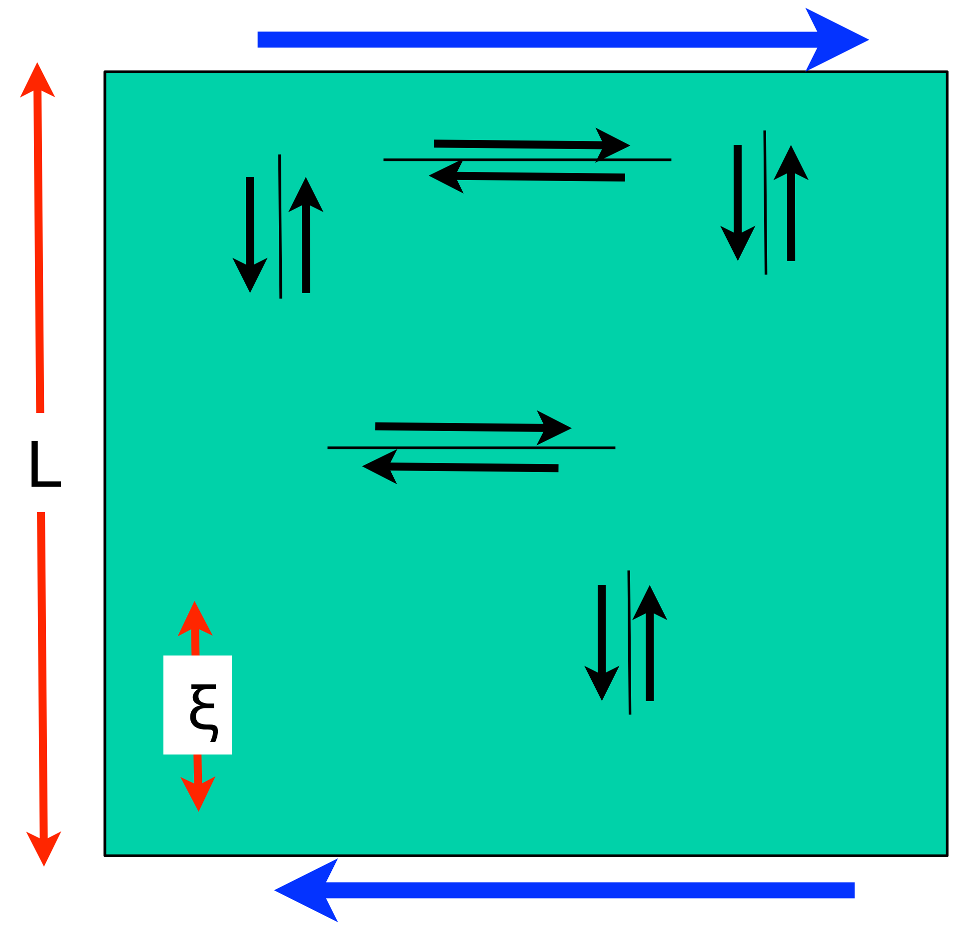
- Lemaitre and Caroli (PRL 2009):
- Assume: deformation from uncorrelated slip lines of length ξ (assume ξ<<L)
- Linear elasticity: $\langle \Delta \mathbf{r}^2 \rangle_{space} \approx \xi^2$. (in 2D)
- Strain (stress) relieved, $\Delta \gamma \approx \xi$ (essentially by construction in the "meso-scale models)
- "Effective diffusion" $\langle \Delta \mathbf{r}^2 \rangle / \Delta \gamma \approx \xi$





Connecting rheology and ξ (scaling theory)

- Lemaitre and Caroli PRL 2009 and Lin et. al. PNAS 2014.
  - $\delta\sigma \sim (d\gamma/dt)\ \tau_{avalanche}$ …
  - $\tau_{avalanche} \sim \xi^z$. (borrowed from depinning)
  - $\xi \sim \delta\sigma^{-v}$. $v=1/(d-d_{fractal})$
  - so $d\gamma/dt \sim \delta\sigma^{1+vz}$. or $\delta\sigma \sim (d\gamma/dt)^{1/(1+vz)}$.
- Lemaitre and Caroli assumed $z \approx 1$, $v \approx 1$.
- This gives HB exponent of 1/2.
- Our data give:
  - v=0.33/0.42=0.79 for "mean drag" (z~2.5)
  - v=0.47/0.60=0.78 for "pair drag" (z~1.25)
- Different values for z:
  (stronger rate dependence for pair drag)
- but same value for v… fractal dimension of shear localization patterns is the same!

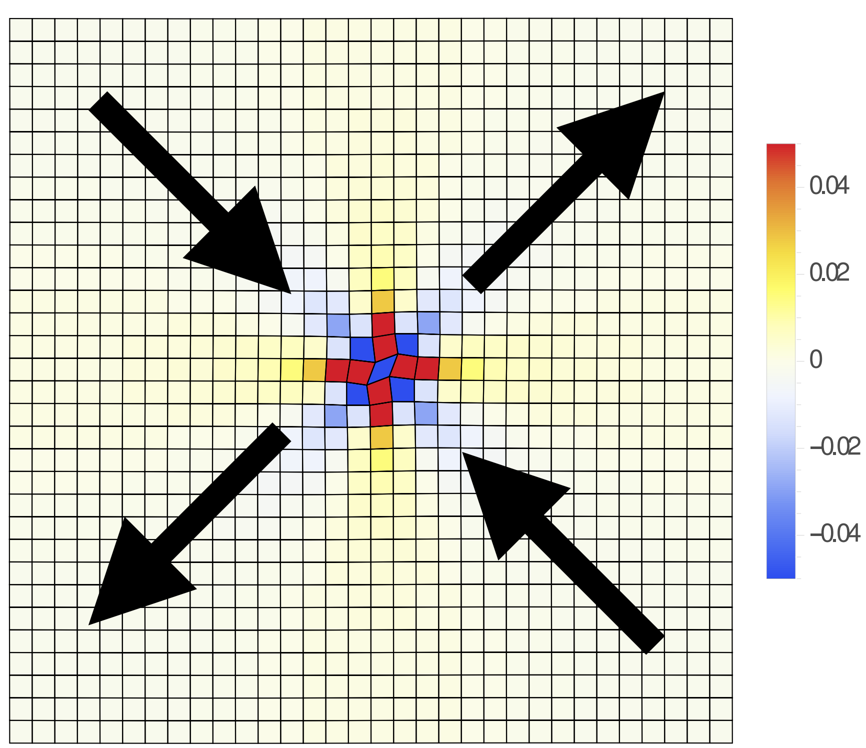


- Roy, Karimi, CEM; PRL Submitted (2016) substantial revision to be submitted.

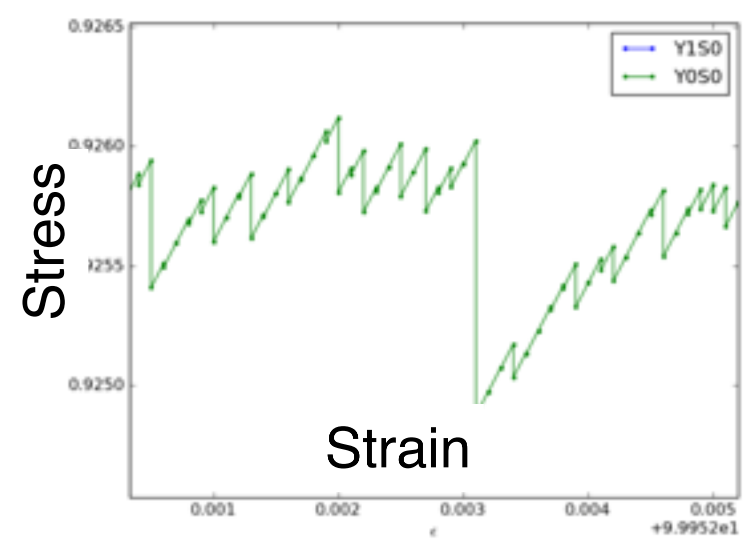
Now throw out the particles!

Meso-scale lattice model (quasi-static version)

- Tile space into squares
- For each square, J, assign energy ϕ_J:
  - $\Phi_J=(K/2)\varepsilon_{1J}^2+(G/2)(\varepsilon_{2J}-\varepsilon_{pJ})^2 + (G/2)\varepsilon_{3J}^2$
  - K: compression modulus
  - G: shear modulus
  - ε_{1J}: volumetric strain at site J
  - ε_{2J}: axial shear strain at site J
  - ε_{3J}: diagonal shear strain at site J
  - ε_{pJ}: plastic strain at site J



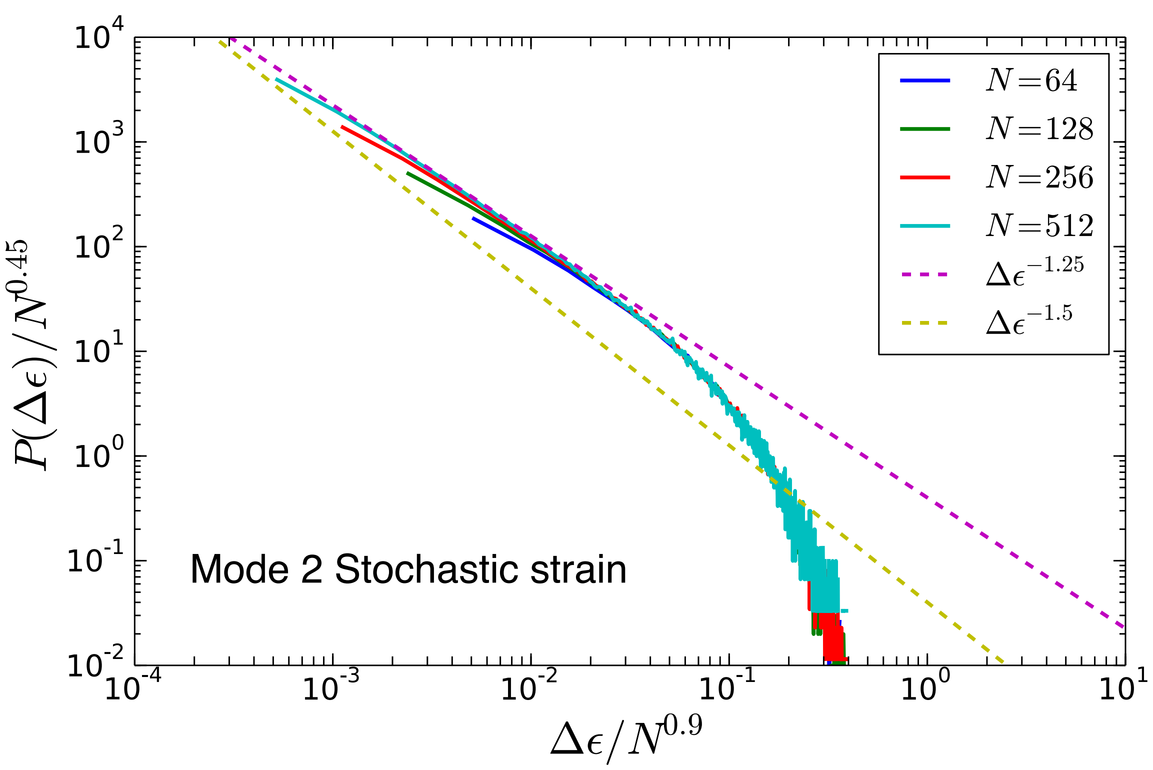
- Strains derived from displacements
- Compatibility is automatic
- Quadratic energy… all elasticity is linear
- Loading:
  - Increment global strain
  - Check for stability ($\sigma_J<\sigma_{yJ}$)
  - Recursively transform sites until stable
  - Repeat

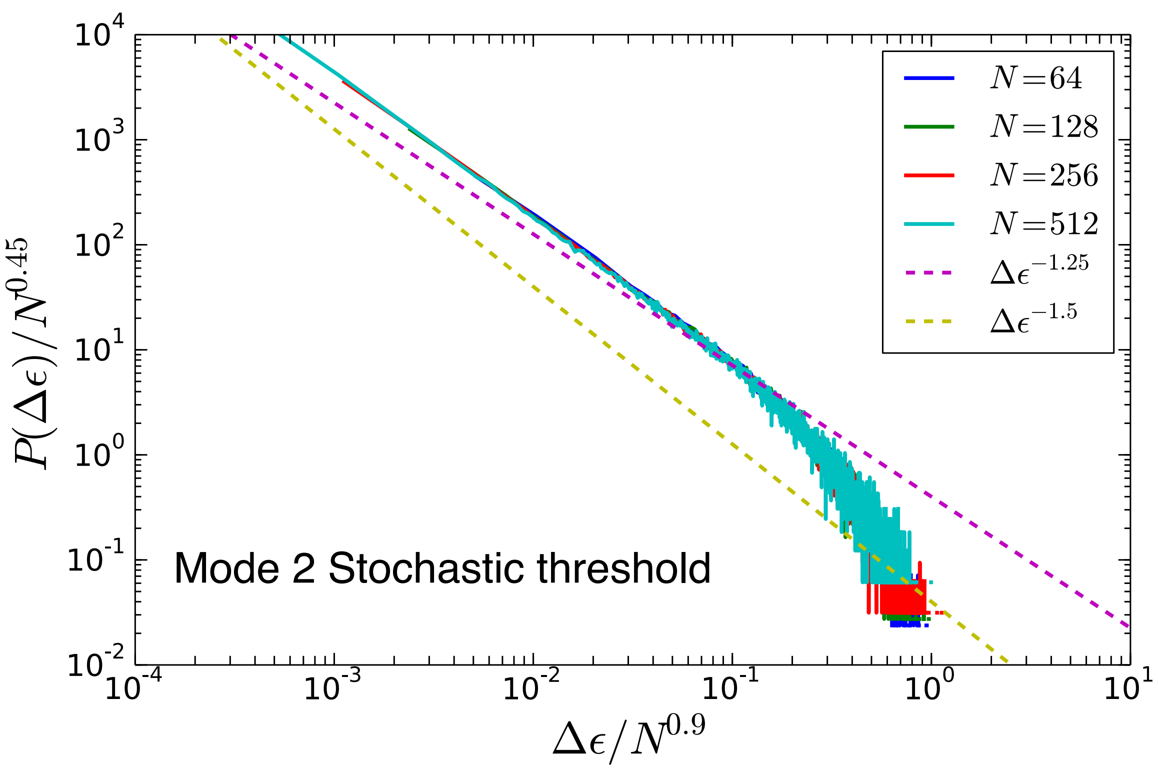


- Flavors:
  - Loading in “mode2” (shown in left) or in “mode1” (45 degrees away)
  - Either random local thresholds or random plastic strain increments
  - “Extremal” protocol or “Synchronous” protocol

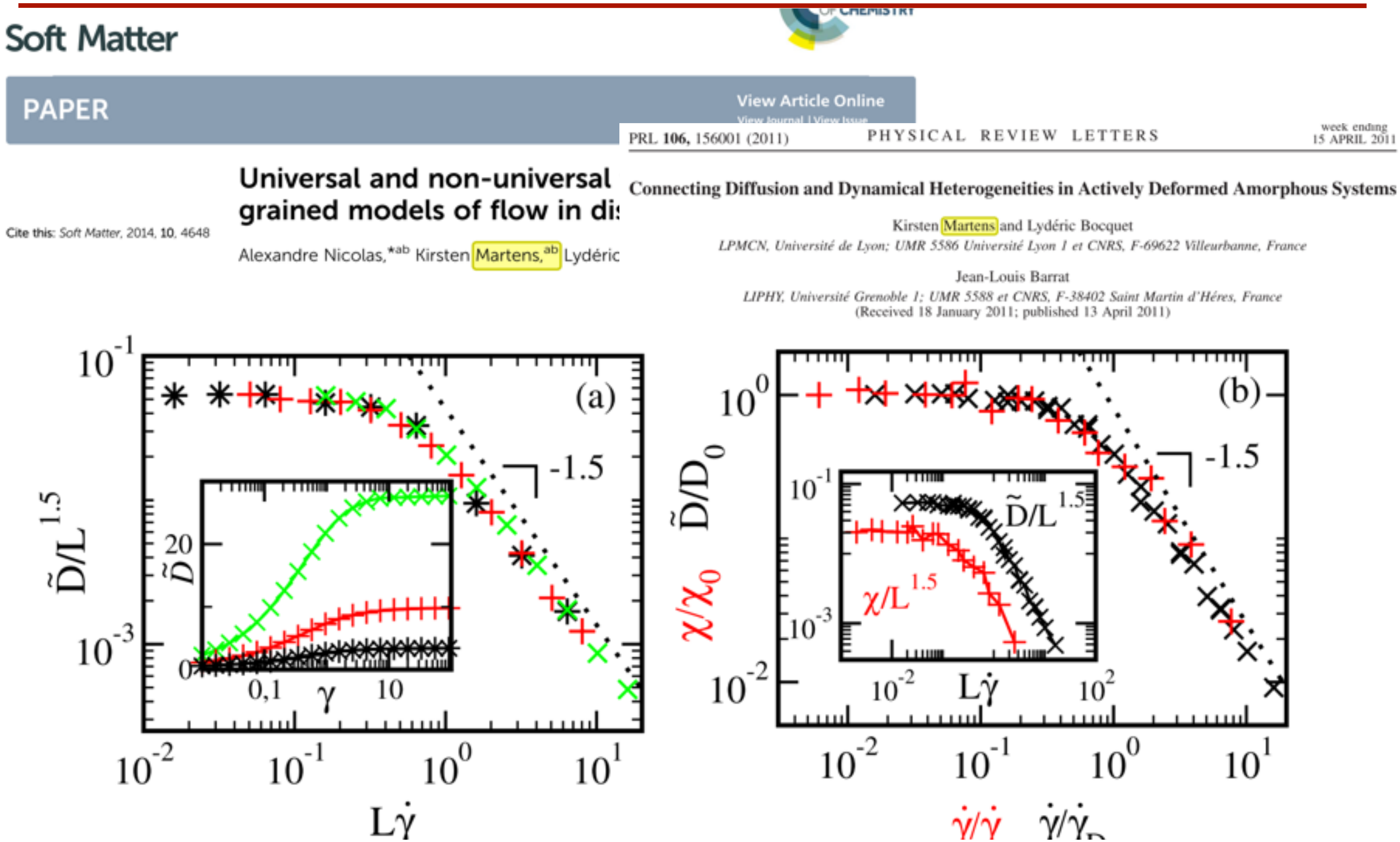
Avalanches strain burst (stress drop) size Δε

- Scaling: $R(\Delta\varepsilon,L)=L^{\beta}g(\Delta\varepsilon/L^{\alpha})$, g~(argument)$^{\tau}$
- MD simulations (Salerno, Maloney, and Robbins PRL 2012)
  - τ=1.25, α=0.9, β=0.2 (for **overdamped**)
- Present results:
  - α=0.9 convincing for all 4 models. Largest strain burst ~ $L^{0.9}$
  - τ=1.25 works well for 3 of the models.
  - β=0.45 related to overall normalization
- Other groups:
  - NYU Group (Lin, Lerner, Rosso, Wyart) PNAS 2014
    - 2D: τ=1.36, α=1.10



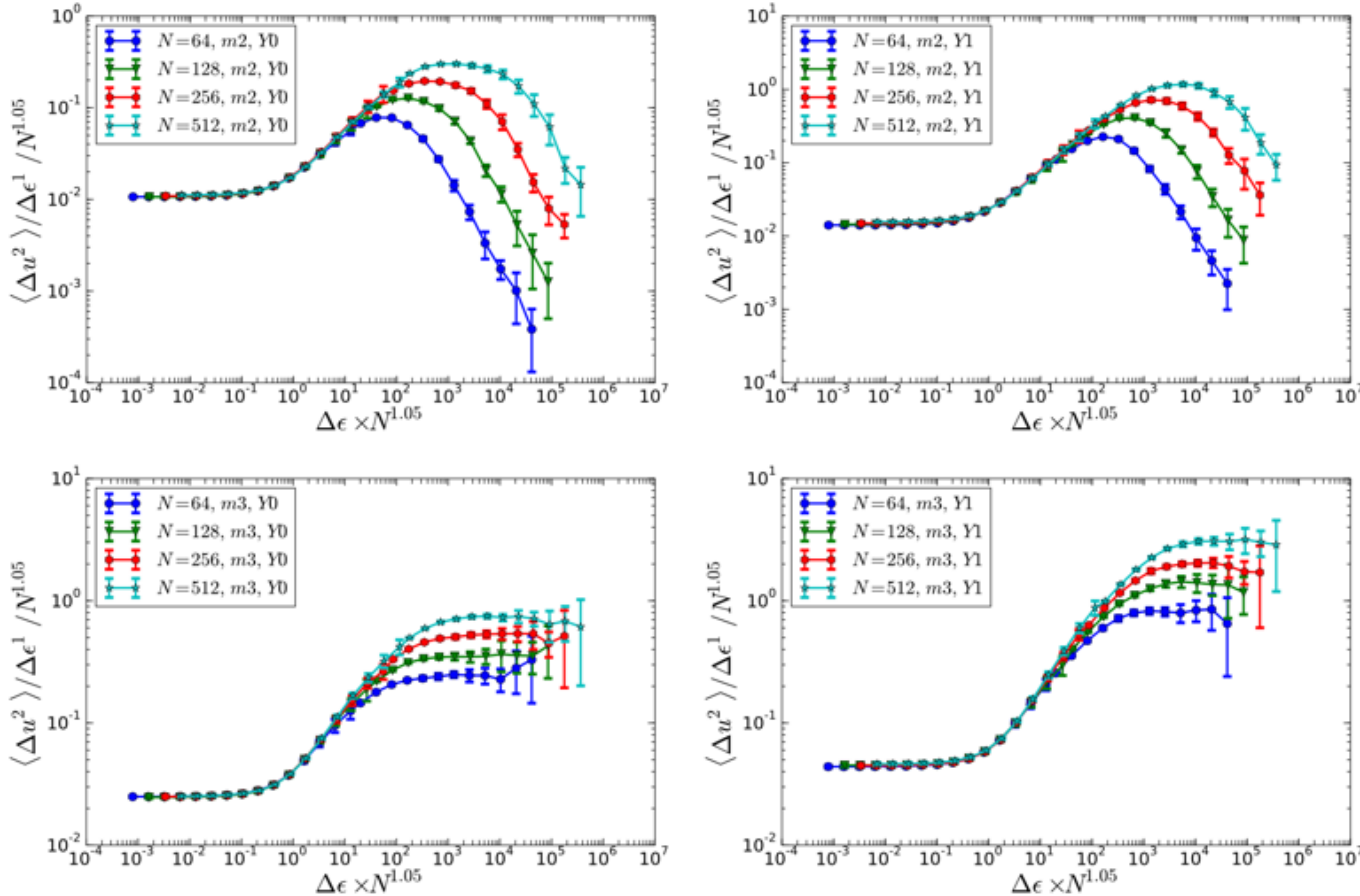


Problem!



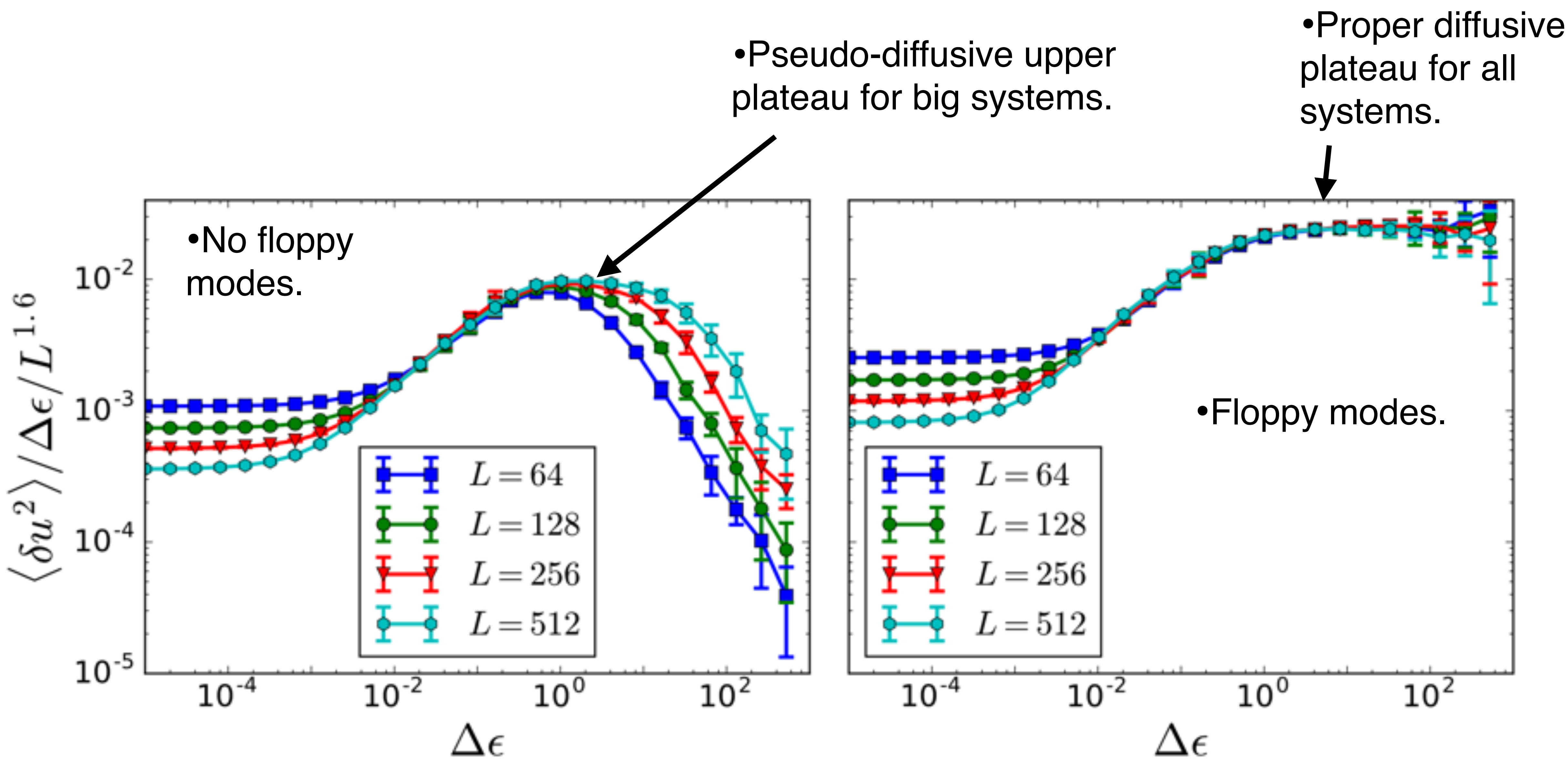
- Big problem!
- Particle simulations (PEM/MD/DEM) show $D \sim L^1$
- Elasto-plastic models show $D \sim L^{1.5}$

Diffusion: two regimes!



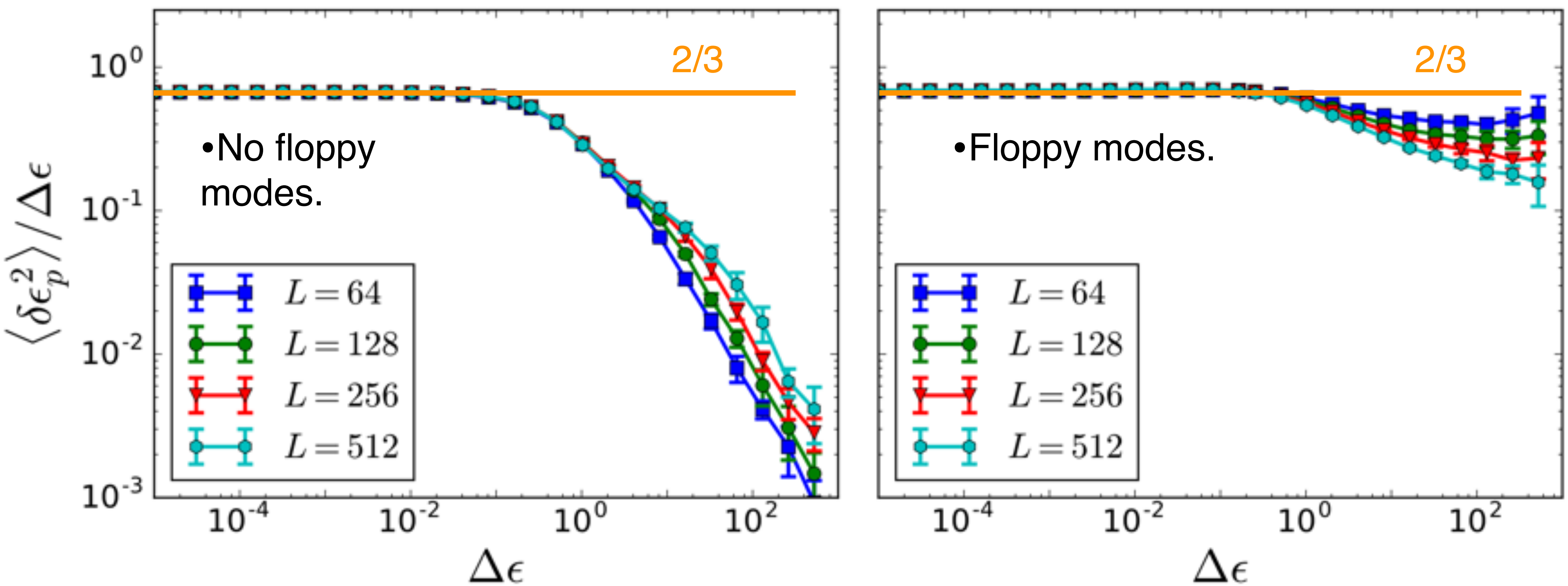
- See $\Delta\gamma$ independent D_e below $\Delta\gamma^* \sim 1/L^{1.05}$. with size dependence, $D_{e0} \sim L^{1.05}$.
- Consistent with particle simulations!
- Above $\Delta\gamma \sim 1$, see $D_e \sim L^{1.5}$ as in Martens et. al.

Diffusion: long time



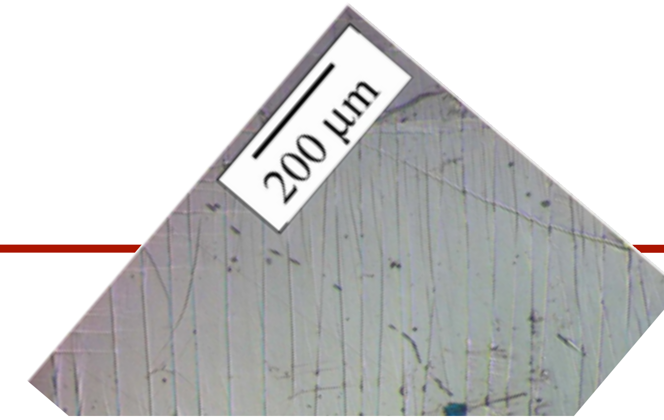
- Bottom line:
  - Long time regime: $L^{1.6}$ with $\Delta\varepsilon_{cross\text{-}over} \sim L^0$. similar to what was seen previously ($L^{1.5}$), but inconsistent with Durian model.
  - Short time: new regime with $D \sim L^{1.05}$. $\Delta\varepsilon_{cross\text{-}over} \sim L^{-1.05}$.

Diffusion of plastic strain field



- Variance of plastic strain field:
  - Independent of L
  - Naive argument at early time: $<\varepsilon_p^2>/\Delta\varepsilon$ =2/3 independent of floppy modes. Great!
  - At long time if there are floppy modes, then $<\varepsilon_p^2>/\Delta\varepsilon$~const, otherwise, $<\varepsilon_p^2>$~const.

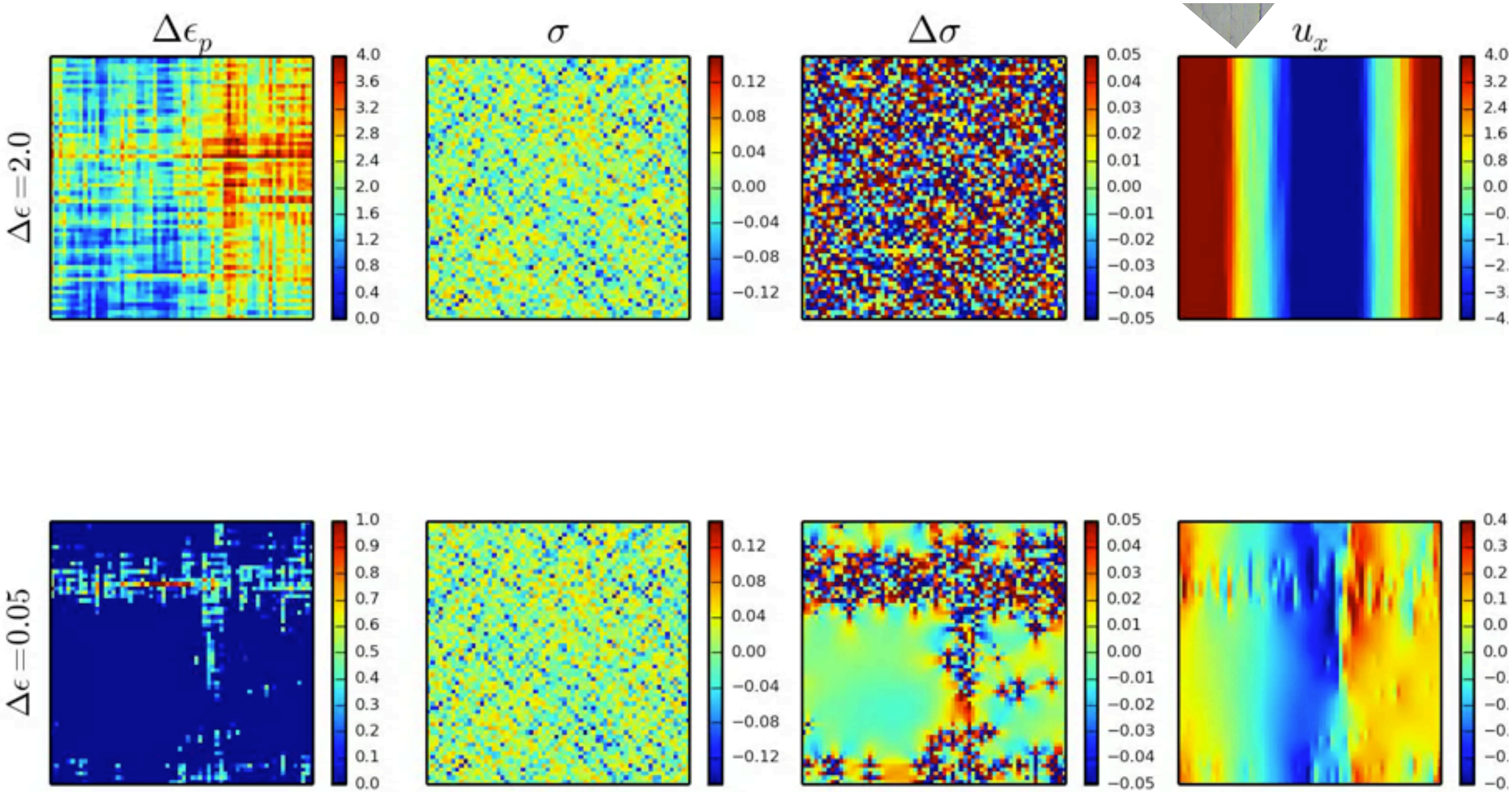
Diffusion and long-time correlations



- Model flavor:
  Mode 3 loading
  Uniform yield thresholds
  Random plastic strain increment

$\epsilon = 20.0$

- Connection with persistent localization?



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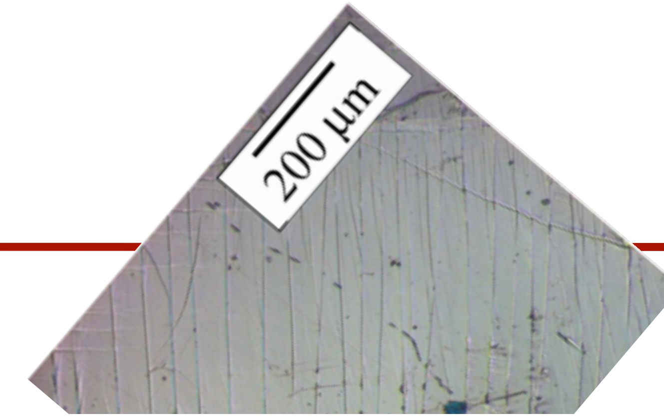

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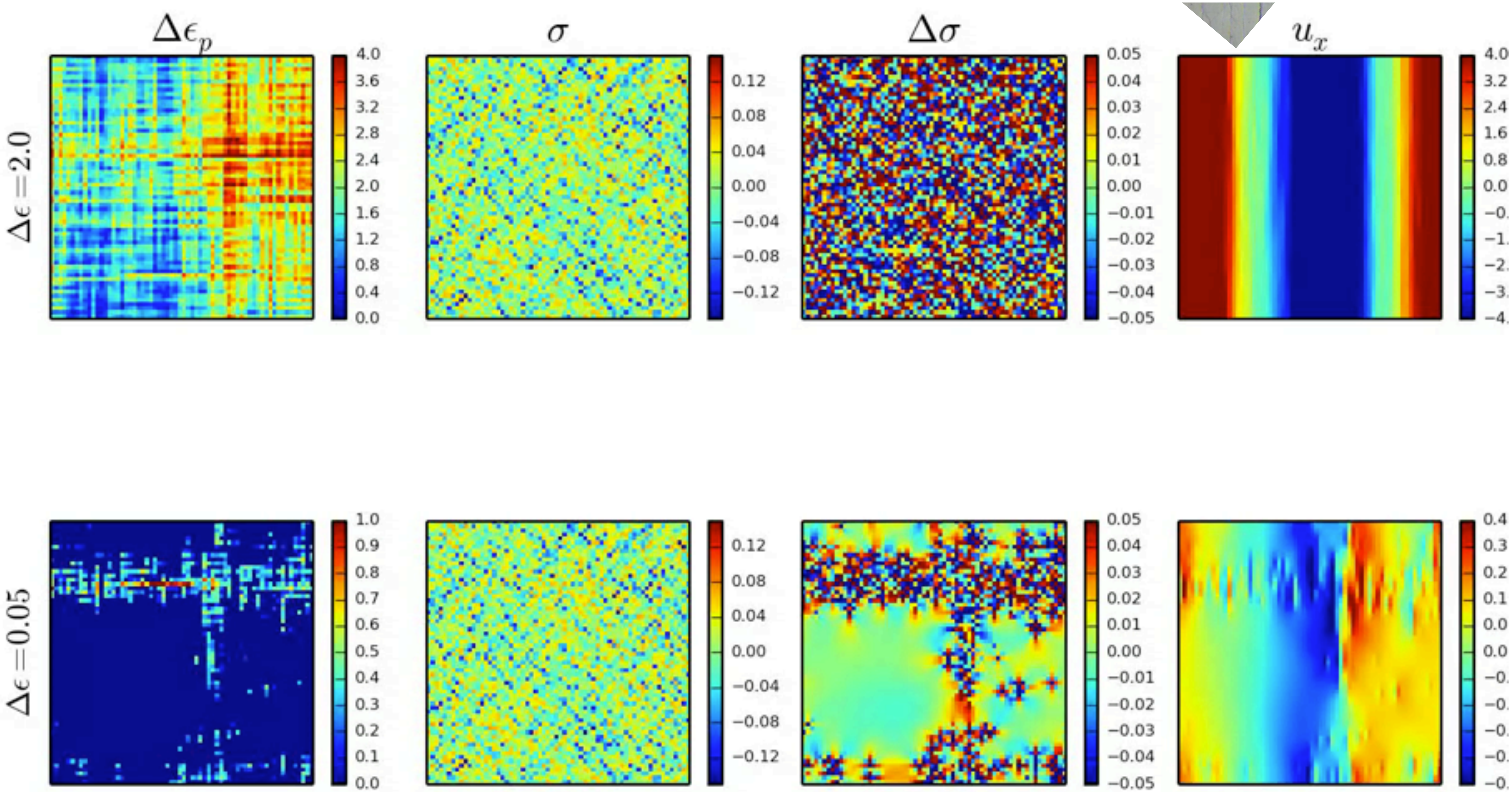
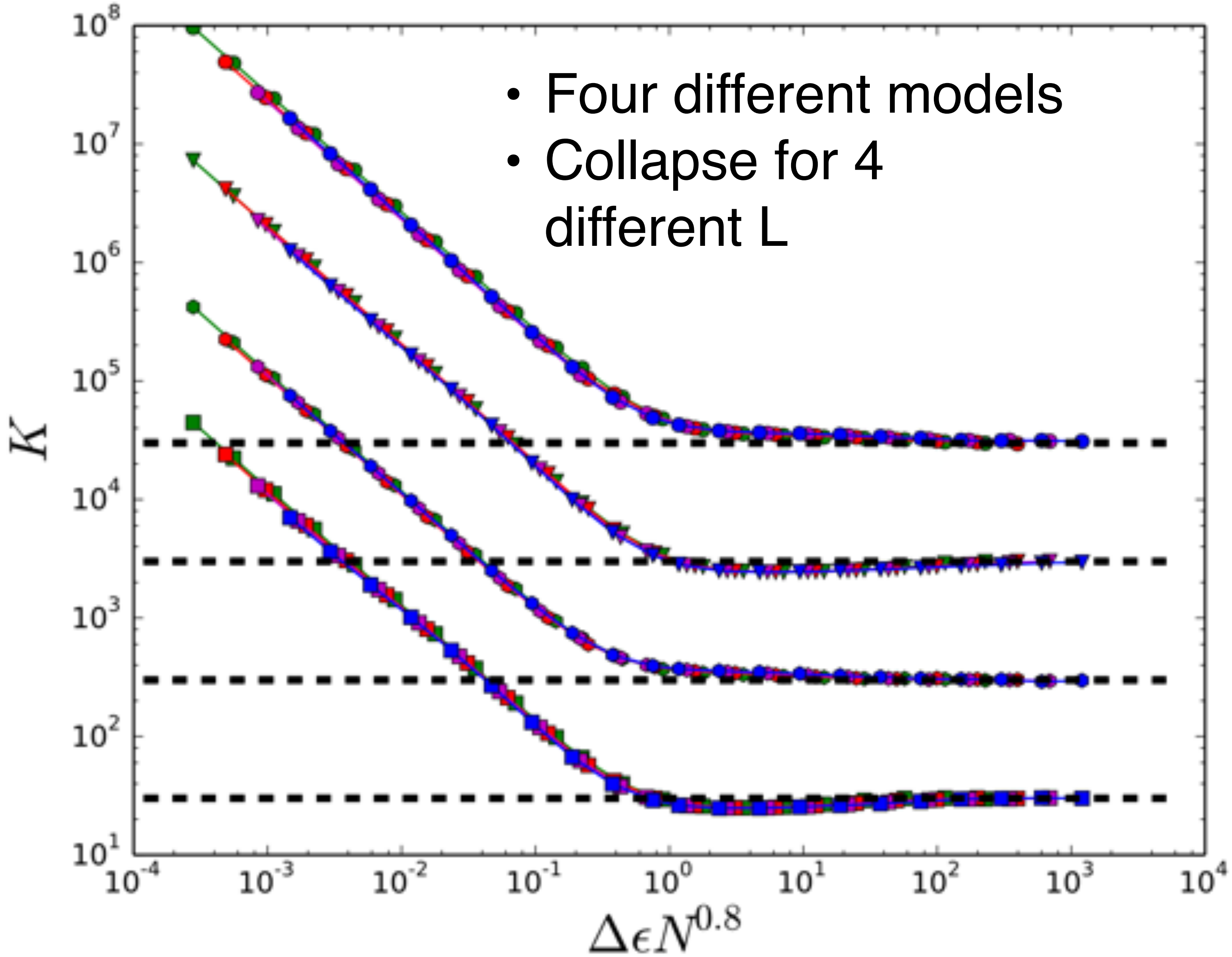
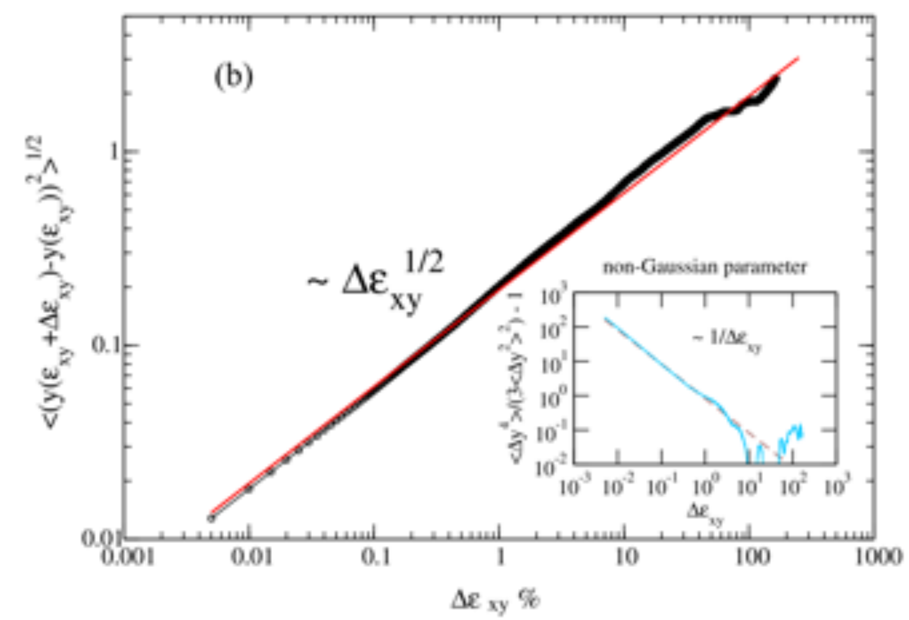


Displacement kurtosis



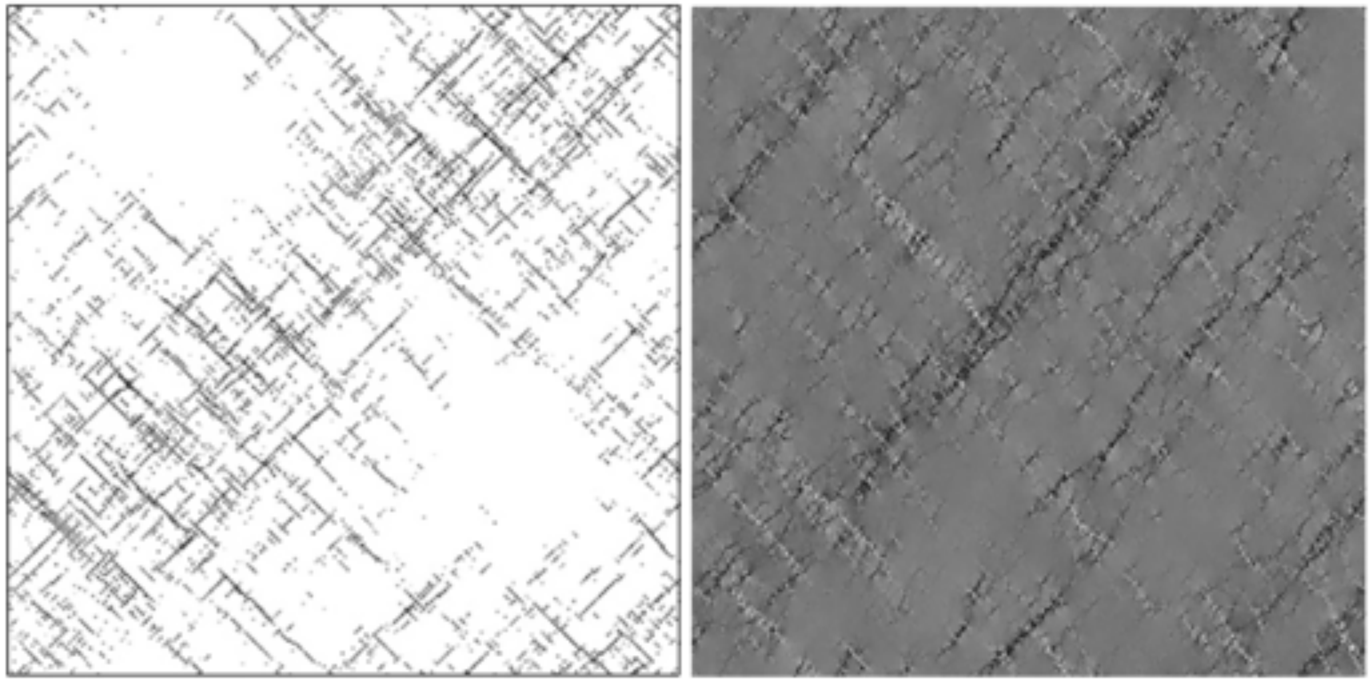
- Four different models
- Collapse for 4 different L

- Kurtosis goes like $\Delta\gamma^{-1}$.
  - (Tanguy, Leonforte, Barrat EPJE 2006)
  - CEM EPL 2015



- Explanation for 1/Δε behavior: shot noise generically gives 1/Δε for any moment ratio.
- But characteristic strain for Gaussian behavior, $\Delta\varepsilon_{kurtosis} \sim L^{-0.8}$. Close to, but not exactly equal to characteristic Δγ from avalanches and particle diffusion.

Conclusions: quasi-static particle -> mesoscale



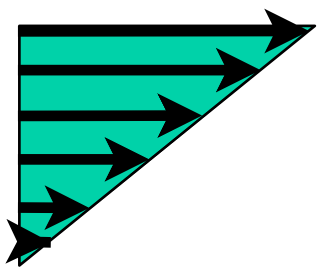
- Universality for avalanche statistics.
- Non-universal behavior for long-time diffusion.
- Depends on local details of interaction kernel.

- Avalanches roughly consistent with particle-simulations:
  $R(X,L)=L^{\beta}g(X/L^{\alpha})$, $g\sim x^{\tau}$
  - $\tau=1.25$, $\alpha=0.9$ (agrees with MD, non MF)
- Below $\Delta\gamma\sim L^{-1.05}$, $D_{e0}\sim L^{1.05}$.
- Beyond $\Delta\gamma\sim 1$, $De\sim L^{1.5}$ (like Martens et. al.)
- Depending on precise near-field form of "eshelby field", beyond $\Delta\gamma$
  - No diffusion without soft modes
  - Diffusion with soft modes.

Working at finite rate is a real drag

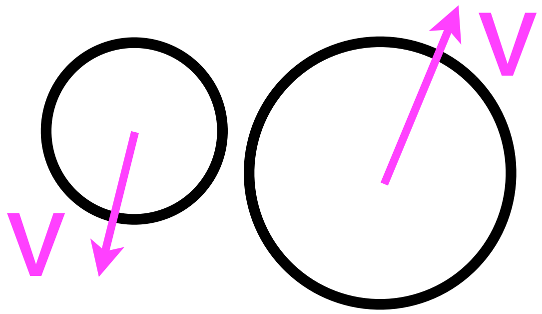
- For both models: $F_{\text{elastic}} = \nabla \cdot \sigma$

"Mean" drag:

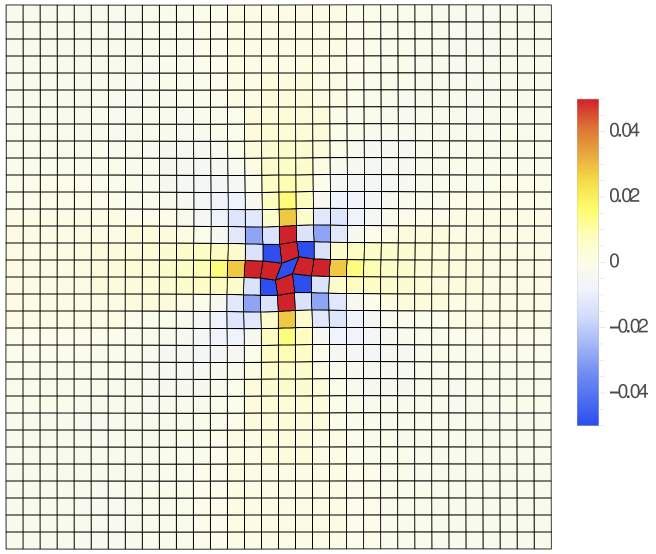


$$F_{\text{visc-mean}} = -bv$$

"Pair" drag: v_{flow} is local



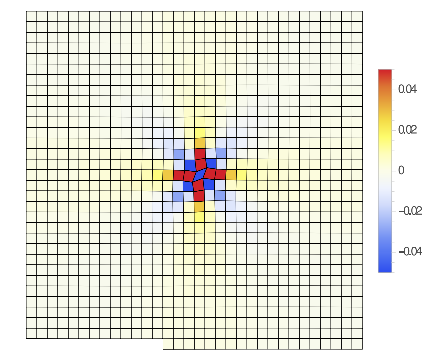
$$F_{\text{visc-pair}} = \eta \nabla^2 v$$

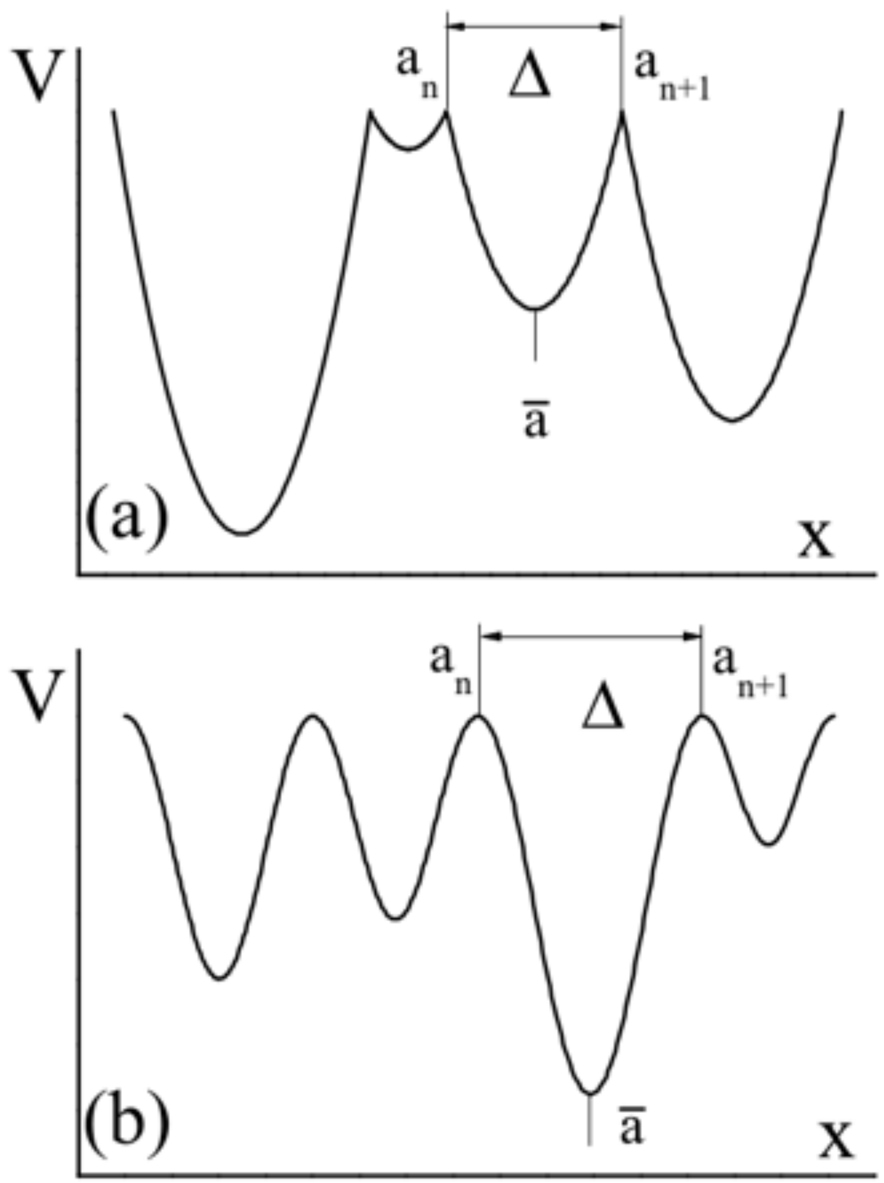


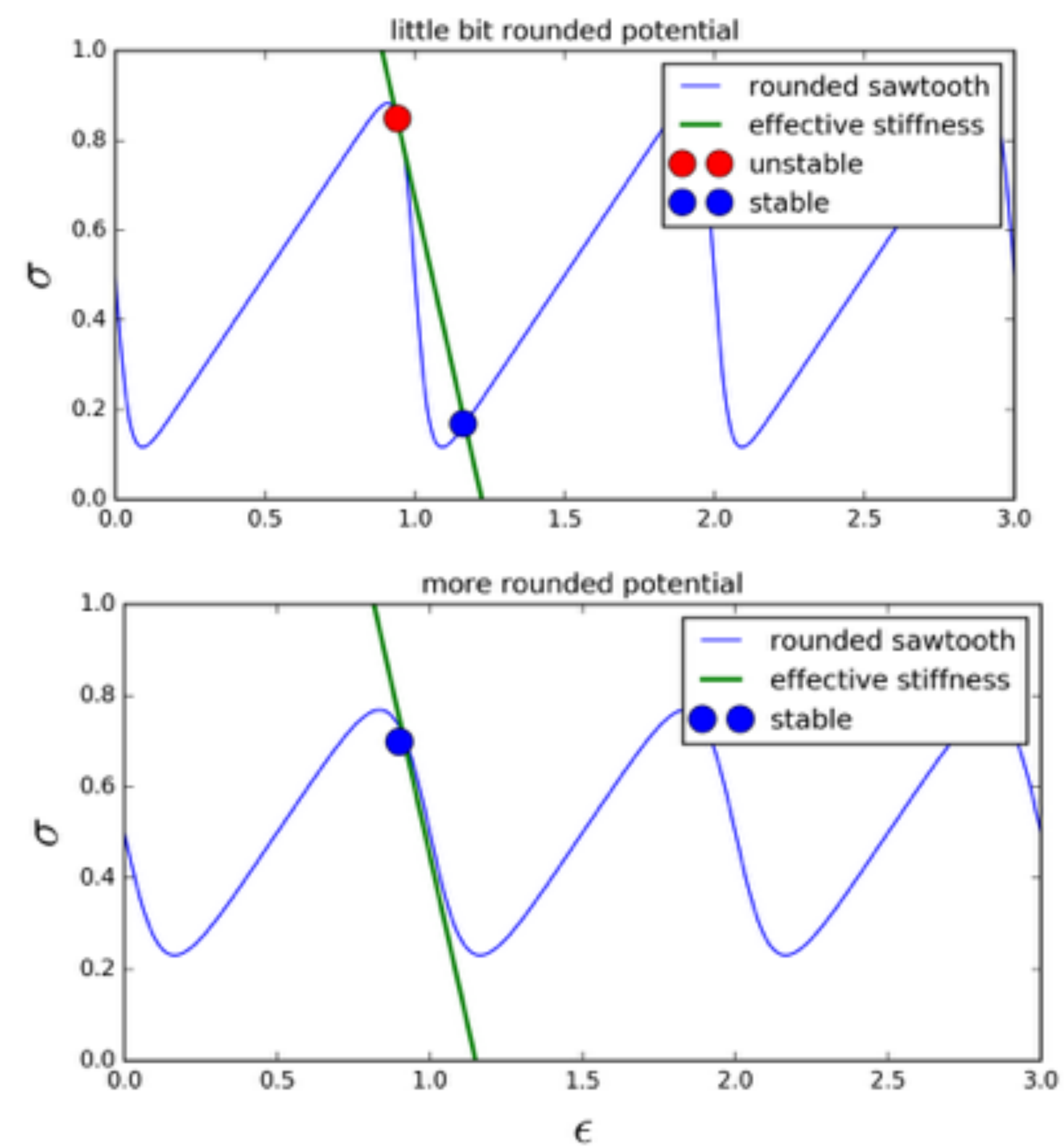
- What others do:
  - Maintain equilibrium of elastic forces at all time with ad-hoc dynamics for local plastic strain
  - Implementing a "physical drag" is crucial to get agreement with particle simulations

Finite rate: what we do

- For each square, J, assign energy ϕ_J: $\Phi_J=(K/2)\varepsilon_{1J}^2+V(\varepsilon_{2J})+(G/2)\varepsilon_{3J}^2$
- Local strain energy function can be piecewise quadratic or smooth.
- Piecewise quadratic gives pathological behavior
- Smooth gives agreement with particle simulations!







- From E. Jagla

Flow curves and diffusion

- For each square, J, assign energy ϕ_J: $\Phi_J=(K/2)\varepsilon_{1J}^2+V(\varepsilon_2 J)+(G/2)\varepsilon_{3J}^2$
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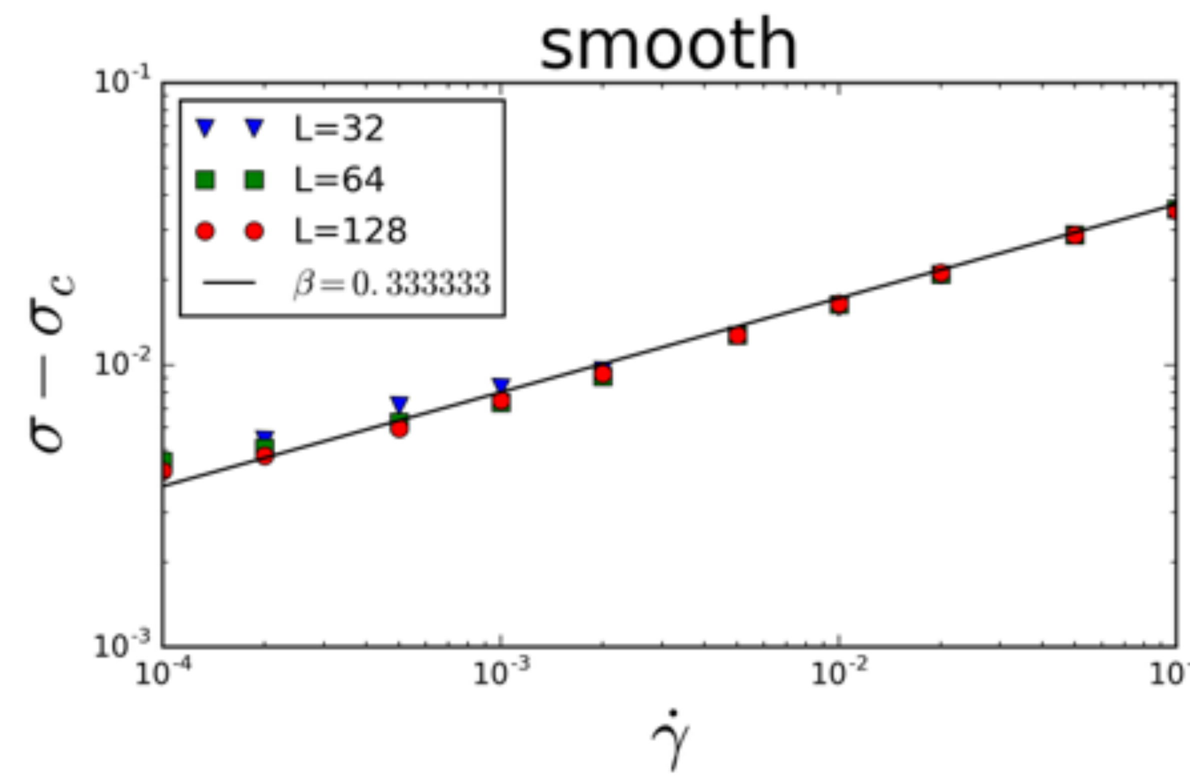
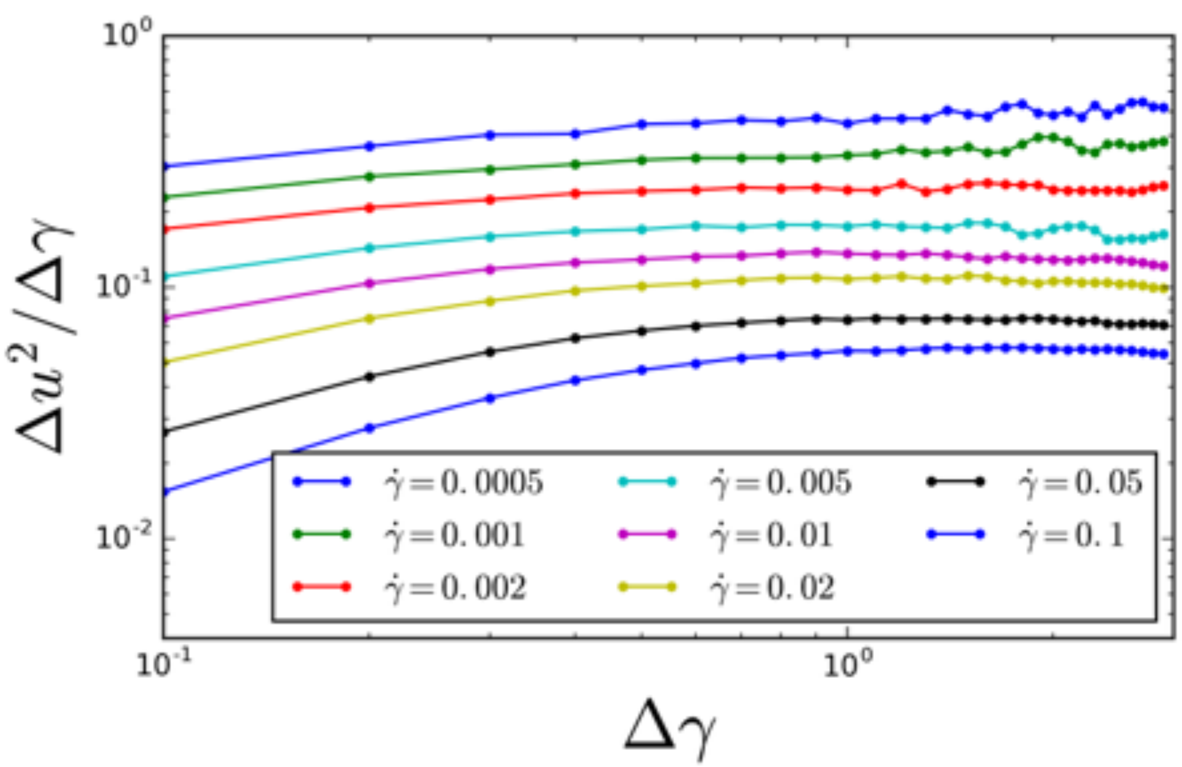
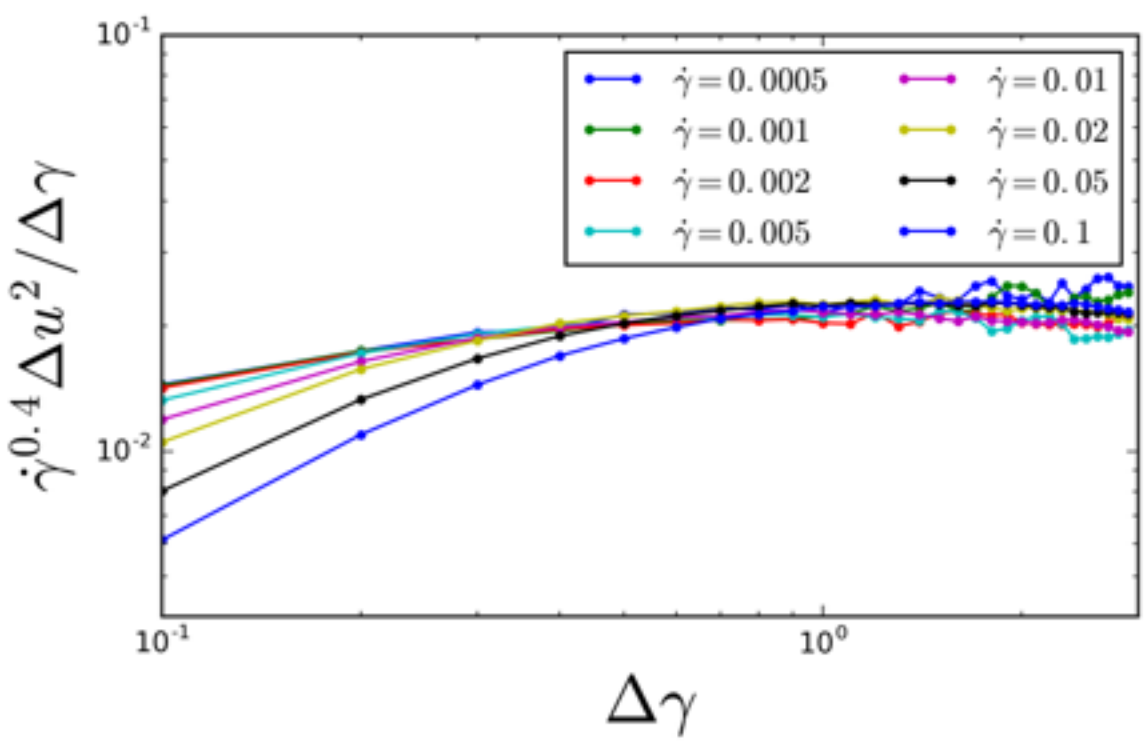
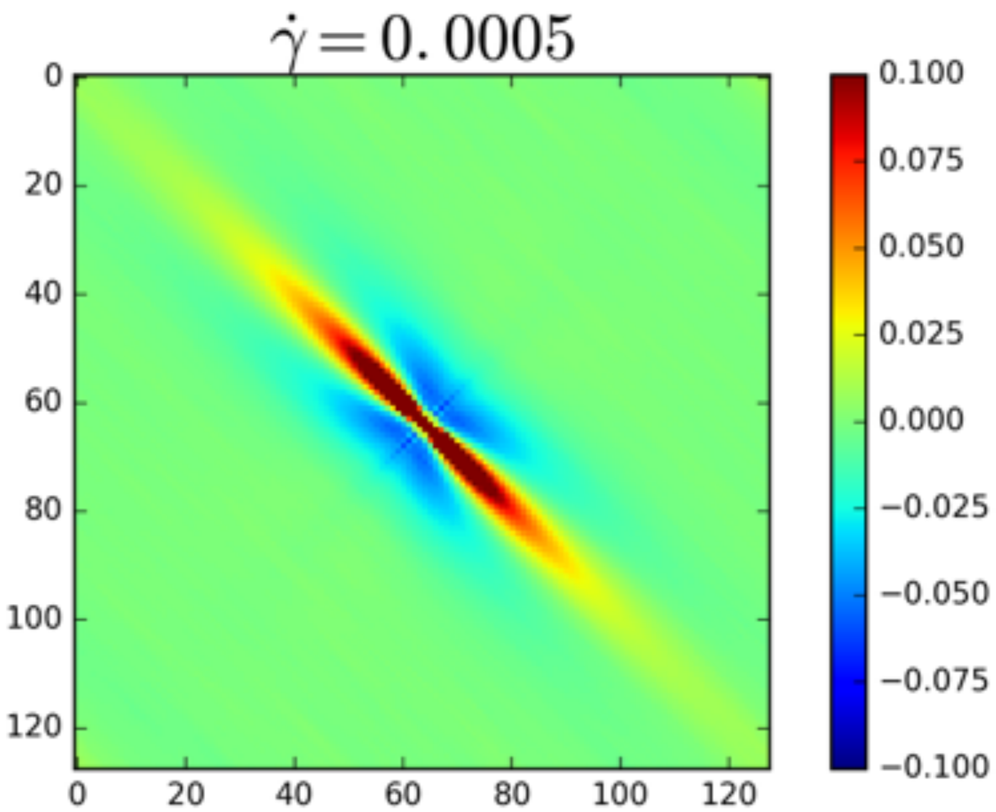




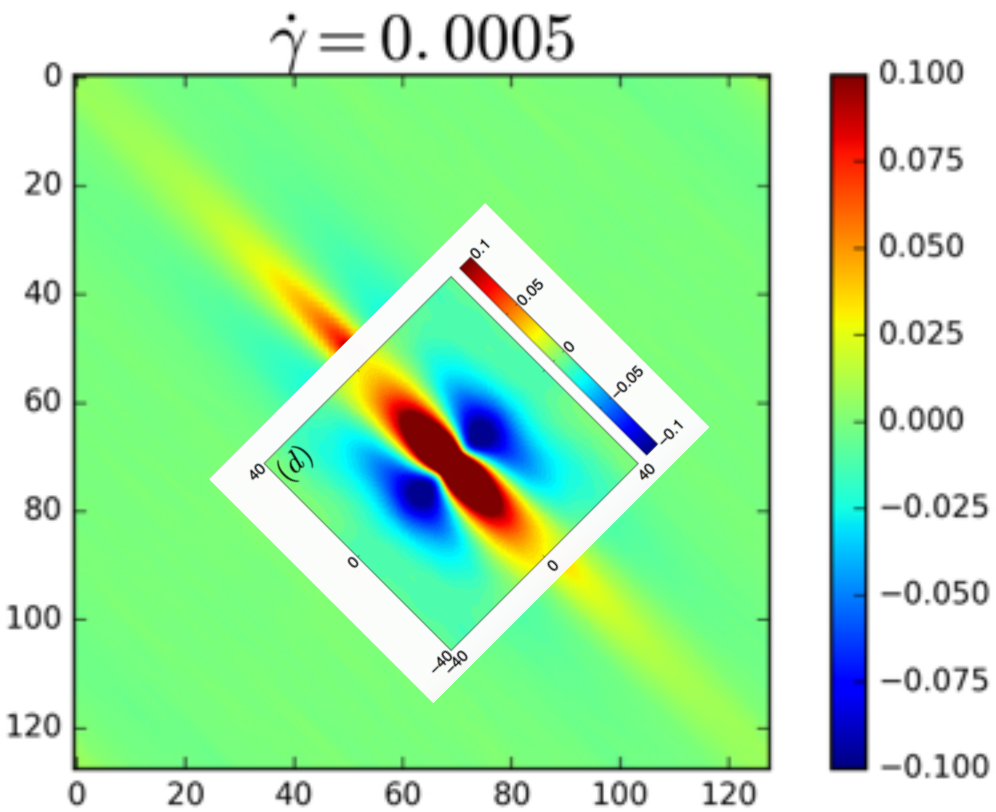


Spatial velocity correlations

- Mesoscale lattice model



- "Mean drag" Durian model at similar ξ

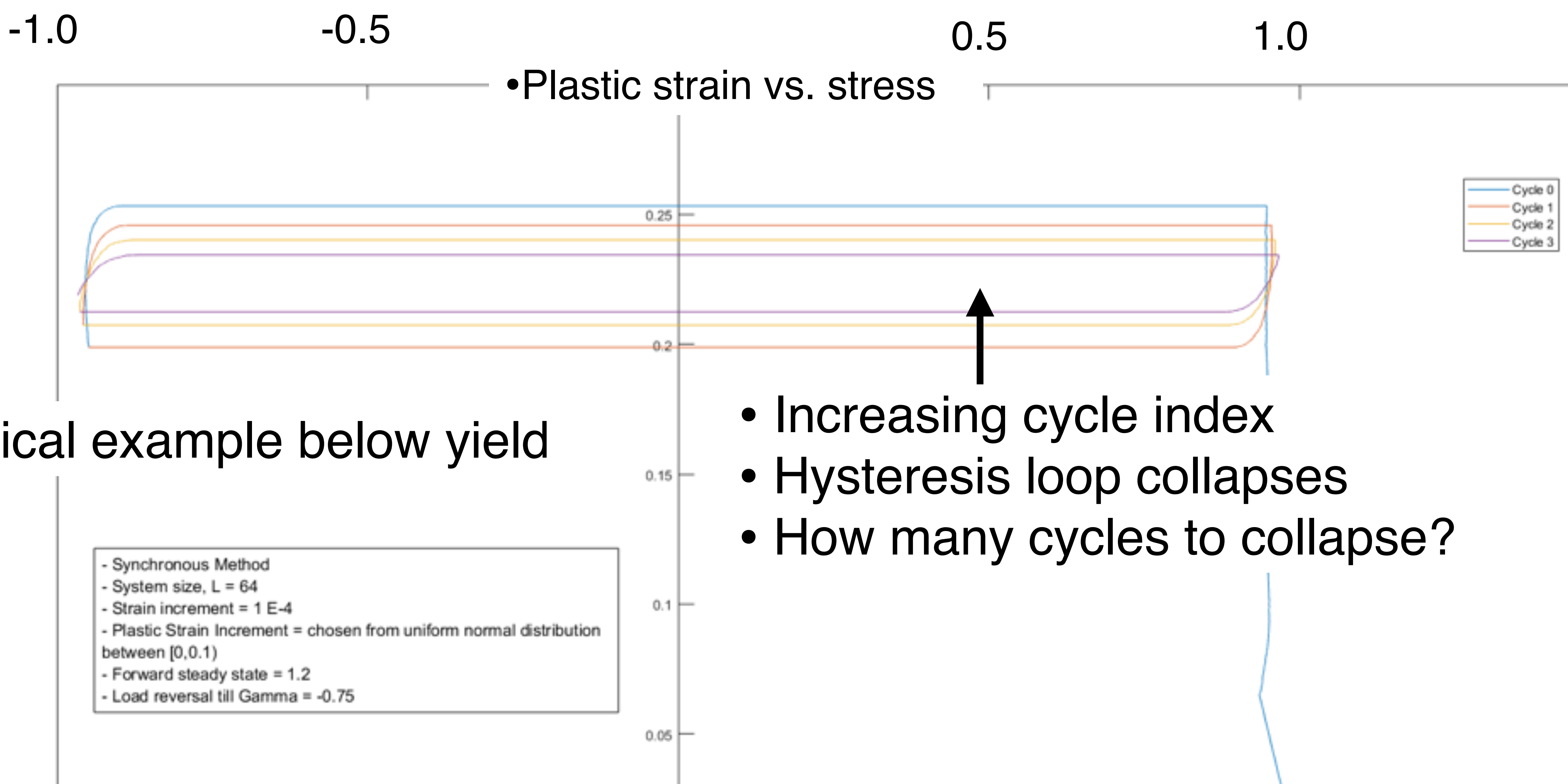


•Future work: pair drag implementation in the lattice model

Hysteresis (quasi-static, piecewise quadratic)

- Protocol:
  - Shear "forward" until steady state.
  - Shear in reverse direction by an amount $2\gamma_{max}$
  - Shear in forward direction by an amount $2\gamma_{max}$
  - Repeat

- Below yield —> "overaging" or "mechanical annealing" or "strain hardening"
- Above yield —> "rejuvenation"



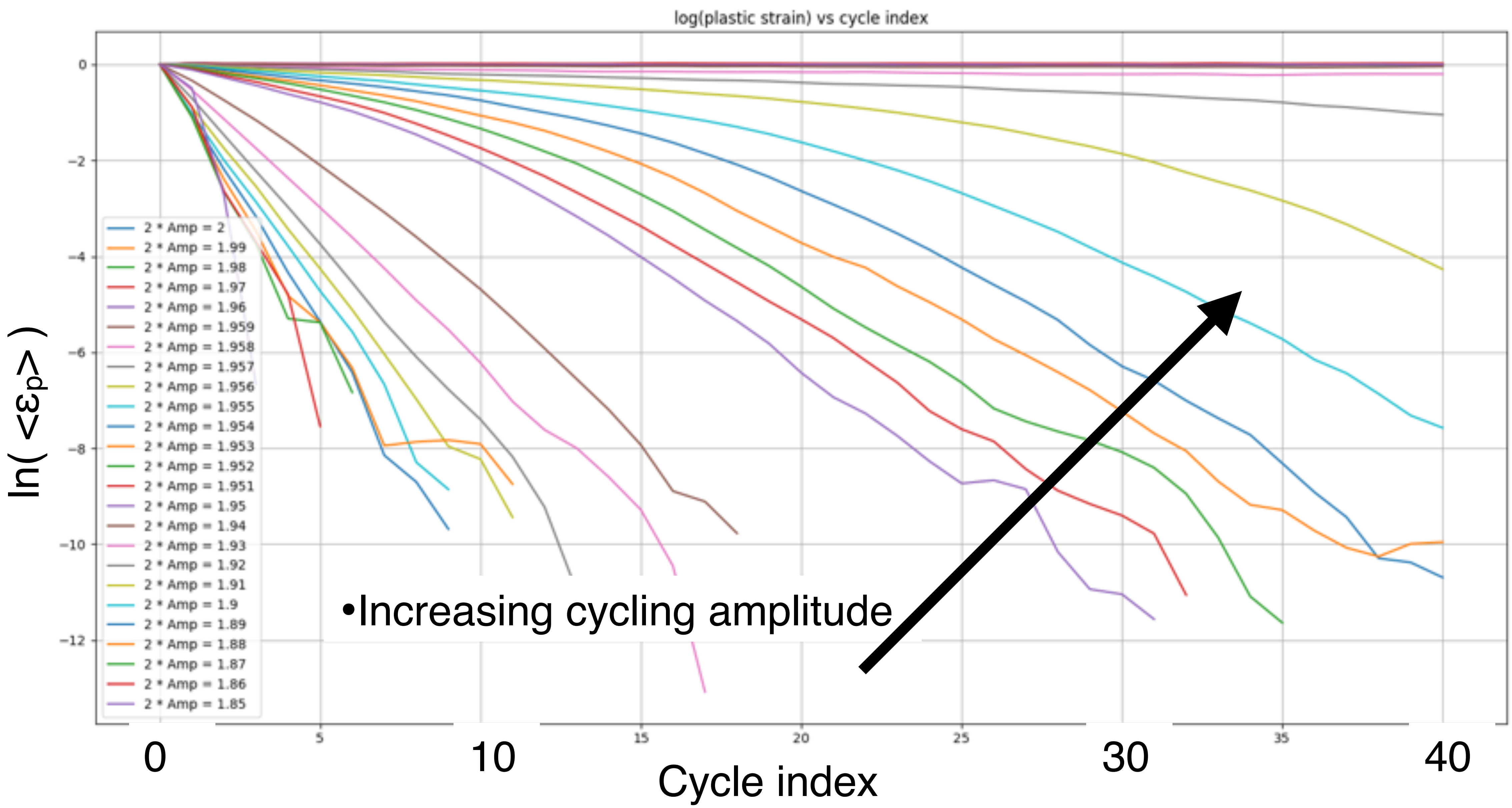
•Plastic strain vs. stress

•Typical example below yield

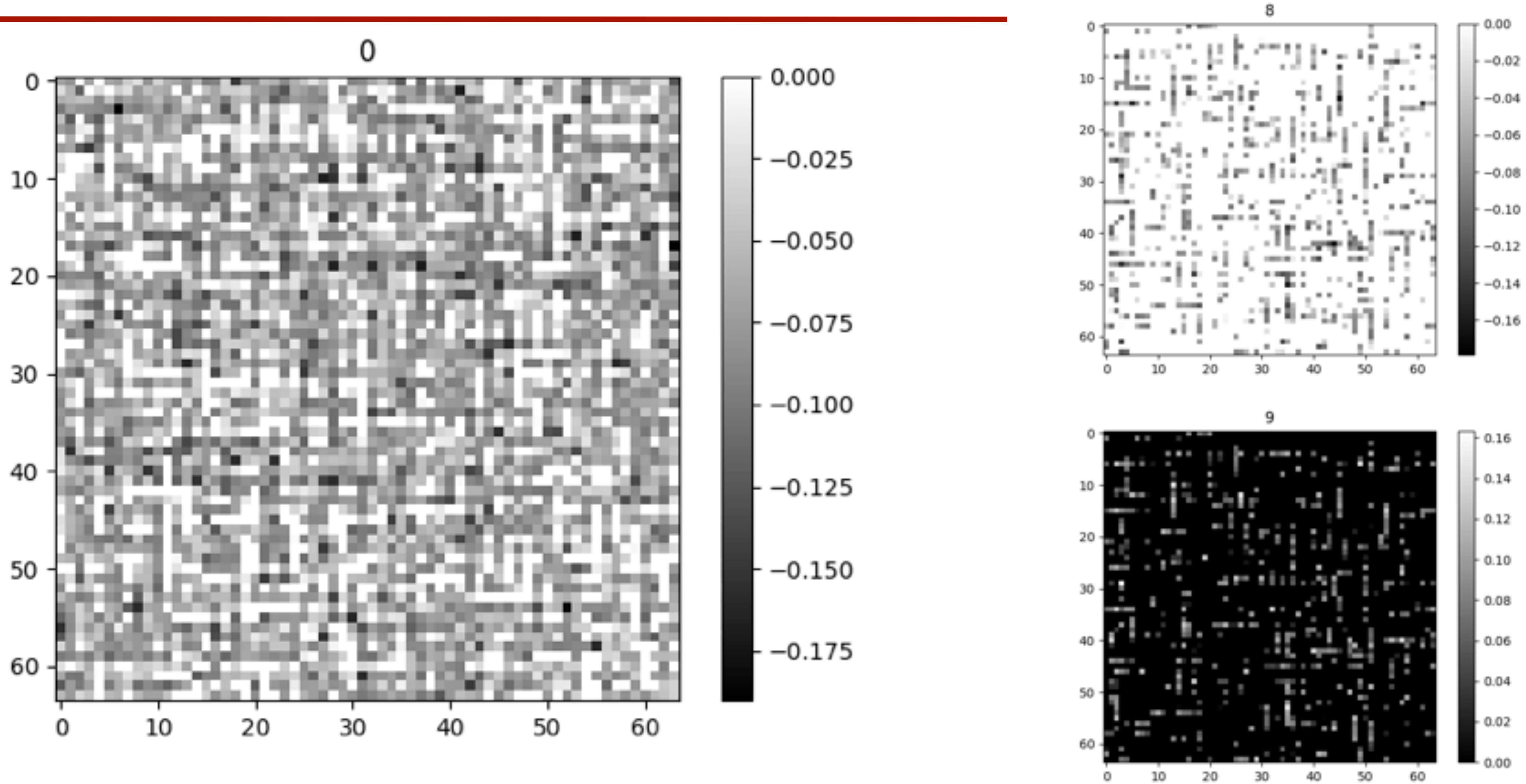
- Increasing cycle index
- Hysteresis loop collapses
- How many cycles to collapse?

Decay of incremental <ε_p> with cycle index

- <ε_p> is essentially width of hysteresis.
- Exponential for low amplitude.
- Non-exponential near yield.
- Diverging strain scale at yield? (Fiocco, et. al. ; Regev et. al.)

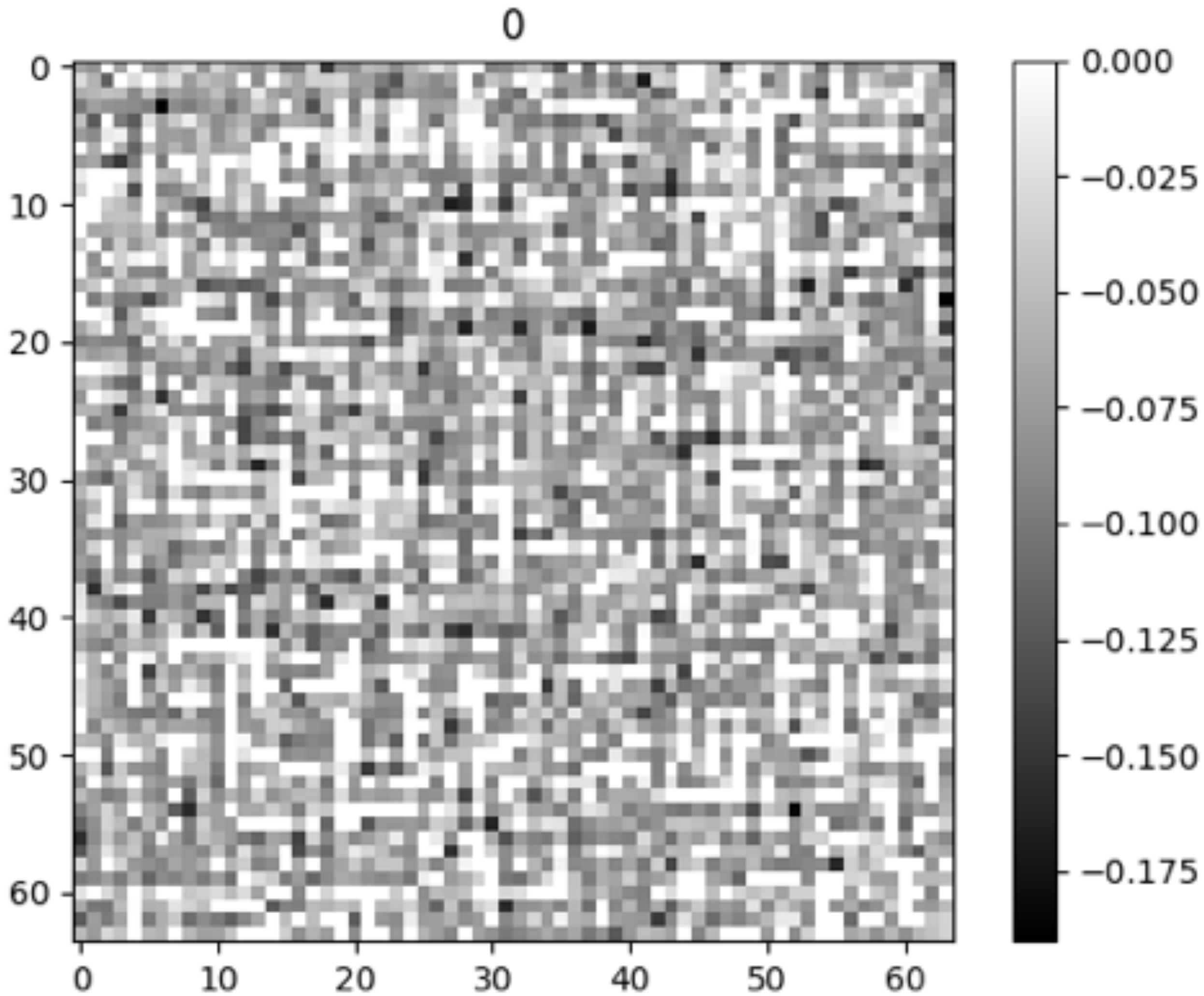


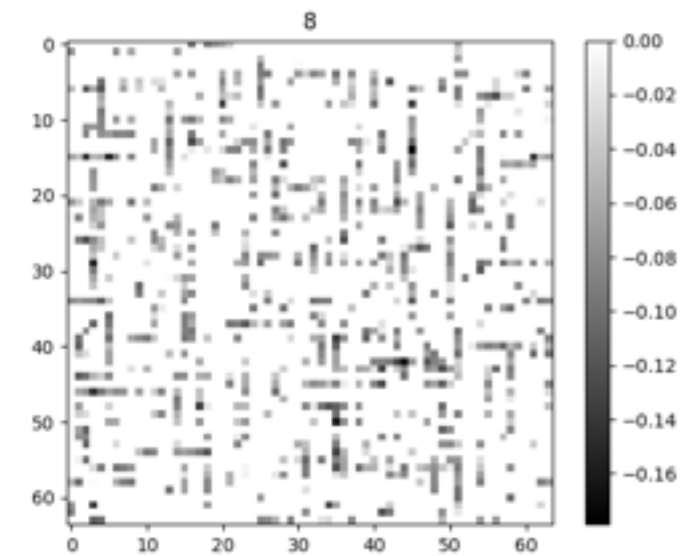
Incremental plastic strain field each half-cycle

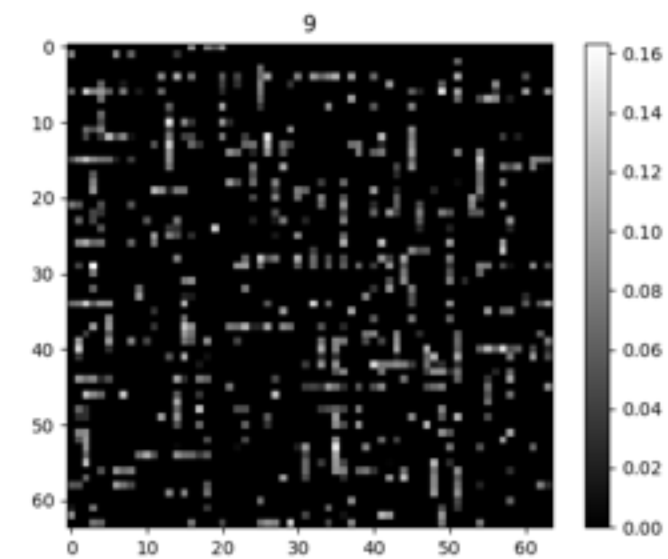


- Organized onto lines as expected.
- Lines are quasi-reversible. Forward one cycle, backward the next.
- Characteristic ξ looks like it may be decreasing with cycle.

Incremental plastic strain field each half-cycle







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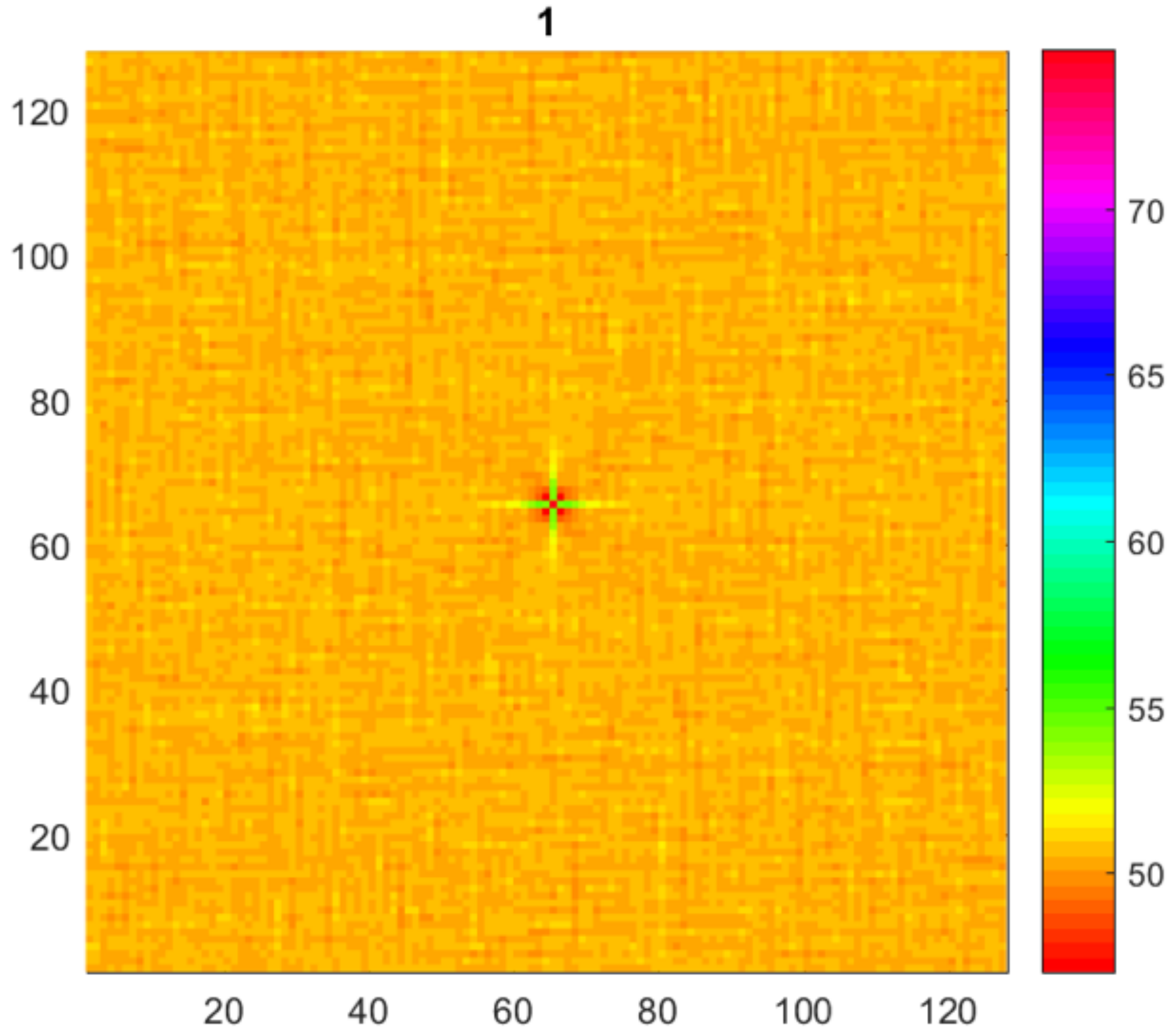
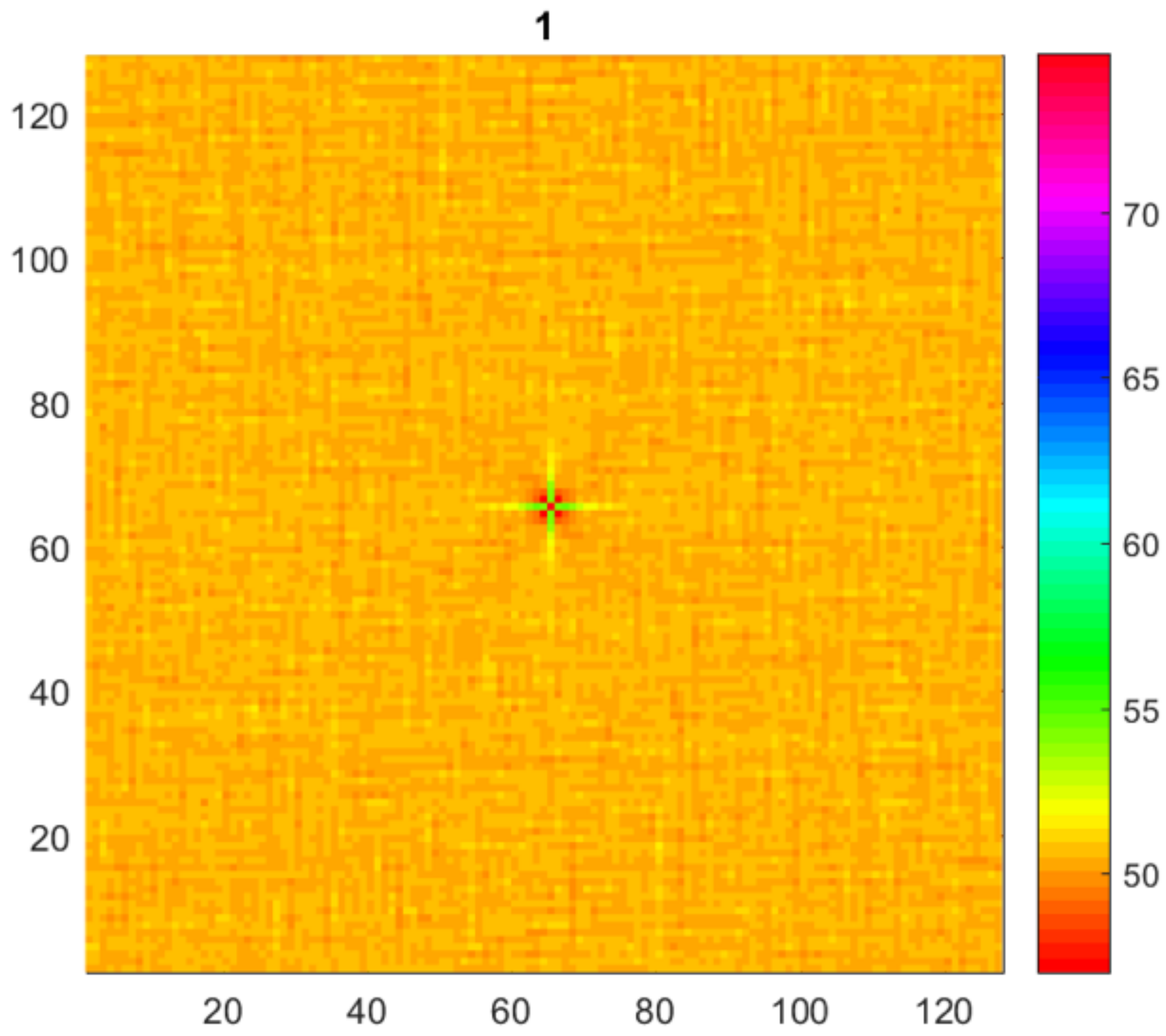
Plastic strain correlations, sub yield, various cycle index

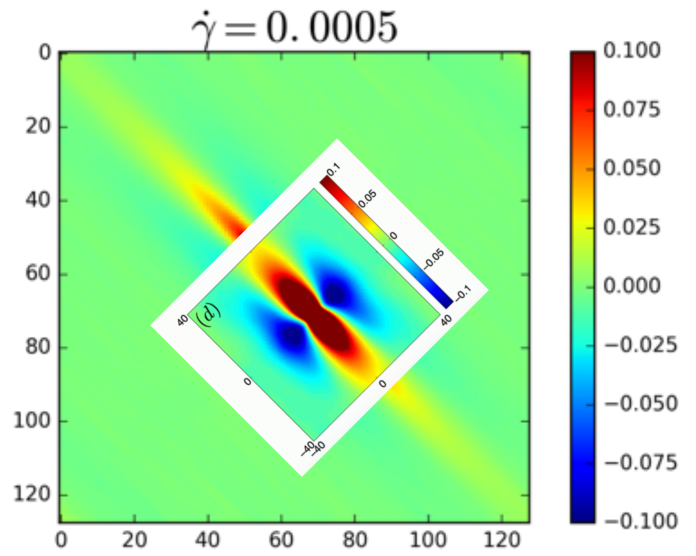


Plastic strain correlations, sub yield, various cycle index



Conclusions

- Part 1: Quasistatic Avalanches/diffusion
  - Identification of early time regime
  - Late time regime similar to earlier work by Martens et. al.
  - Late time regime respects Tyukodi et. al. argument about soft modes.
  - Scaling exponents agree with particle simulations



- Part 2: Rheology
  - Non-linear (smooth) strain energy function and "real" drag necessary to get agreement with Durian model.
  - Scaling laws for the σ, De, and ξ agree with "mean drag" Durian.
  - Todo: "pair drag".

- Part 3: Hysteresis (or "work hardening" or "over-aging")
  - When cycling below yield, all plasticity eventually goes away.
  - Plastic strain field consists of lines with a characteristic length which vanishes as the number of cycles increases.
  - Characteristic number of cycles to "forget" increases (diverges?) at yield. (Consistent with Fiocco et. al. and Regev et. al.)