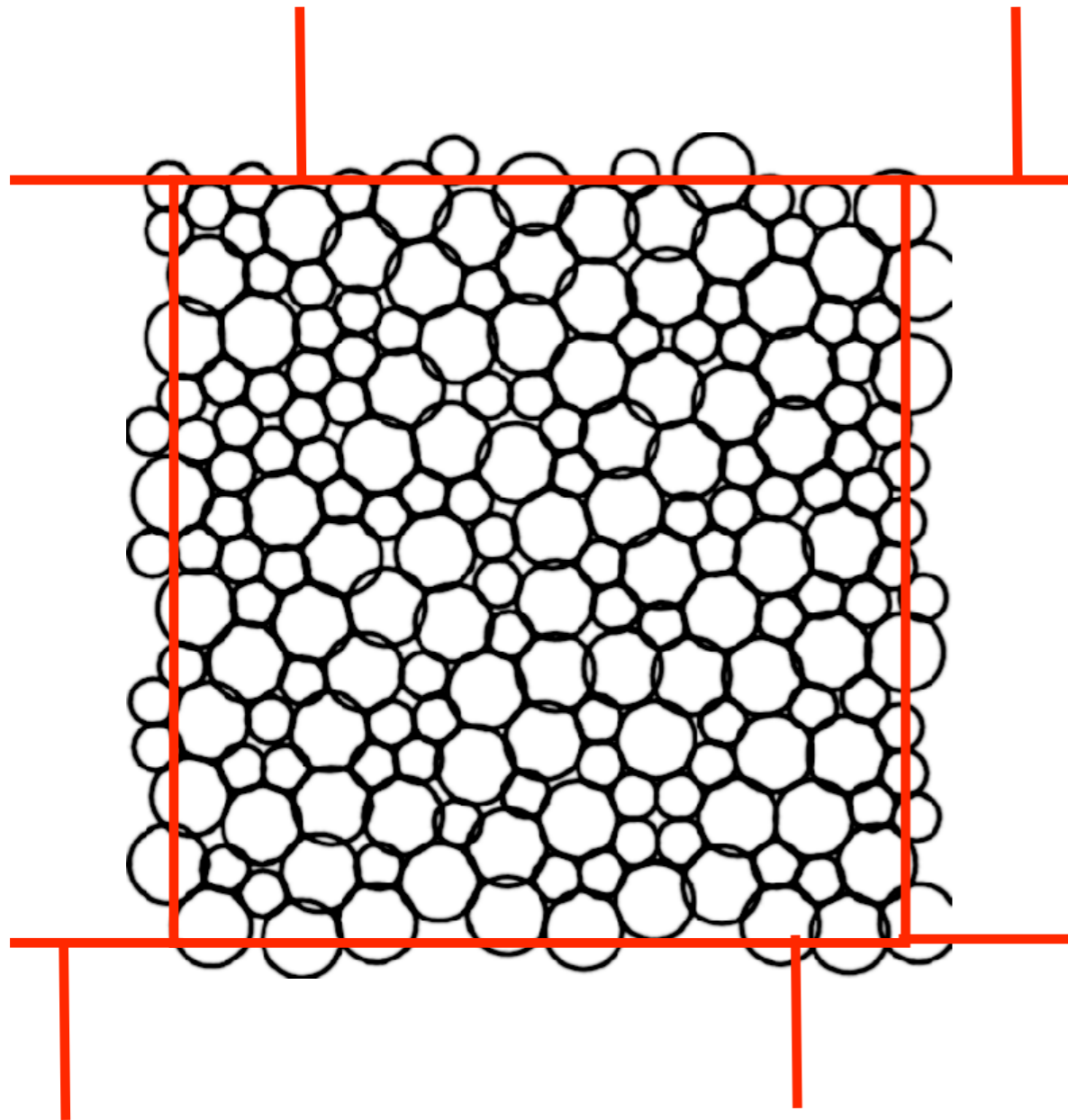


Avalanches and Diffusion in Amorphous Solids Under Athermal, Quasistatic Shear



Craig Maloney

Collaborators:
M. O. Robbins (Hopkins)

Funding:
NSF DMR-0454947 and
PHY99-07949

KITP

June 2010

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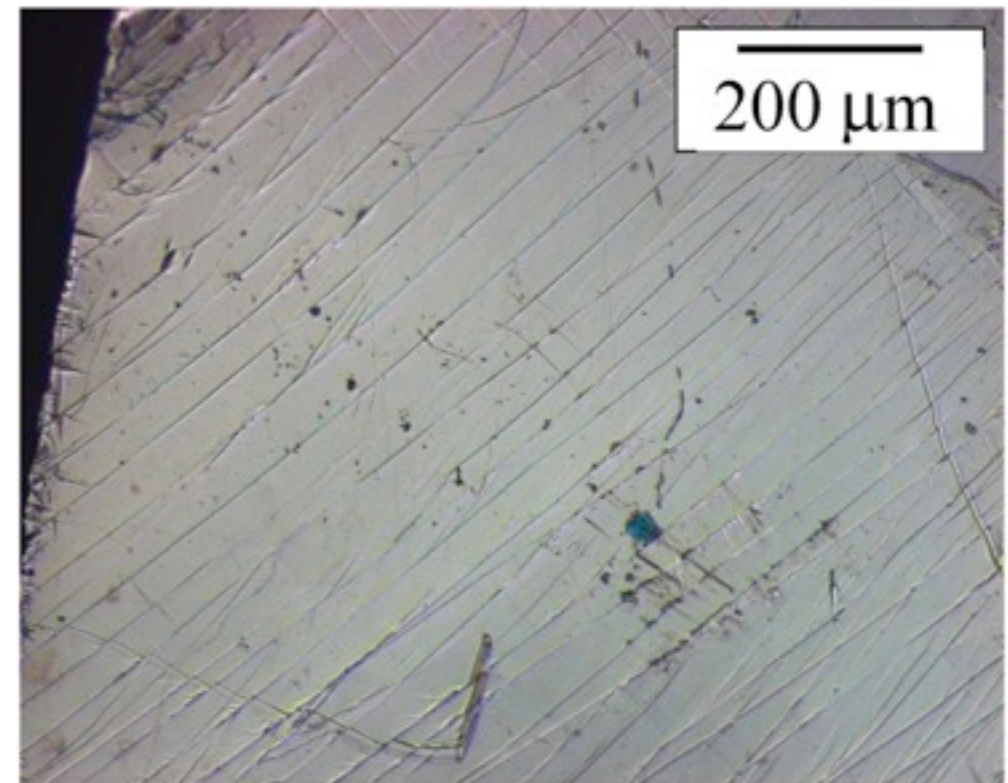
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Outline

- **Amorphous solids**
 - Types
 - Athermal quasistatic shear (AQS)
- **Slip lines in Lennard-Jones solids**
 - CEM + M.O. Robbins (J. Phys 2008, PRL 2009)
 - Spatial structure of plasticity
 - Effective diffusion
- **Jamming**
 - (CEM. PRL Submitted)
 - Bubble model / critical scaling near jamming
 - Effective diffusion
 - Avalanches

The question(s) I am asking

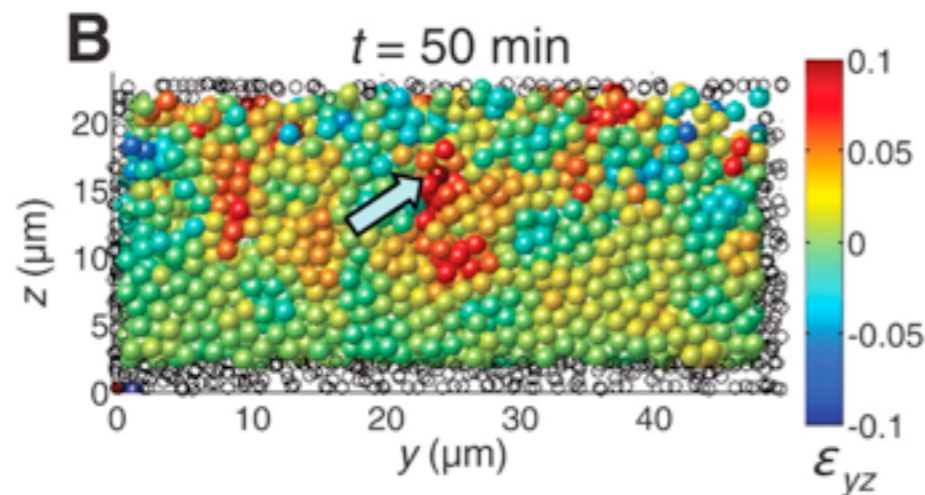
- For “simple” amorphous solids in AQS:
 - What is the elementary mechanism(s) which accommodates applied shear?
 - How are they organized in space and time?
 - ~~(How does this impact viscoplastic rheology)?~~



Types of amorphous solids

- Types
 - Emulsions / Foams
 - Granular packings
 - Colloidal suspensions
 - Atoms / Molecules

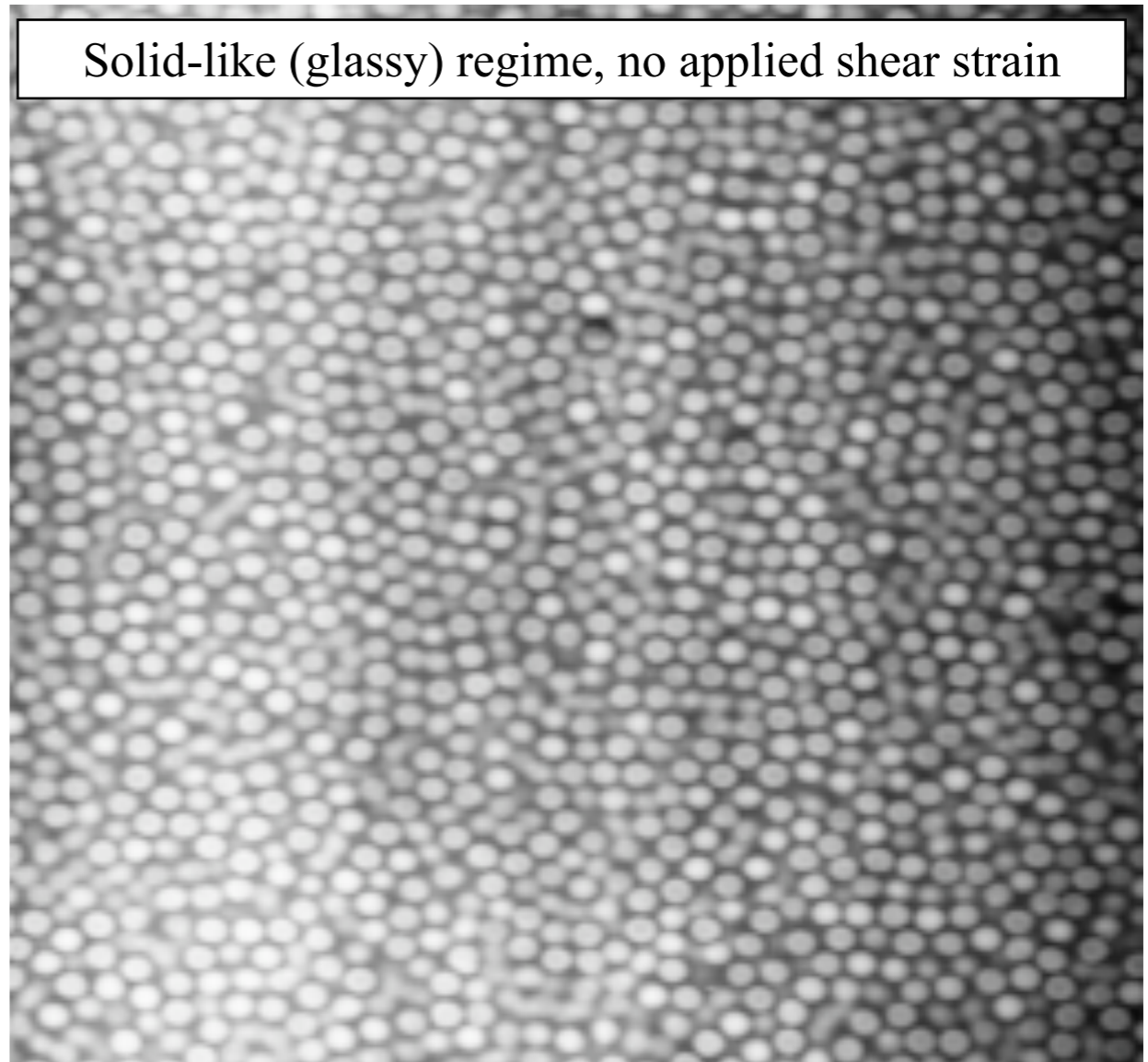
Local shear strain under driving:



(Schall et. al.)

Polydisperse PMMA spheres in density-matched solvent

Solid-like (glassy) regime, no applied shear strain



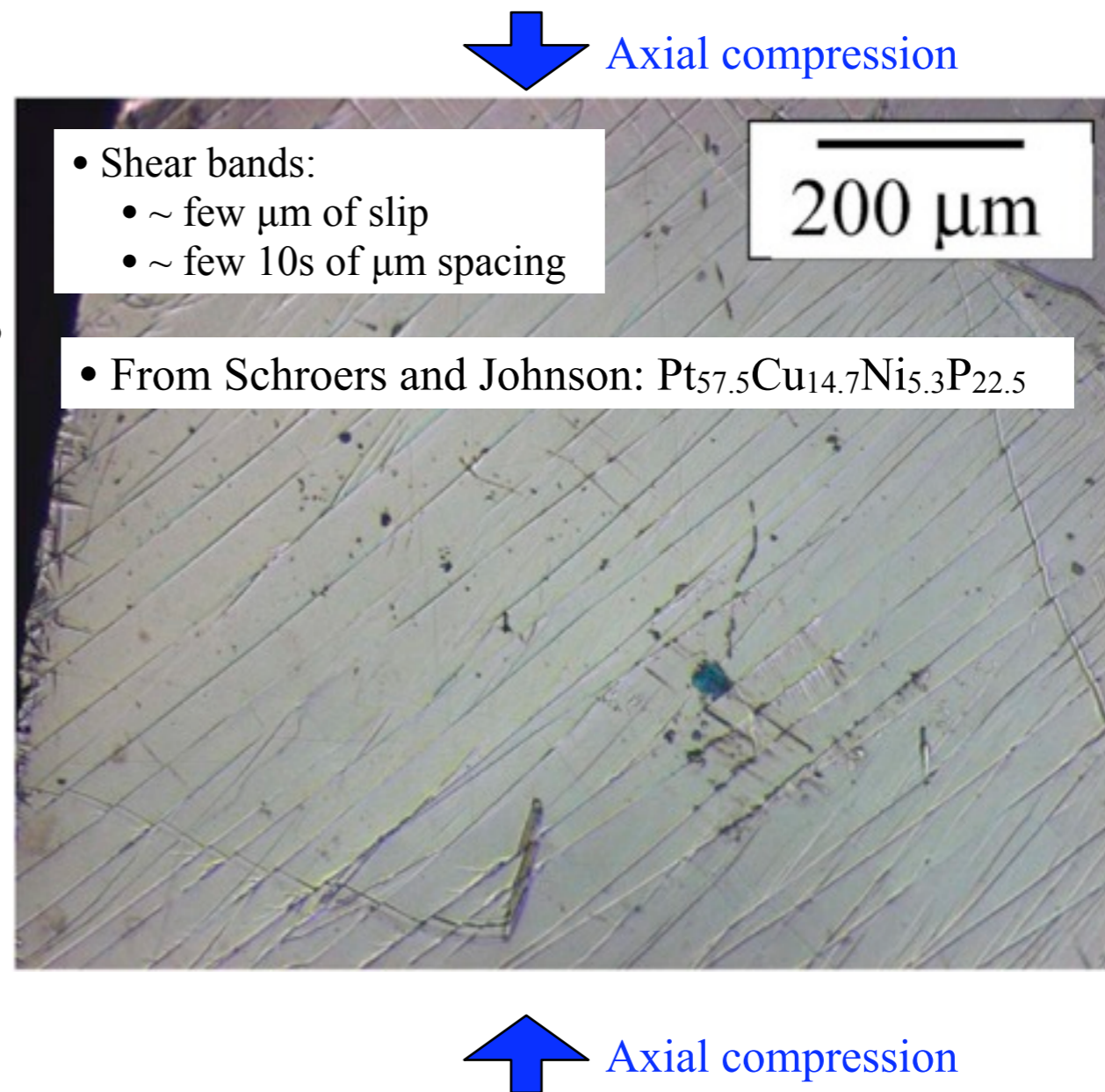
(Weeks et. al.)

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Types of amorphous solids

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Athermal, quasistatic shear (AQS)

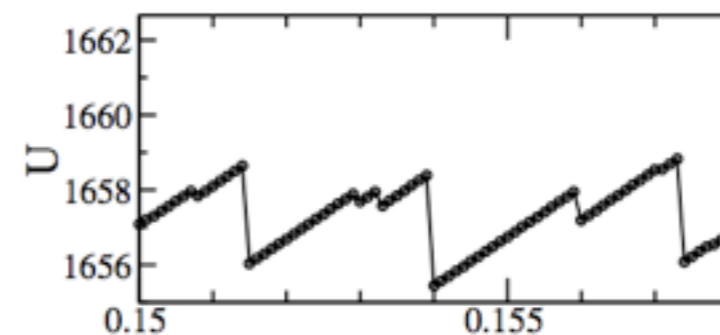
- Differences in particle-scale physics (do they matter?):
 - Inertial or overdamped?
 - “Real” temperature
 - Dissipation mechanisms / hydrodynamics
 - Attractive forces / adhesion
 - Coulomb friction / covalent bonding

- Energy landscape picture of AQS (Malandro and Lacks)



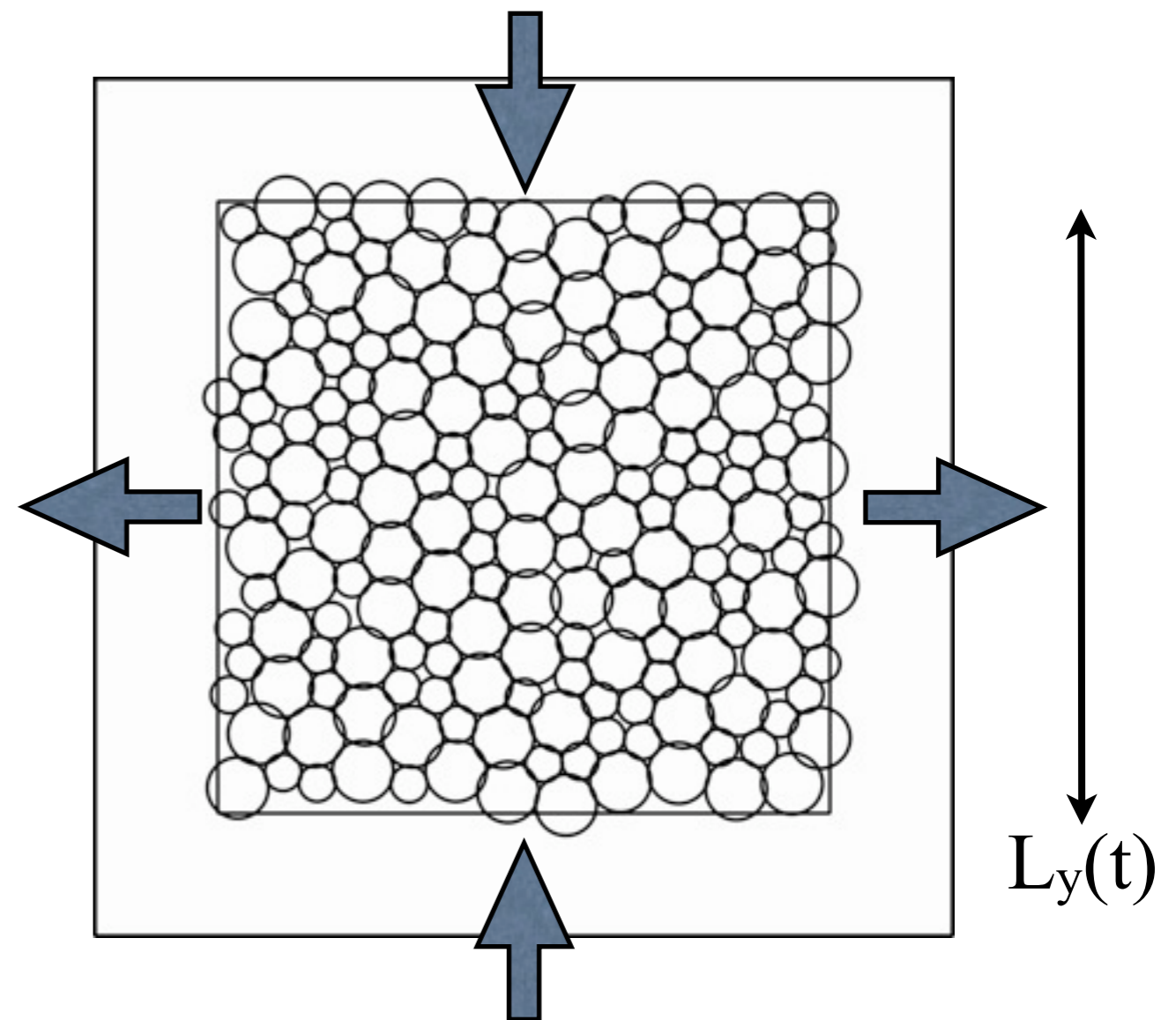
Increasing shear →

- $t_{\text{thermal}} \gg t_{\text{shear}} \gg t_{\text{rearrange}}$
- first Temperature to zero, then shear rate to zero.



Zero temperature molecular dynamics

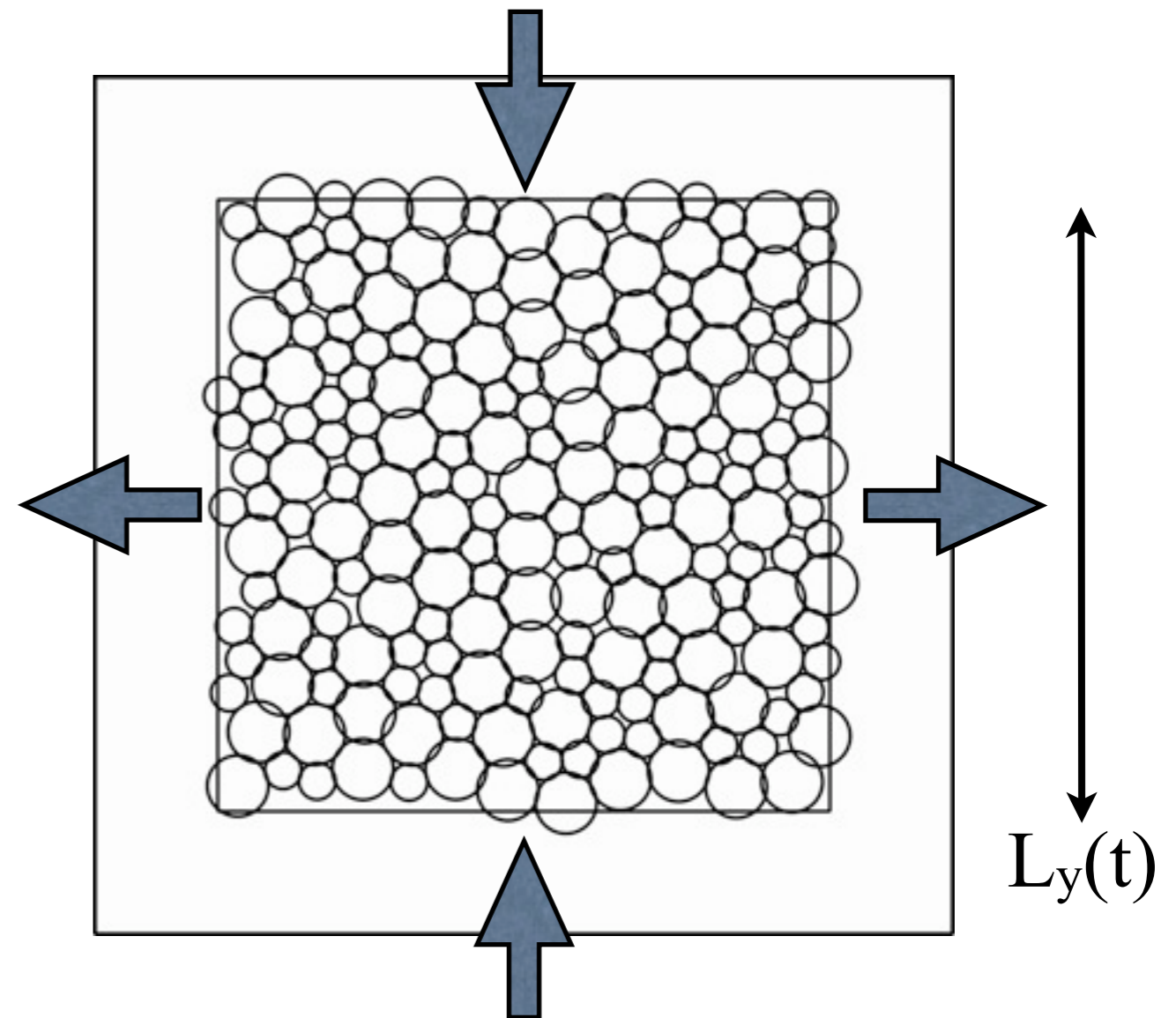
control: $L_y(t)$, $L_x(t)$
conserve area



Zero temperature molecular dynamics

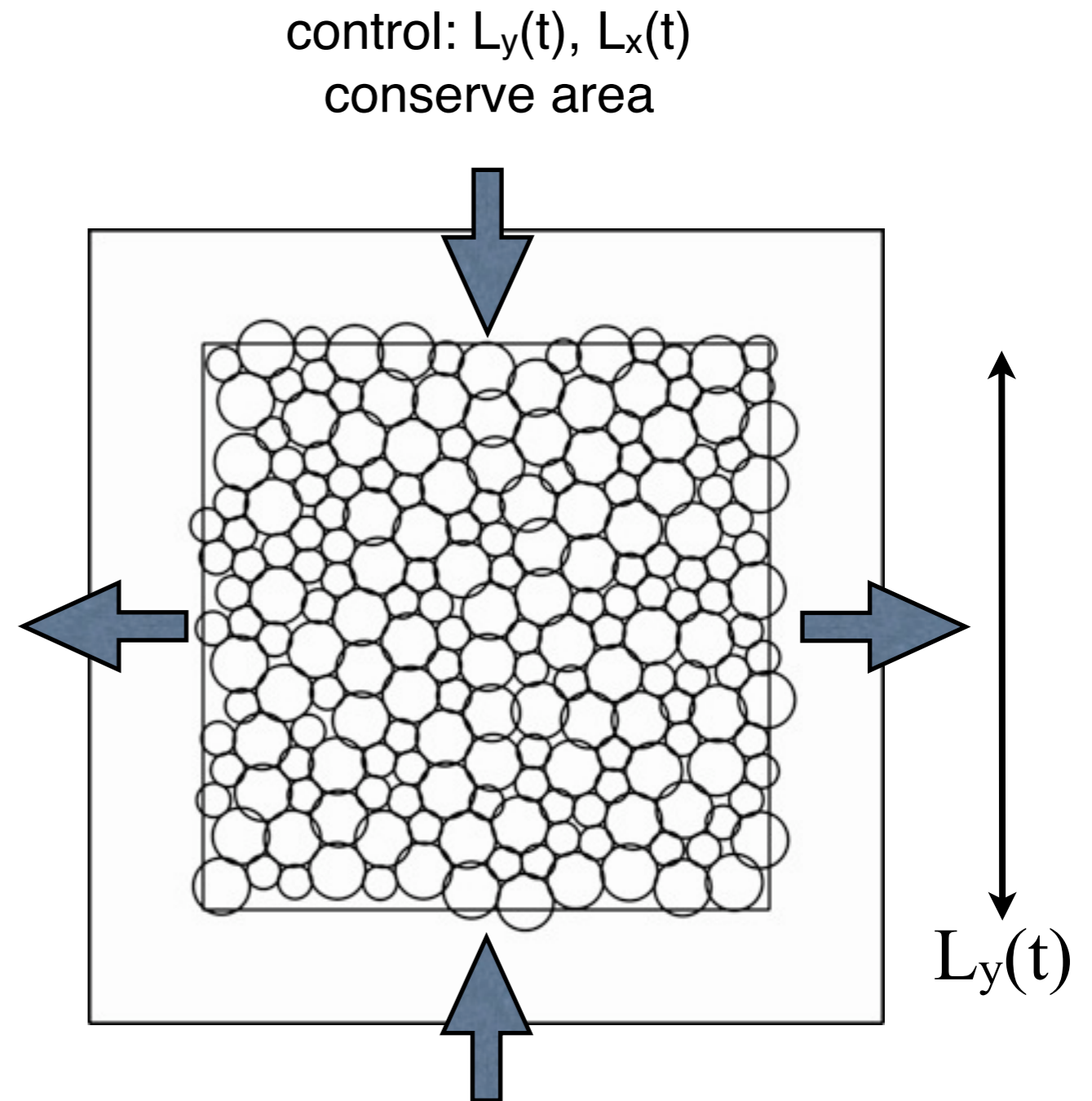
- 2D Molecular Dynamics:

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conserve area



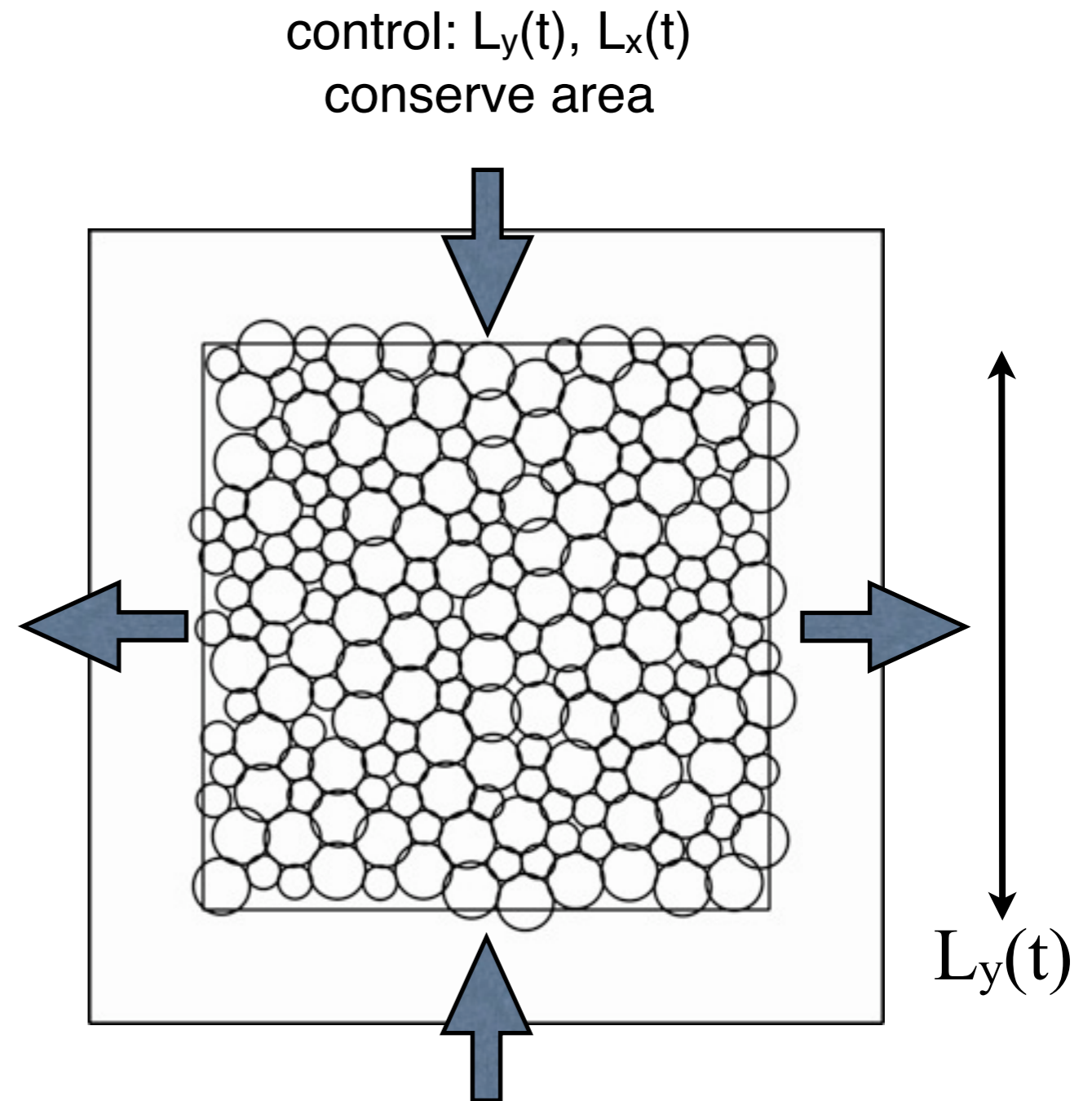
Zero temperature molecular dynamics

- 2D Molecular Dynamics:
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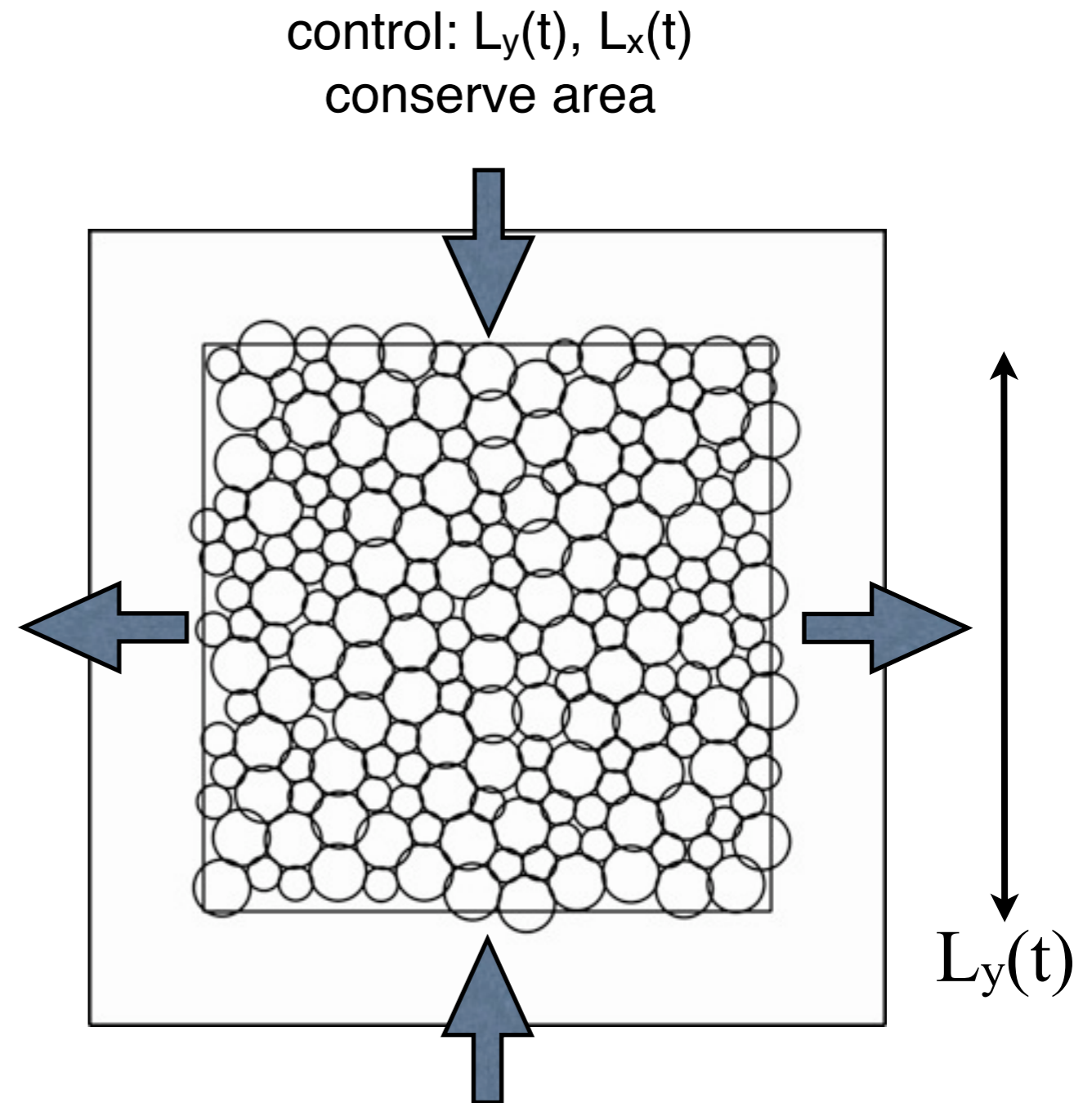
Zero temperature molecular dynamics

- 2D Molecular Dynamics:
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- quenched at Pressure=0



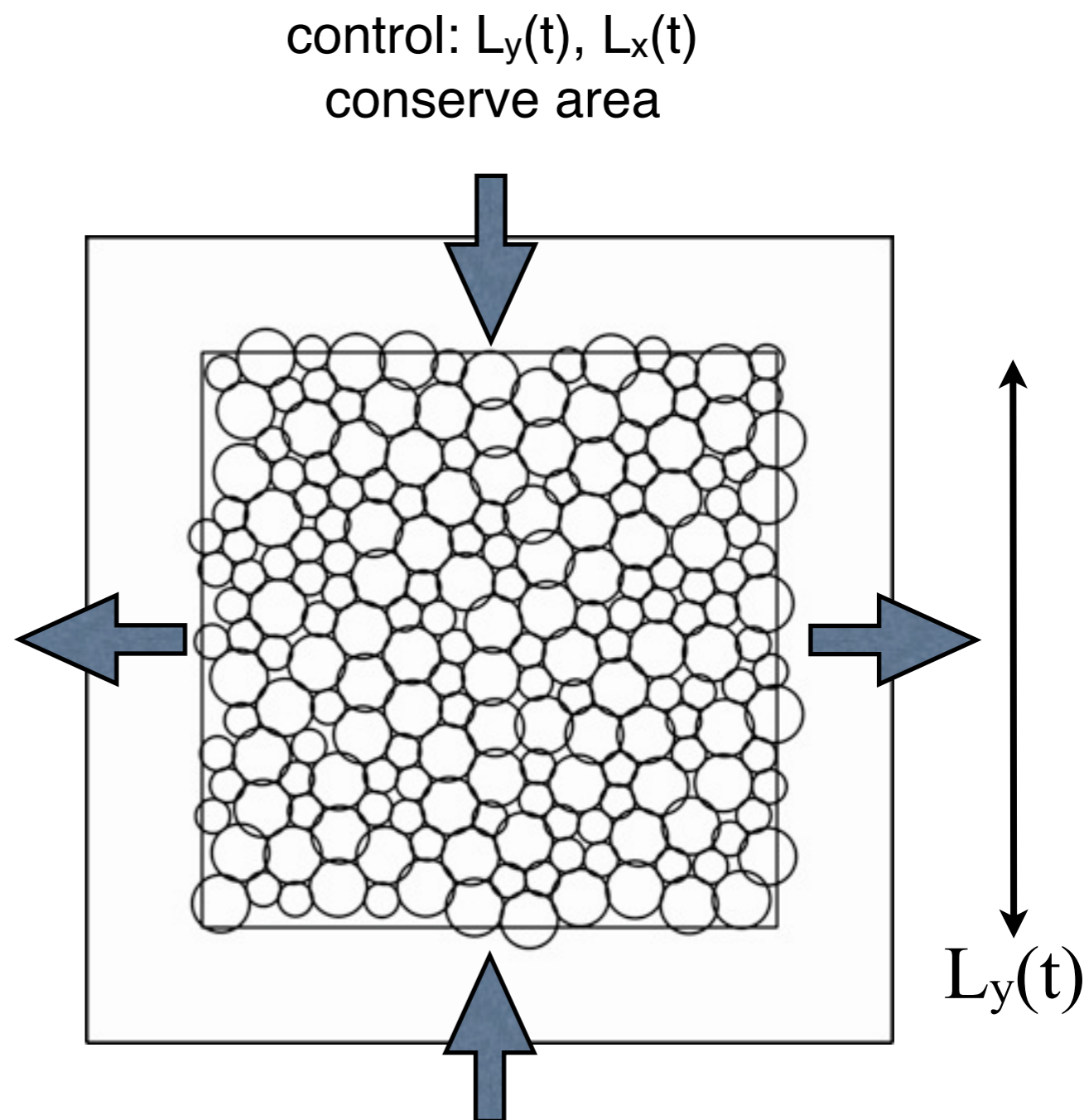
Zero temperature molecular dynamics

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- quenched at Pressure=0
- damp relative velocity (Kelvin/
DPD)



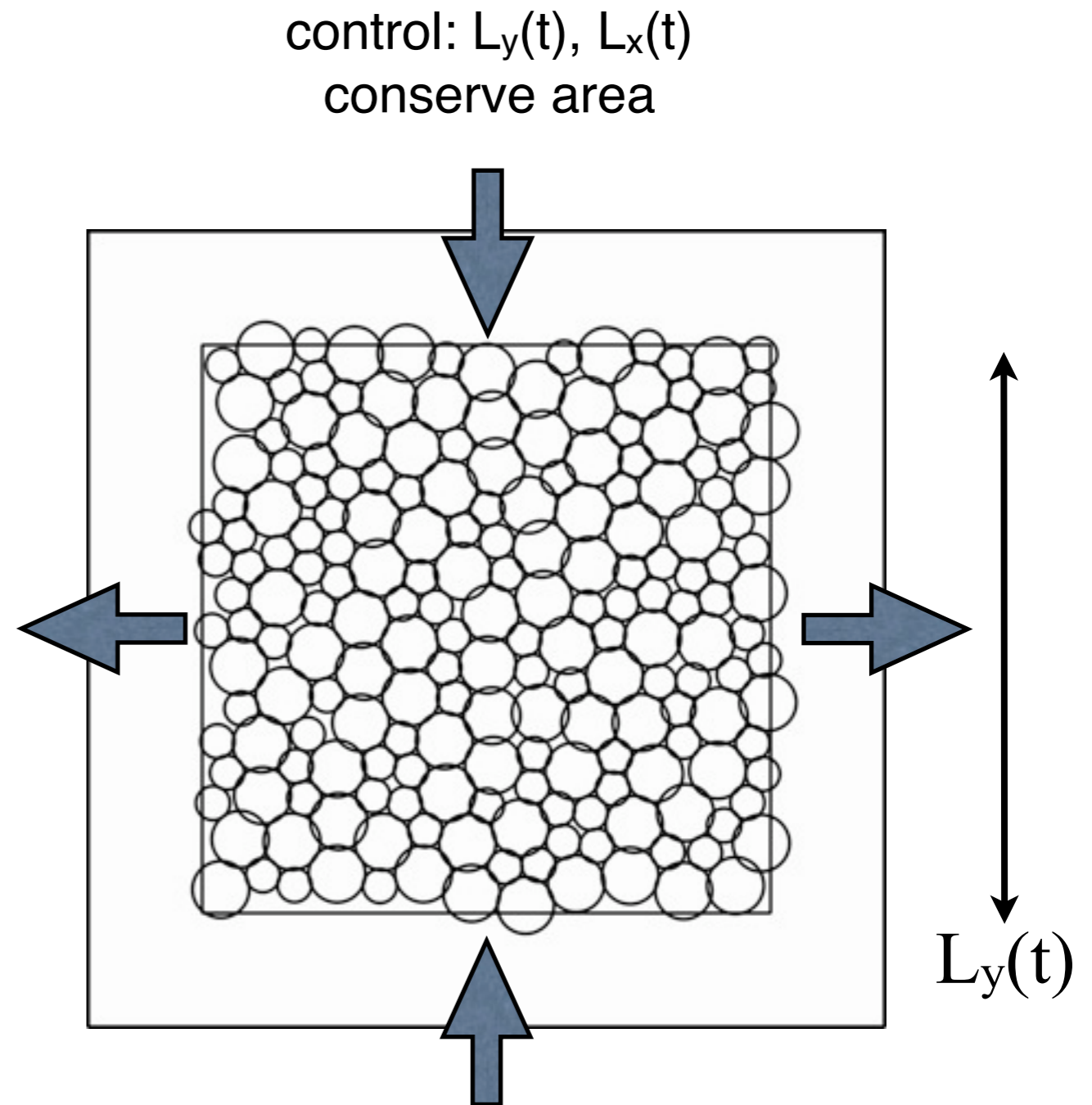
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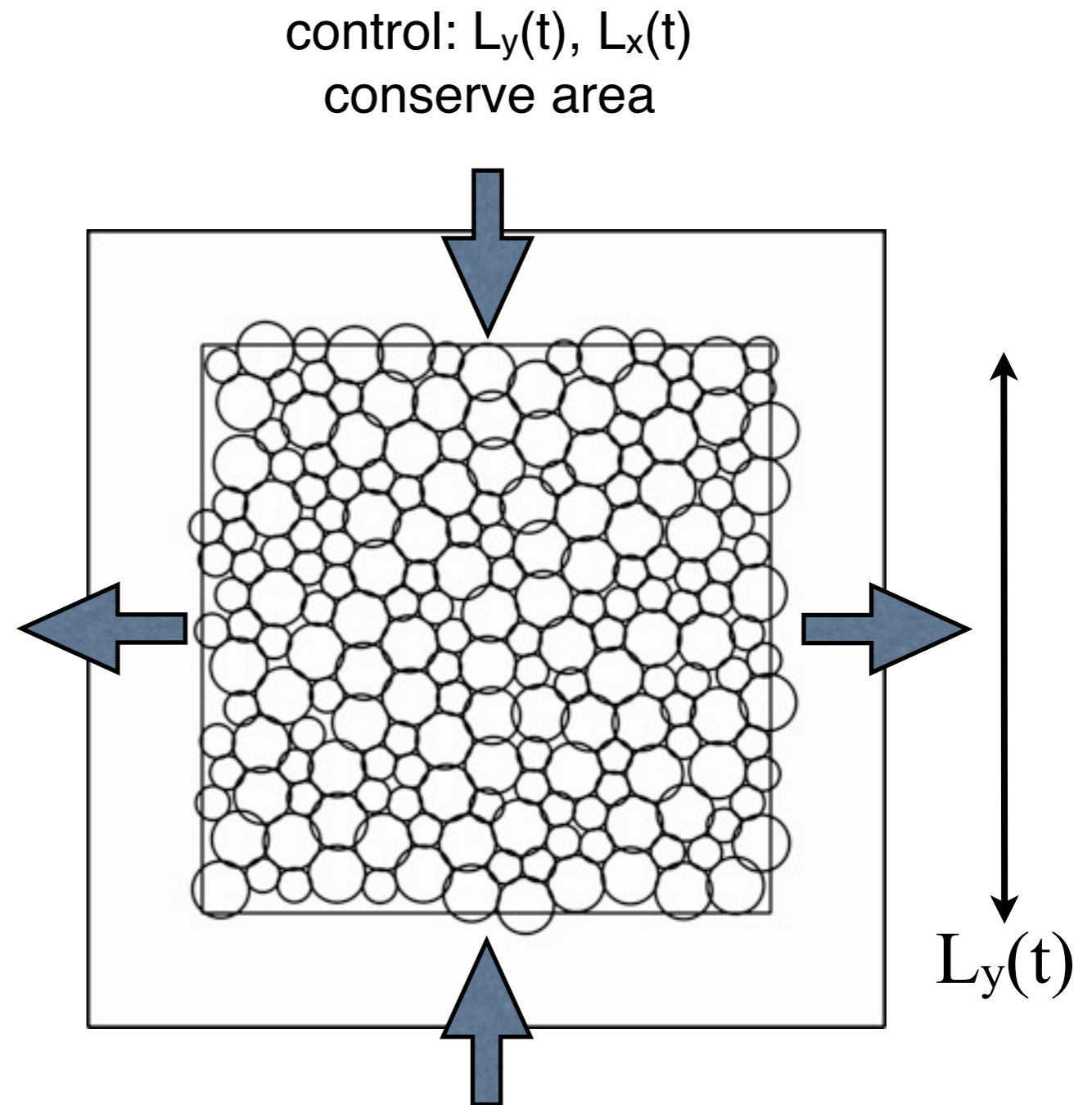
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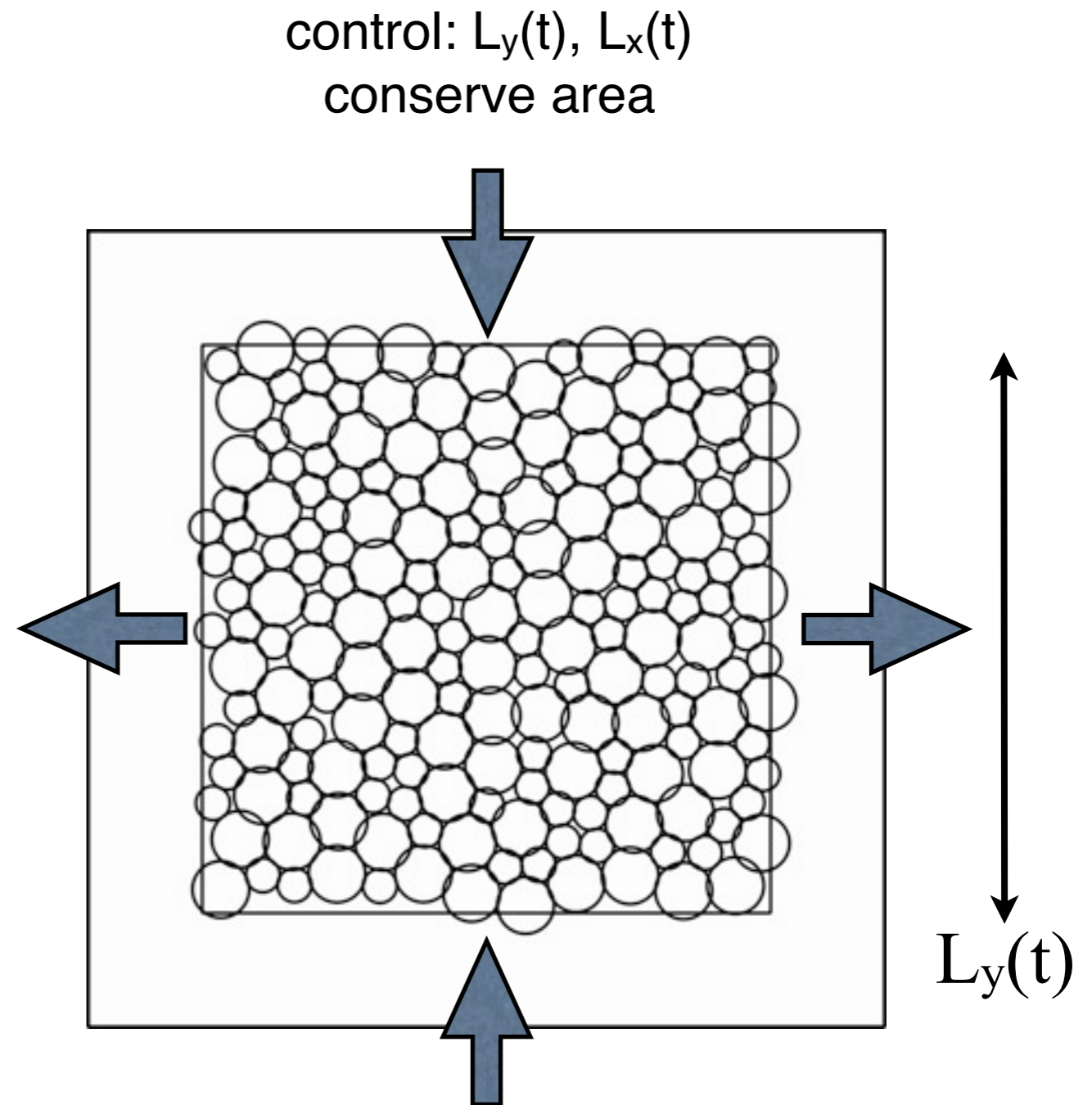
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~ 10M particles



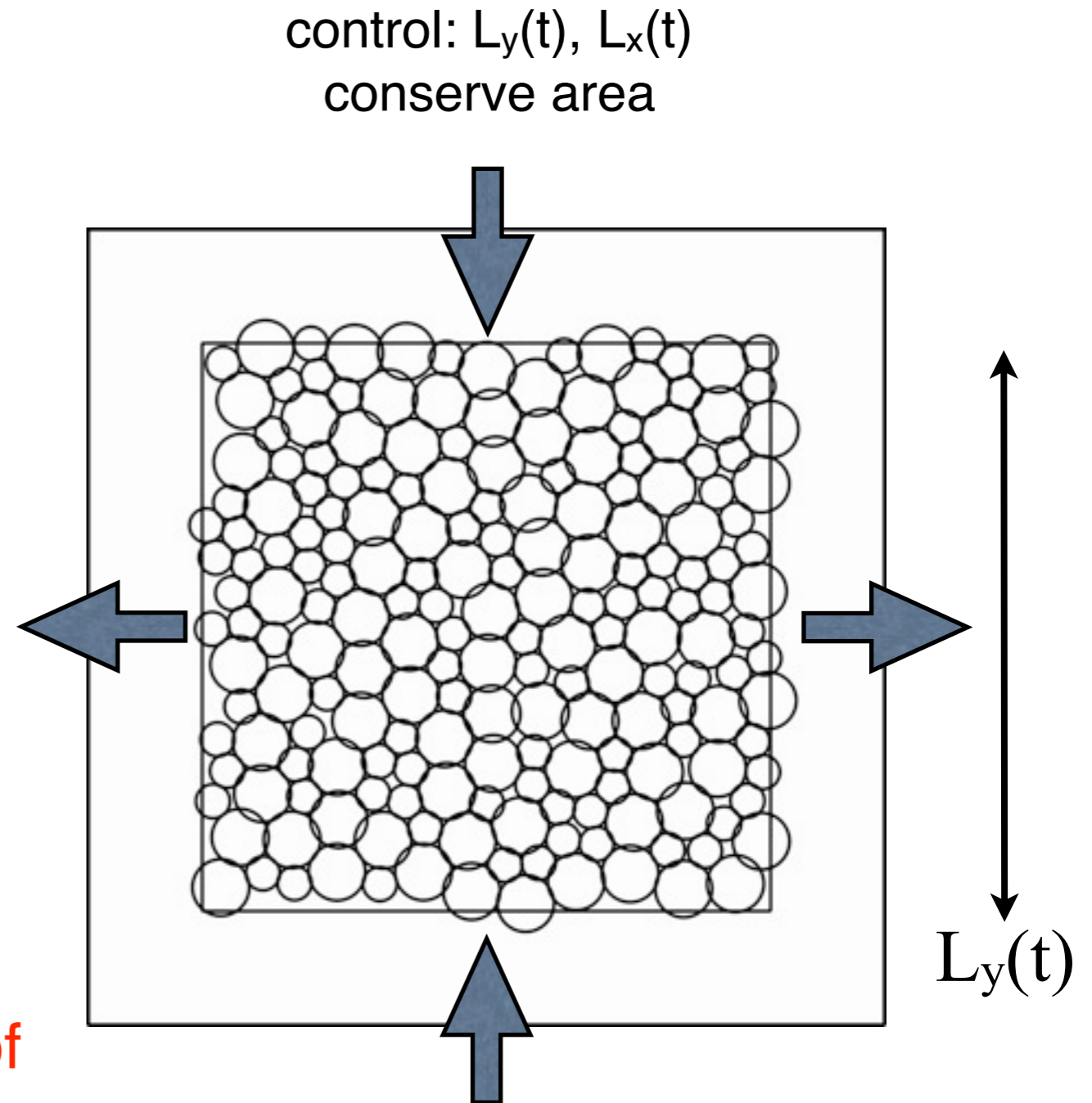
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Zero temperature molecular dynamics

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- Quasi-static limit (about 500 CPU days / run)
- **Strain window, $\Delta\gamma$, plays role of time!**



Local vorticity, ω

For each triangle:

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

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

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

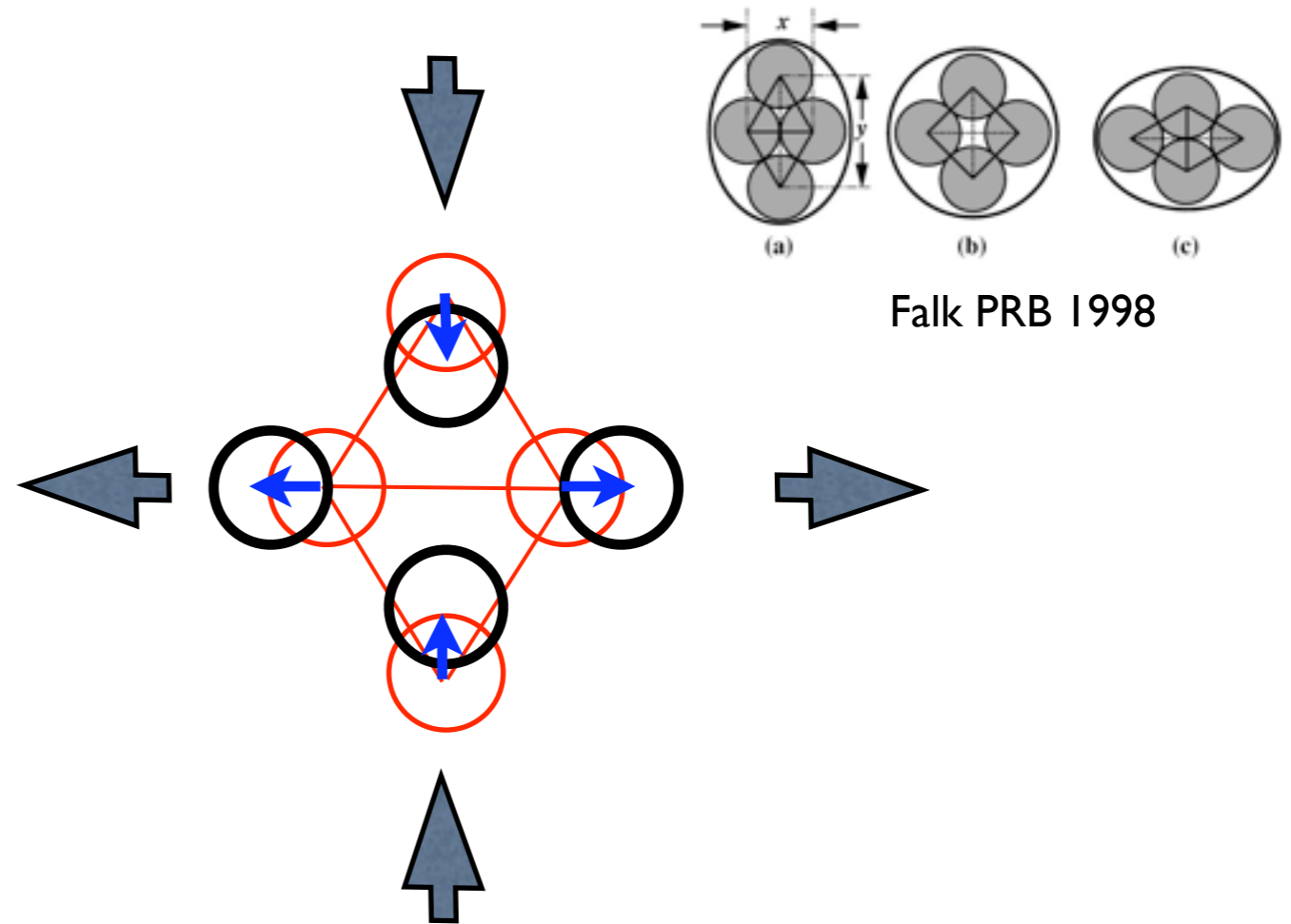
Invariants:

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

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

“Canonical” atomistic Eshelby
shear transformation:

pure shear $\epsilon_1 > 0$ $\epsilon_2 = 0$ $\omega = 0$



Local vorticity, ω

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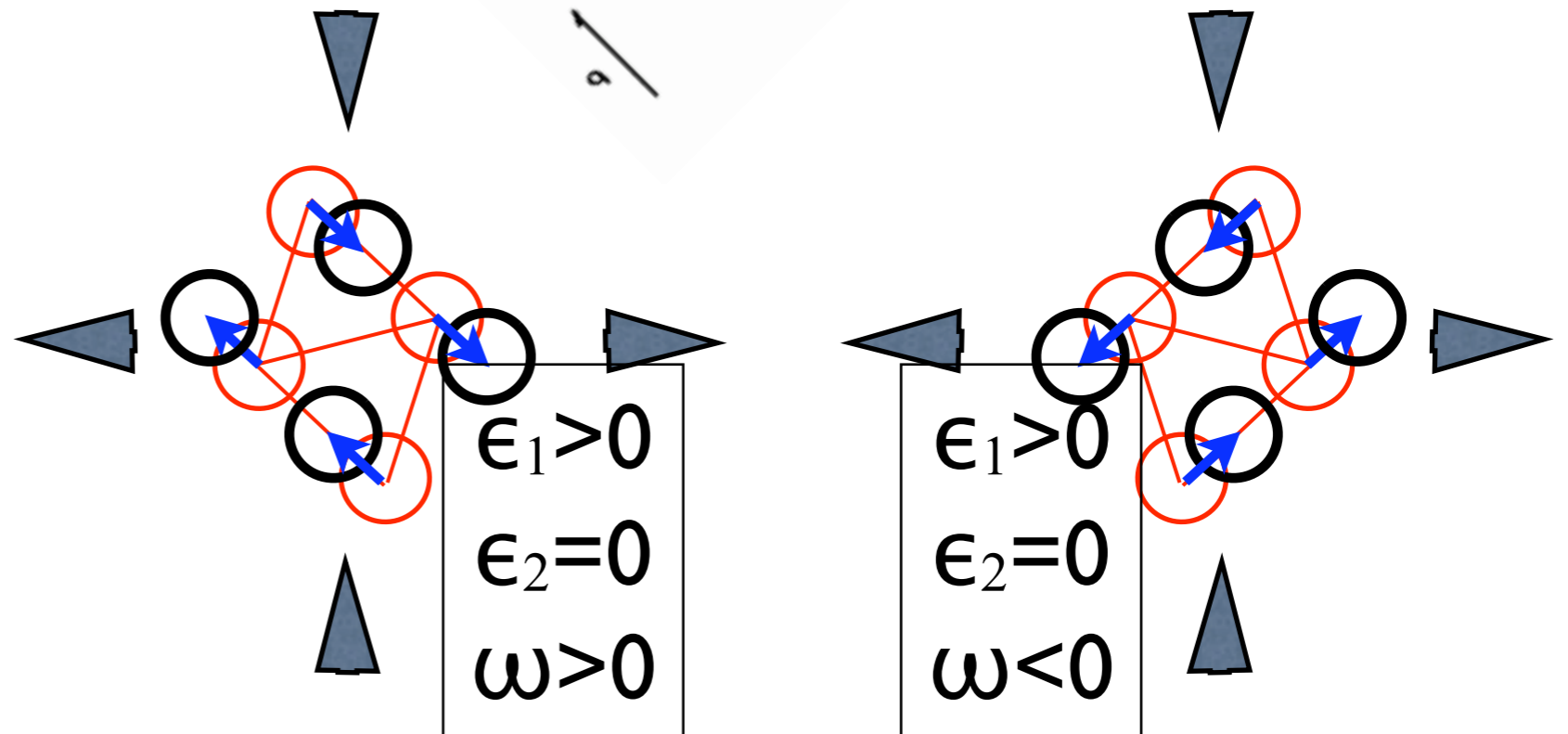
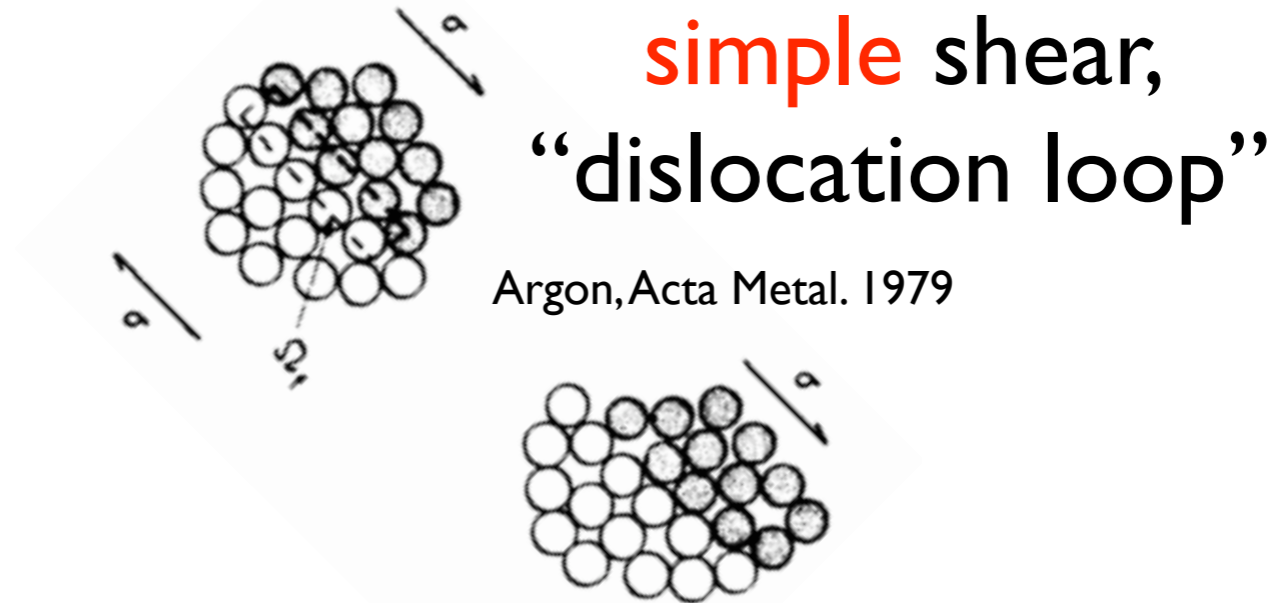
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Correlations in steady state

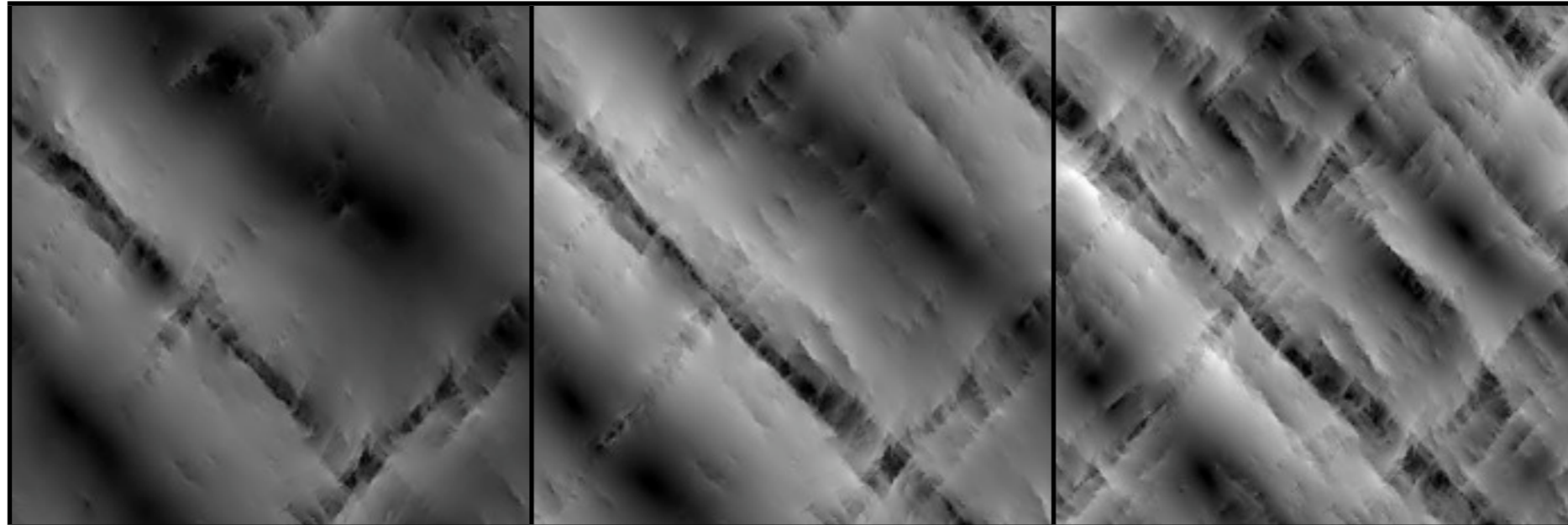
γ :

6.0% to 6.1%

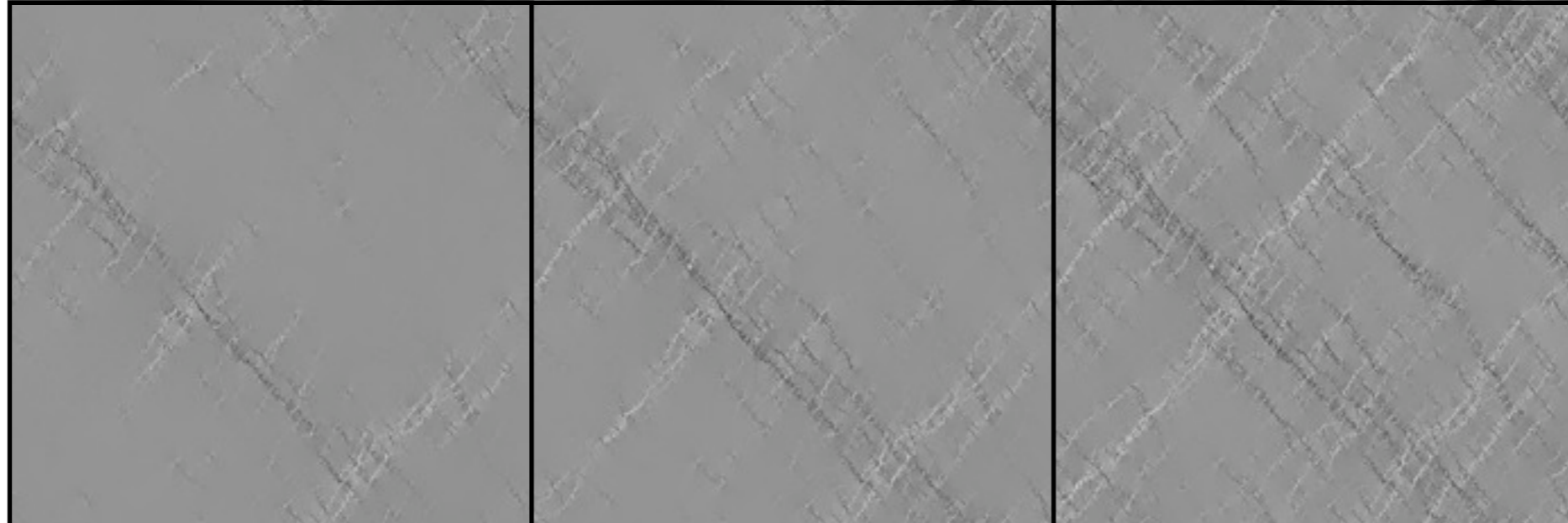
6.0% to 6.2%

6.0% to 6.4%

$|\Delta r|$



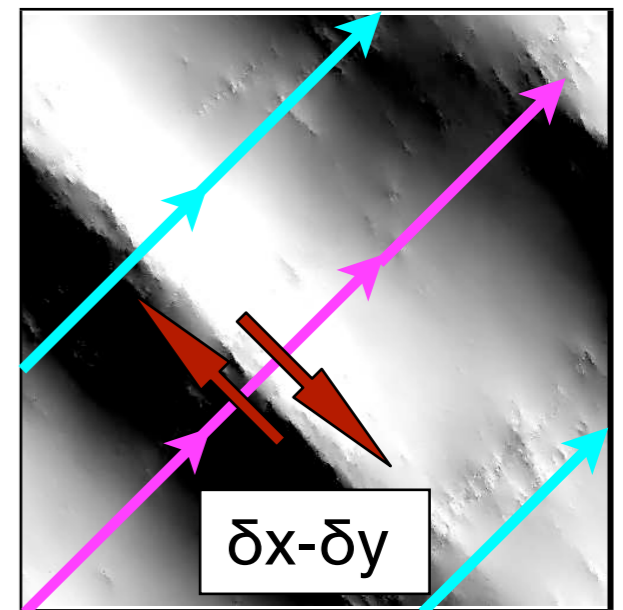
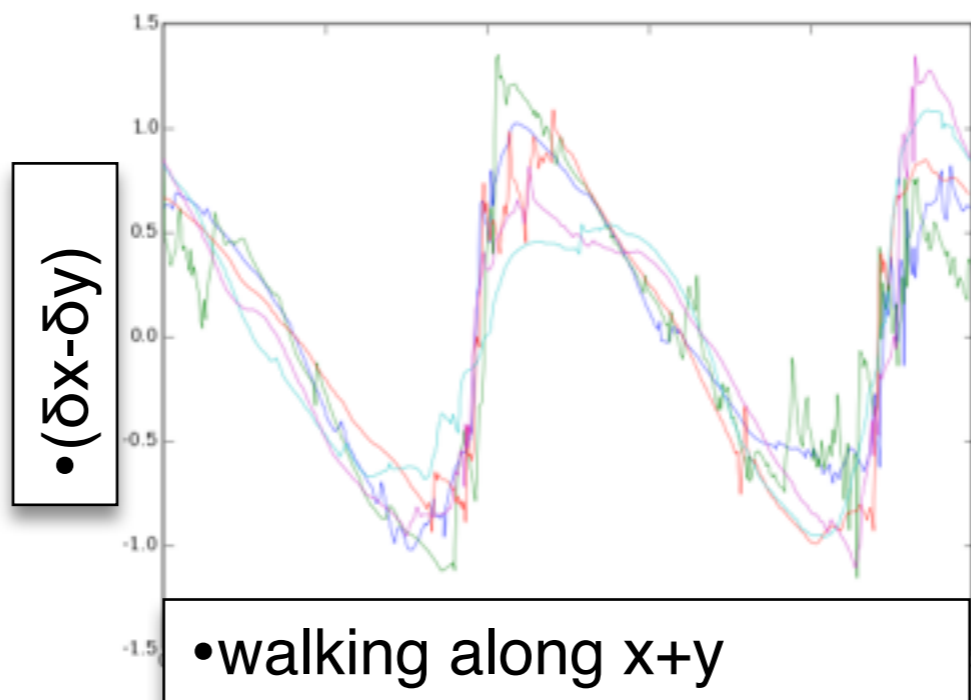
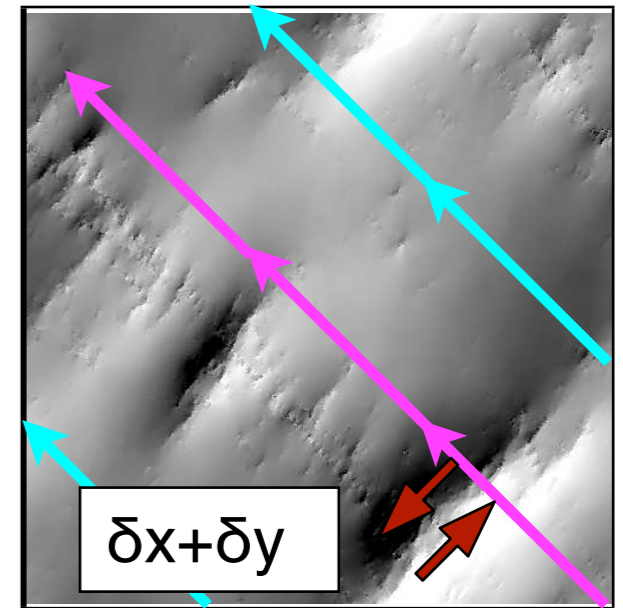
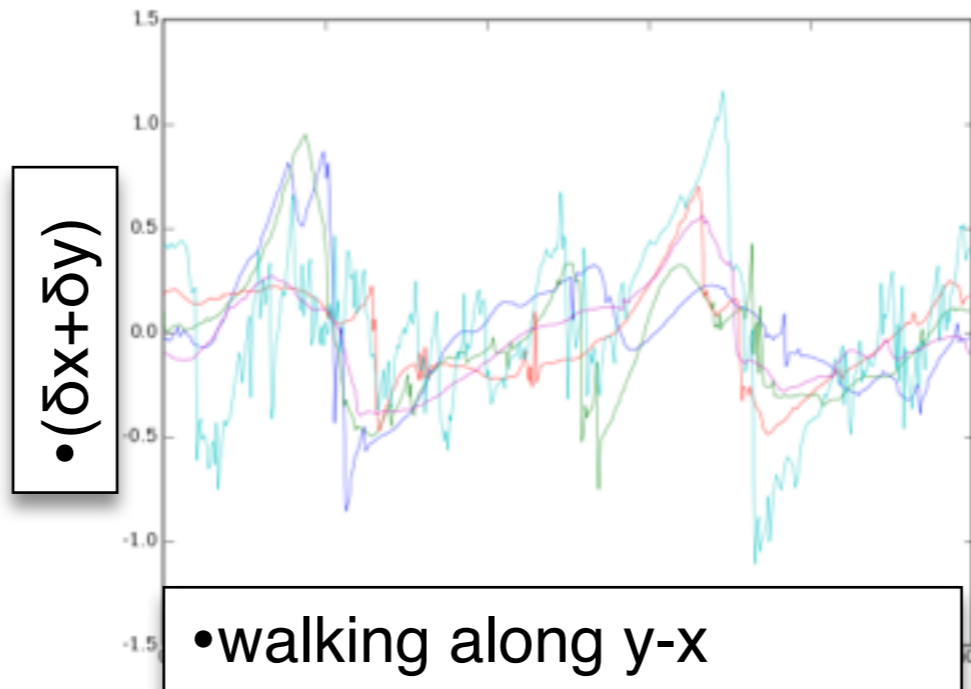
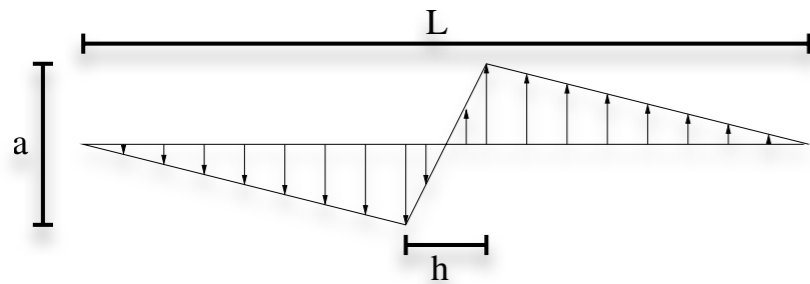
ω



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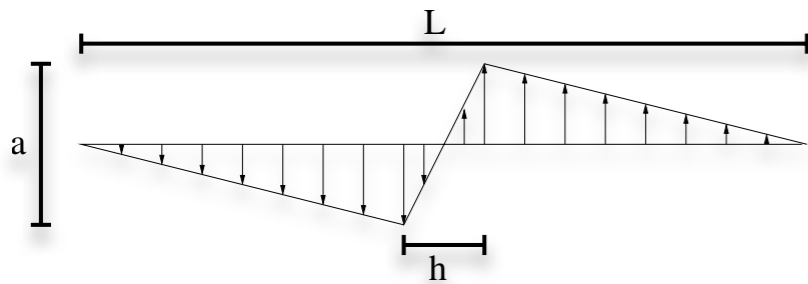
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Transverse displacement traces (6.1% -> 6.2%)



Transverse displacement traces (6.1% -> 6.2%)

$L \sim 1000\sigma_0$



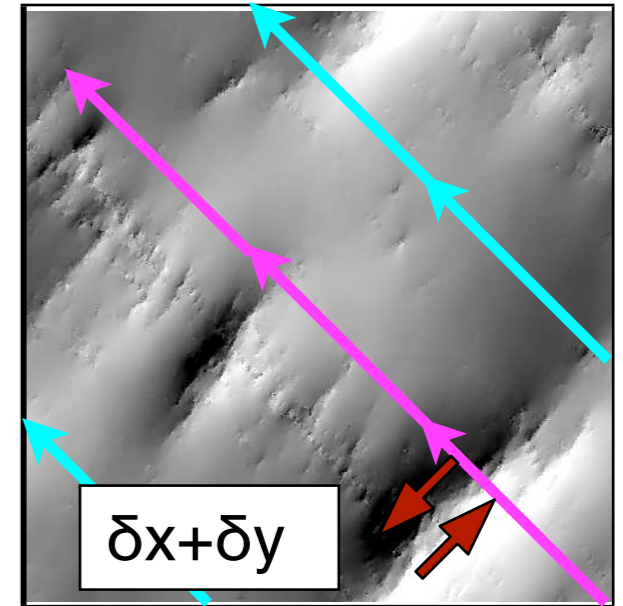
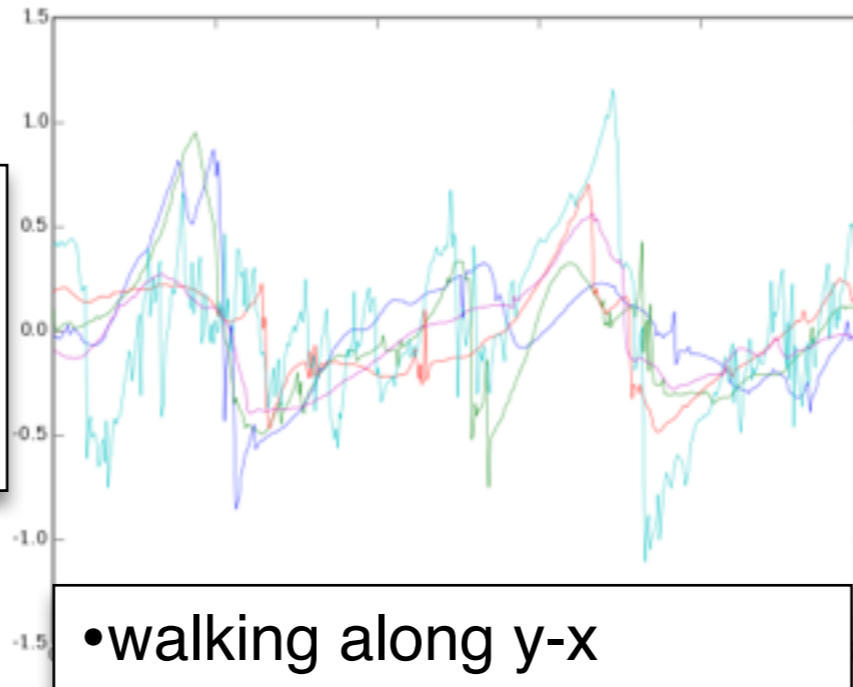
width, $h \sim 50\sigma_0$

strain in shear zone $\sim 2\%$ to 4%

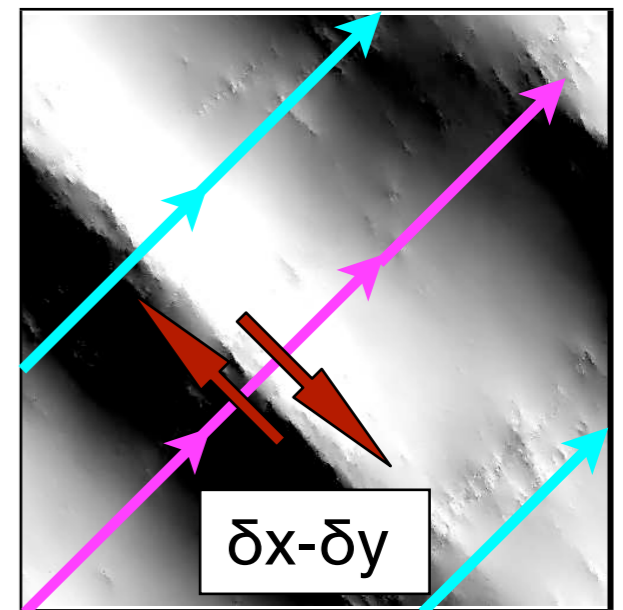
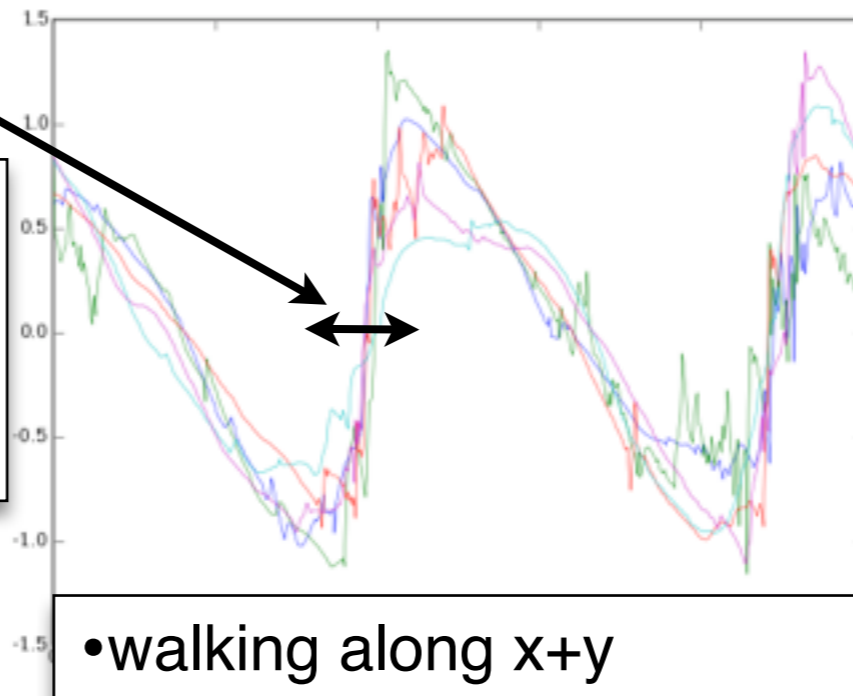
$a \sim 1$ to $2\sigma_0$

unloaded $\sim a/L \sim 0.1\%$ to 0.2% globally

$\bullet (\delta x + \delta y)$



$\bullet (\delta x - \delta y)$

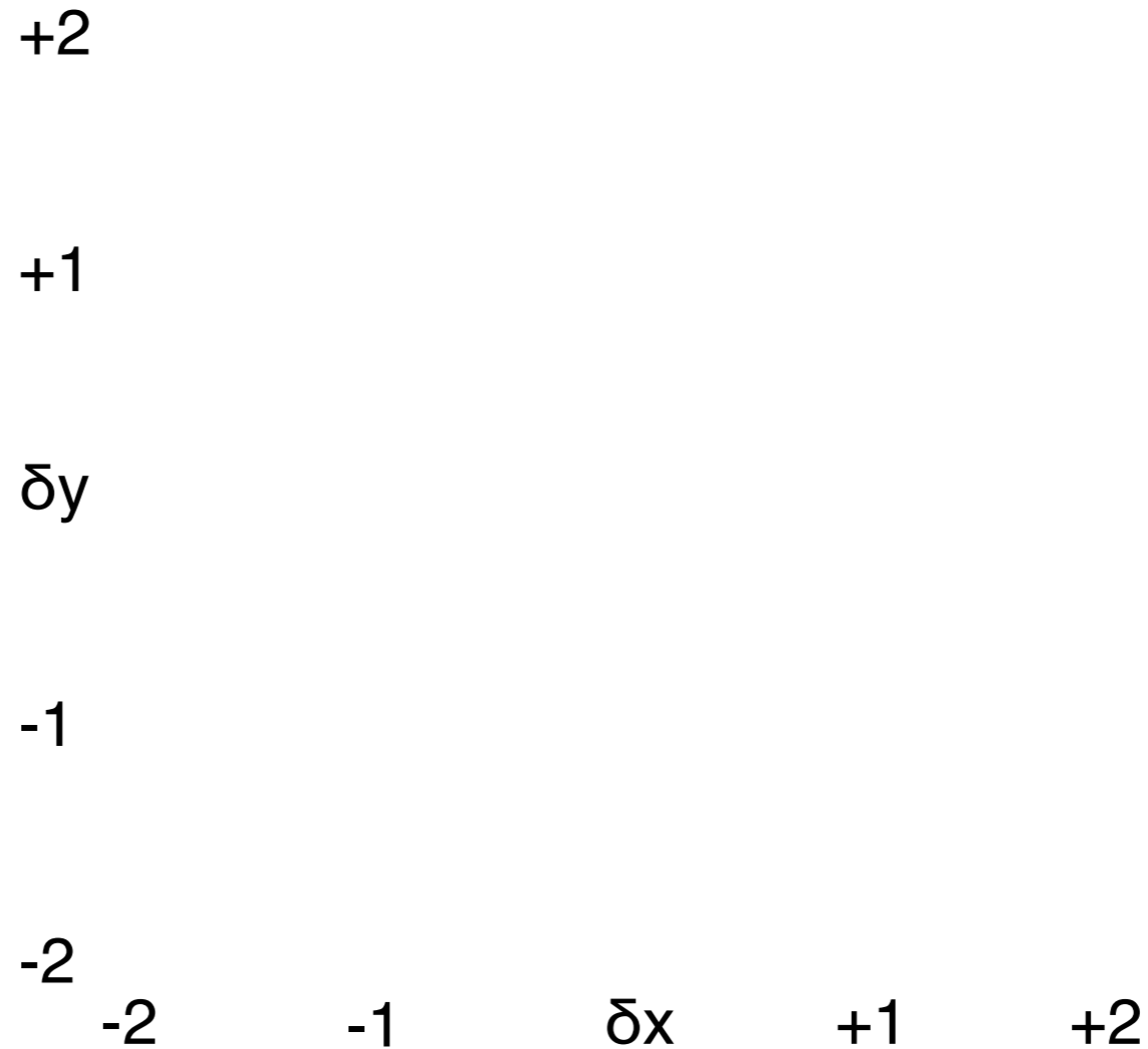


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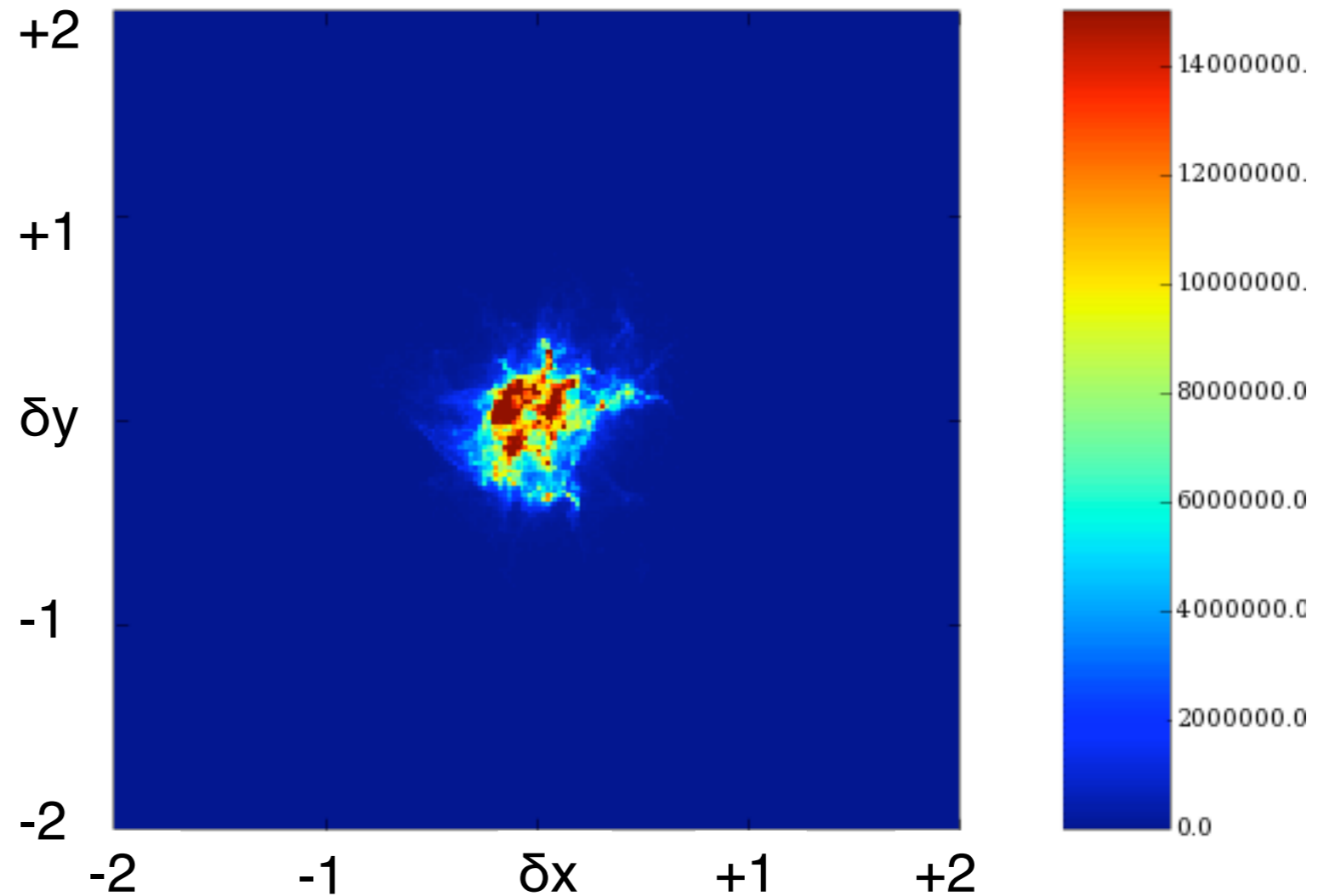
$P(\delta x, \delta y)$ for 8 consecutive $\Delta y = 0.001$ windows

- System is either:
 - active along $\delta x = \delta y$
 - active along $\delta x = -\delta y$
 - or quiescent



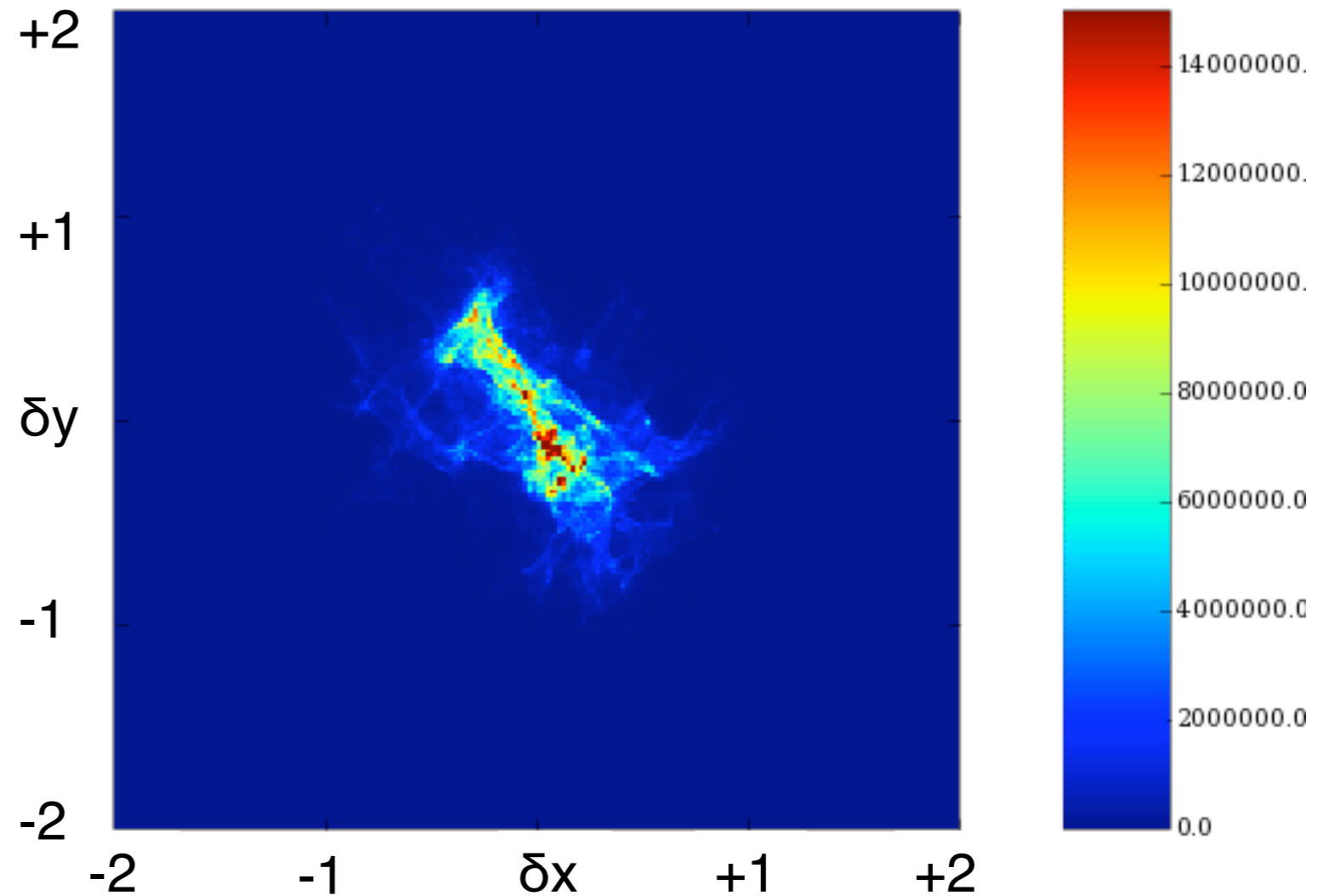
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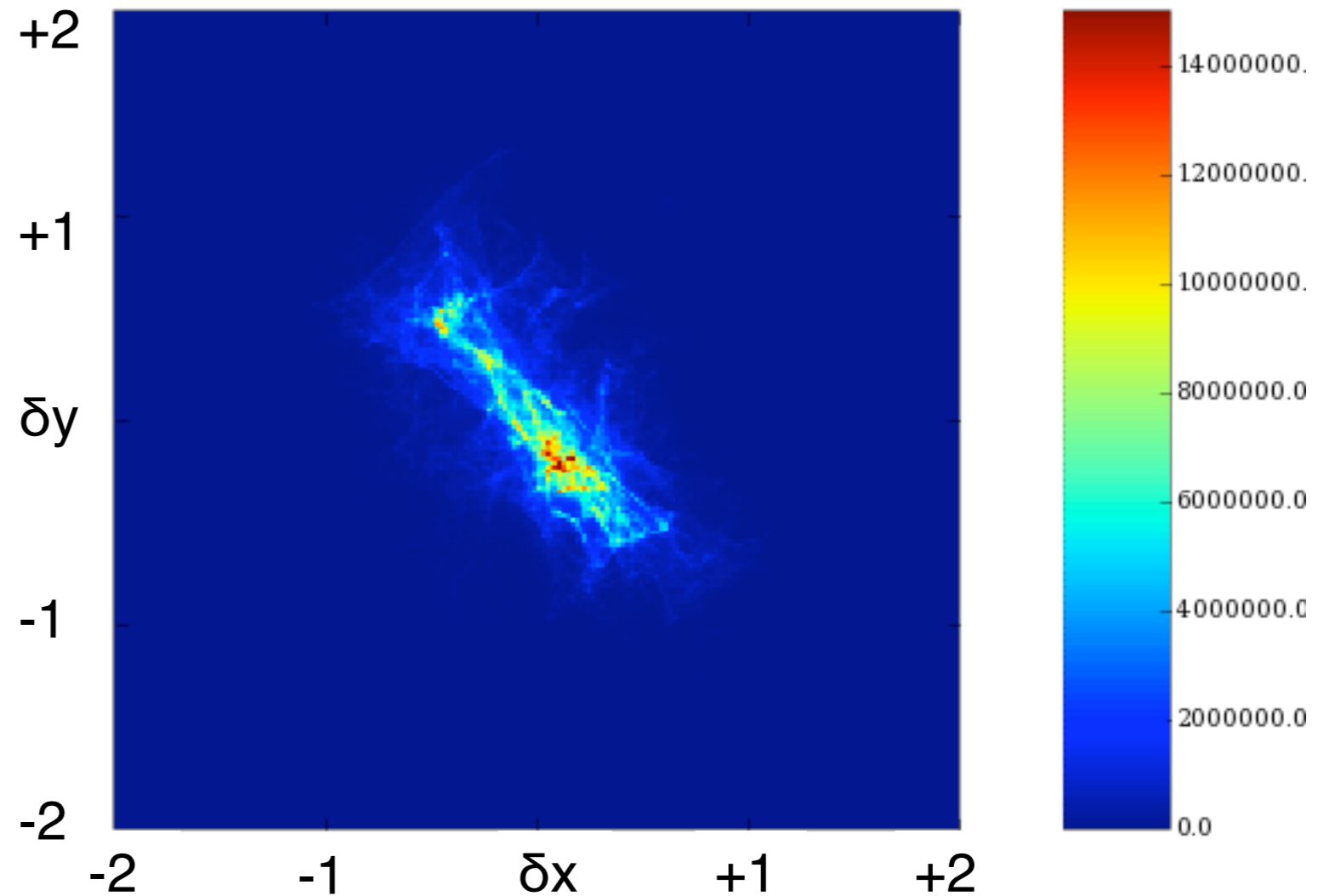
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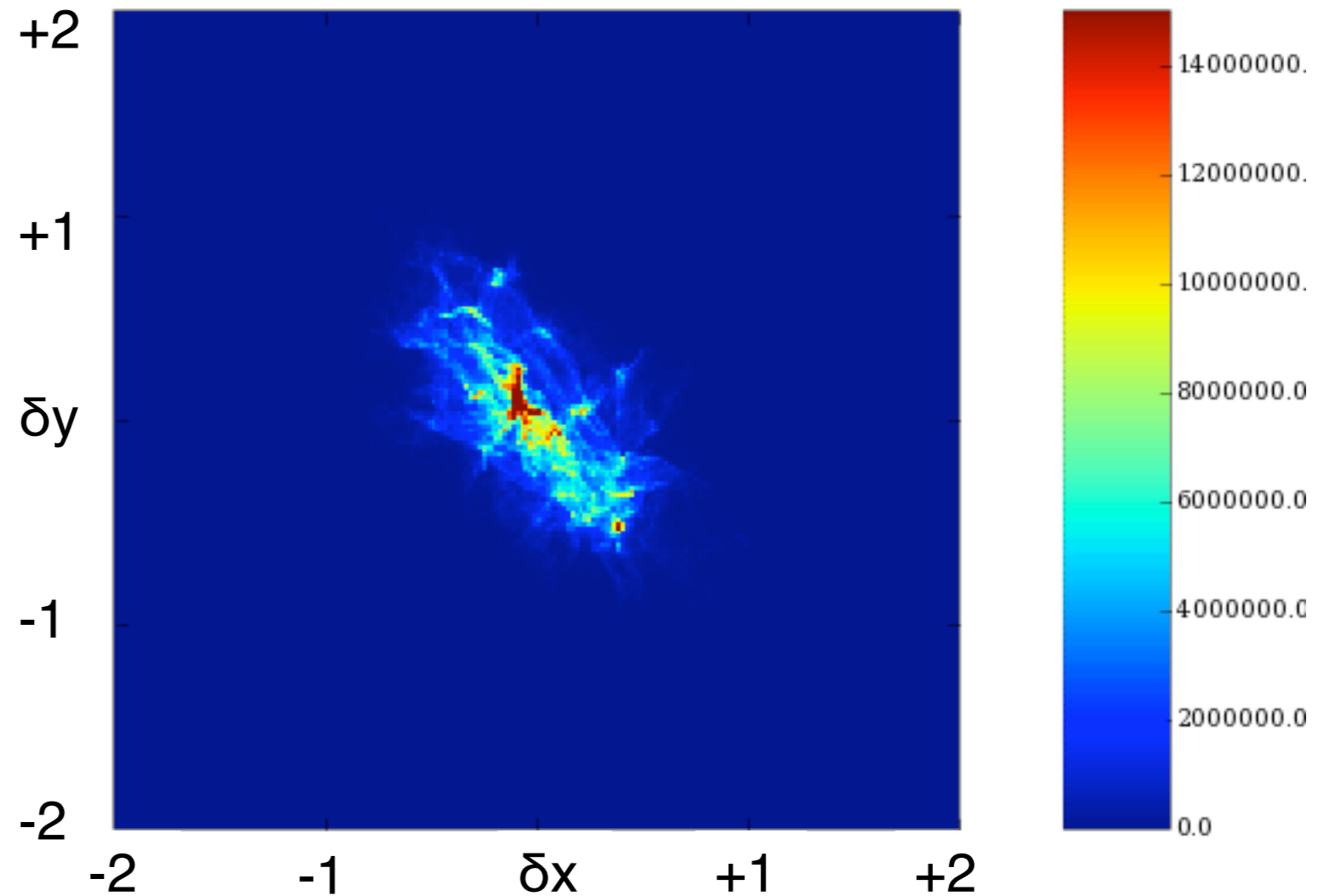
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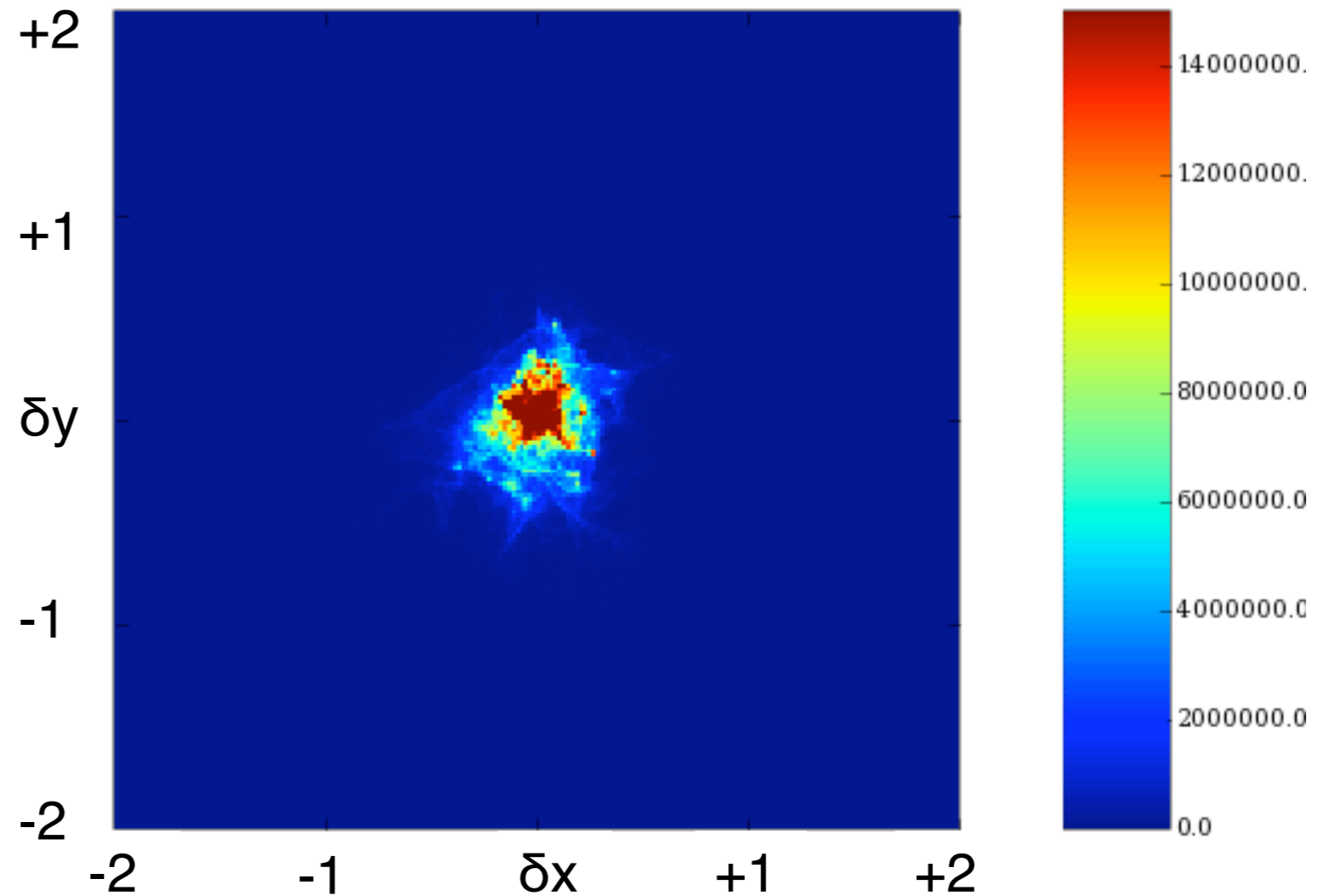
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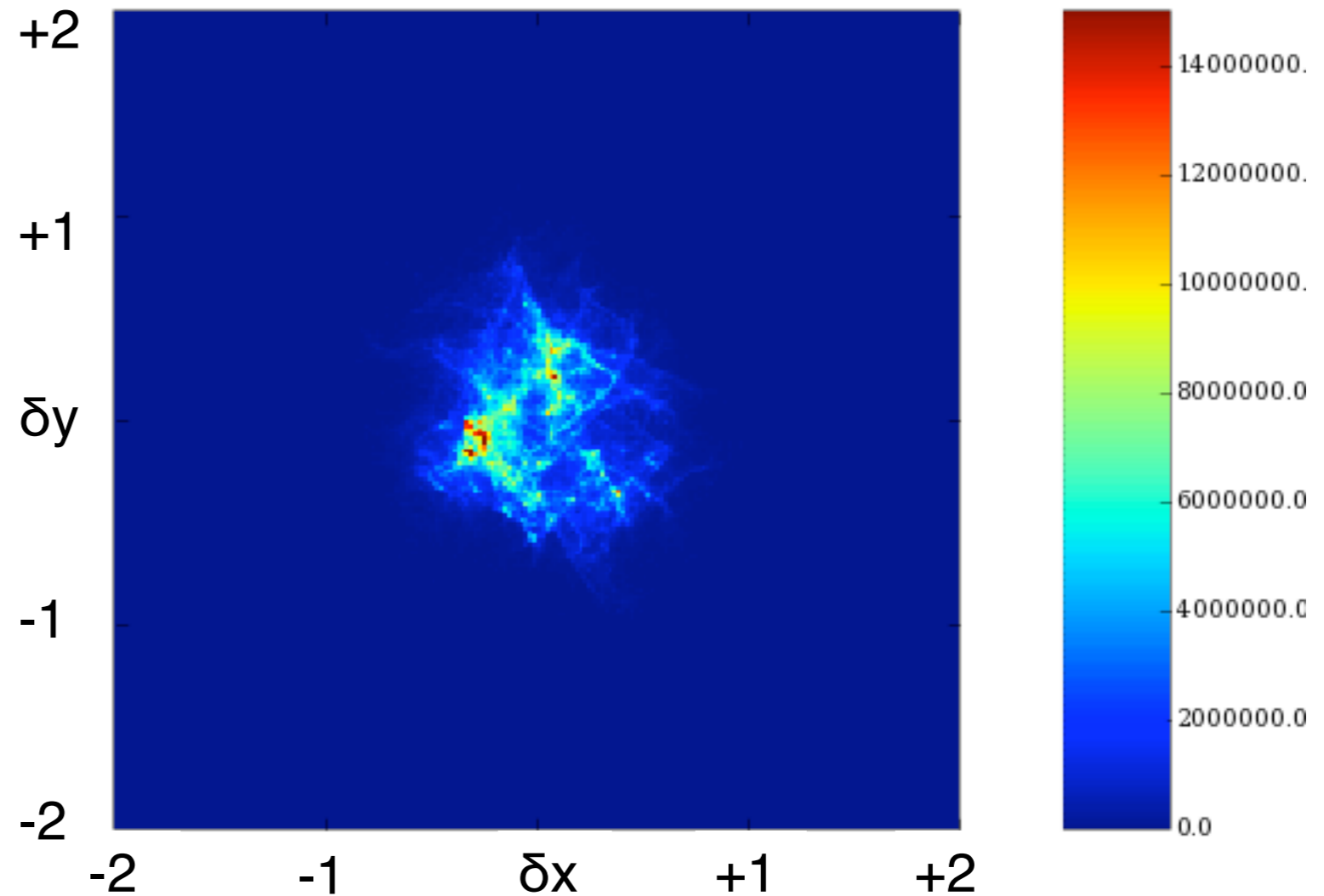
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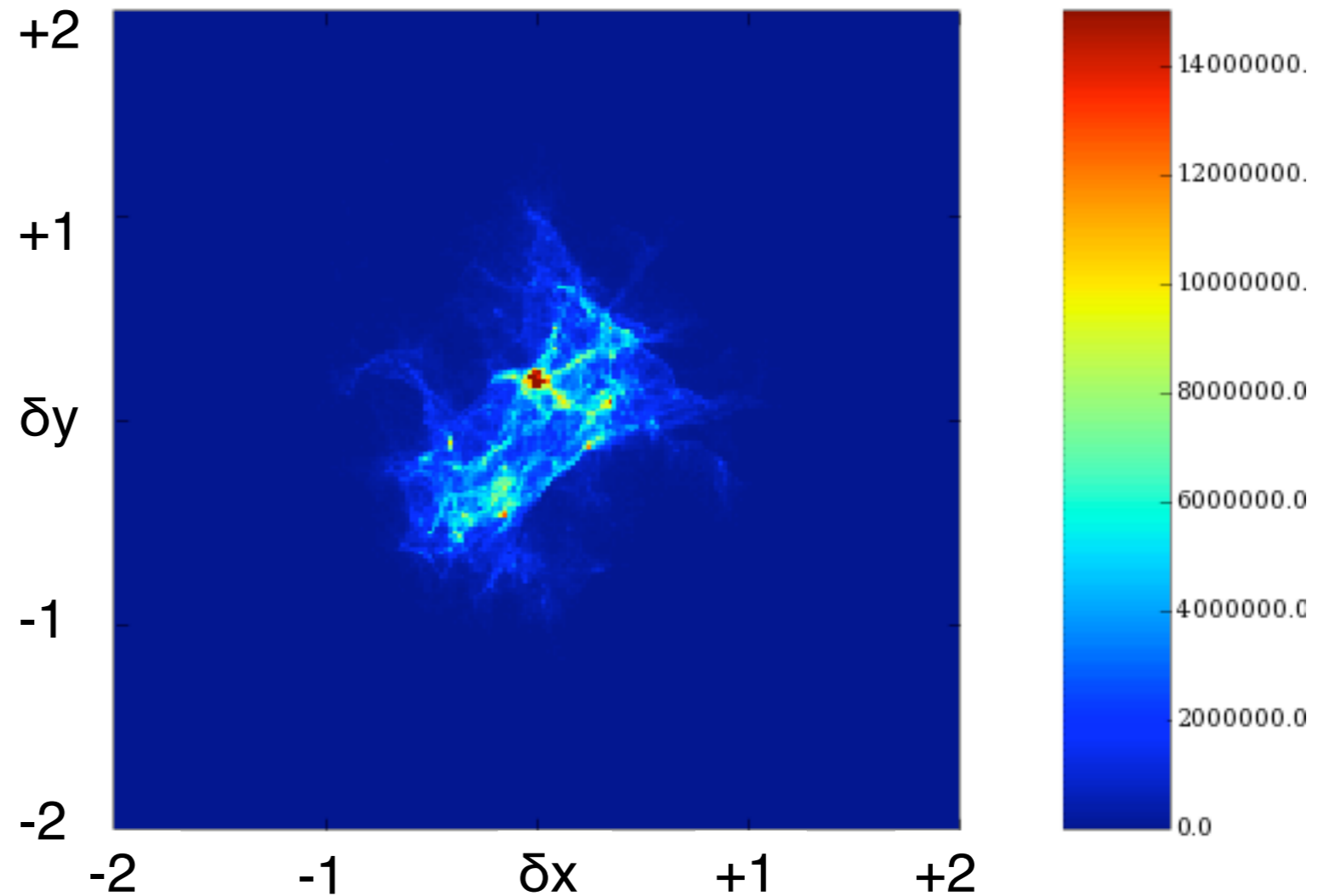
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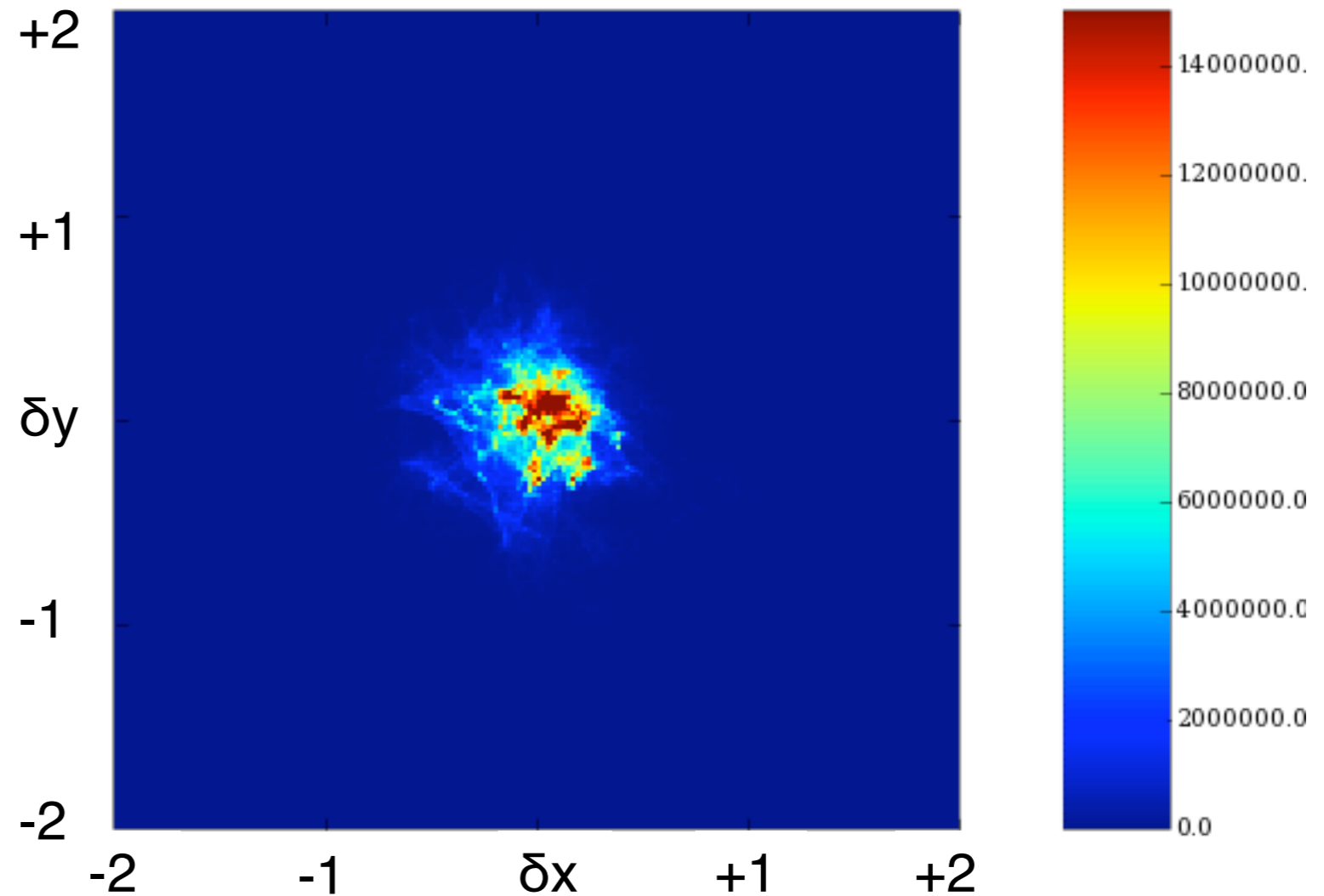
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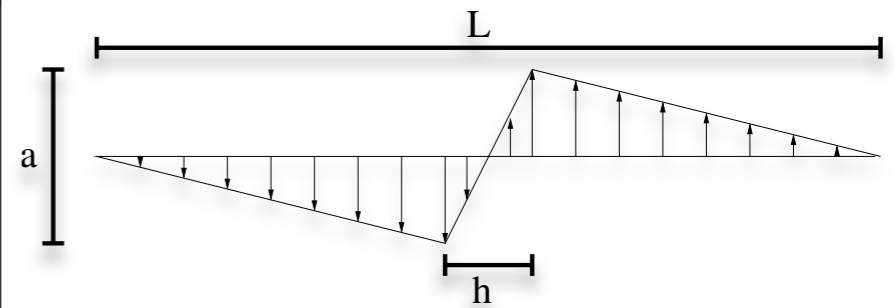
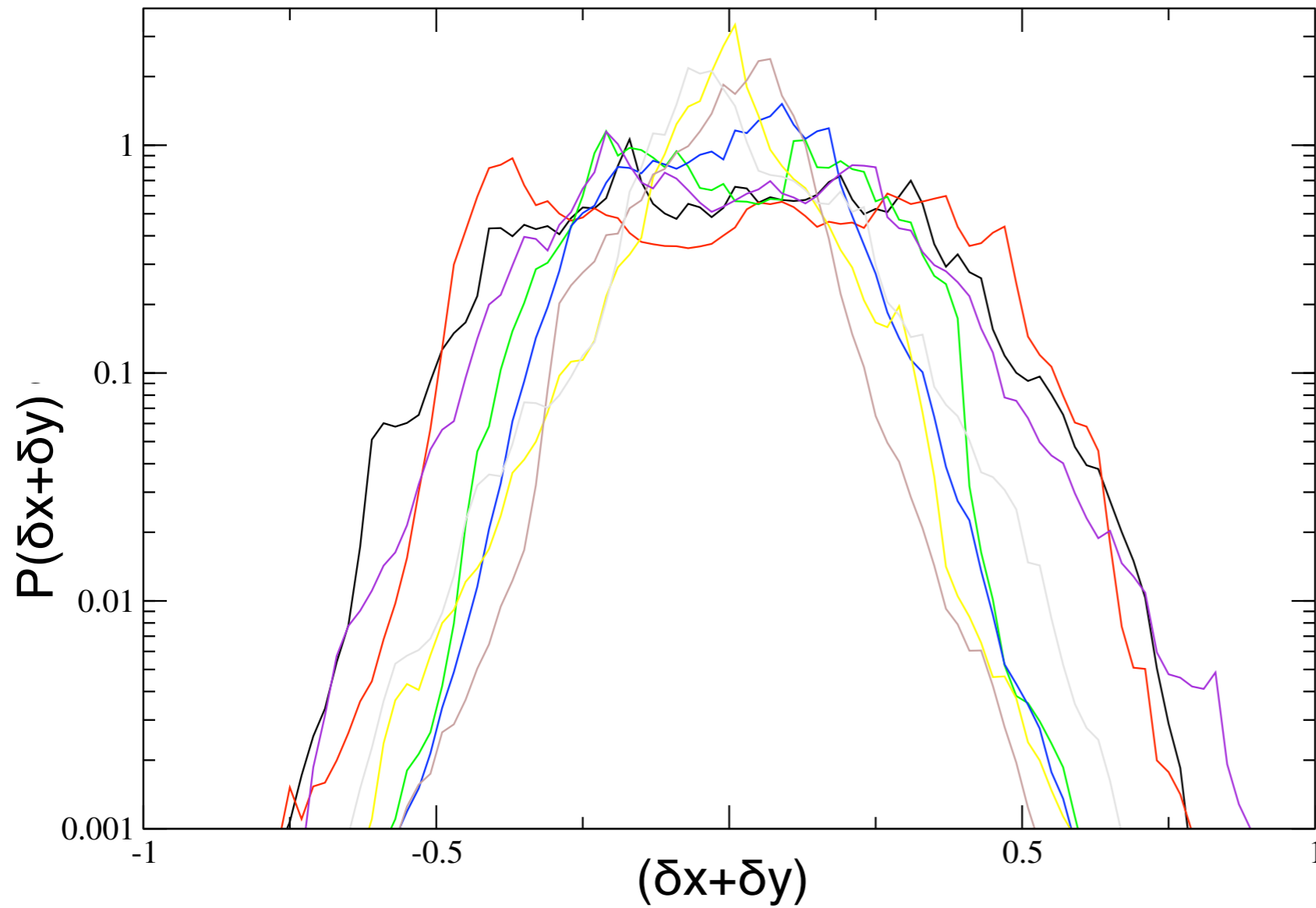


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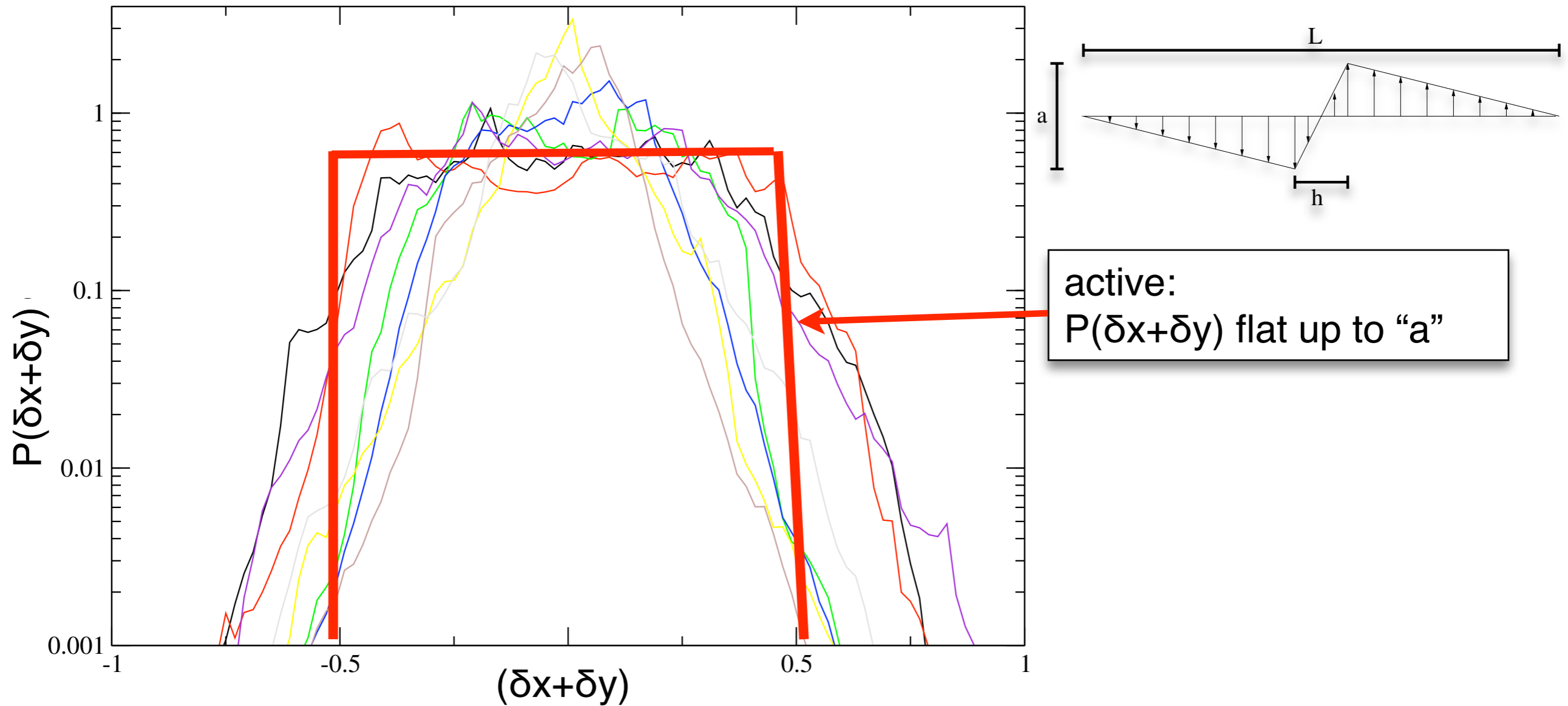
$P(\delta x + \delta y)$ for 8 consecutive $\Delta\gamma = 0.001$ windows



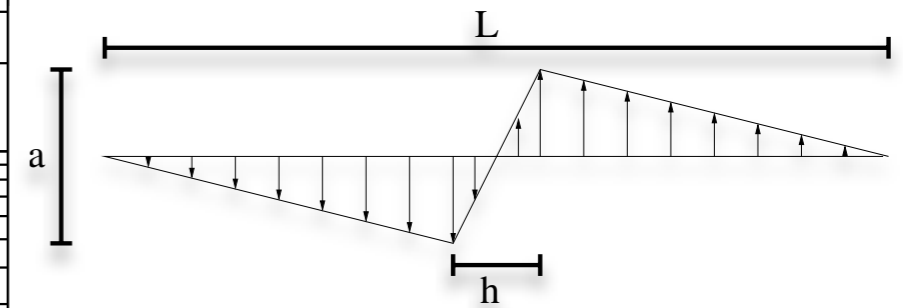
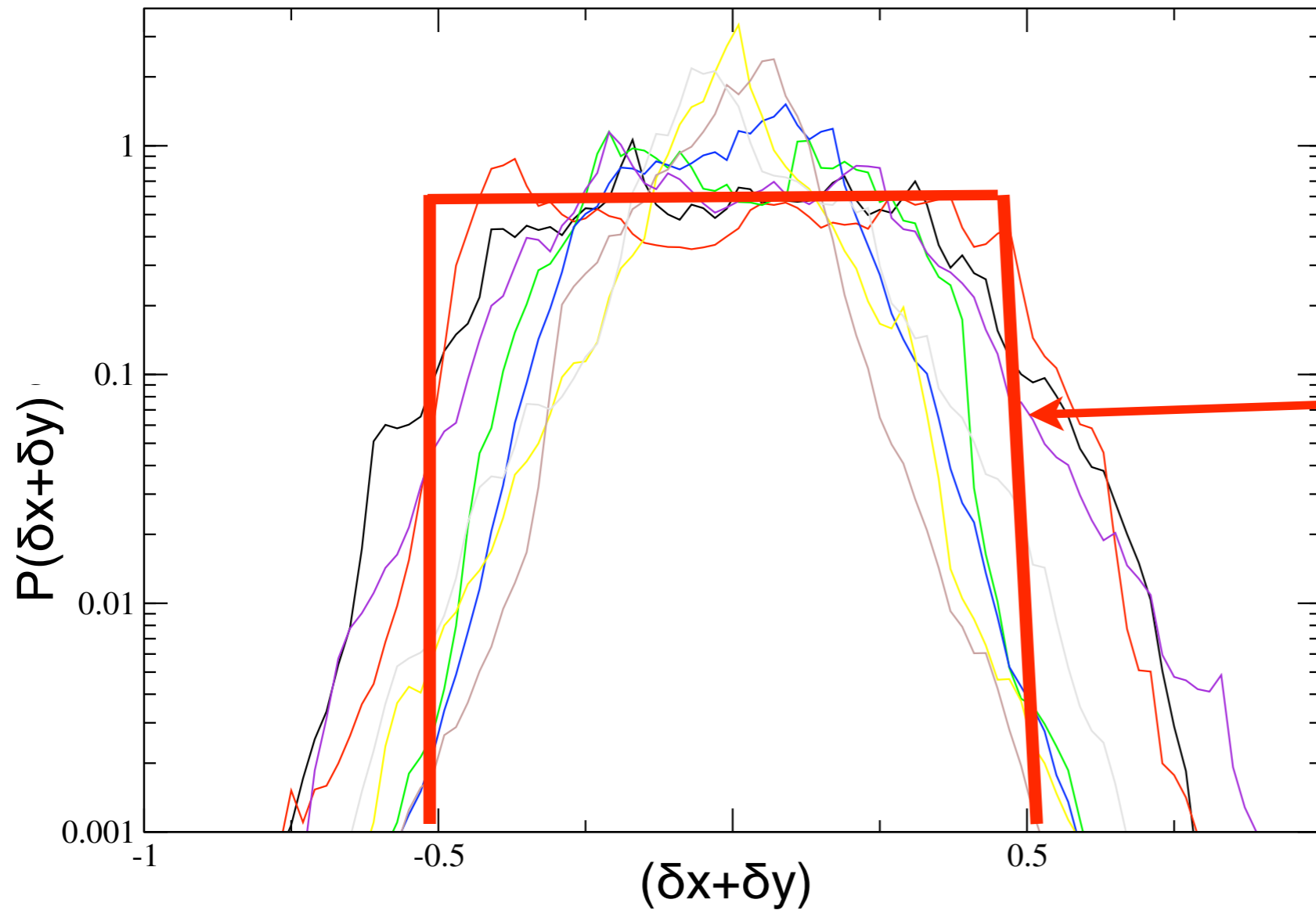
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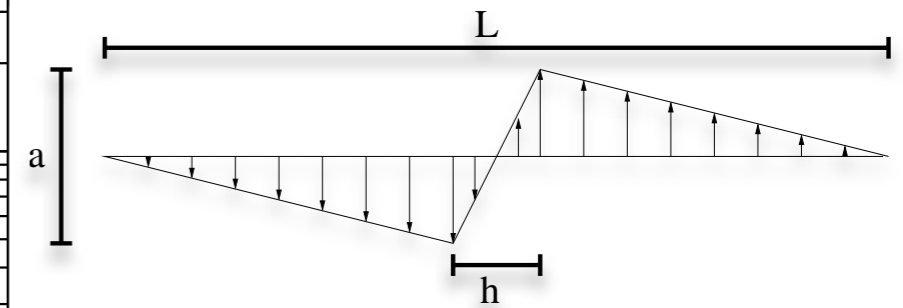
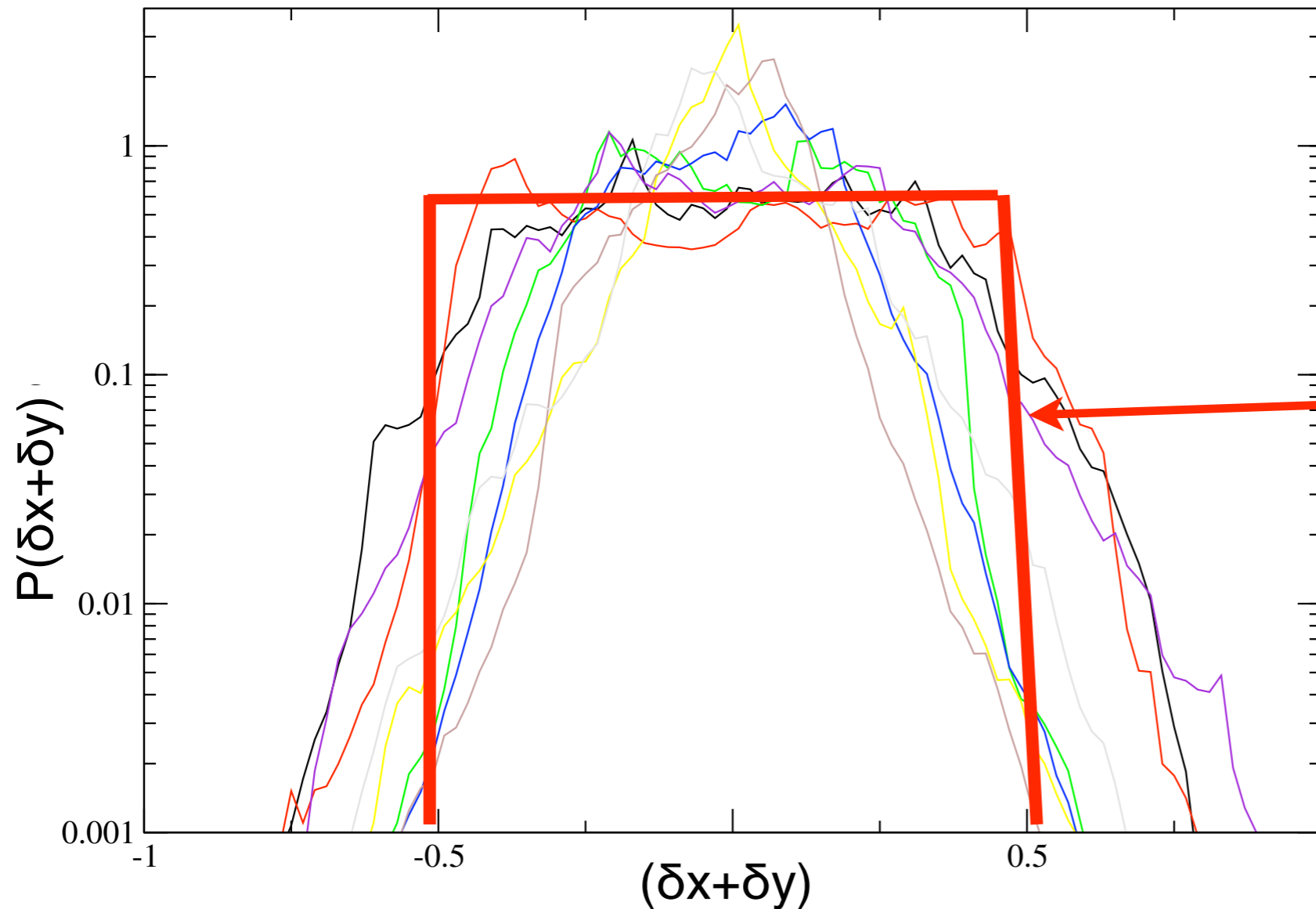
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active:
 $P(\delta x + \delta y)$ flat up to "a"

Elementary slip lines
have $\langle \Delta r^2 \rangle_{\text{elem.}} \sim a^2/12$

$P(\delta x + \delta y)$ for 8 consecutive $\Delta\gamma = 0.001$ windows

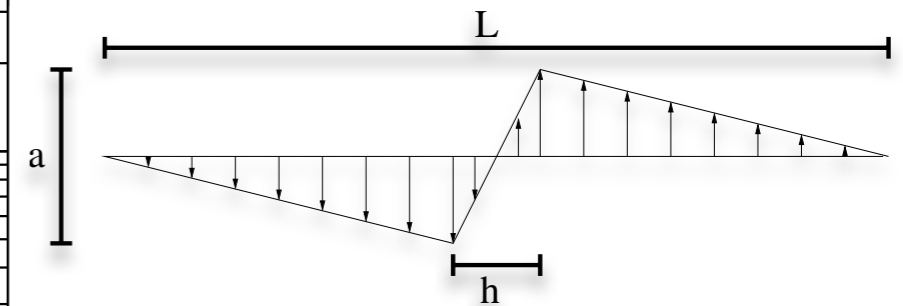
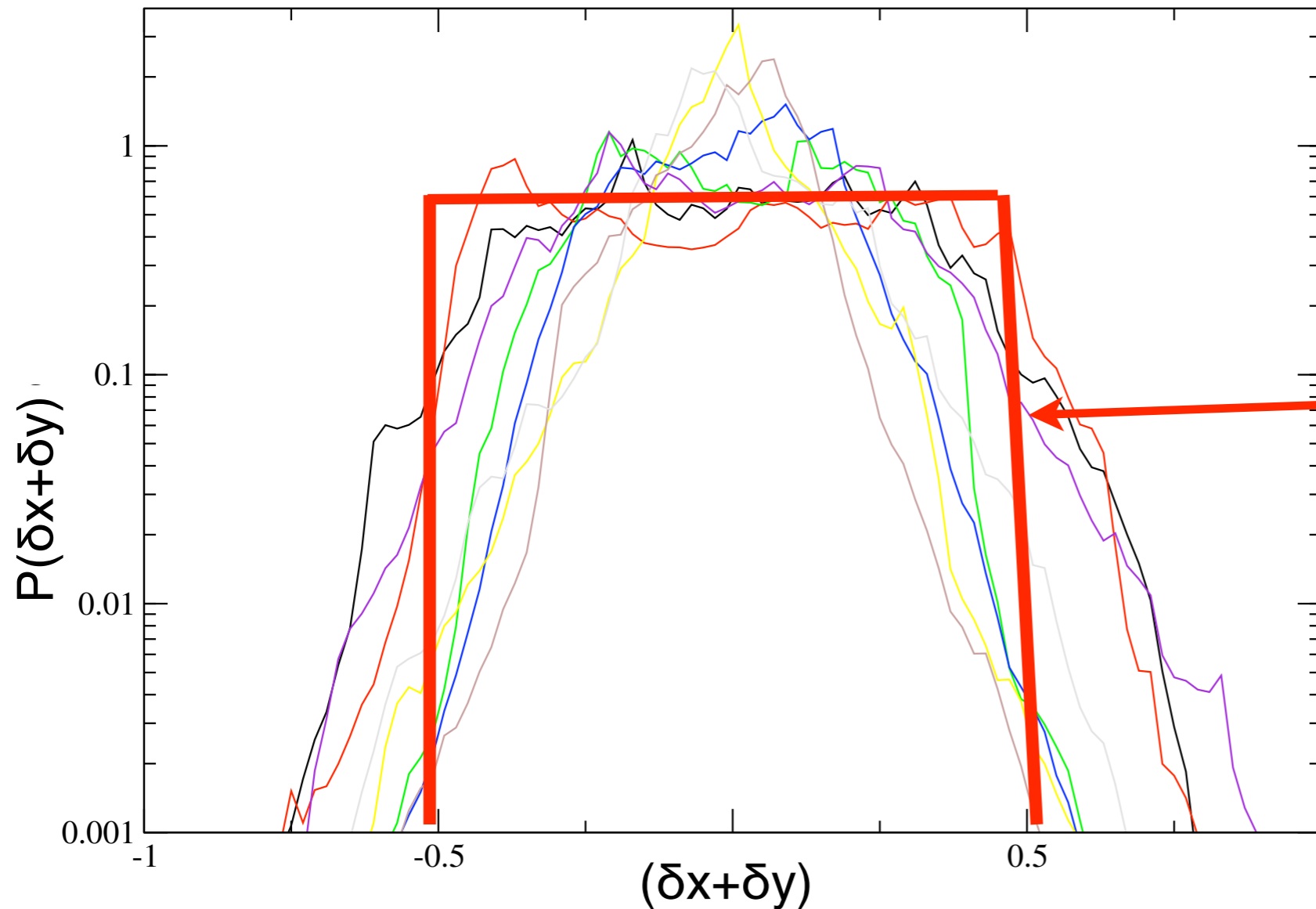


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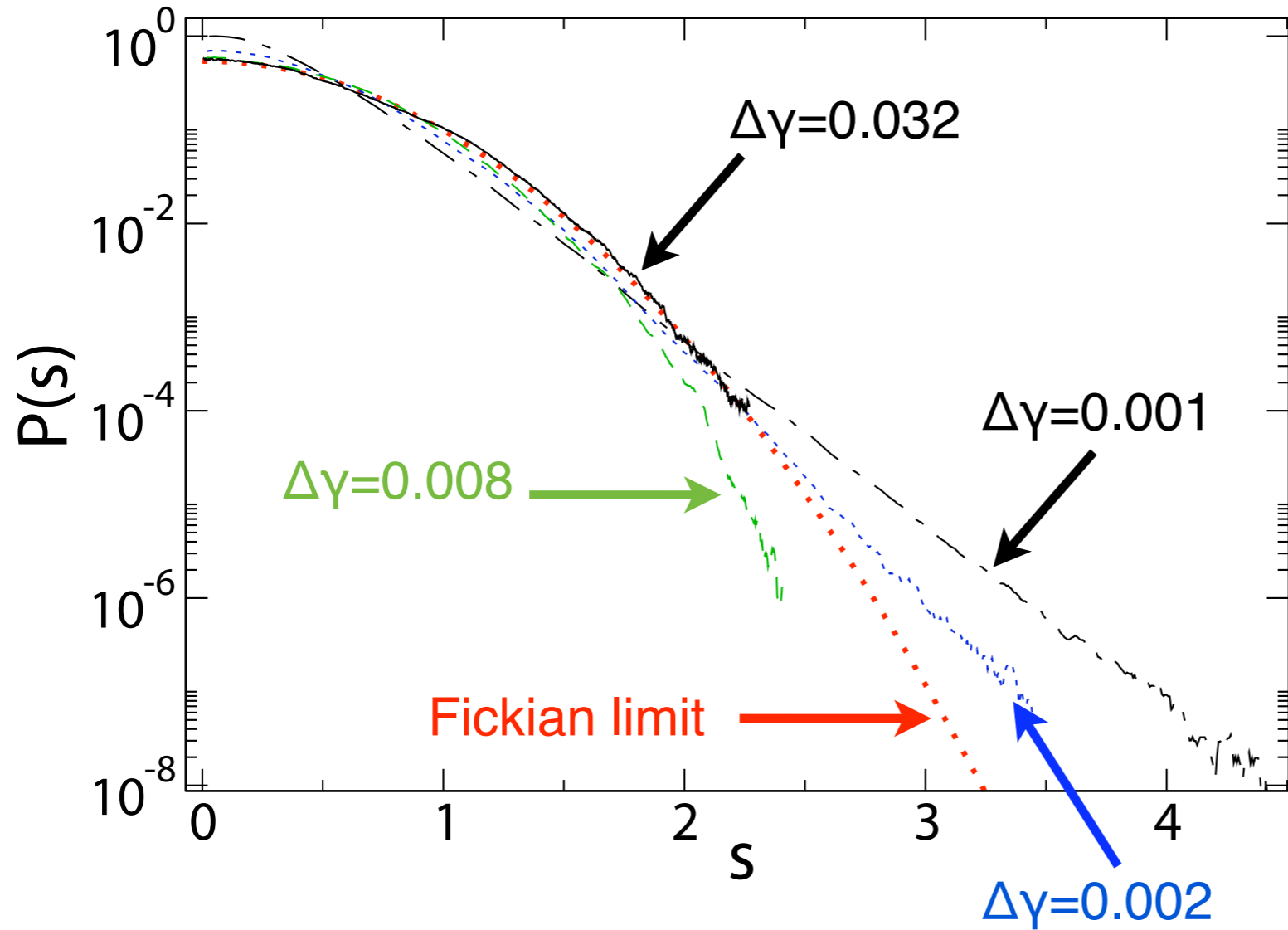
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 incoherently

$$\langle \Delta r^2 \rangle = \{N_{\text{events}}\} \{ \langle \Delta r^2 \rangle_{\text{elem.}} \} = \{ \Delta\gamma / (a/L) \} \{ a^2/12 \} = La/12 \Delta\gamma$$

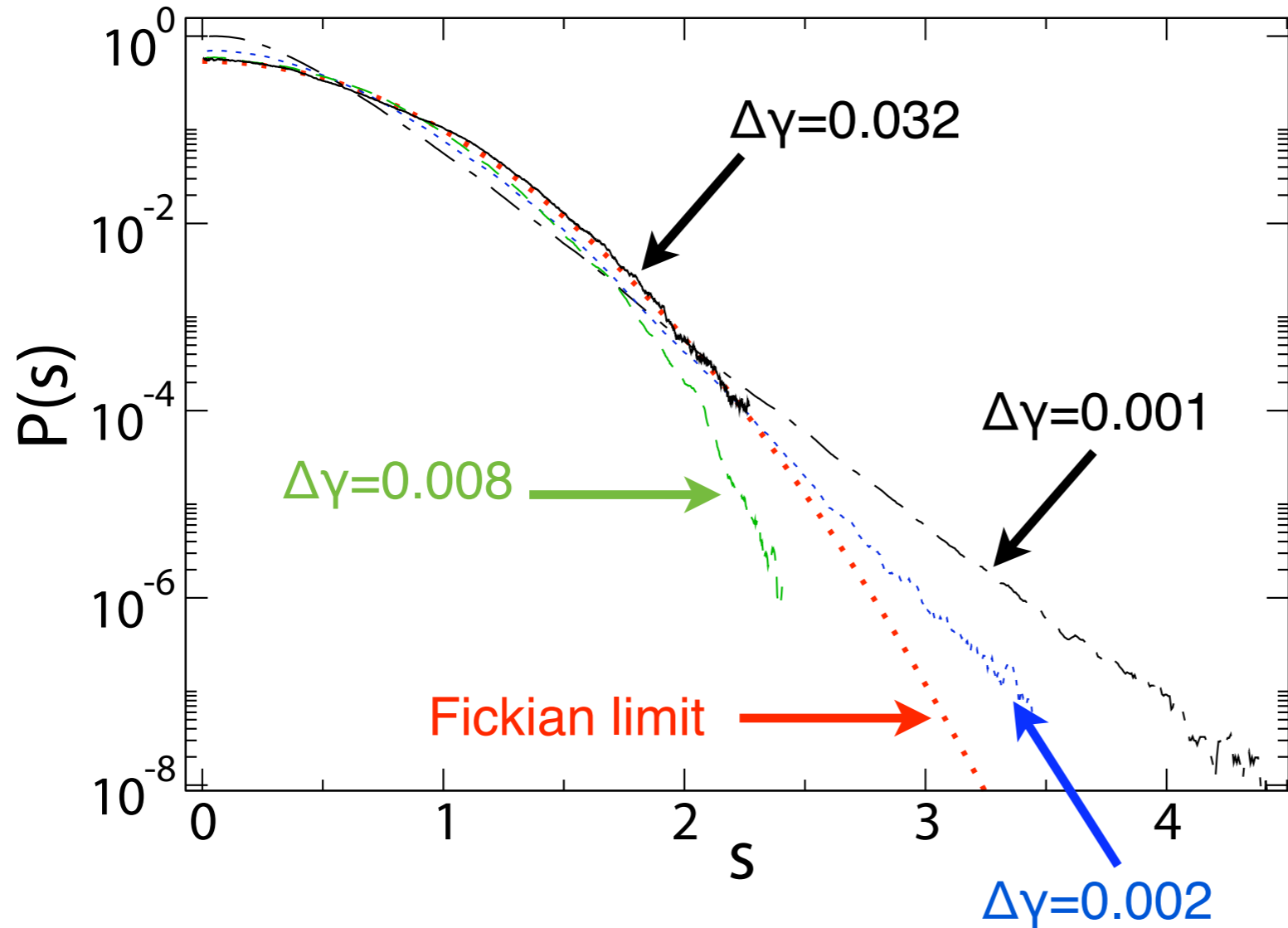
$P(\Delta r)$ for various $\Delta\gamma$



All distributions rescaled
by Fickian expectation:

$$s = \langle \Delta r^2 \rangle / \Delta\gamma$$

$P(\Delta r)$ for various $\Delta\gamma$



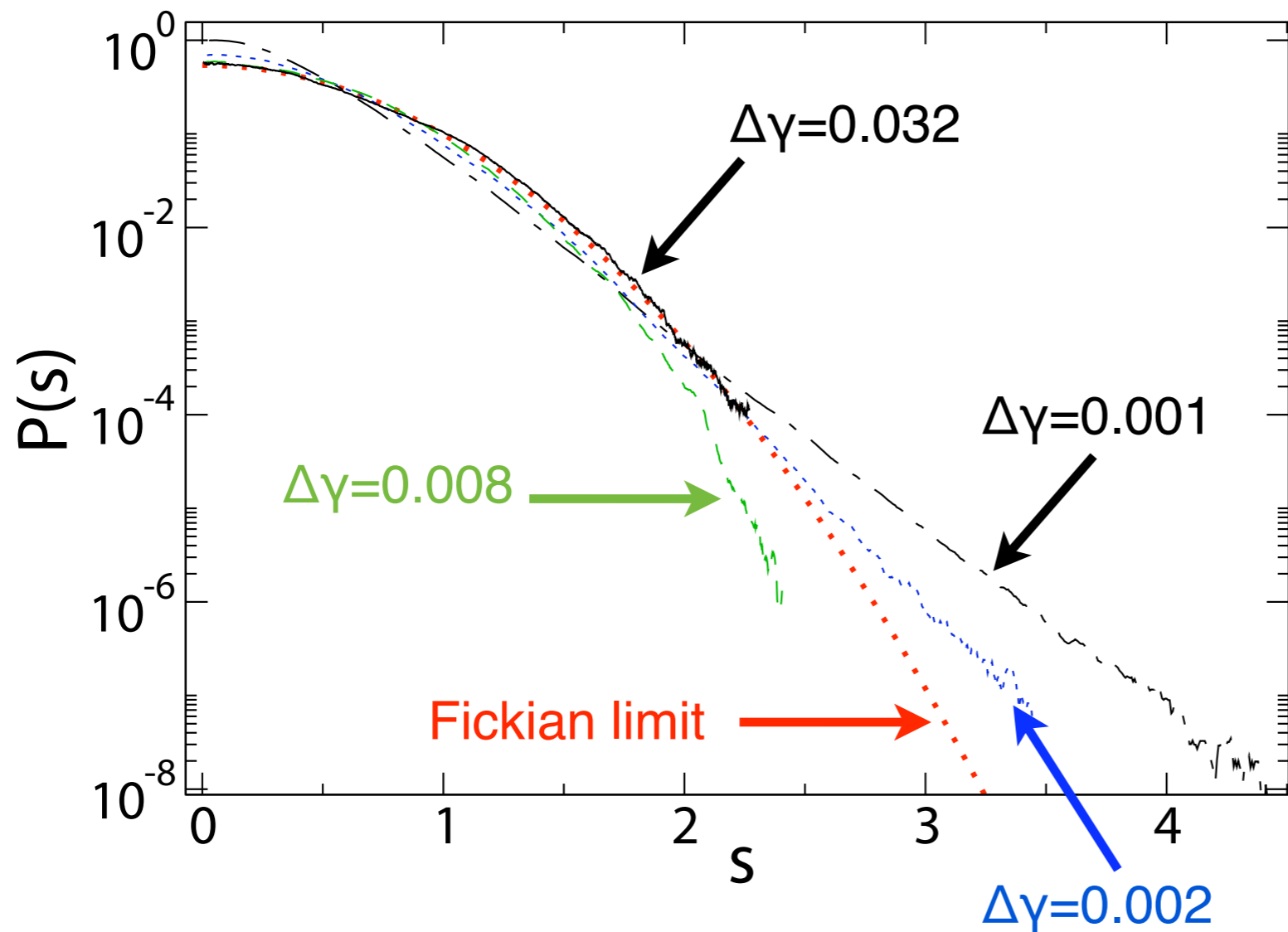
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Looks Fickian but:

- spatial correlations
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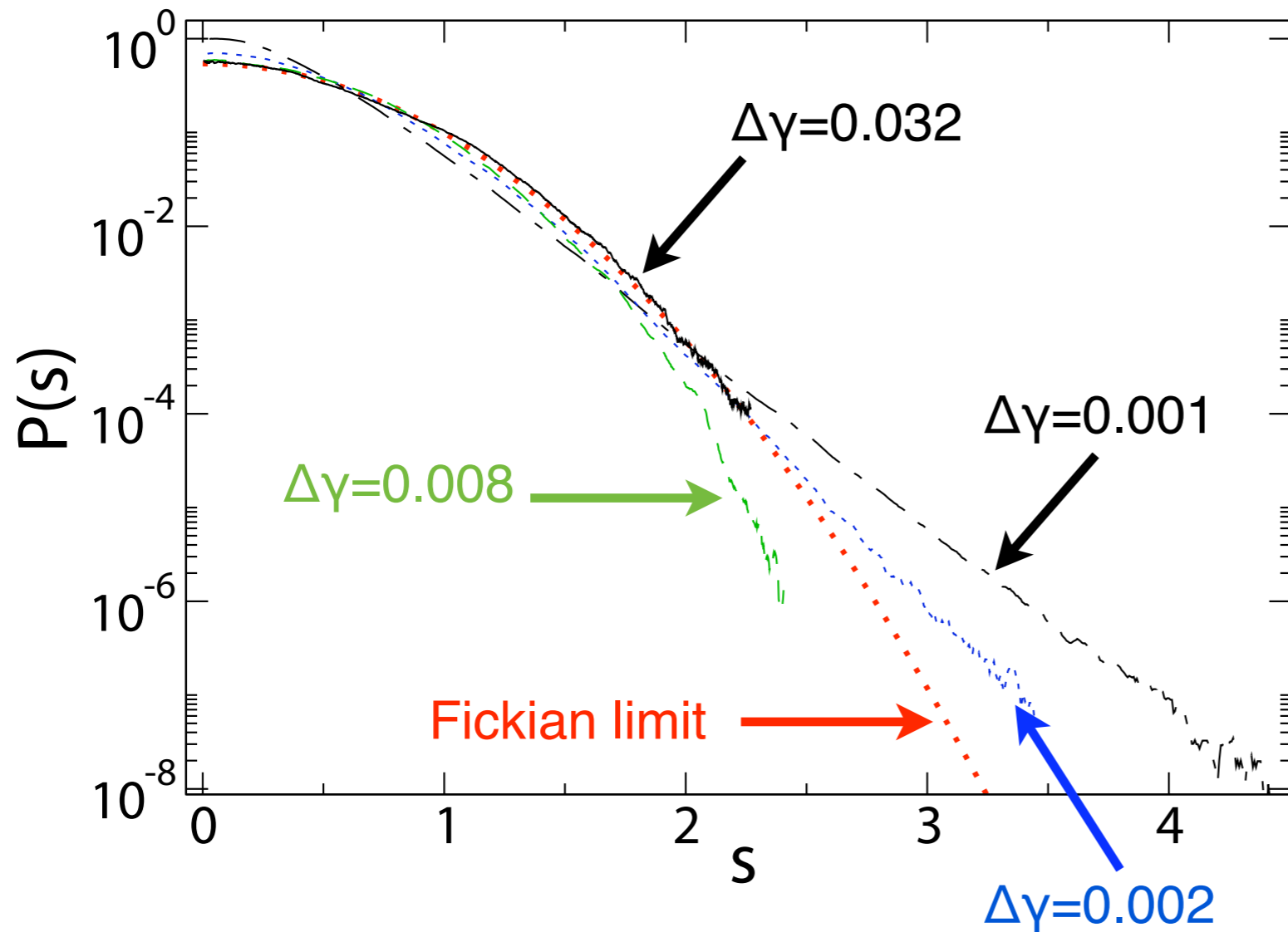
At $\Delta\gamma=0.001$, $P(\Delta r)$ is exponential for 7 decades!

Crossover to Fickian ($\Delta\gamma \sim 0.032$) consistent with thick bands filling space

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$P(\Delta r)$ for various $\Delta\gamma$



All distributions rescaled by Fickian expectation:

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Looks Fickian but:

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- $\langle \Delta r^2 \rangle / \Delta\gamma$ depends on L

• Slip line argument:

$$a = (12s/L) \sim 0.7\sigma_0$$

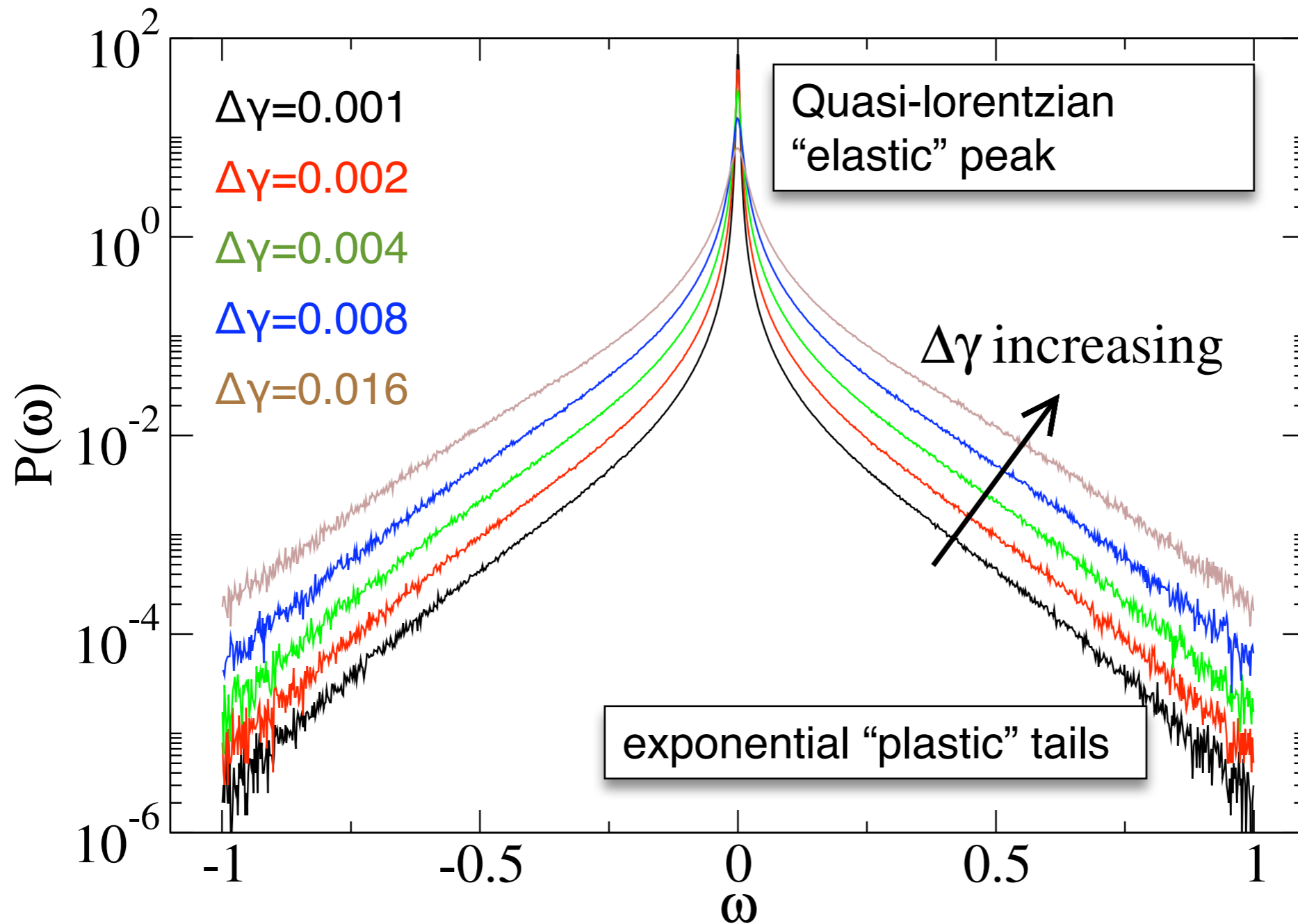
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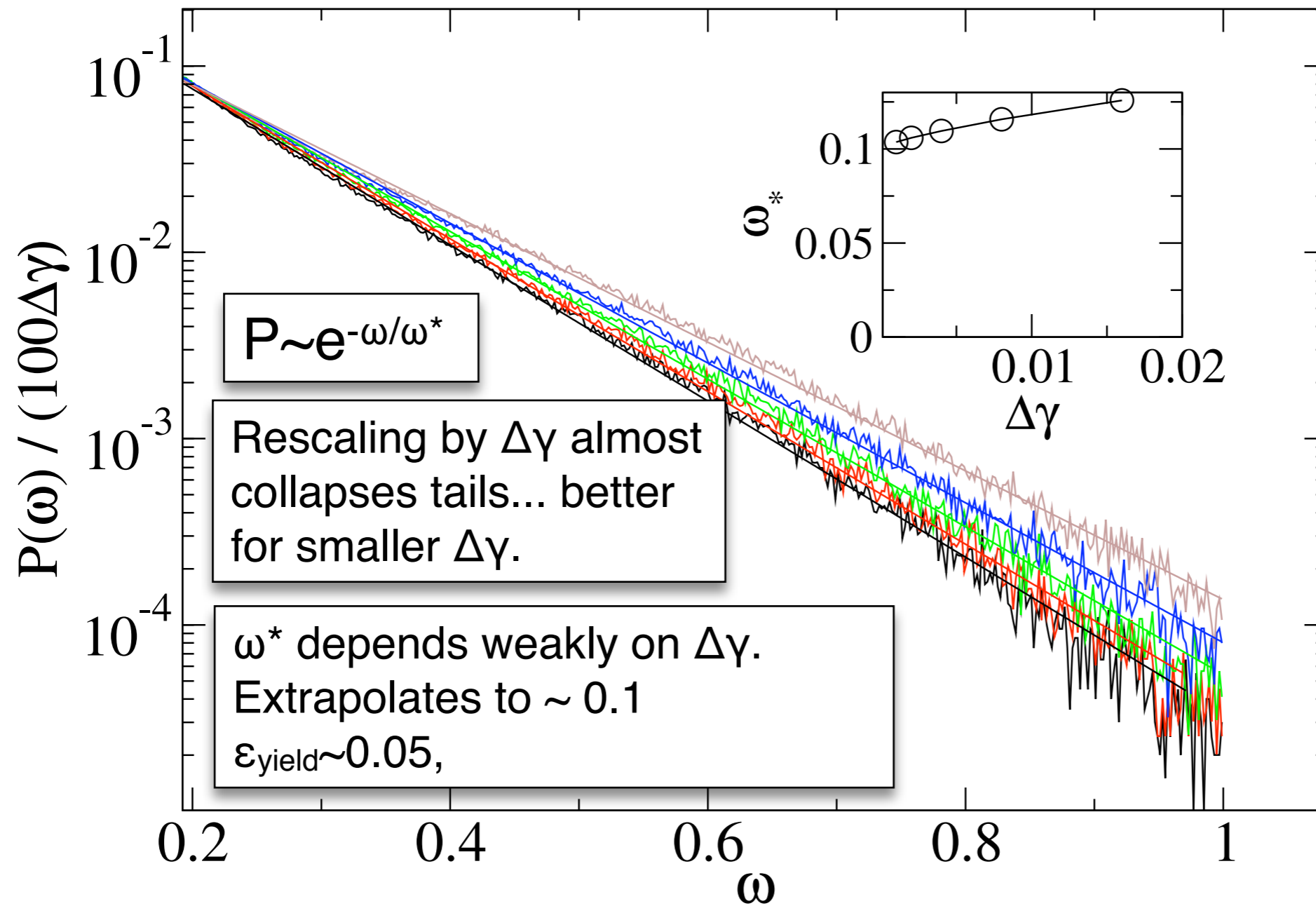
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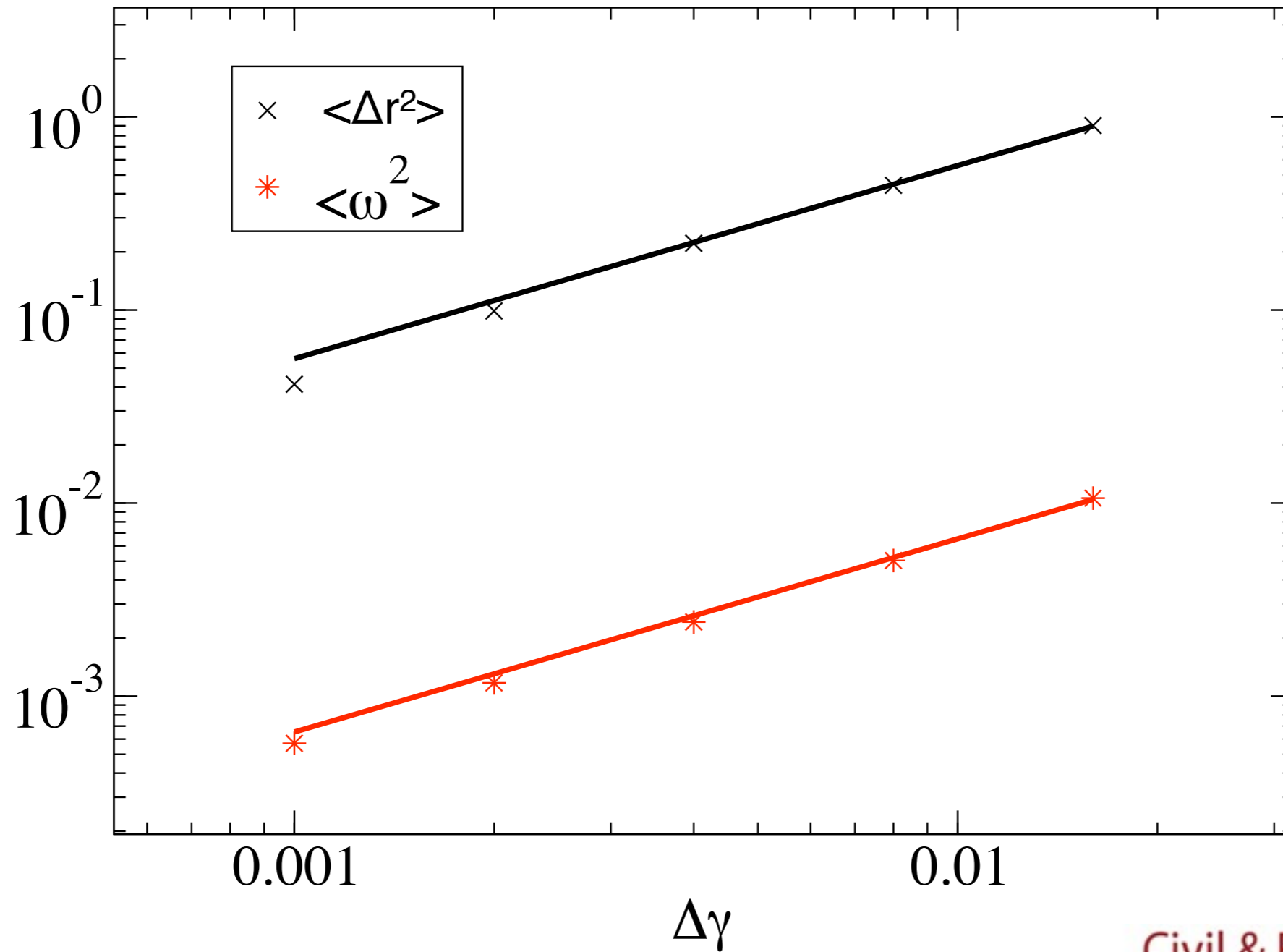
$P(\omega; \Delta\gamma)$



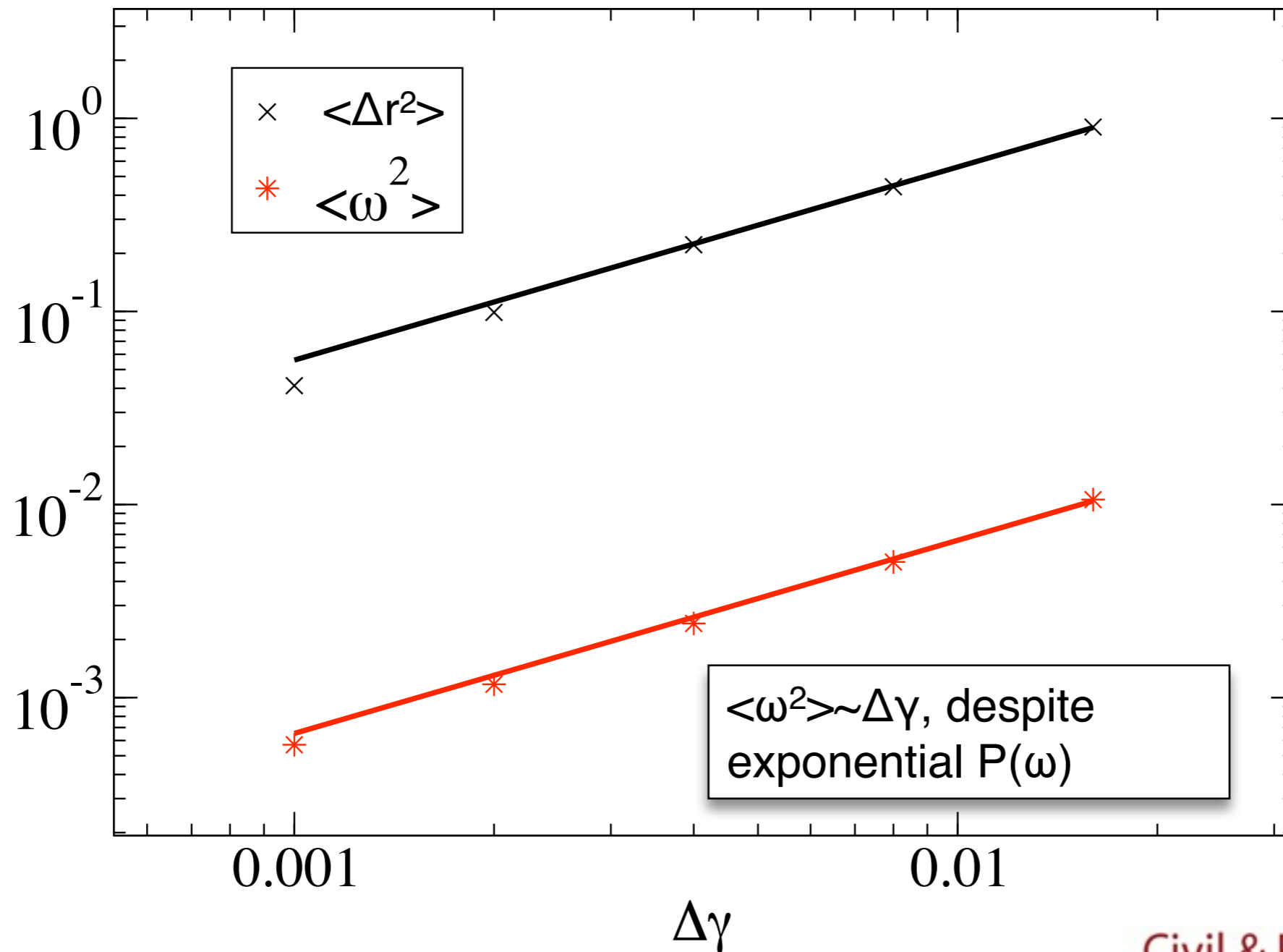
$P(\omega; \Delta\gamma)$. Scale by $\Delta\gamma$, fit to $e^{-\omega/\omega^*}$



RMS ω vs $\Delta\gamma$



RMS ω vs $\Delta\gamma$



Effective diffusion in Lennard-Jones

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Effective diffusion in Lennard-Jones

- Slip in bands: $a \sim \sigma_0$, $h \sim 50\sigma_0$, $\gamma_{\text{band}} \sim 1\%$ (for $L \sim 1000$)

Effective diffusion in Lennard-Jones

- Slip in bands: $a \sim \sigma_0$, $h \sim 50\sigma_0$, $\gamma_{\text{band}} \sim 1\%$ (for $L \sim 1000$)
- (**system size dependent**) “time” scale $\Delta\gamma = a/L \sim 1/1000 \sim 0.001$

Effective diffusion in Lennard-Jones

- Slip in bands: $a \sim \sigma_0$, $h \sim 50\sigma_0$, $\gamma_{\text{band}} \sim 1\%$ (for $L \sim 1000$)
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- A flat “elementary” $P(\Delta r)$ gives: $D_{\text{eff}} = \langle \Delta r^2 \rangle / \Delta\gamma = (La/12)$

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- $P(\Delta r^2)$ Gaussian at $\Delta\gamma \sim 0.032$

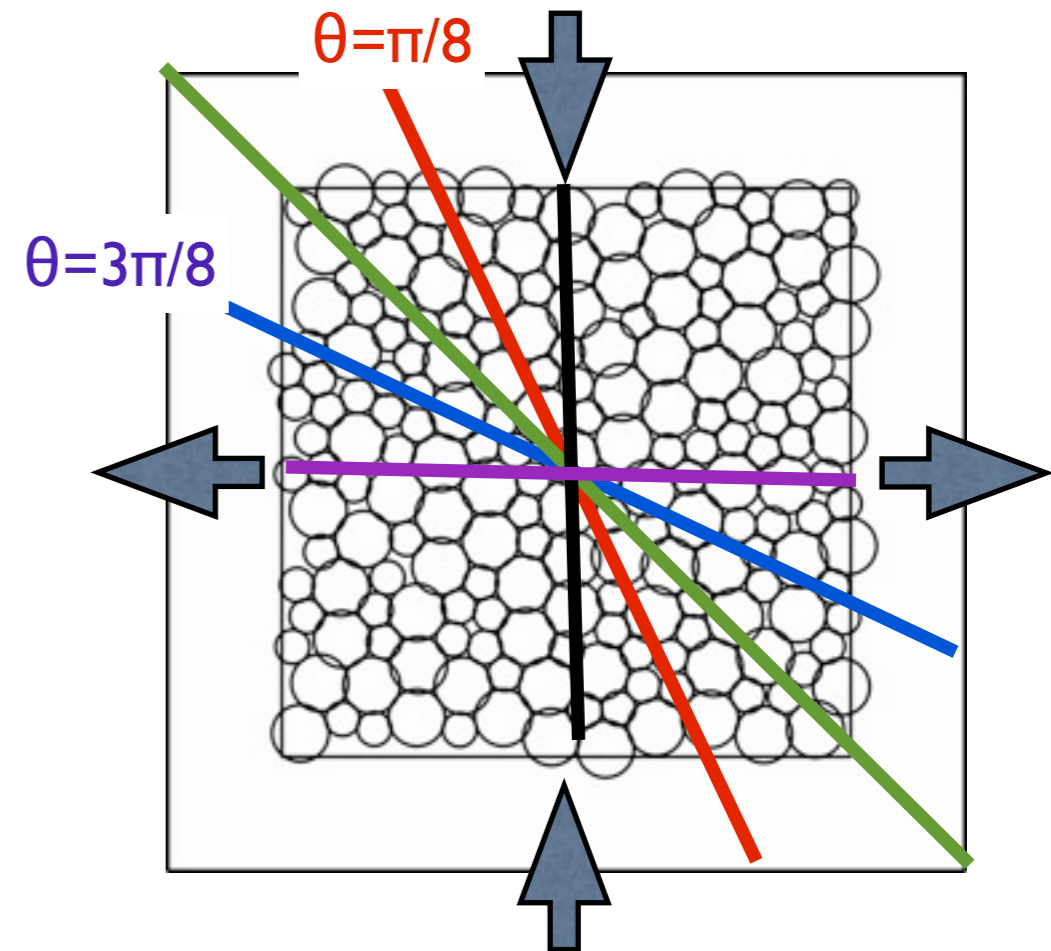
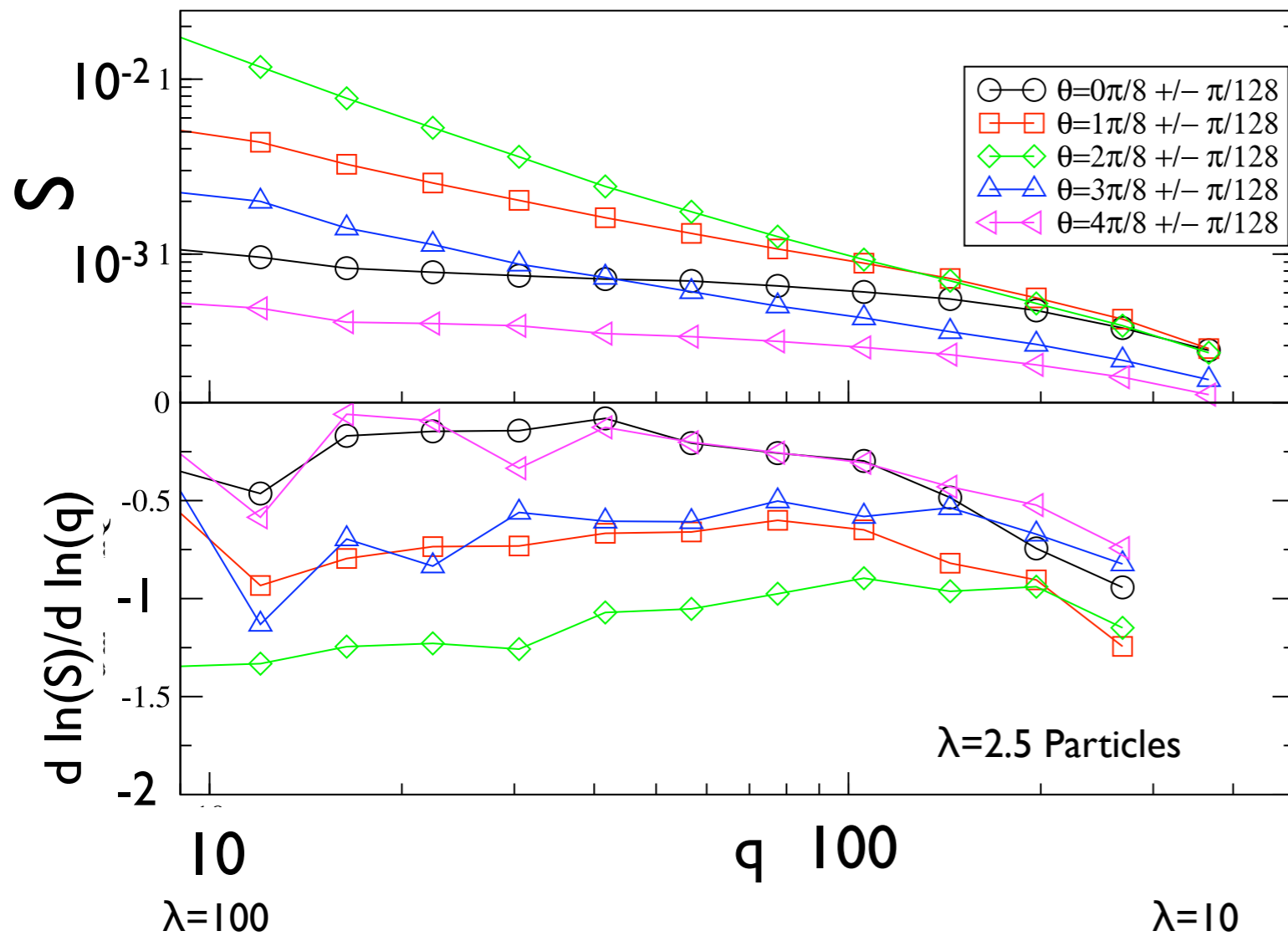
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- $\langle \omega^2 \rangle \sim \Delta\gamma$, BUT, $P(\omega)$ highly non-Gaussian: $P \sim e^{\omega/\omega^*}$
- $\omega^* \sim 0.1$ compatible with yield strain $\epsilon_{\text{yield}} \sim 0.05$

Structure factor for $\Delta\gamma=0.04$ $S(\vec{q}) = \left| \int \omega(\vec{r}) \exp[i\vec{q} \cdot \vec{r}] d\vec{r} \right|^2$

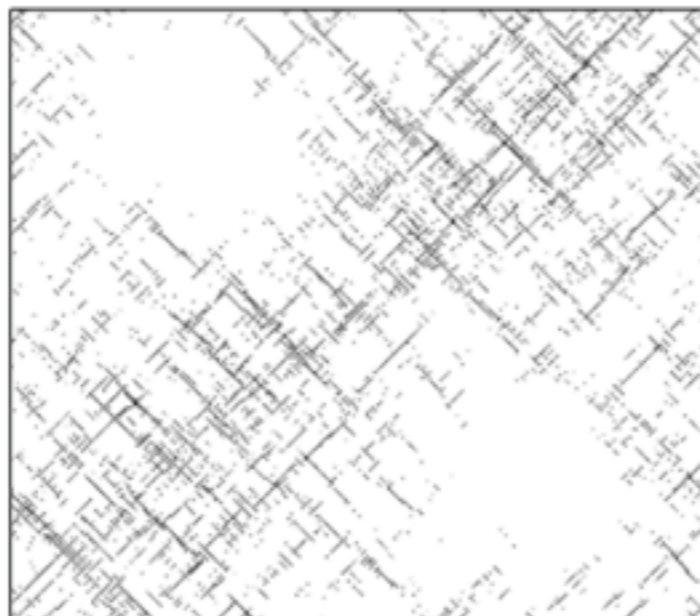
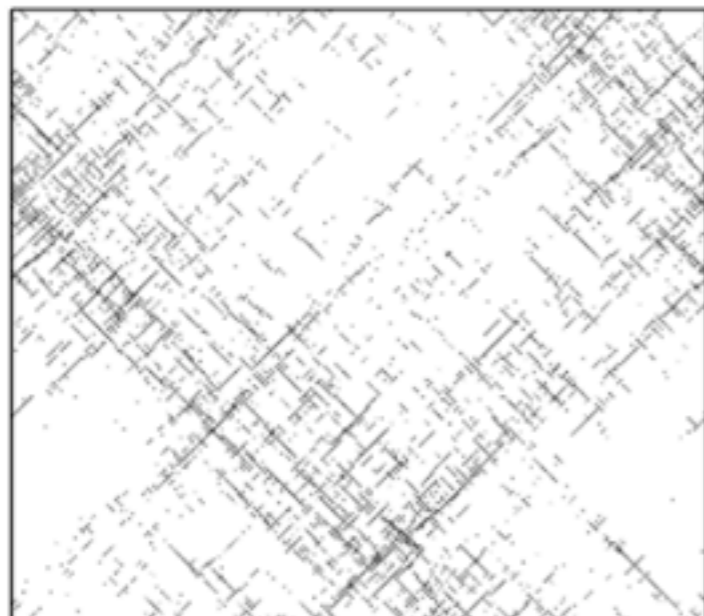
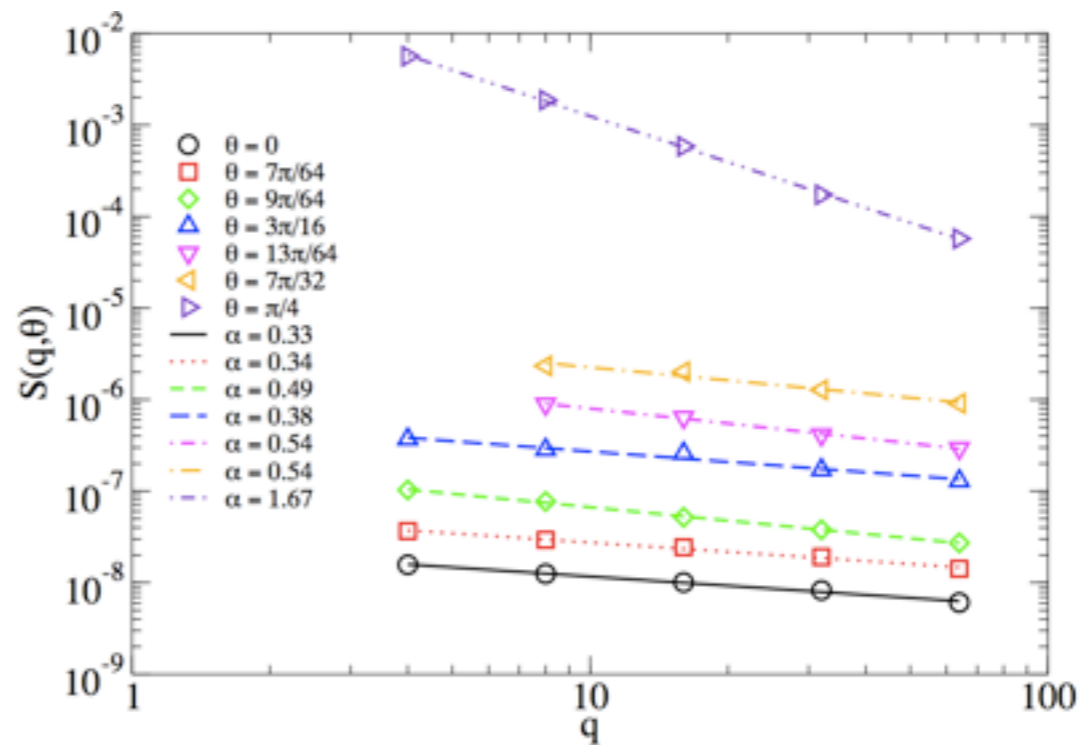
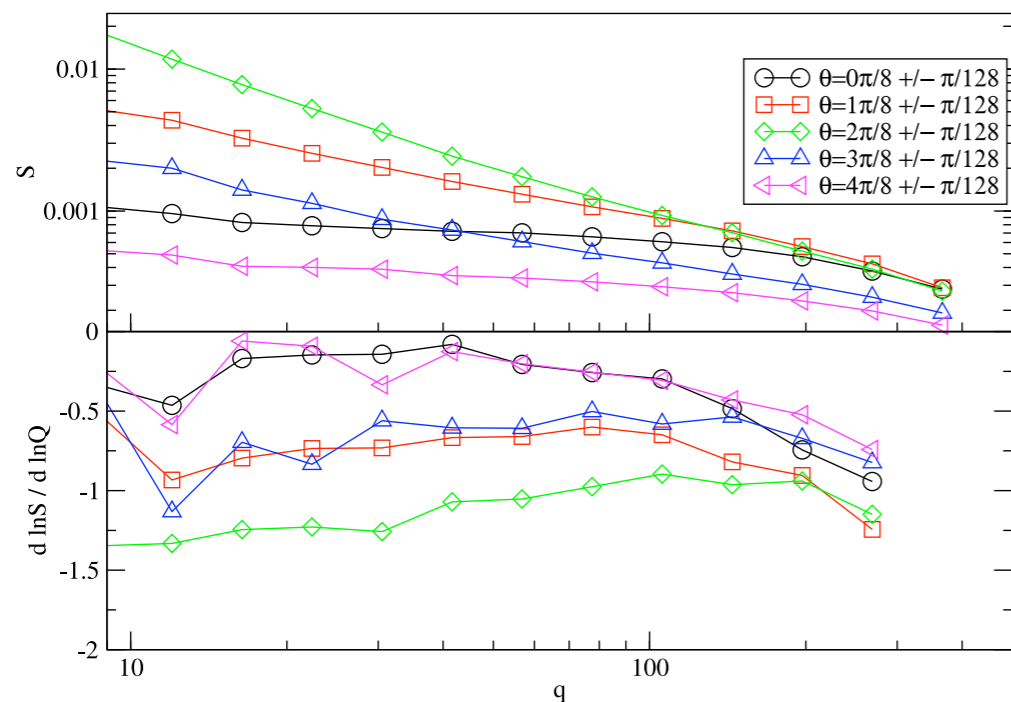


$\theta=\pi/8$ and $\theta=3\pi/8$ have same shear stress, different normal stress.

$$S(q;\theta) = A(\theta) q^{-\alpha(\theta)}$$

α depends on angle!
 α : has "shear" symmetry
 θ : does not

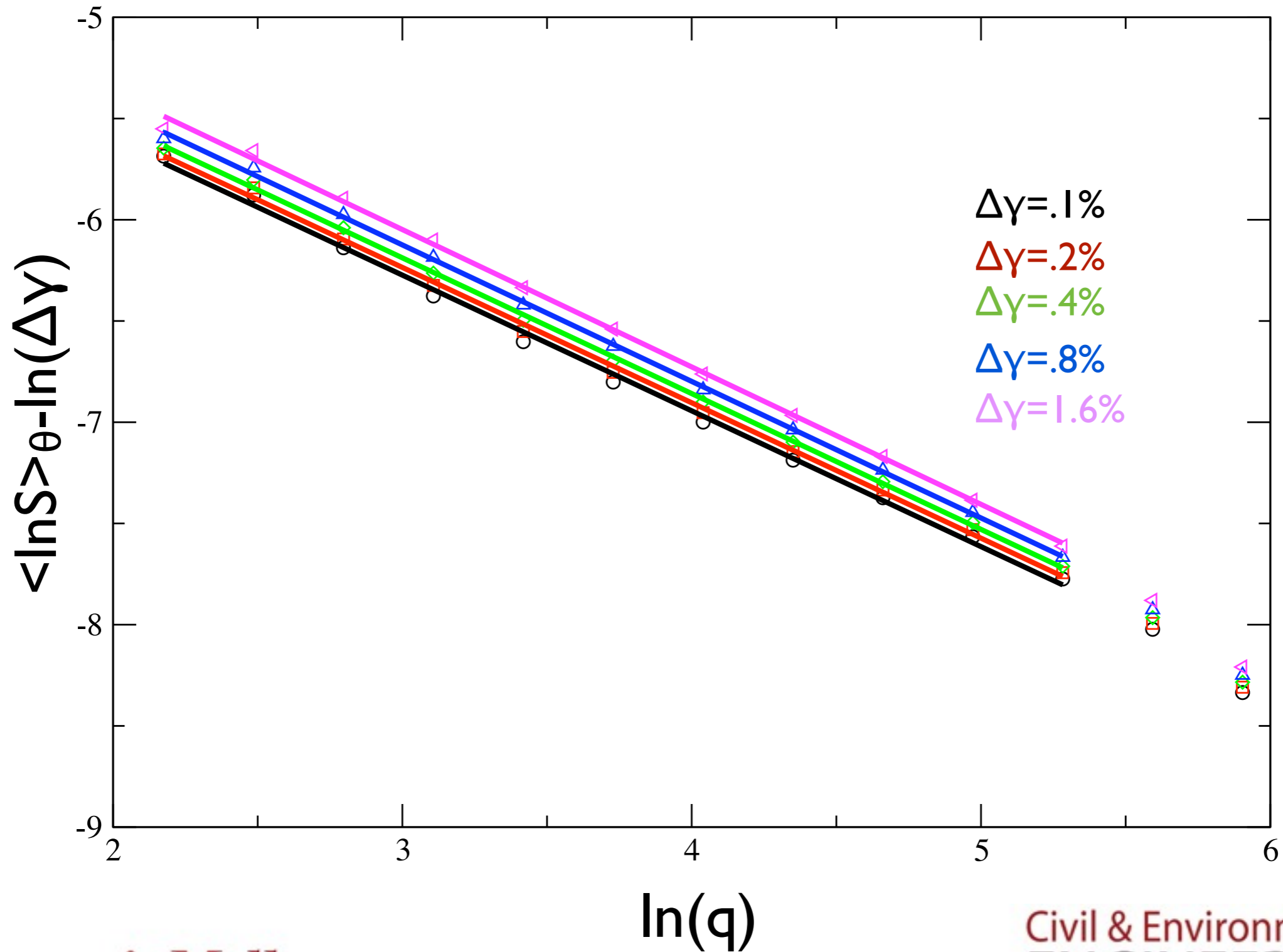
Compare to Talamali et. al. (Vandembroucq talk)



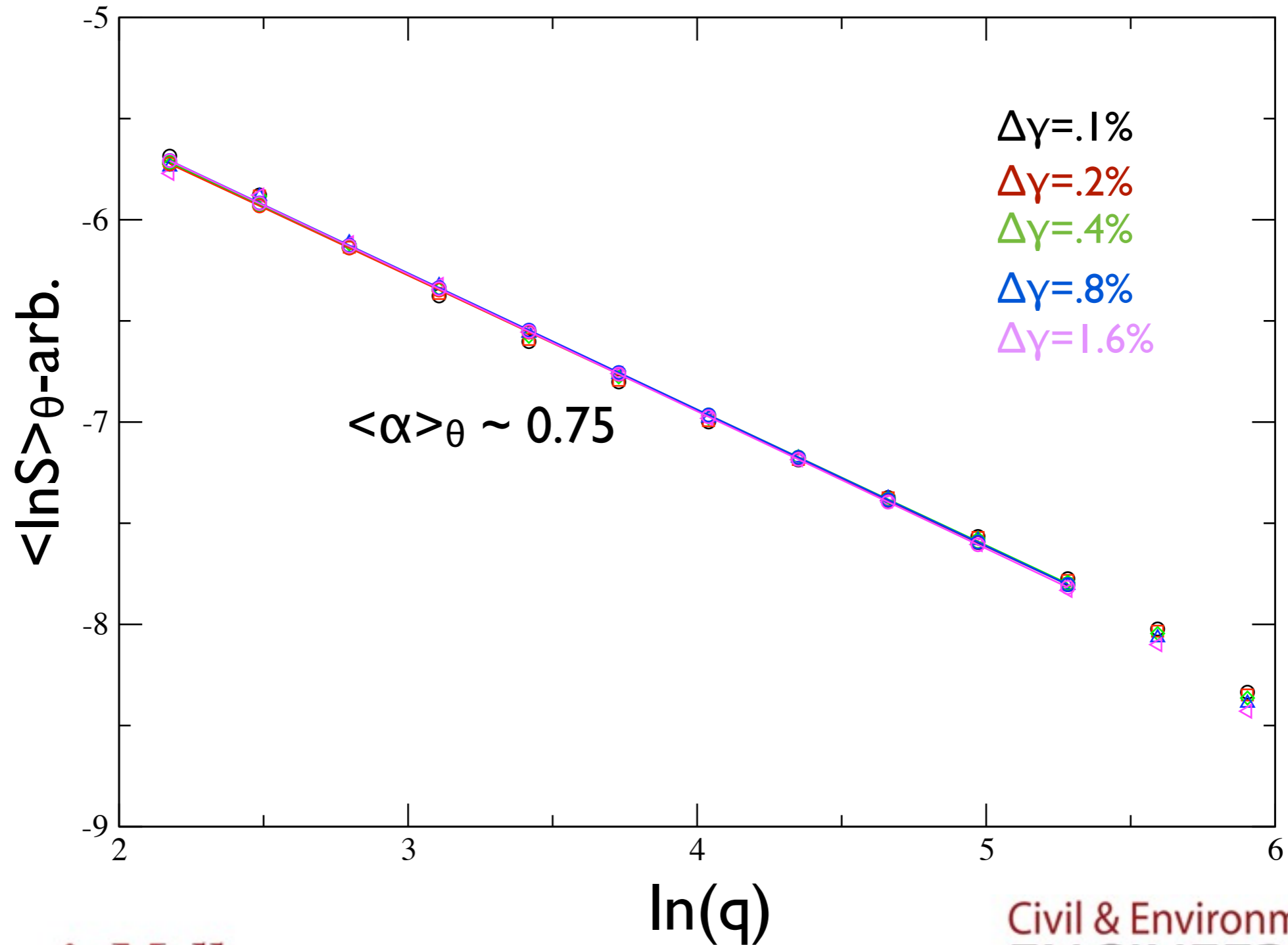
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$\langle \text{Log}S \rangle_\theta$ scaled by $\Delta\gamma$

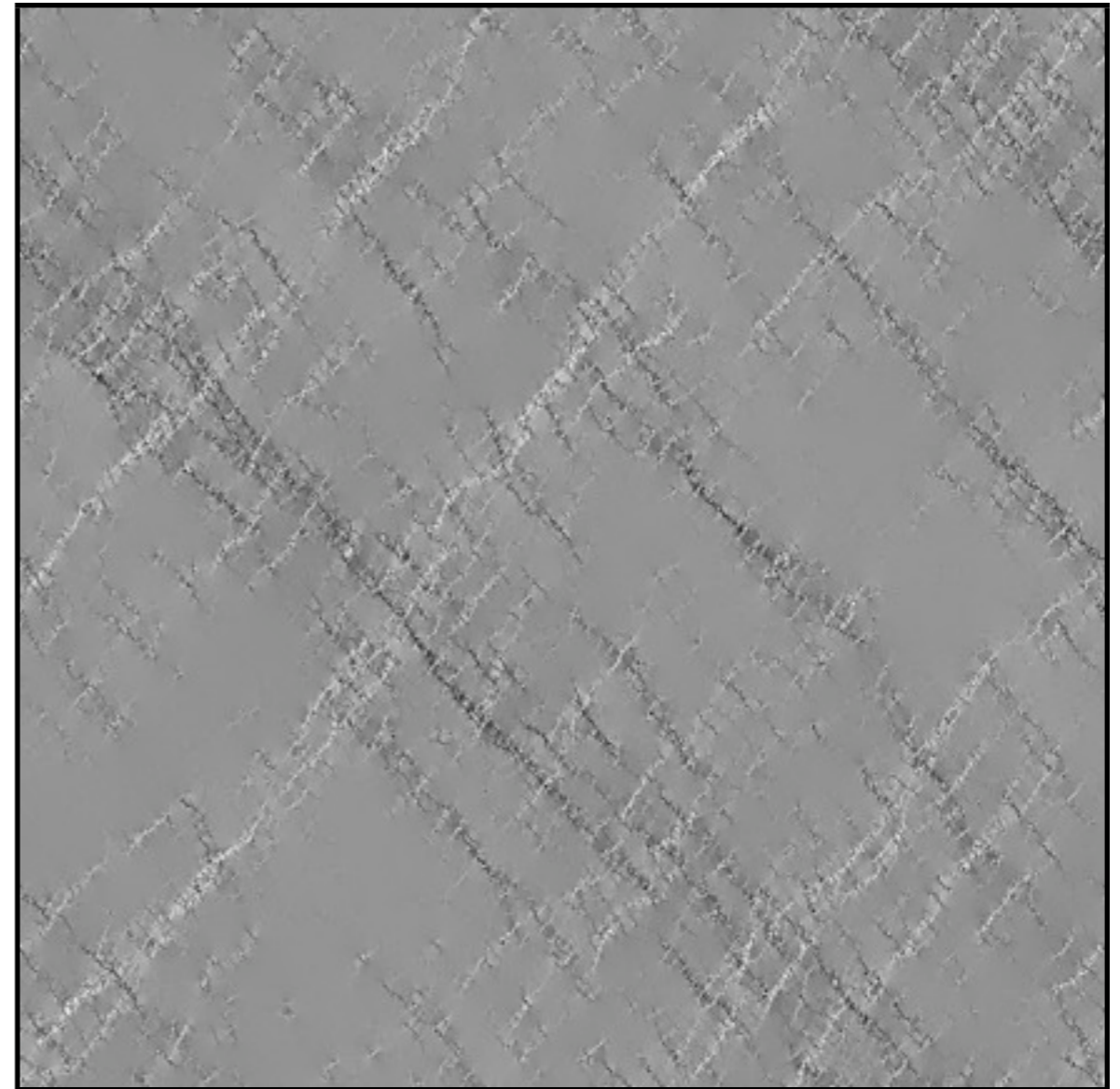


$\langle \text{Log}S \rangle_\theta$ best-rescaling

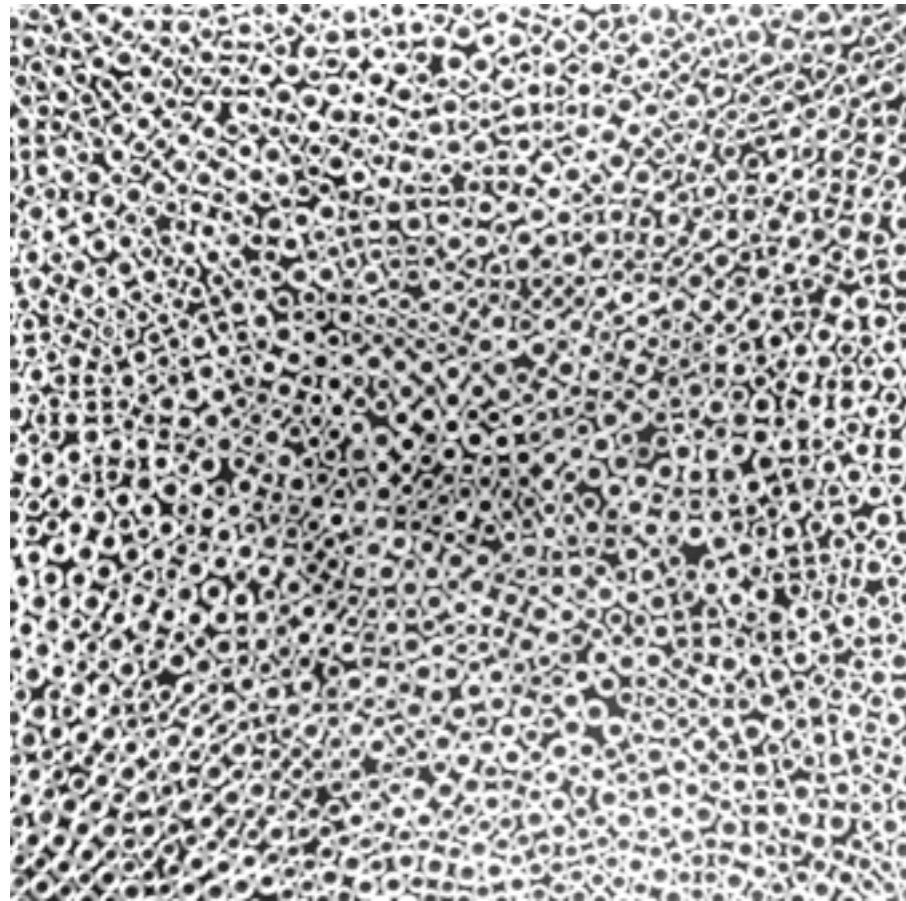


Summary: Spatial structure of strain

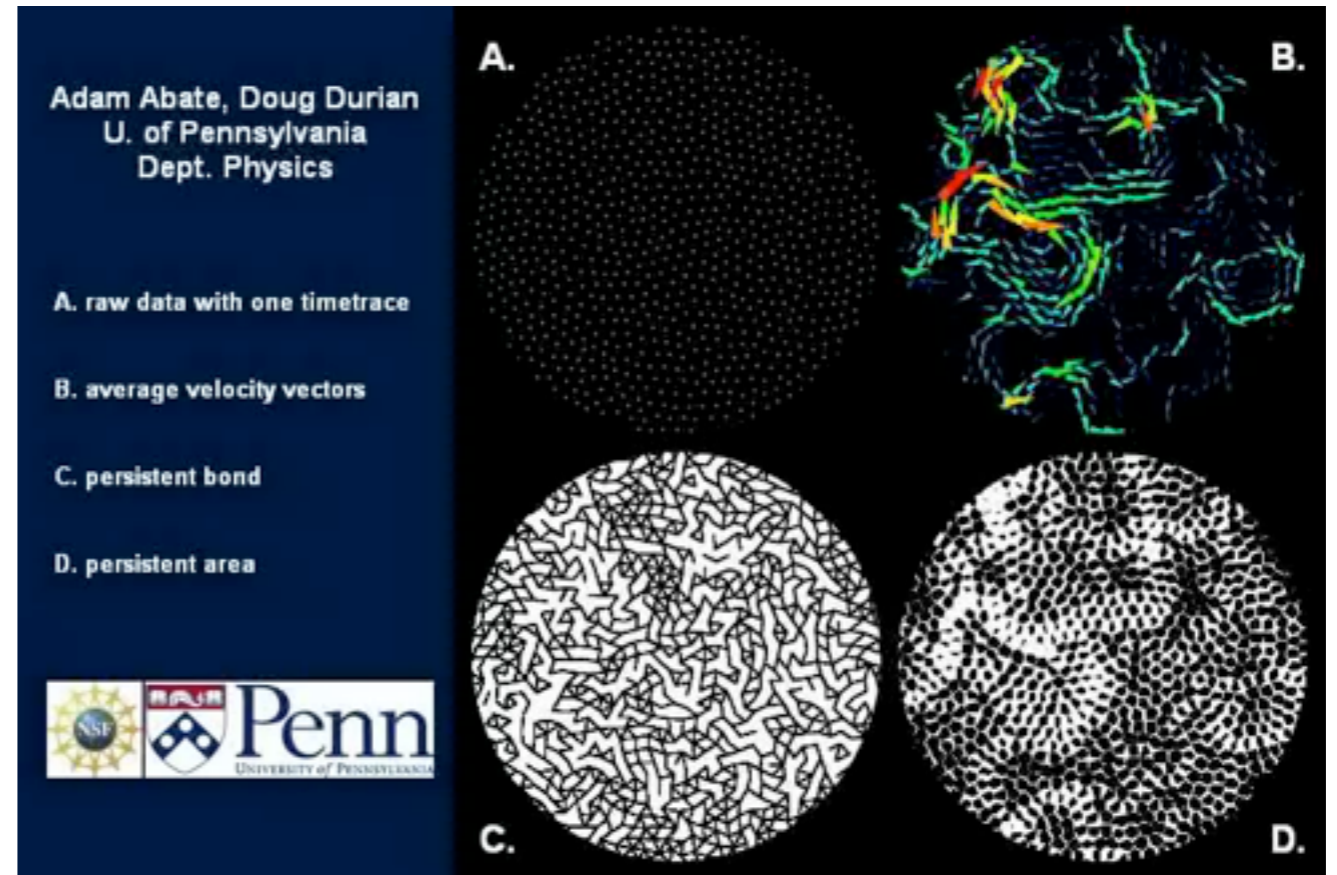
- Measured vorticity, ω , for various, $\Delta\gamma$
- In steady state, $S(q,\theta)=A(\theta)q^\alpha$
(θ)
- α has “shear symmetry”
- $A(\theta)$: Mohr-Coulomb effect
- $S/\Delta\gamma$ collapse implies: ω is de-correlated



Jammed systems

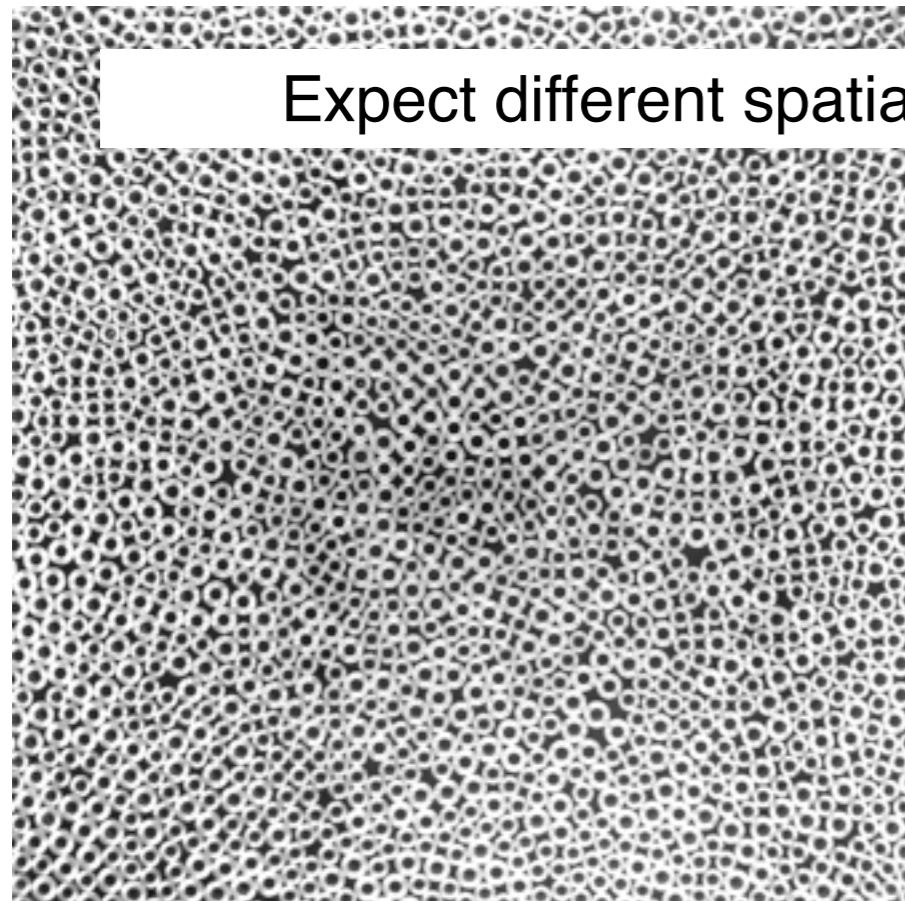


From F. Lechenault

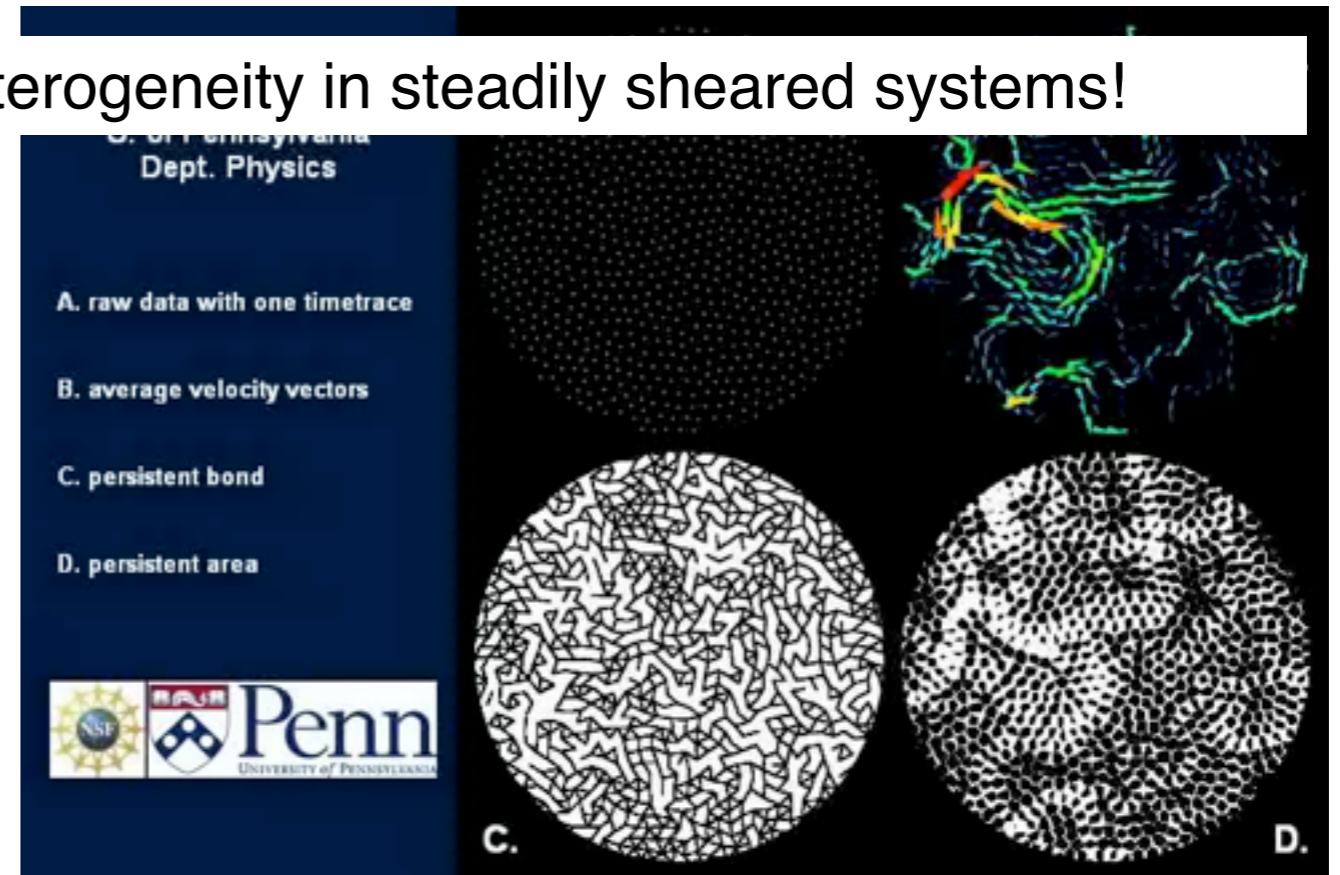


From A. Abate

Jammed systems



Expect different spatial heterogeneity in steadily sheared systems!

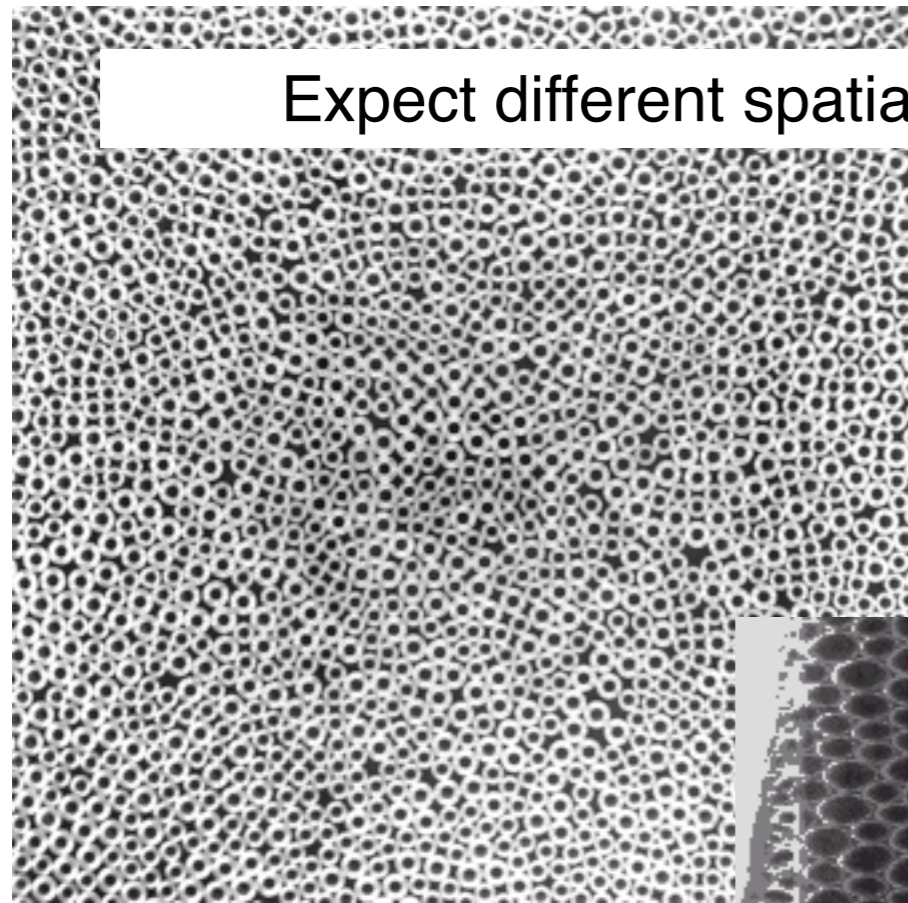


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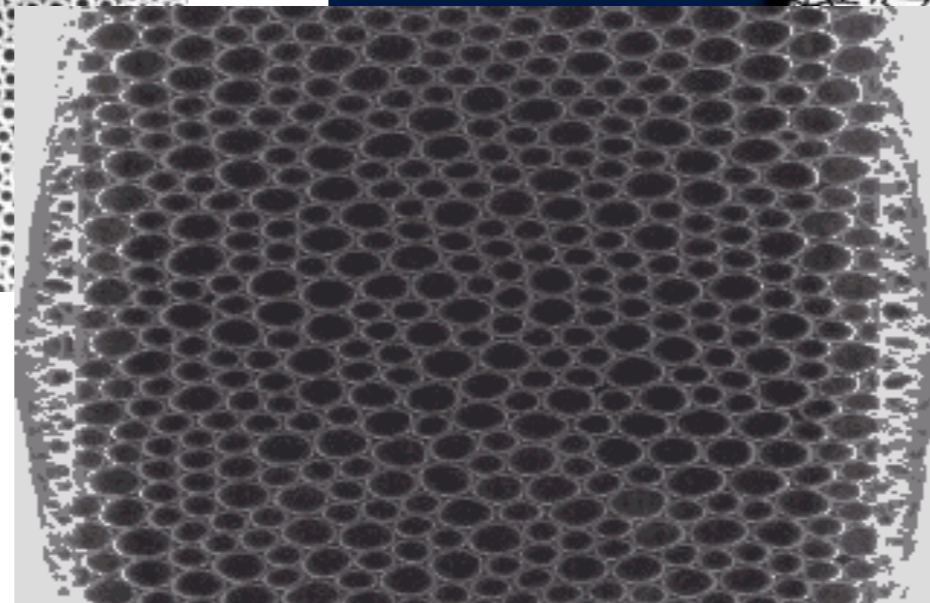
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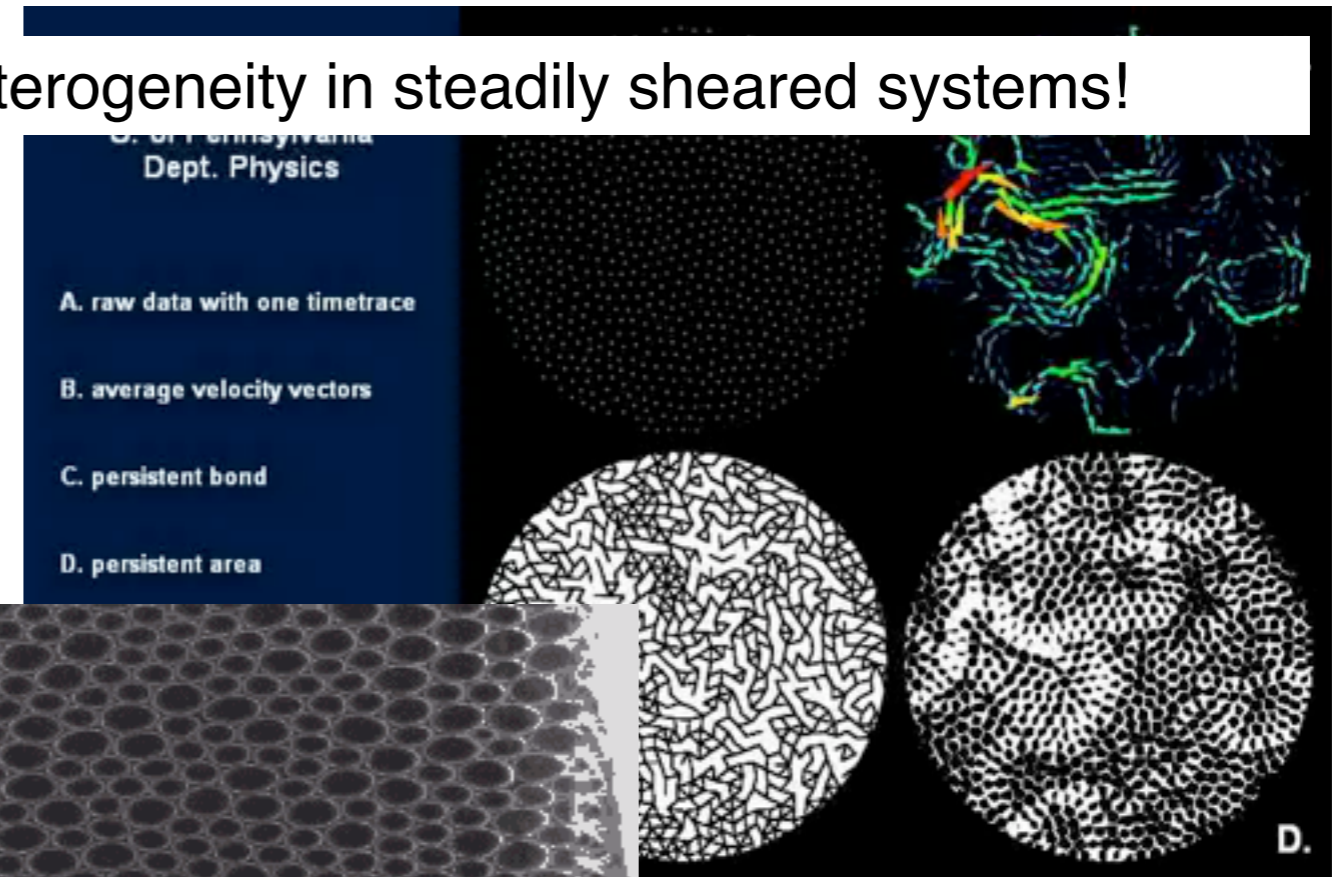


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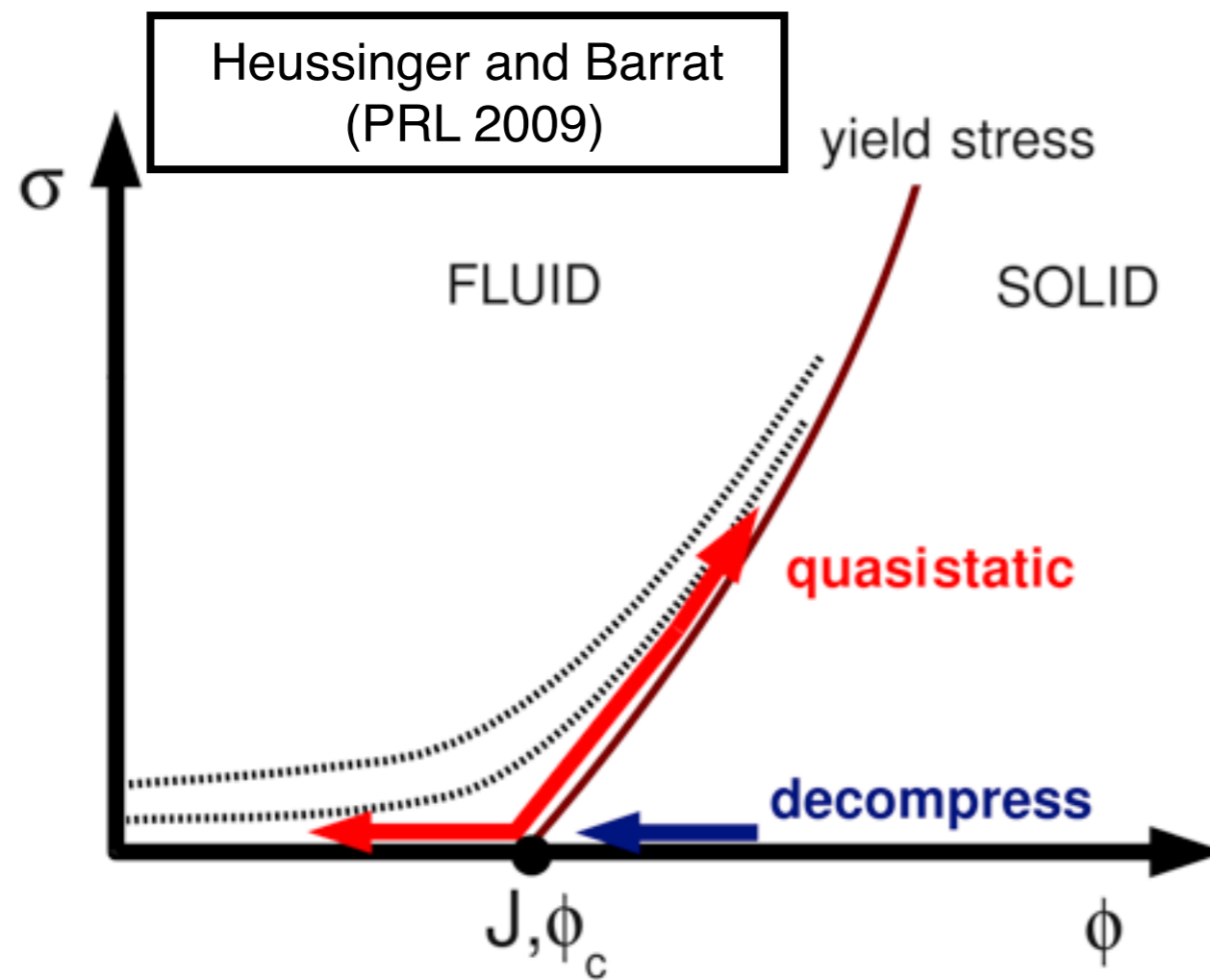
Layer of polydisperse soap bubbles on water

vanHecke group

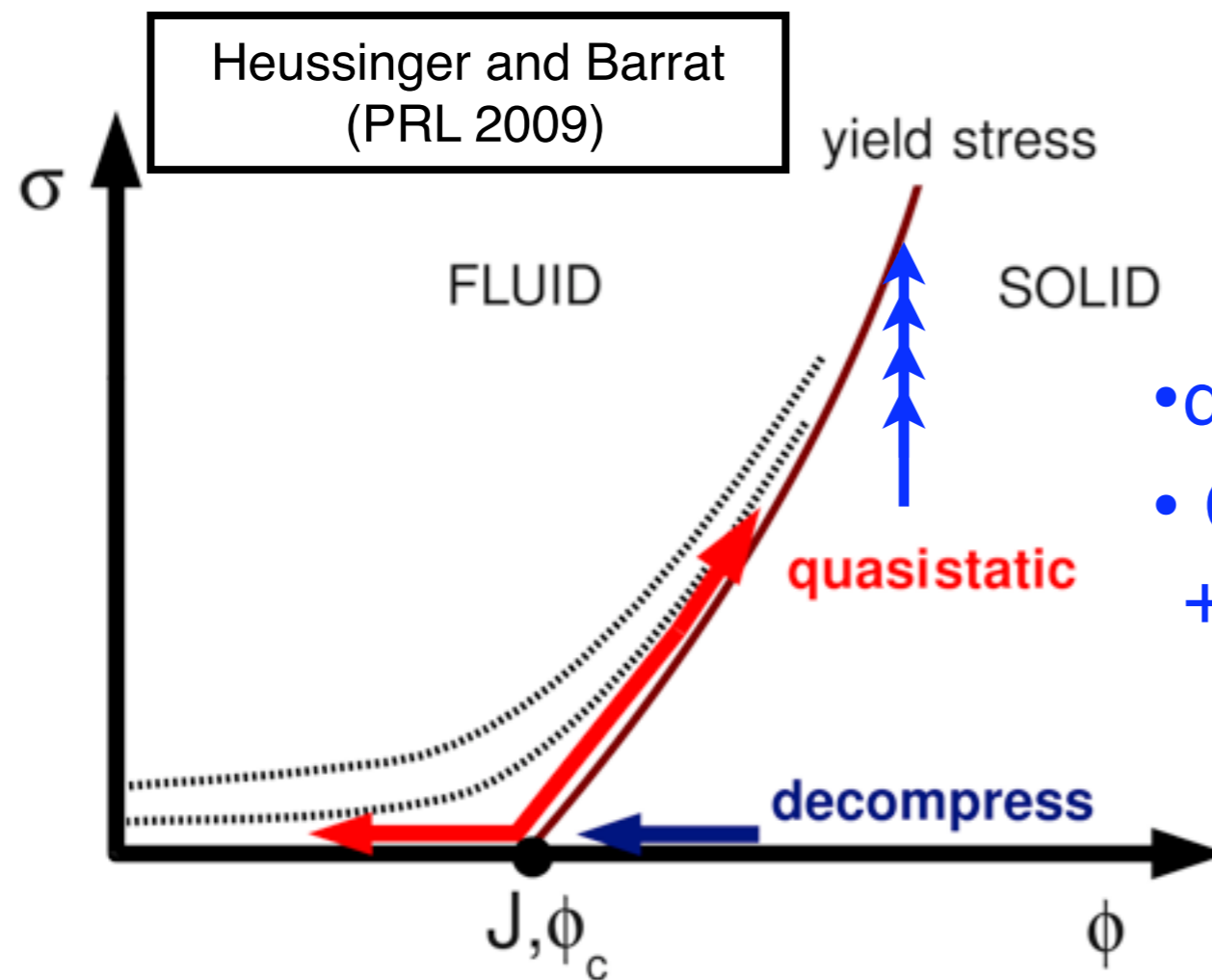


From A. Abate

Jamming and critical scaling at ϕ_c

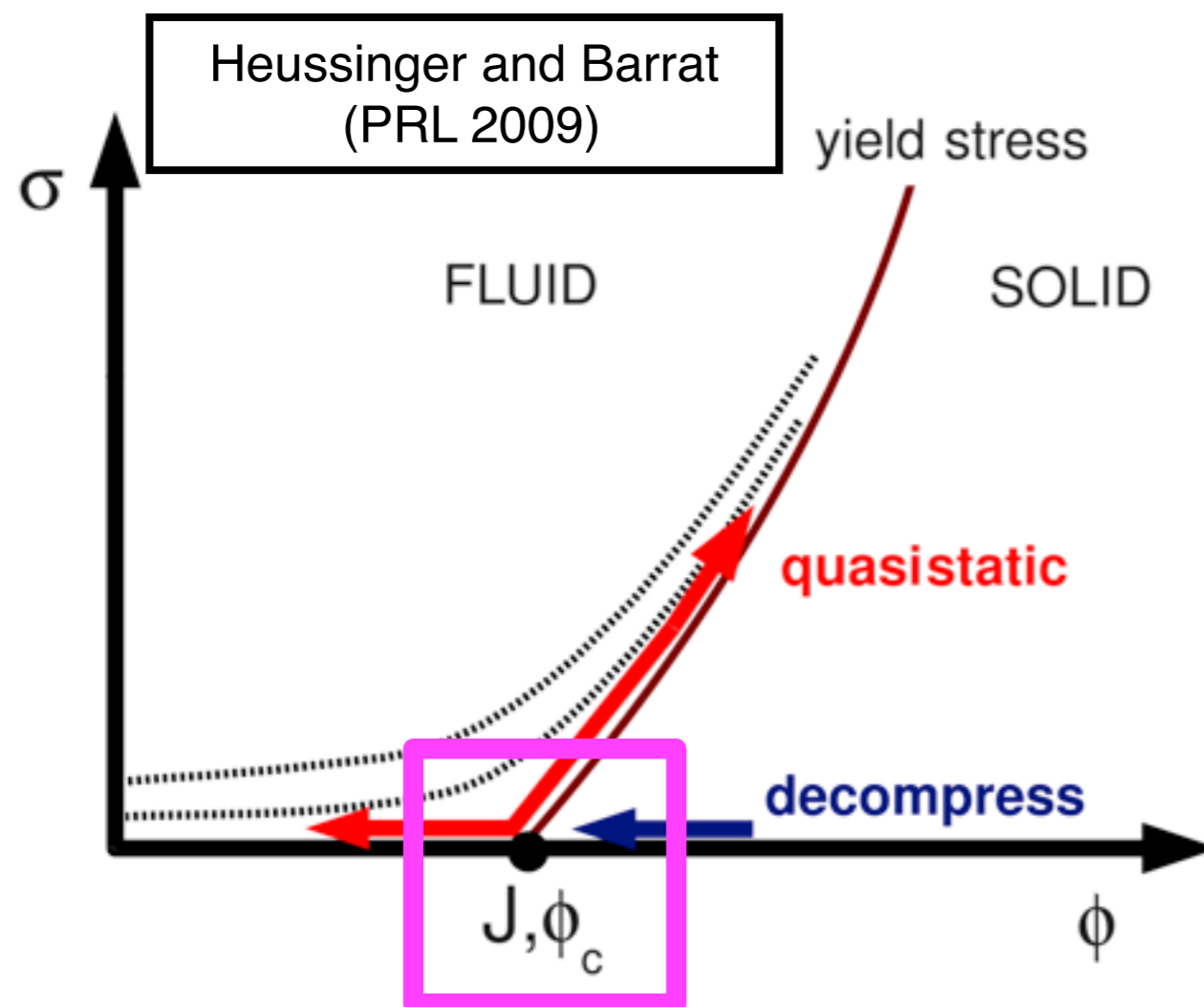


Jamming and critical scaling at ϕ_c



- quasistatic avalanches
- CEM+Robbins / Lemaître +Caroli

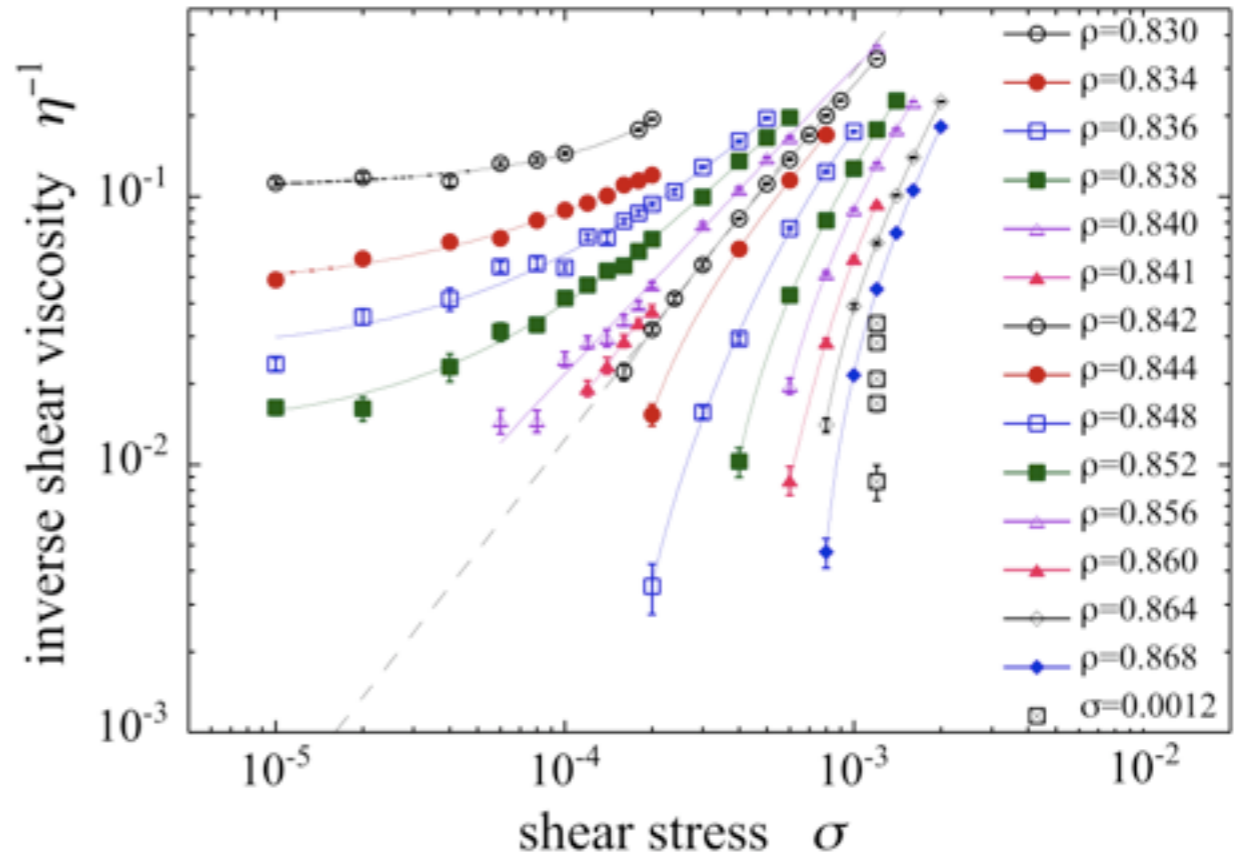
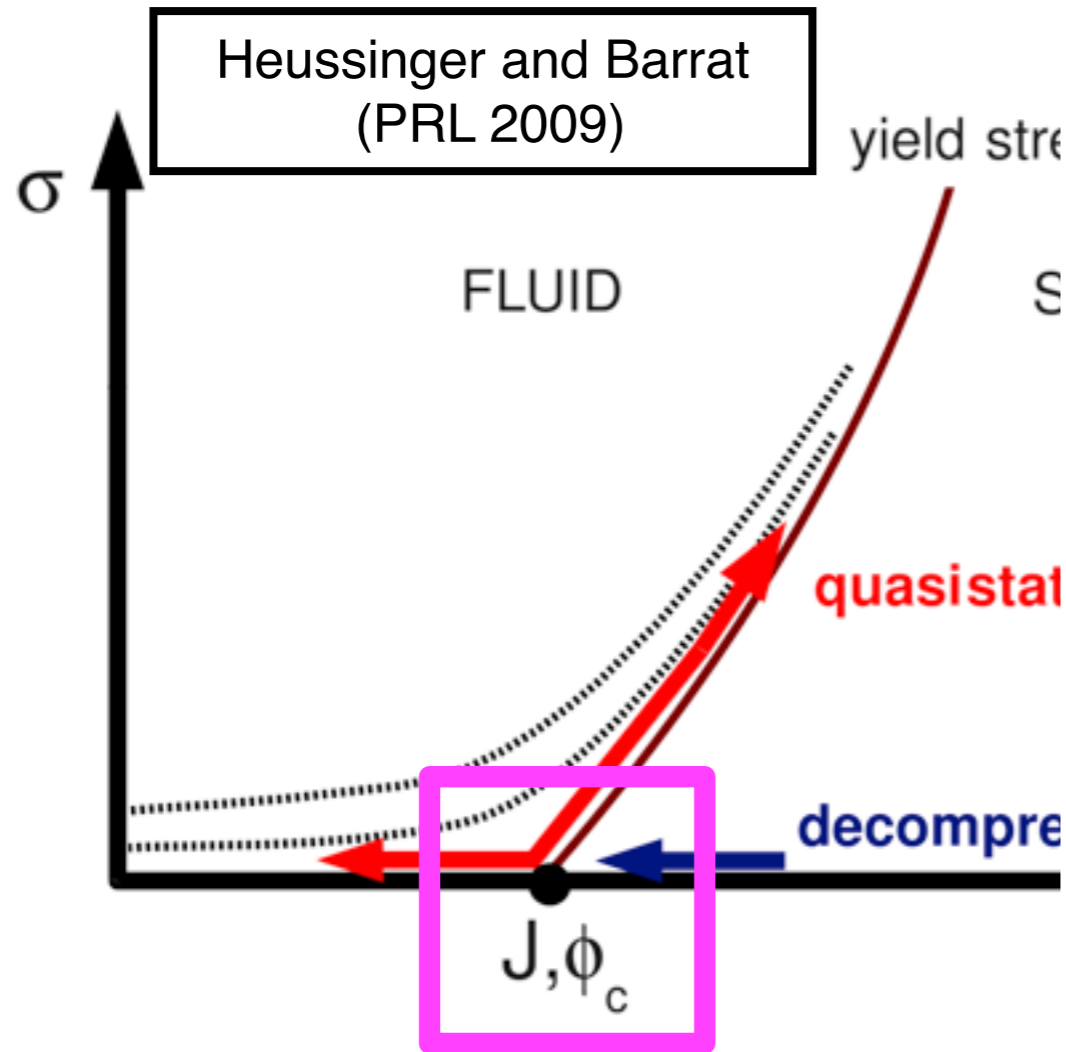
Jamming and critical scaling at ϕ_c



•Olsson and Teitel PRL 2008

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

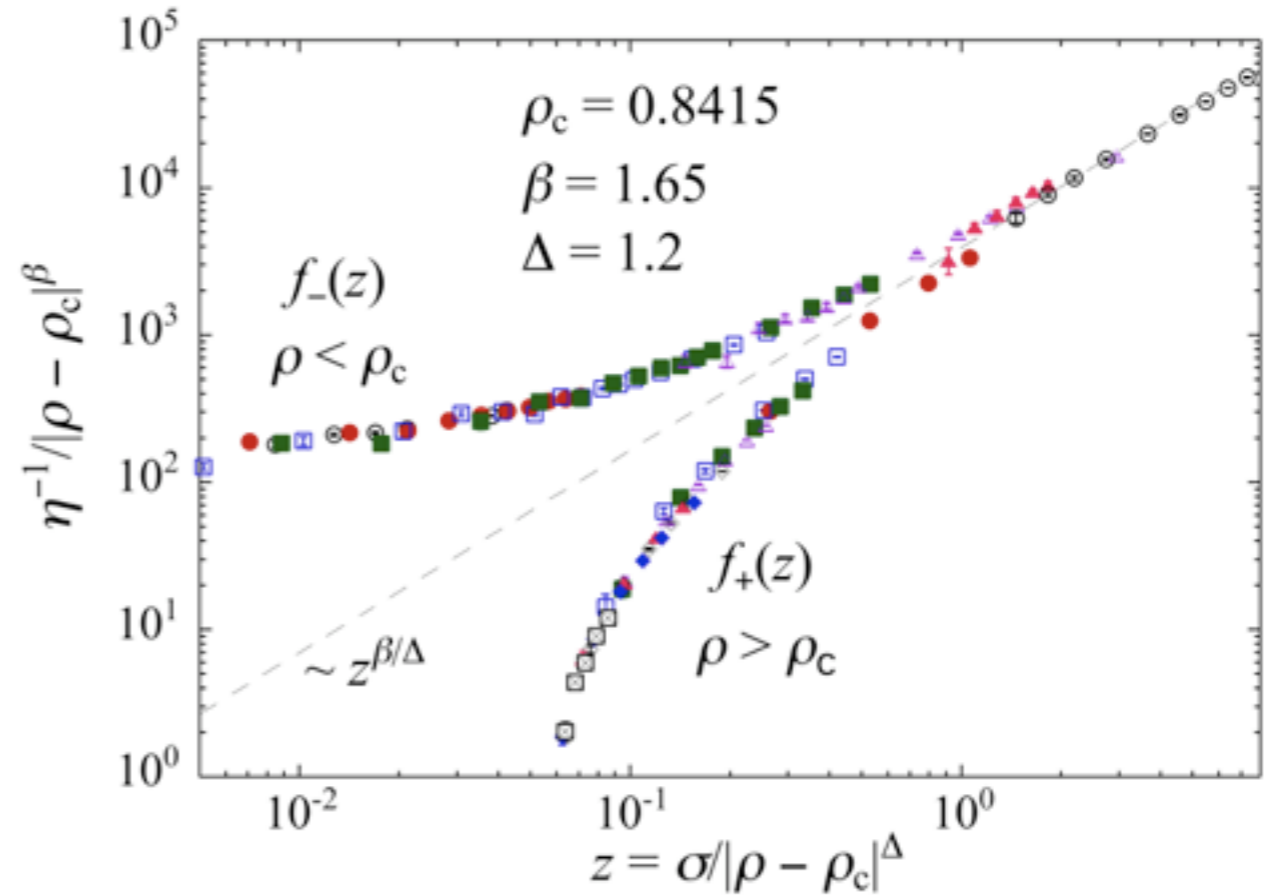
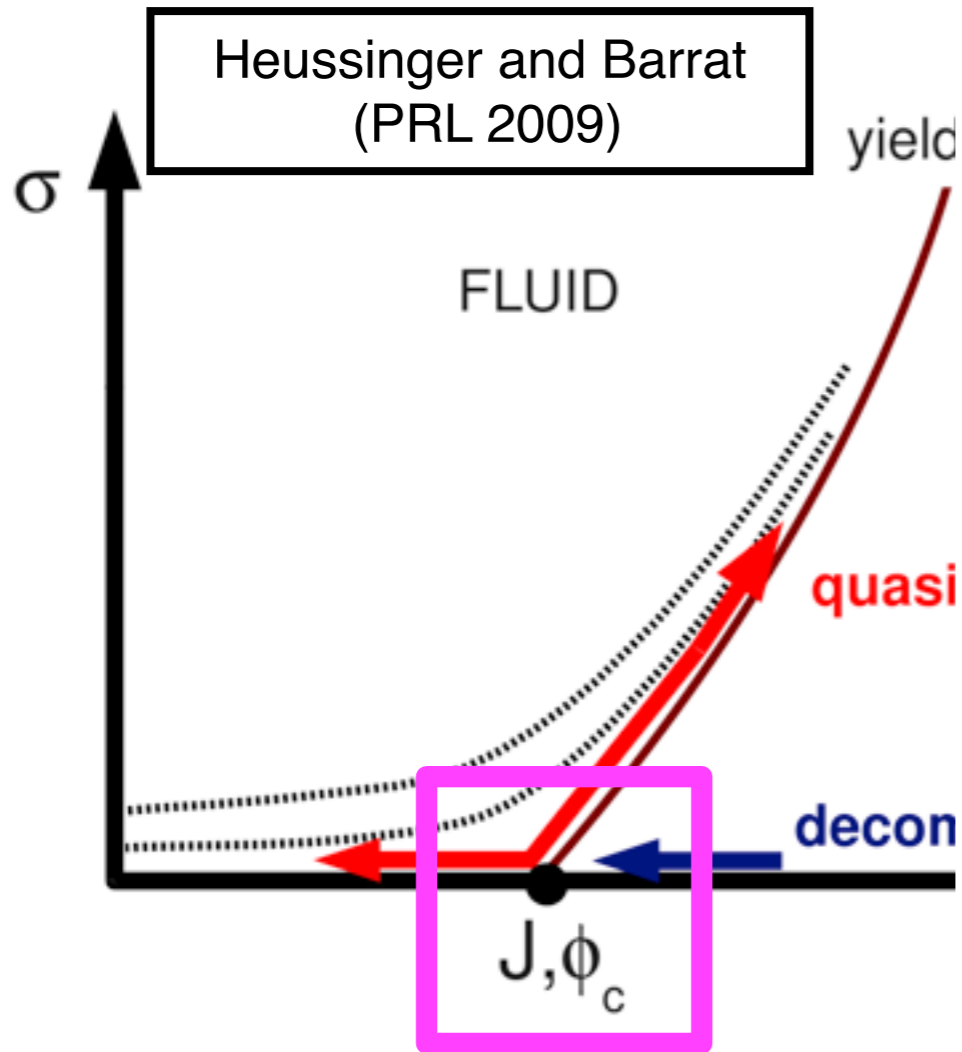
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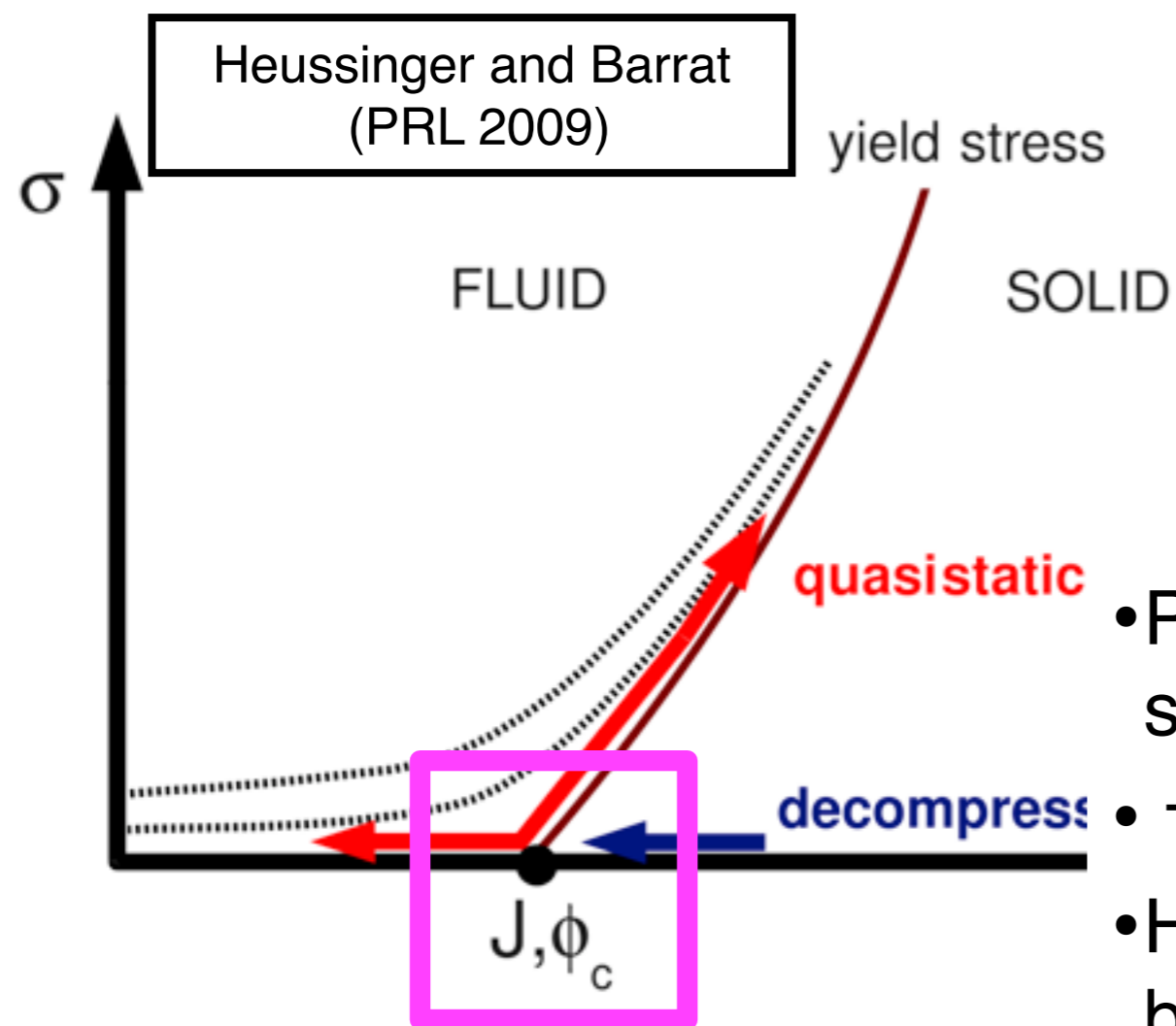
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Jamming and critical scaling at ϕ_c



- Point J scaling implies: $\phi - \phi_c$ sets stress and **time** scale.

- $\tau_J = (\phi - \phi_c)^{\Delta - \beta}$

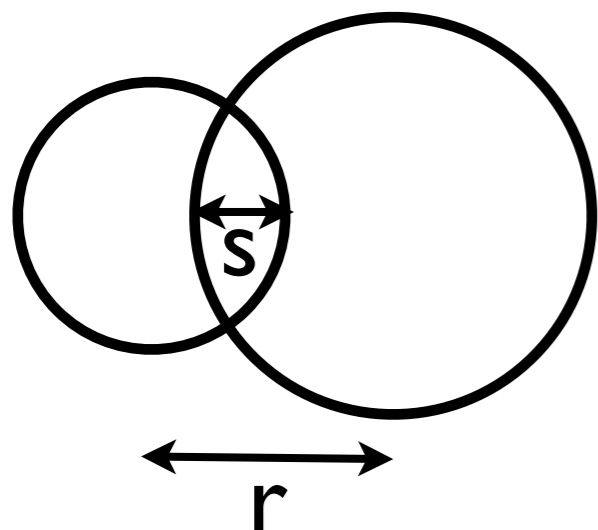
- How does this affect quasistatic behavior?

- ϕ, σ rheology scaling near “point J”

- Olsson and Teitel (bubbles), Hatano (grains)...

Bubble model

$$\delta \vec{v}_i = \vec{F}_i / D; \quad \delta \vec{v}_i = \vec{v}_i - y_i \dot{\gamma} \hat{x}; \quad \dot{\vec{r}}_i = \vec{v}_i$$

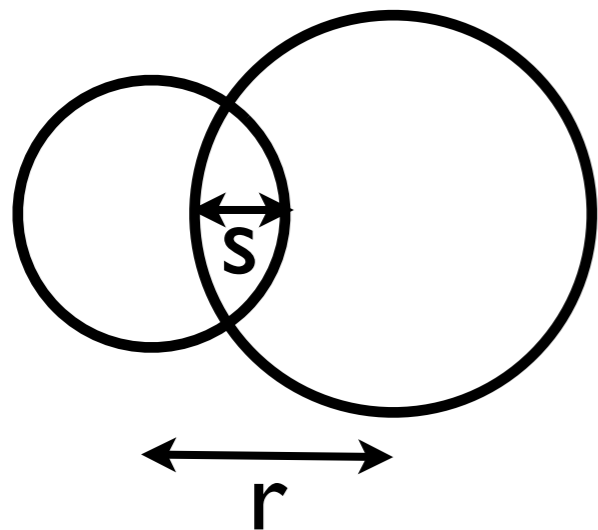


$$a = \frac{(R_i + R_j) - r_{ij}}{R_i + R_j}$$

$$U = \frac{\epsilon}{2} a^2$$

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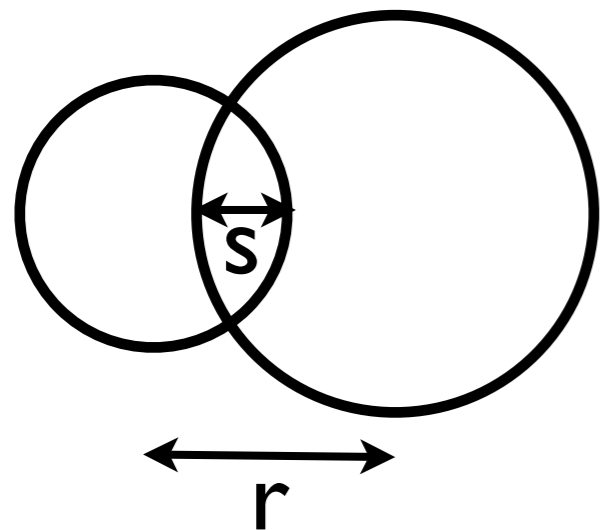
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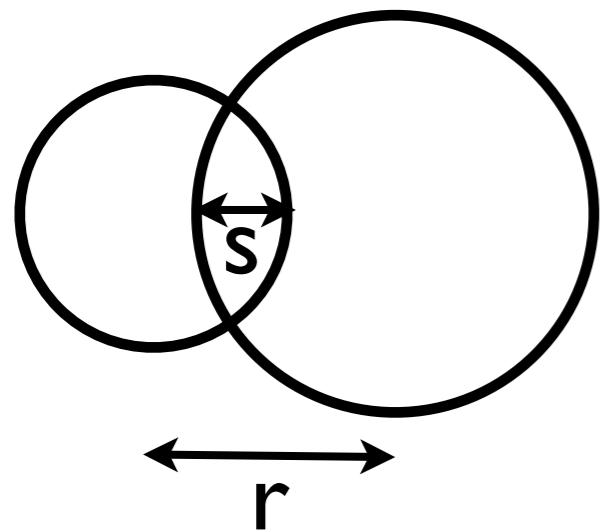
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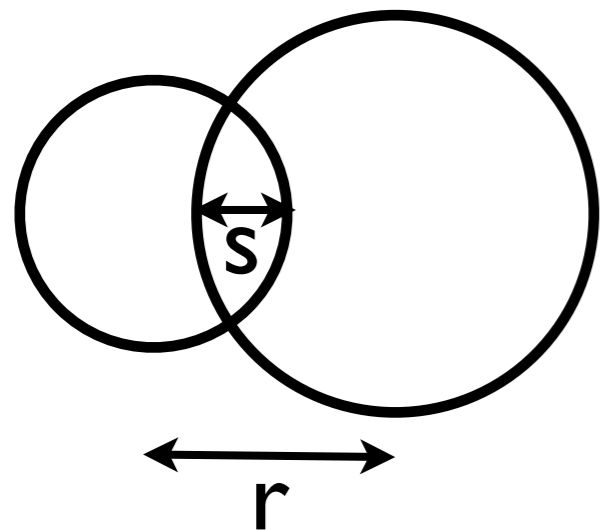
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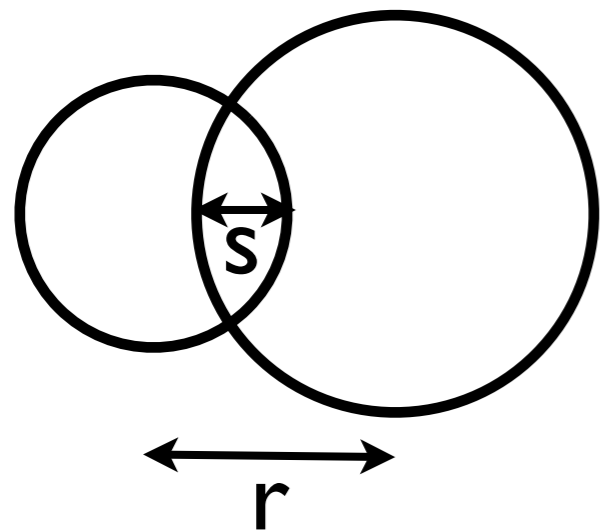
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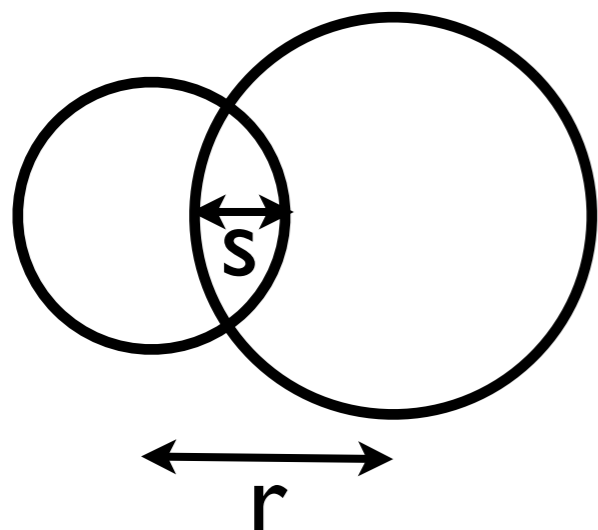
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- Only single timescale in model:
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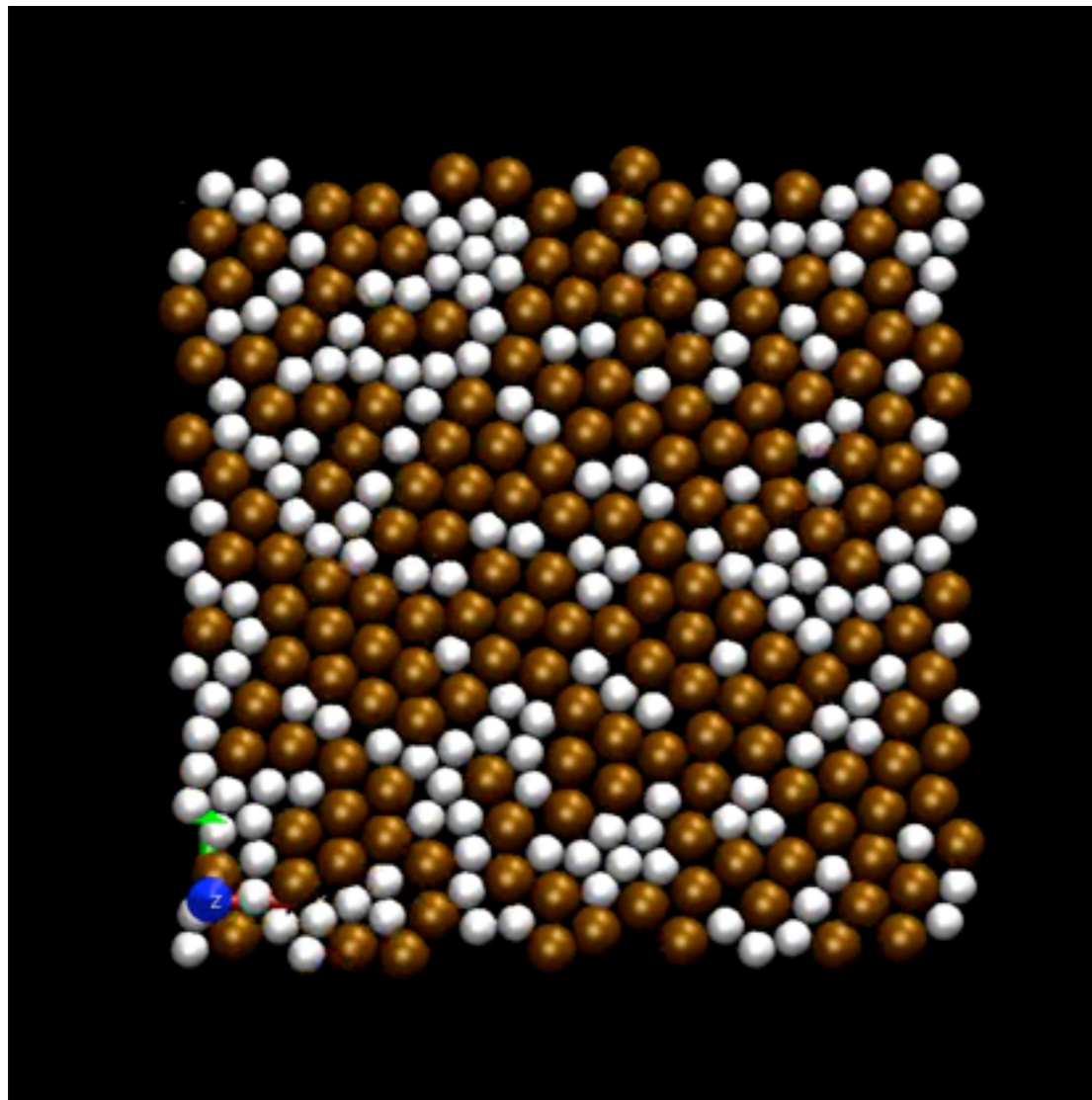
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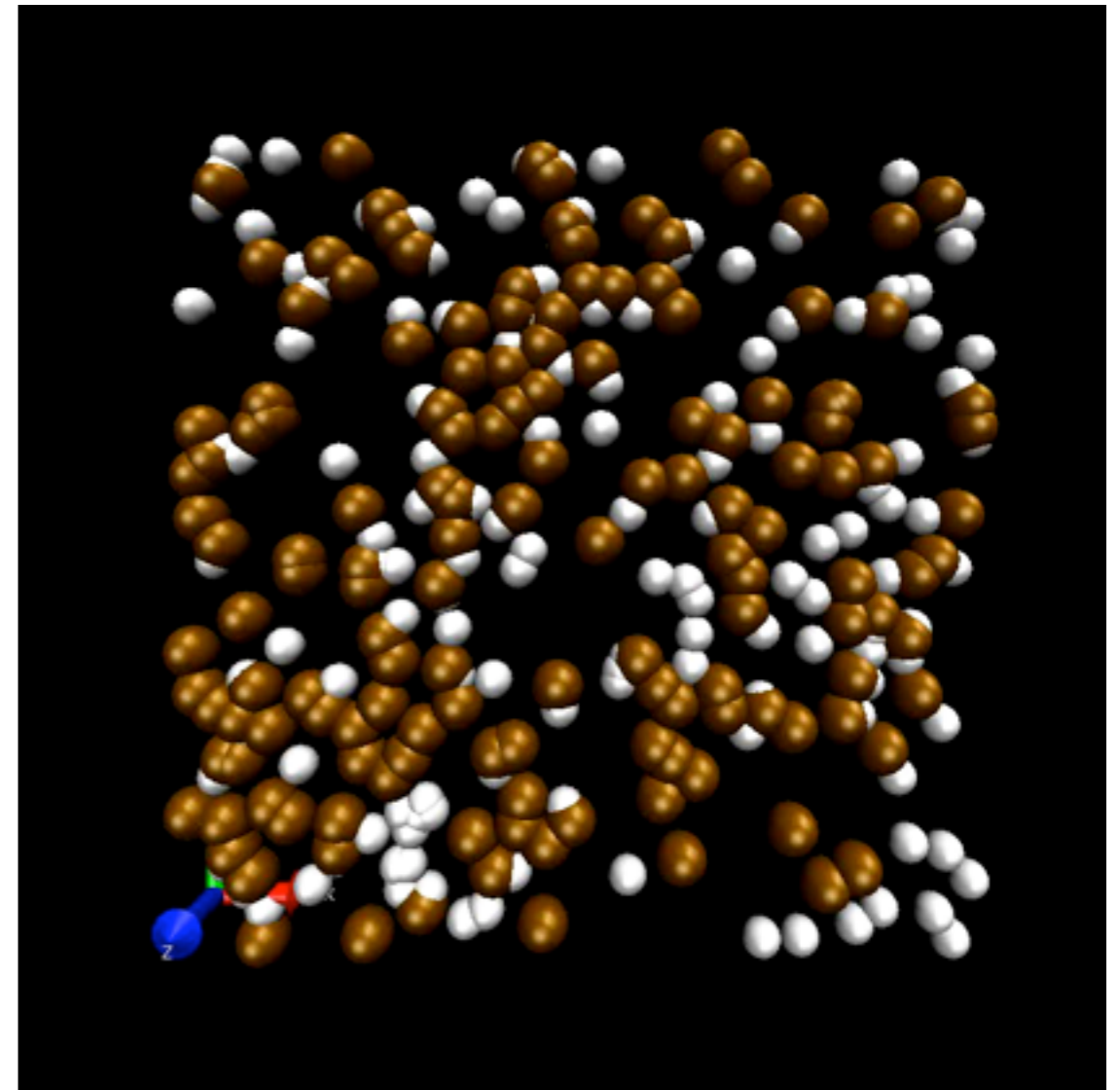
$$\tau_D \doteq D\sigma_0^2 / \epsilon$$

"Slow" shear at various density



$\phi=1.0$

$dy/dt=1.25 \times 10^{-6}$



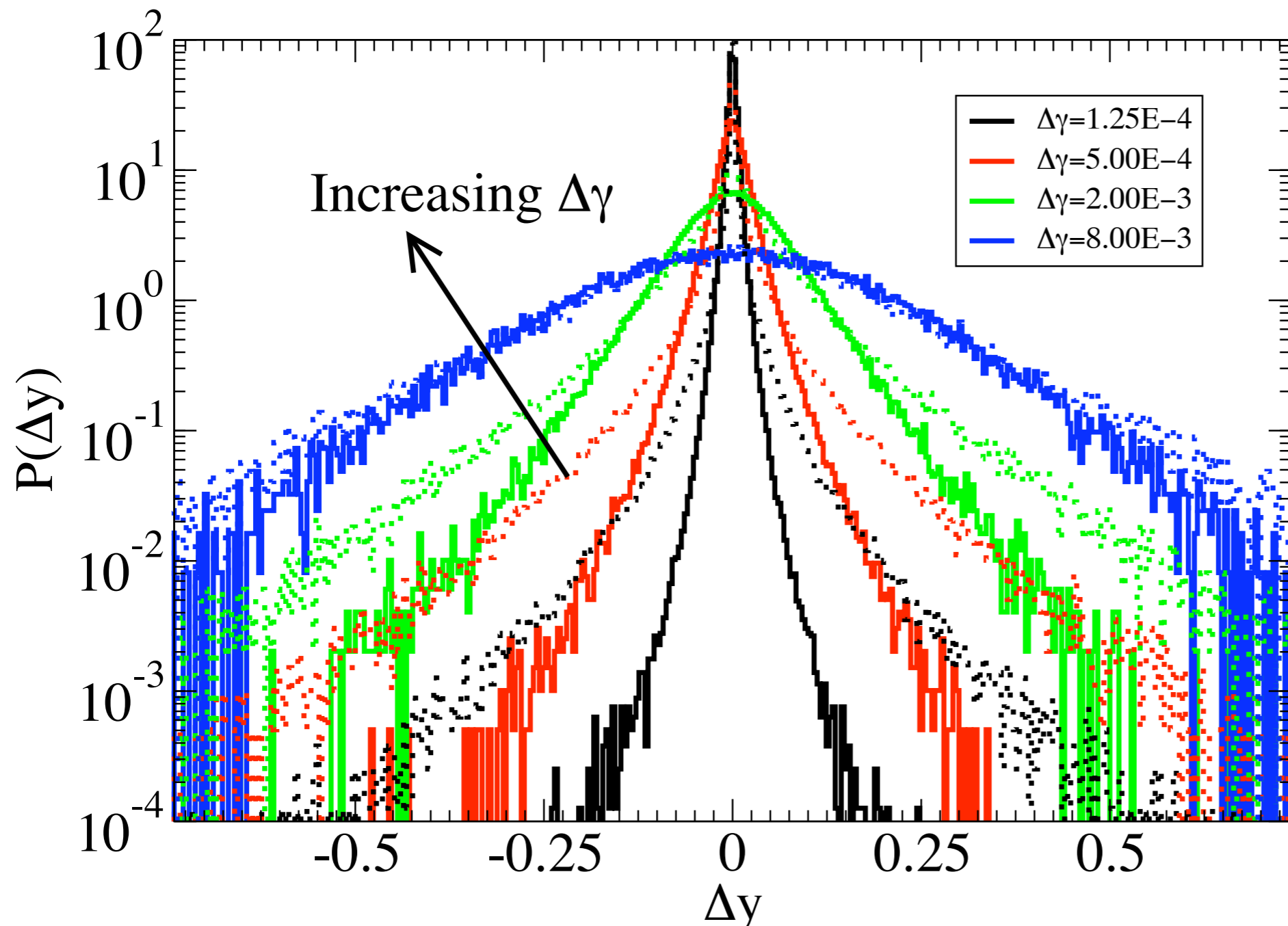
$\phi=0.85$

How are they different?

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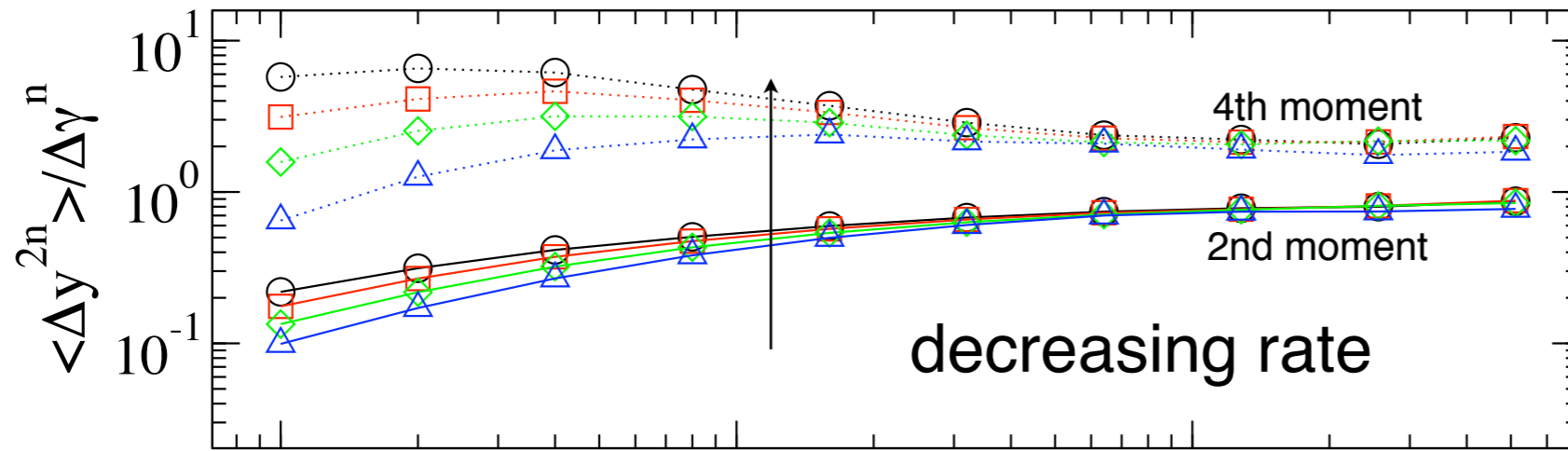
Transverse displacement distribution



$P(\Delta y)$ much broader for $\phi=1.0$ than $\phi=0.85$ at early $\Delta\gamma$

$P(\Delta y)$ similar for $\phi=1.0$ and $\phi=0.85$ at late $\Delta\gamma$

2nd and 4th moments ($\varphi=1.0$)

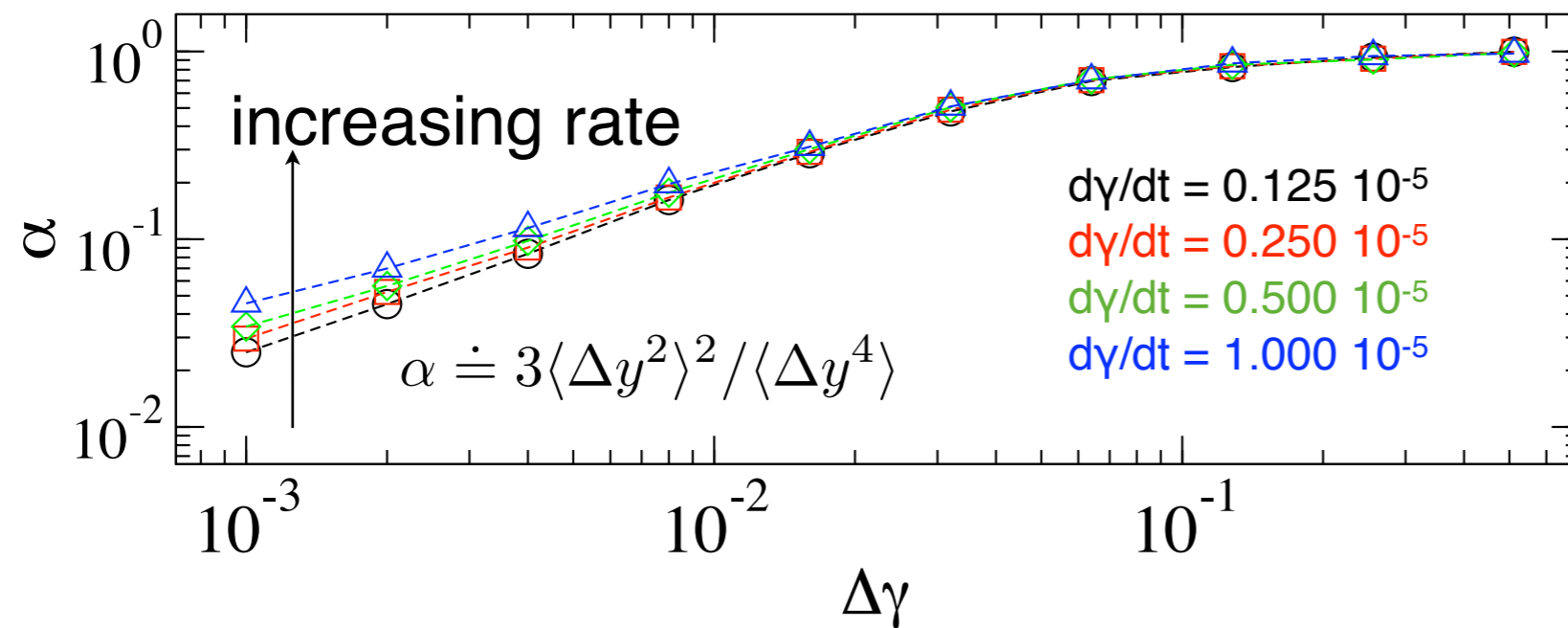


no rate dependence
at plateau,
we're quasistatic!

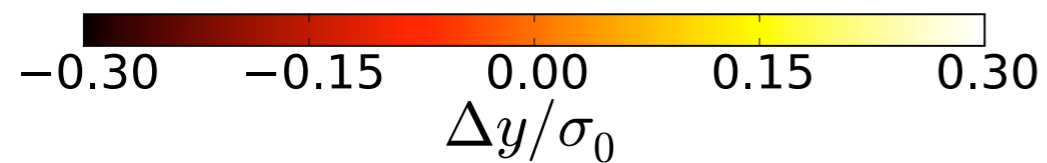
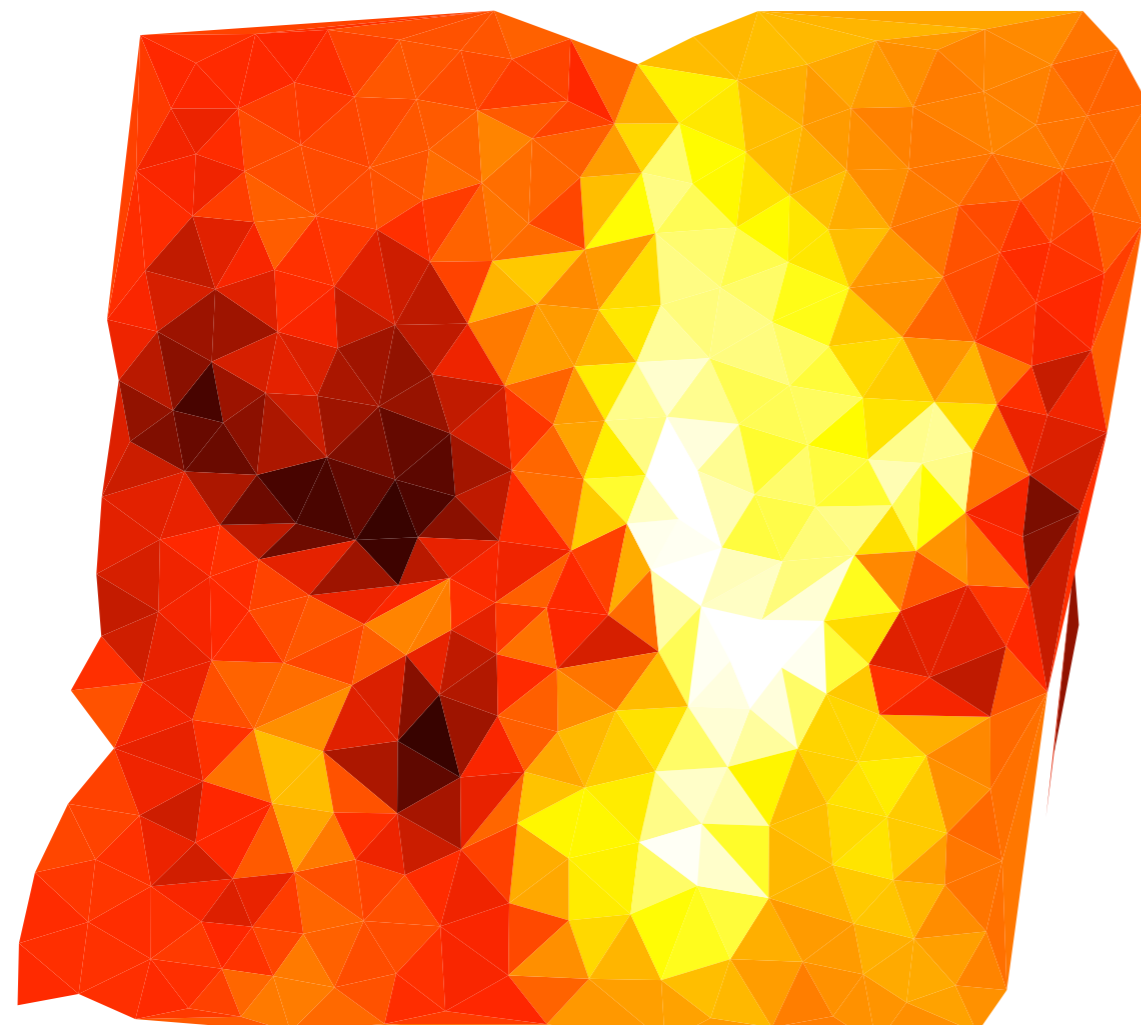
From LJ slip-line
arguments:
 $D_{\text{eff}} \sim La/12$

$$a \sim 0.8\sigma$$

$$\Delta \gamma^* \sim a/L \sim .05$$



Typical displacement over $\Delta\gamma \sim 0.05$



From LJ slip-line arguments:

$$D_{\text{eff}} \sim La/12$$

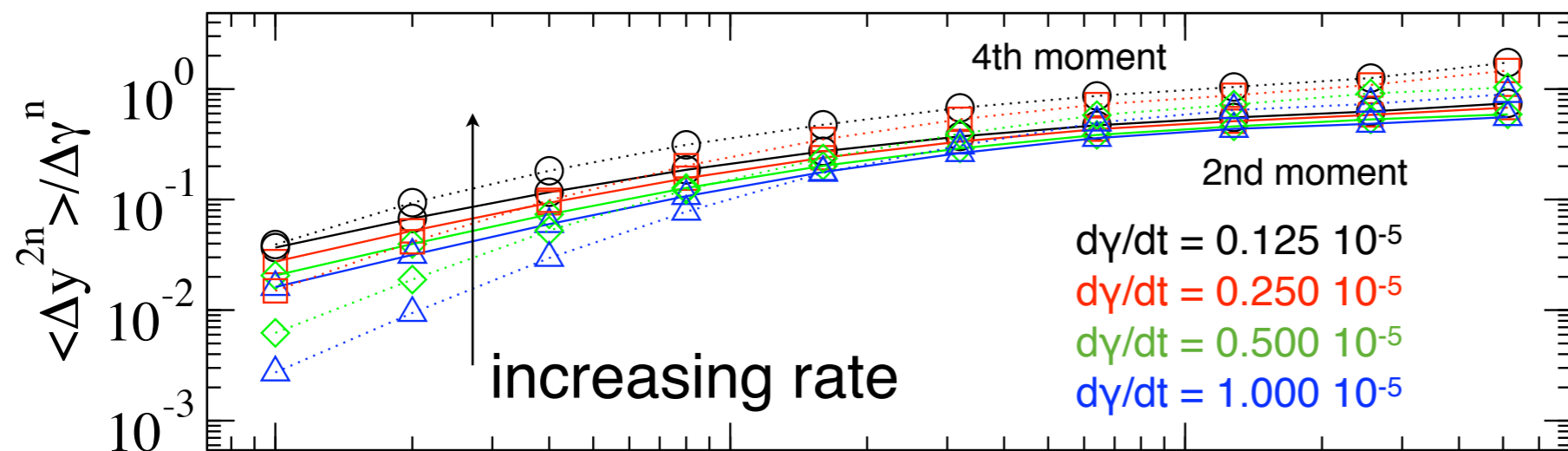
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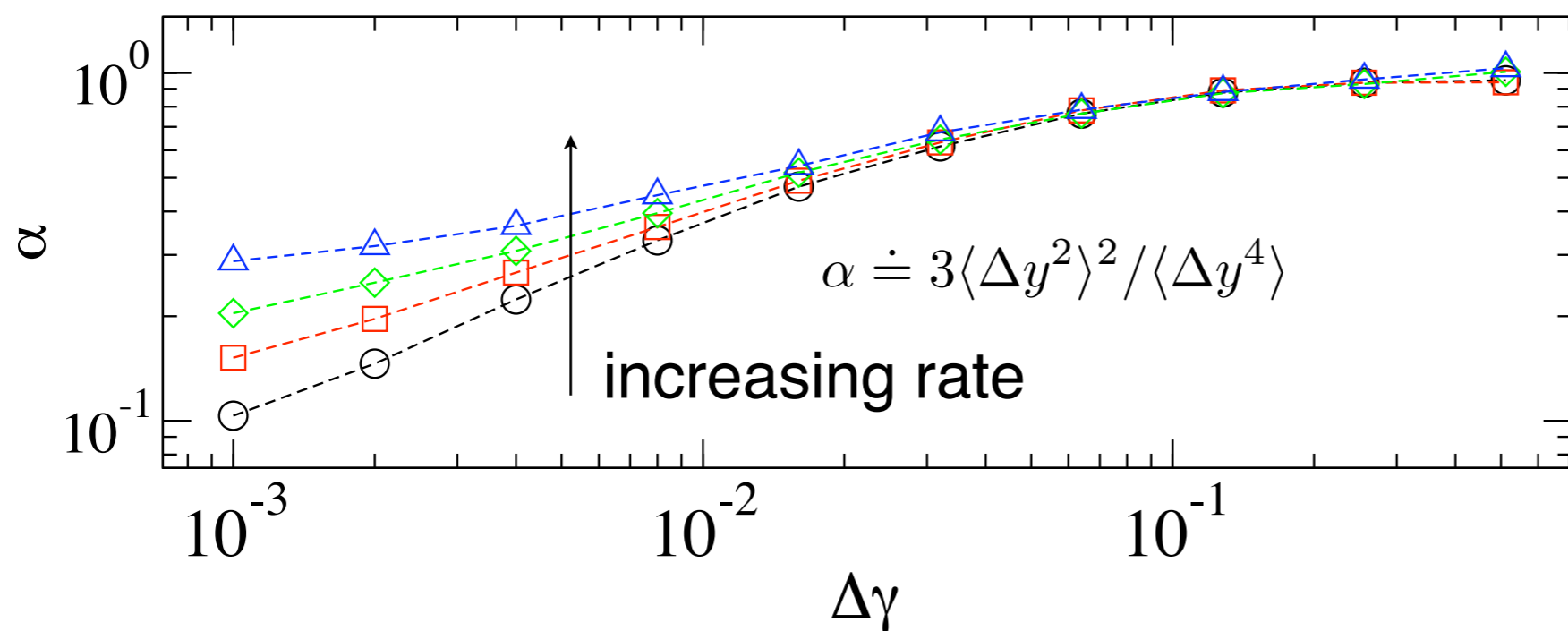
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2nd and 4th moments ($\phi=0.85$)

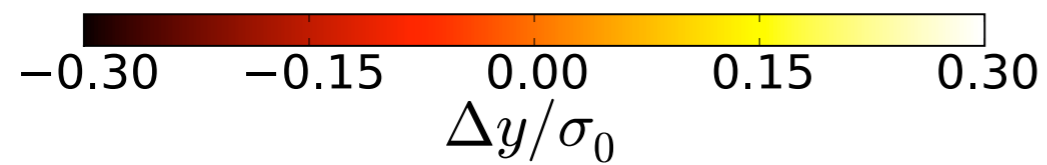
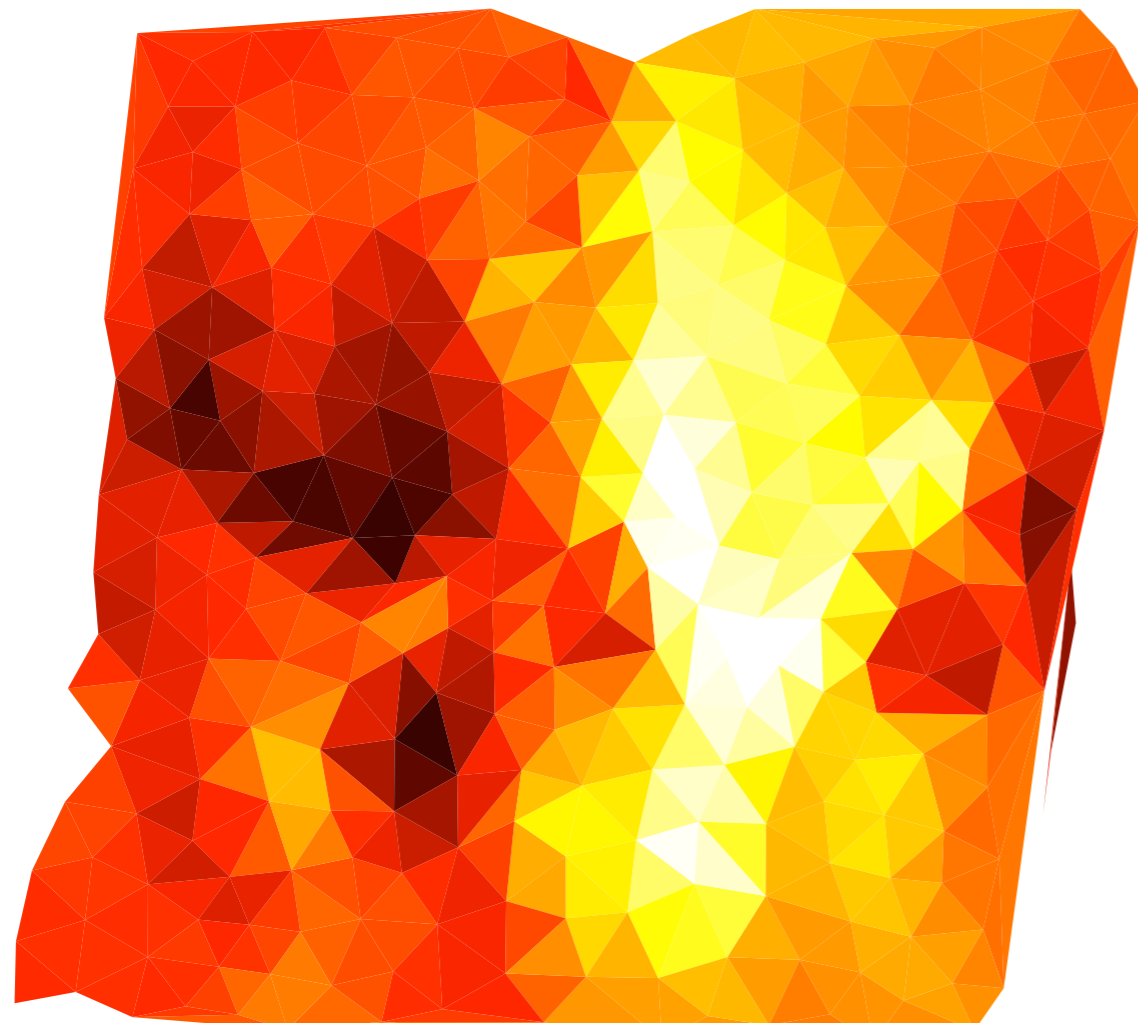


slight rate dependence at plateau

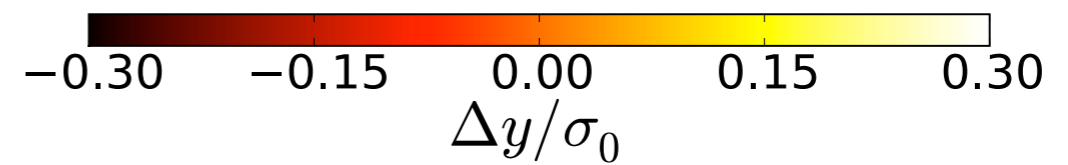
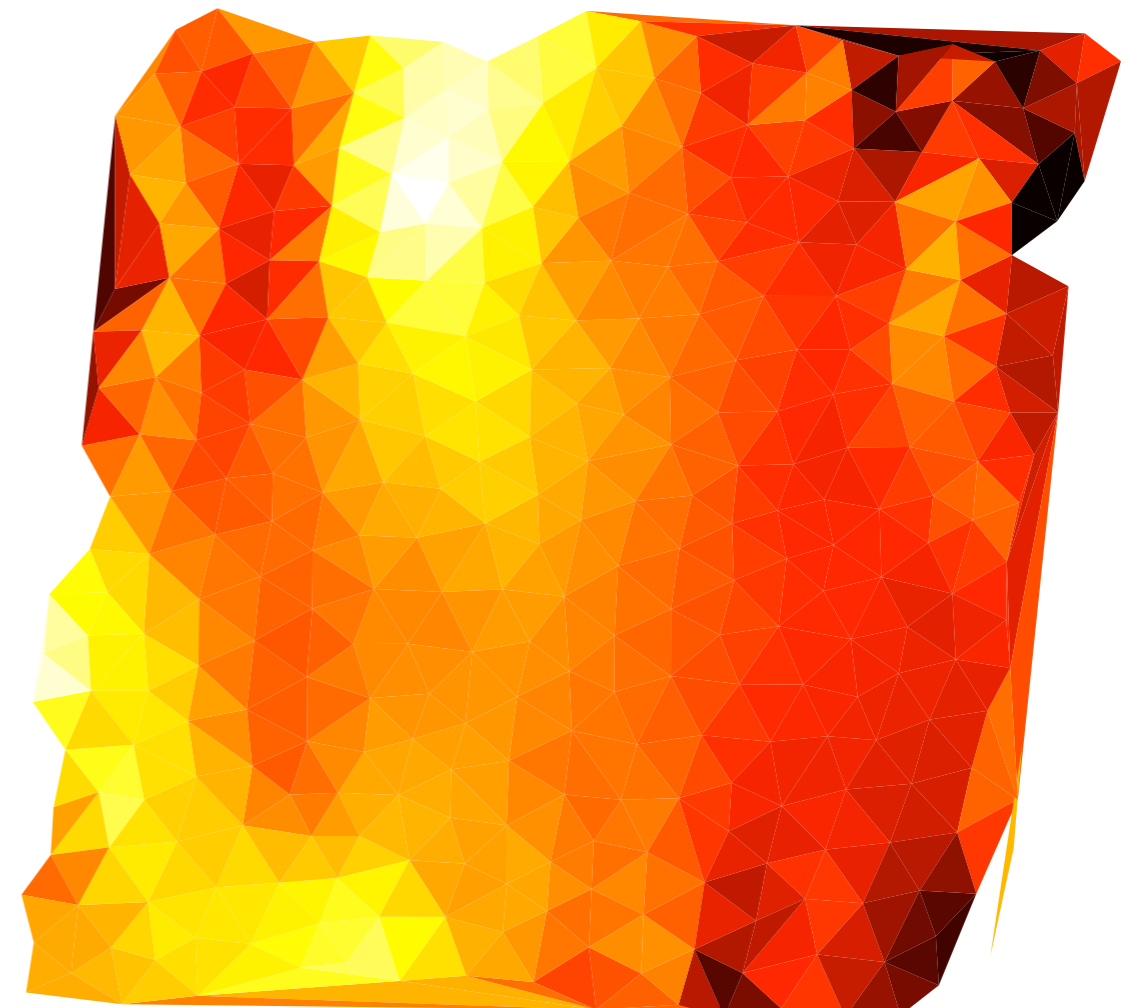
at slowest rate, D_{eff} within 10% of D_{eff} for $\phi=1.0$



Typical displacement over $\Delta\gamma \sim 0.05$



$\phi = 1.0$

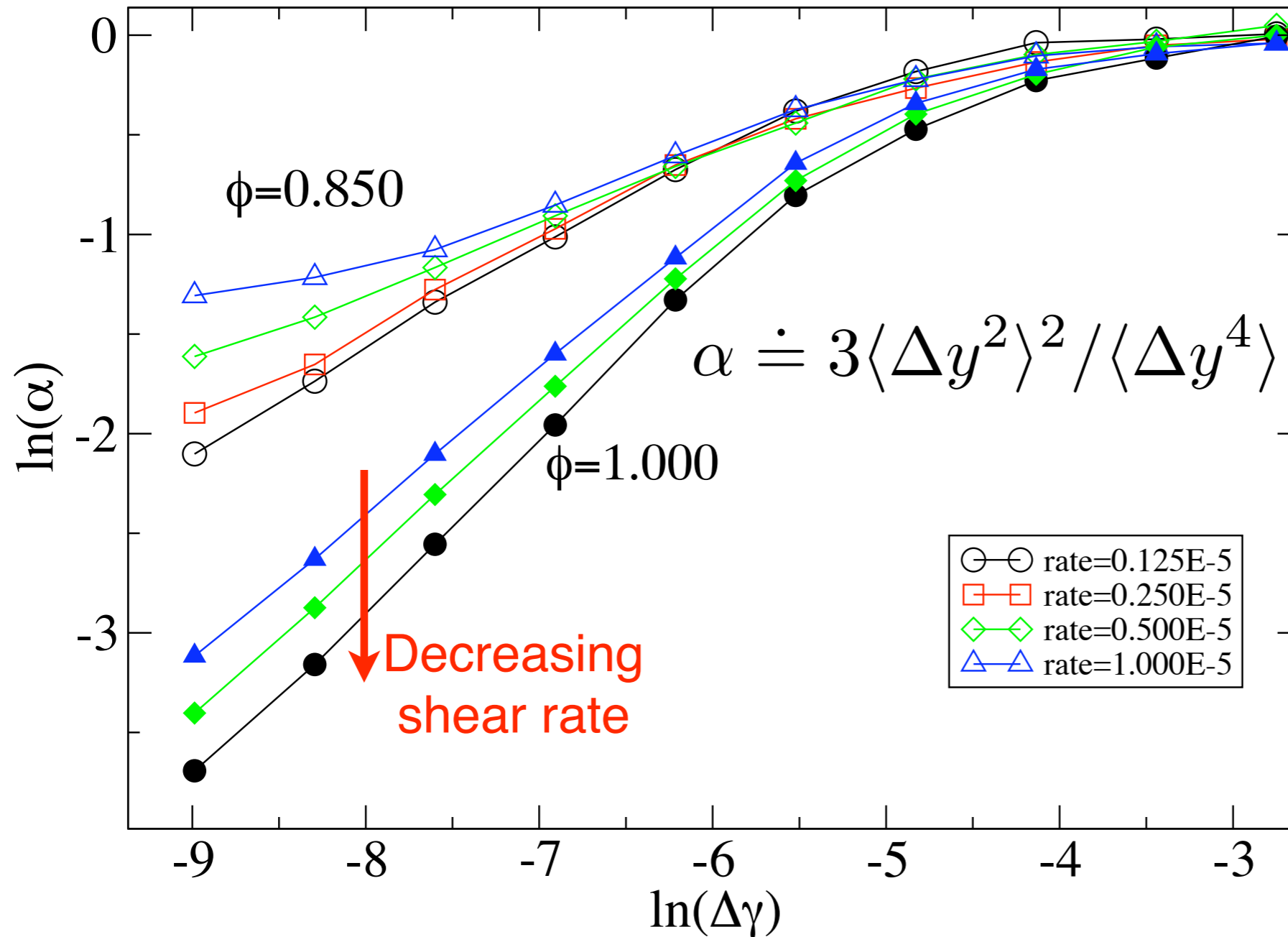


$\phi = 0.85$

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Non-gaussian parameter, α



cross-over to Gaussian is roughly independent of ϕ and dy/dt .

Conclusion (Diffusion)

- Slip lines argument gives:
 - slip amplitude = $a \sim 0.8\sigma$
 - strain quantum = $\Delta\gamma^* \sim a/L \sim 0.05$
- Displacement fields at $\Delta\gamma \sim 0.05$ look like slip lines with consistent slip amplitude
- Seems surprisingly robust with respect to ϕ !
 - systems near ϕ_c much less intermittent at small $\Delta\gamma$
 - but surprisingly similar in Fickian regime!

Dissipation

$$\frac{dU}{dt} = \left. \frac{\partial U}{\partial \gamma} \right|_s \dot{\gamma} + \sum_i \frac{\partial U}{\partial \vec{s}_i} \dot{\vec{s}}_i = \sigma \dot{\gamma} - \sum_i \vec{F}_i \cdot \delta \vec{v}_i$$

Dissipation

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- Energy change under affine deformation = σ

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- Energy change under affine deformation = σ

- Identify as input power
- Identify as dissipation rate

Dissipation

$$\frac{dU}{dt} = \boxed{\frac{\partial U}{\partial \gamma} \Big|_s} \dot{\gamma} + \sum_i \frac{\partial U}{\partial \vec{s}_i} \dot{\vec{s}}_i = \boxed{\sigma \dot{\gamma}} - \boxed{\sum_i \vec{F}_i \cdot \delta \vec{v}_i}$$

- Energy change under affine deformation = σ

- Identify as input power
- Identify as dissipation rate

$$\Gamma \dot{\gamma} = \sigma \dot{\gamma} - \frac{dU}{dt} = \sum_i \vec{F}_i \cdot \delta \vec{v}_i = D \sum_i \delta v_i^2$$

Dissipation

$$\frac{dU}{dt} = \left[\frac{\partial U}{\partial \gamma} \right]_s \dot{\gamma} + \sum_i \frac{\partial U}{\partial \vec{s}_i} \dot{\vec{s}}_i = \sigma \dot{\gamma} - \sum_i \vec{F}_i \cdot \delta \vec{v}_i$$

- Energy change under affine deformation = σ

- Identify as input power
- Identify as dissipation rate

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$$\langle \Gamma \rangle = \langle \sigma \rangle = \frac{DN}{\dot{\gamma}} \langle \delta v^2 \rangle$$

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- Γ is energy dissipated **per unit strain**

Dissipation

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- Ono *et. al.* PRE 2003

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Dissipation

$$\frac{dU}{dt} = \left[\frac{\partial U}{\partial \gamma} \right]_s \dot{\gamma} + \sum_i \frac{\partial U}{\partial \vec{s}_i} \dot{\vec{s}}_i = \sigma \dot{\gamma} - \sum_i \vec{F}_i \cdot \delta \vec{v}_i$$

- Energy change under affine deformation = σ

- Identify as input power
- Identify as dissipation rate

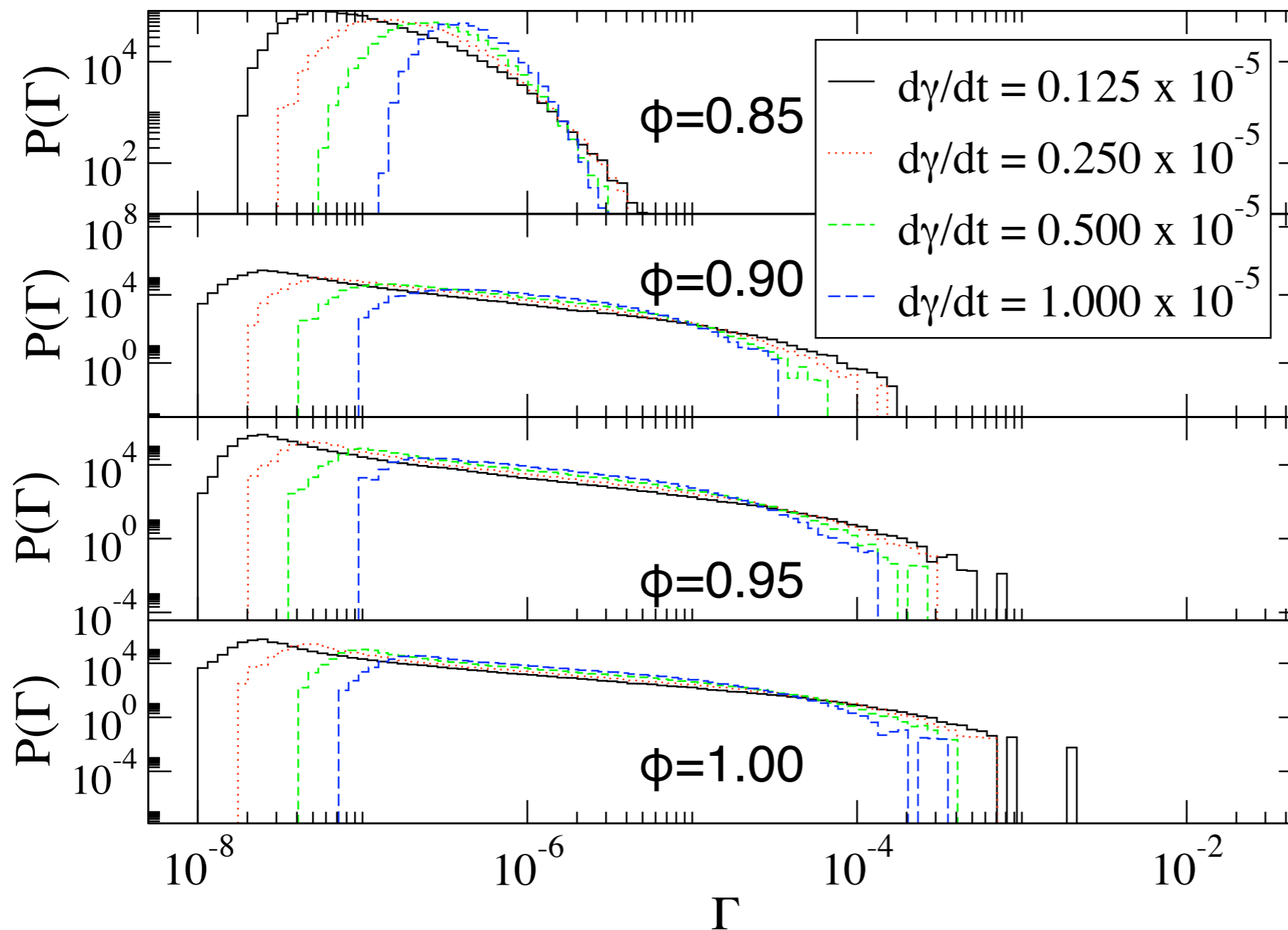
$$\Gamma \dot{\gamma} = \sigma \dot{\gamma} - \frac{dU}{dt} = \sum_i \vec{F}_i \cdot \delta \vec{v}_i = D \sum_i \delta v_i^2$$

$$\langle \Gamma \rangle = \langle \sigma \rangle = \frac{DN}{\dot{\gamma}} \langle \delta v^2 \rangle$$

- Ono *et. al.* PRE 2003
- Rheology = fluctuations

- Γ is energy dissipated **per unit strain**

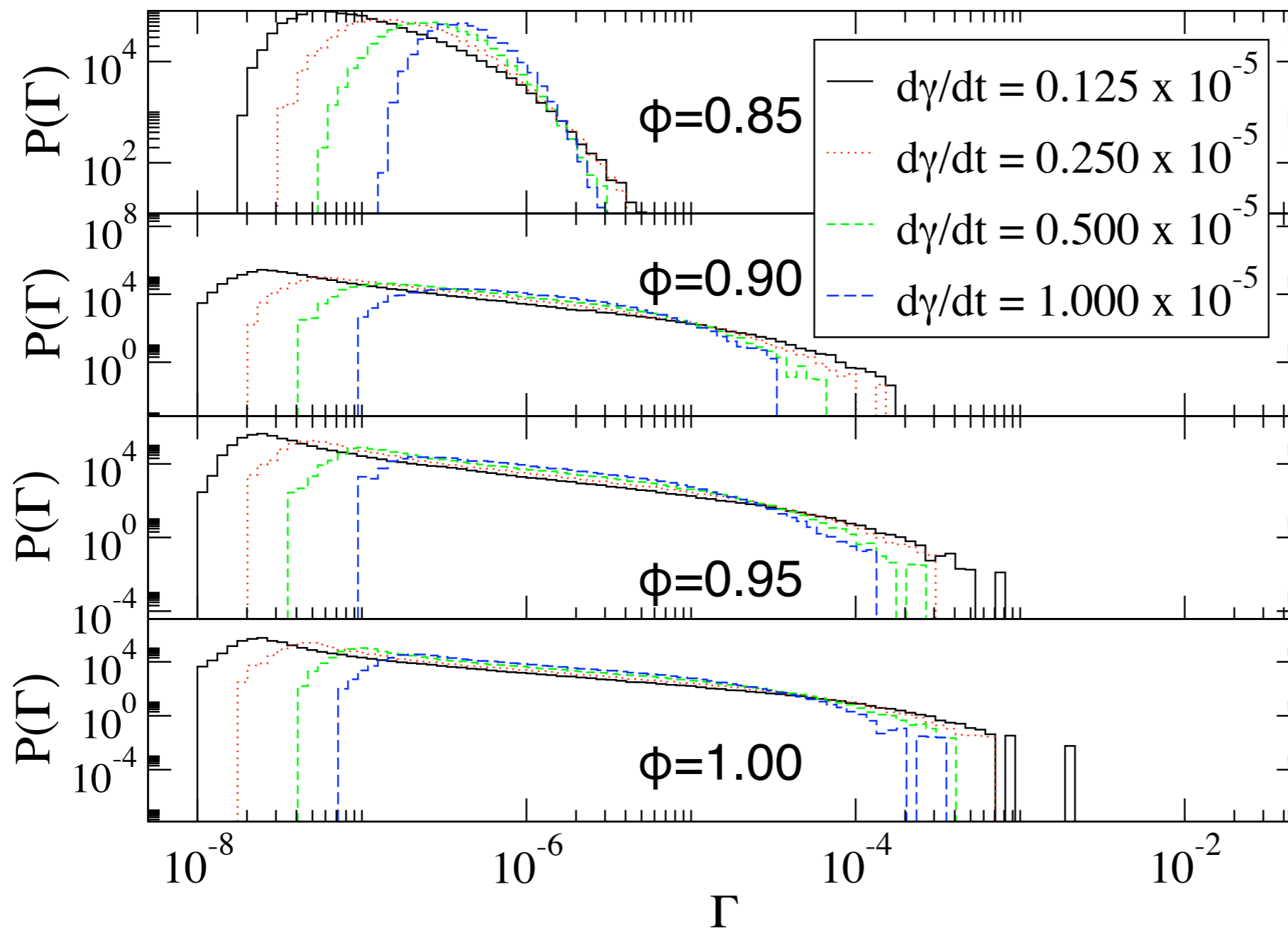
Γ distribution (like acoustic emission spectrum)



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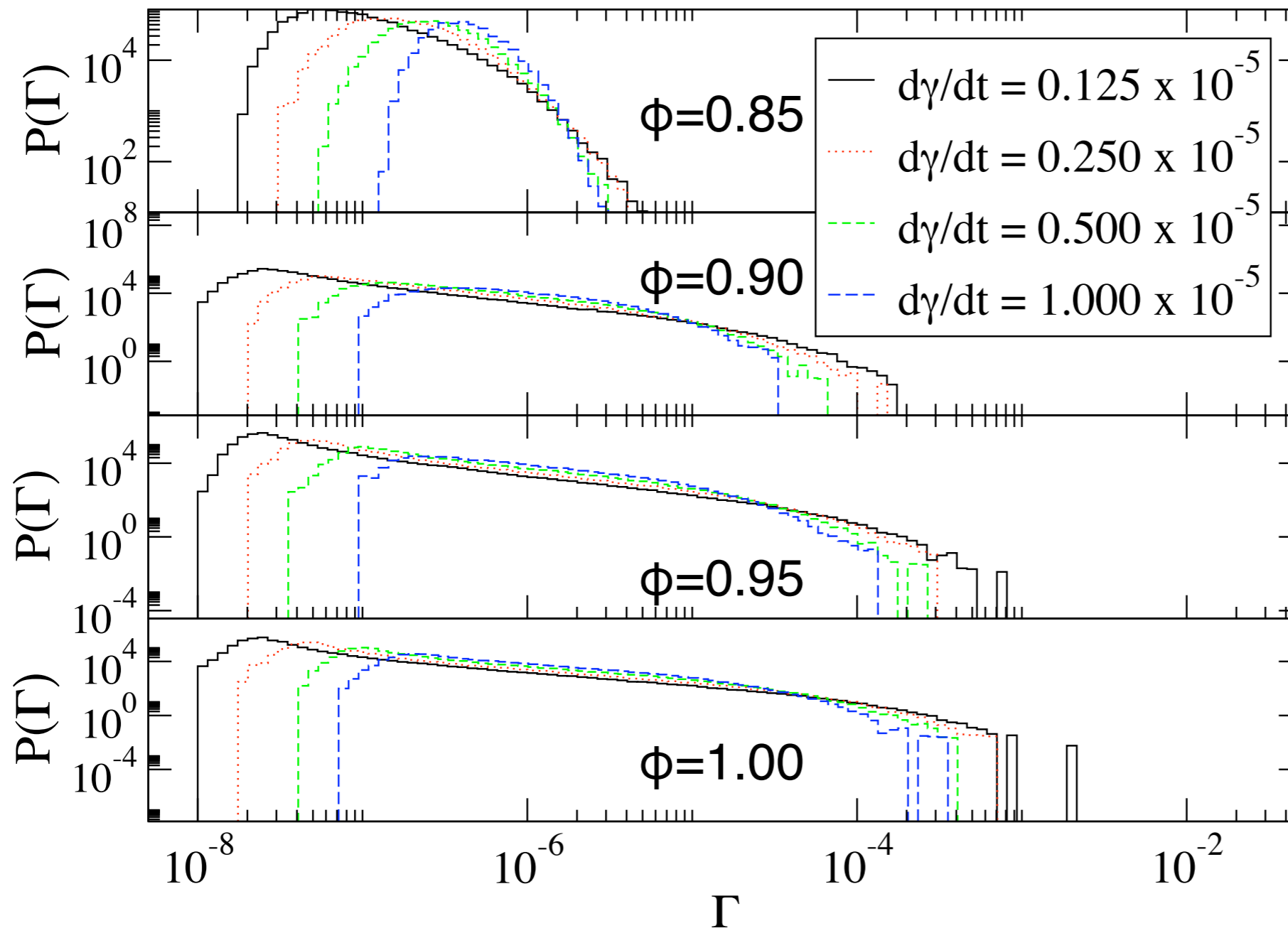
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Γ distribution (like acoustic emission spectrum)



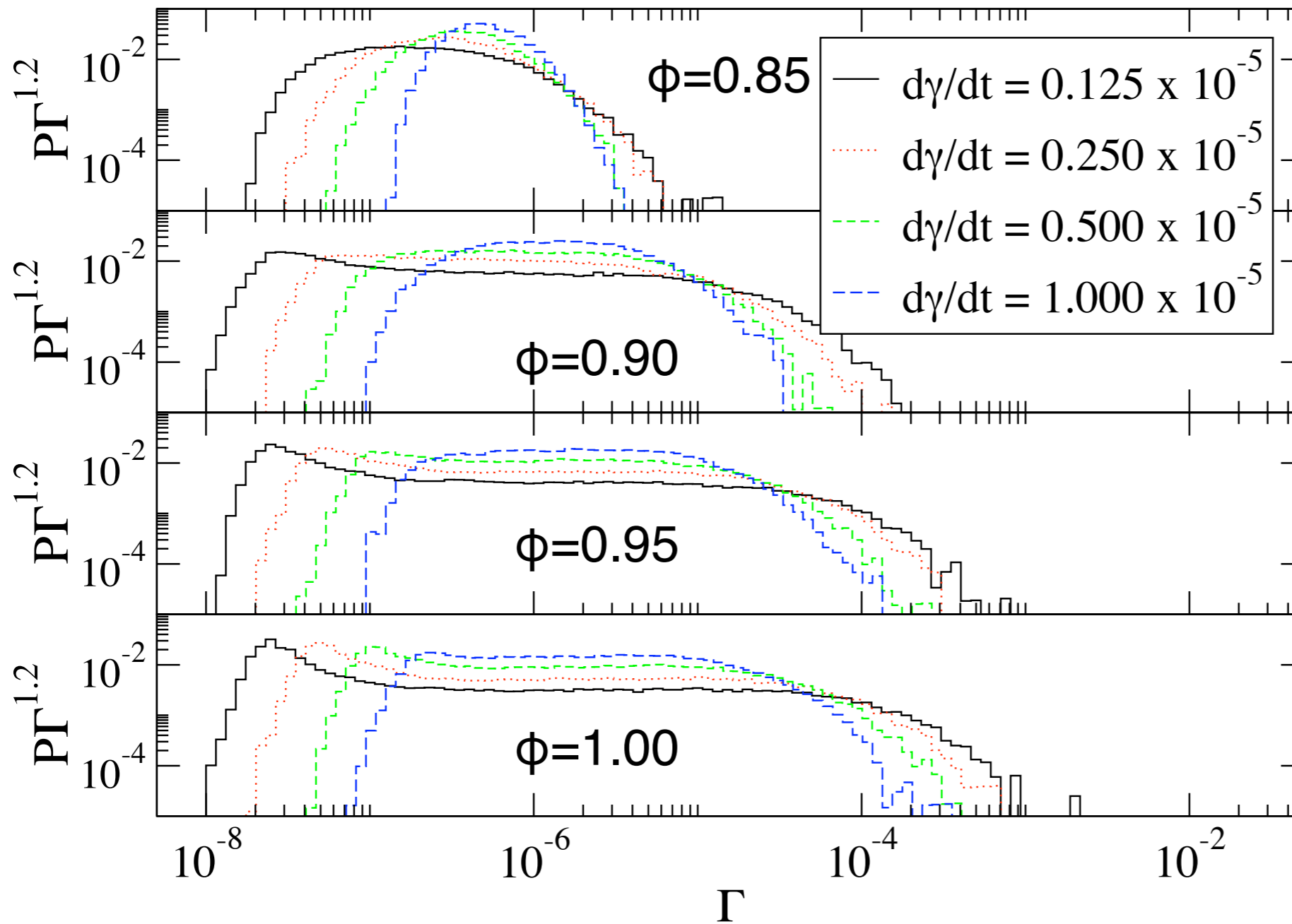
• power-law regime

Γ distribution (like acoustic emission spectrum)

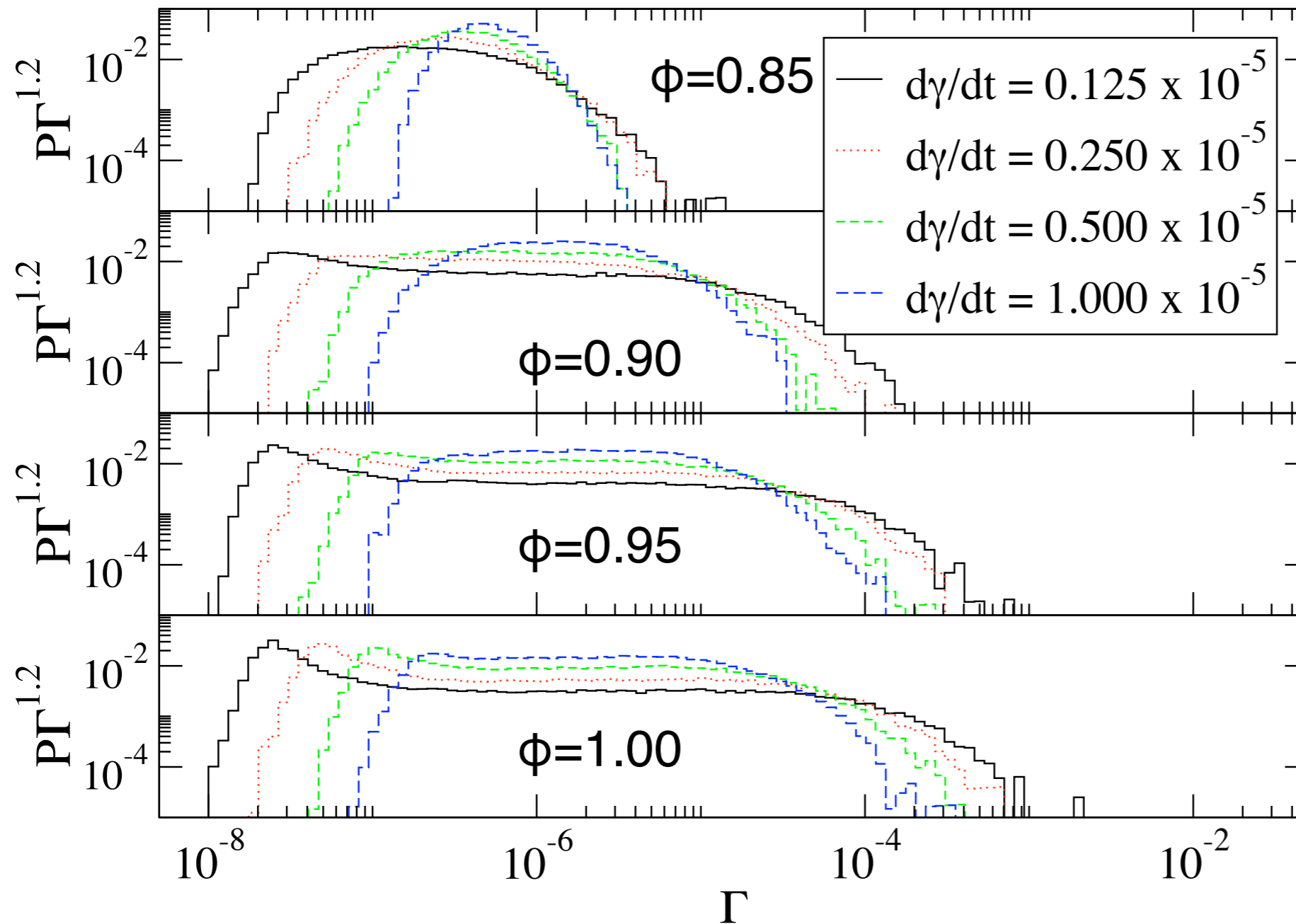


- power-law regime
- exponent ~ -1.2

Γ distribution power-law rescaling

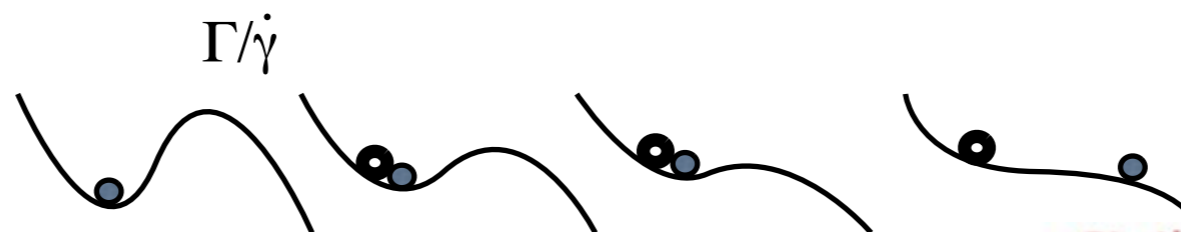
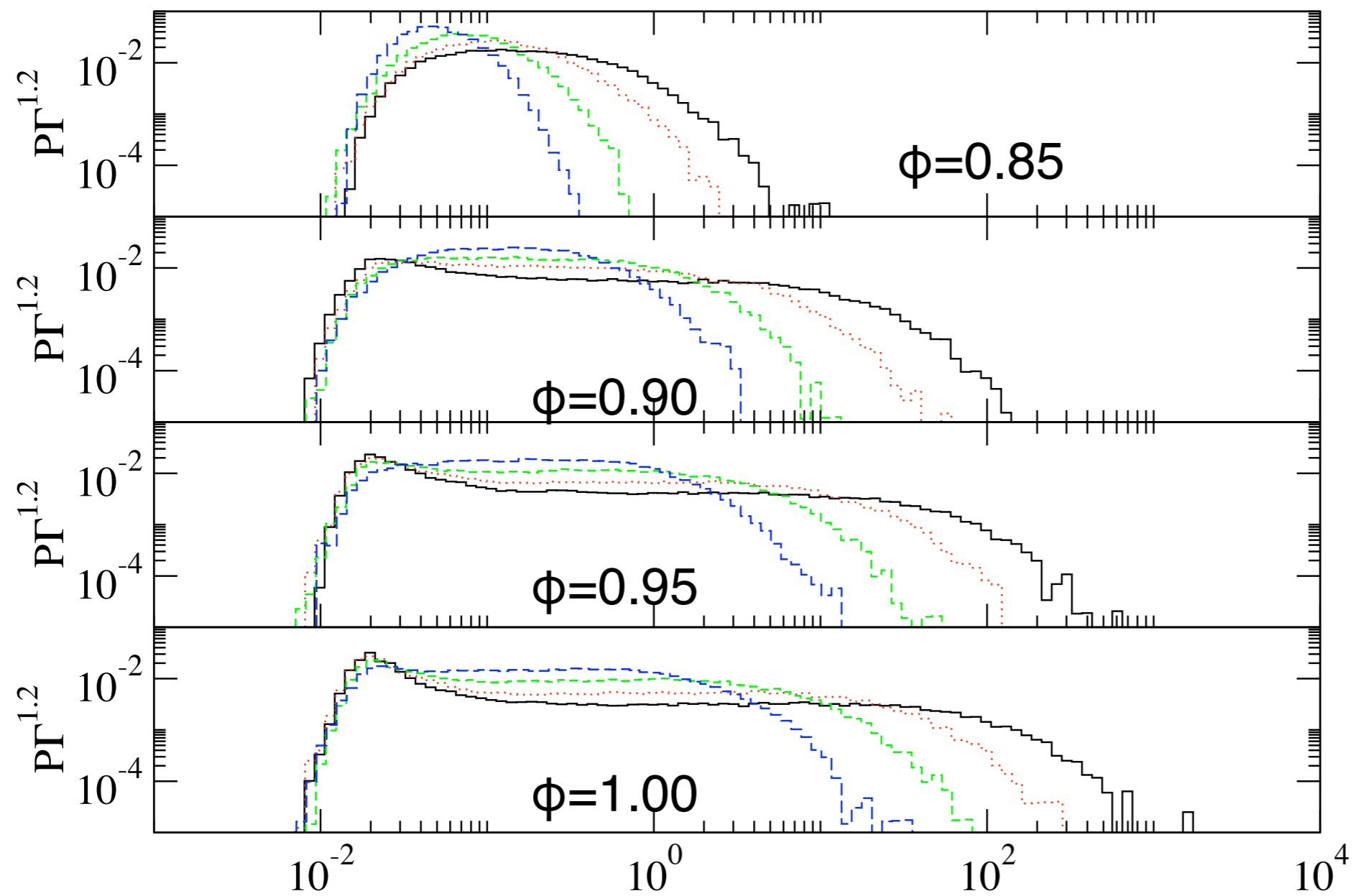


Γ distribution power-law rescaling

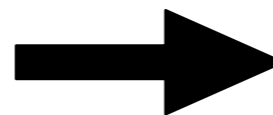


- Scale P by $\Gamma^{-1.2}$

Γ distribution kinematic QS rescaling



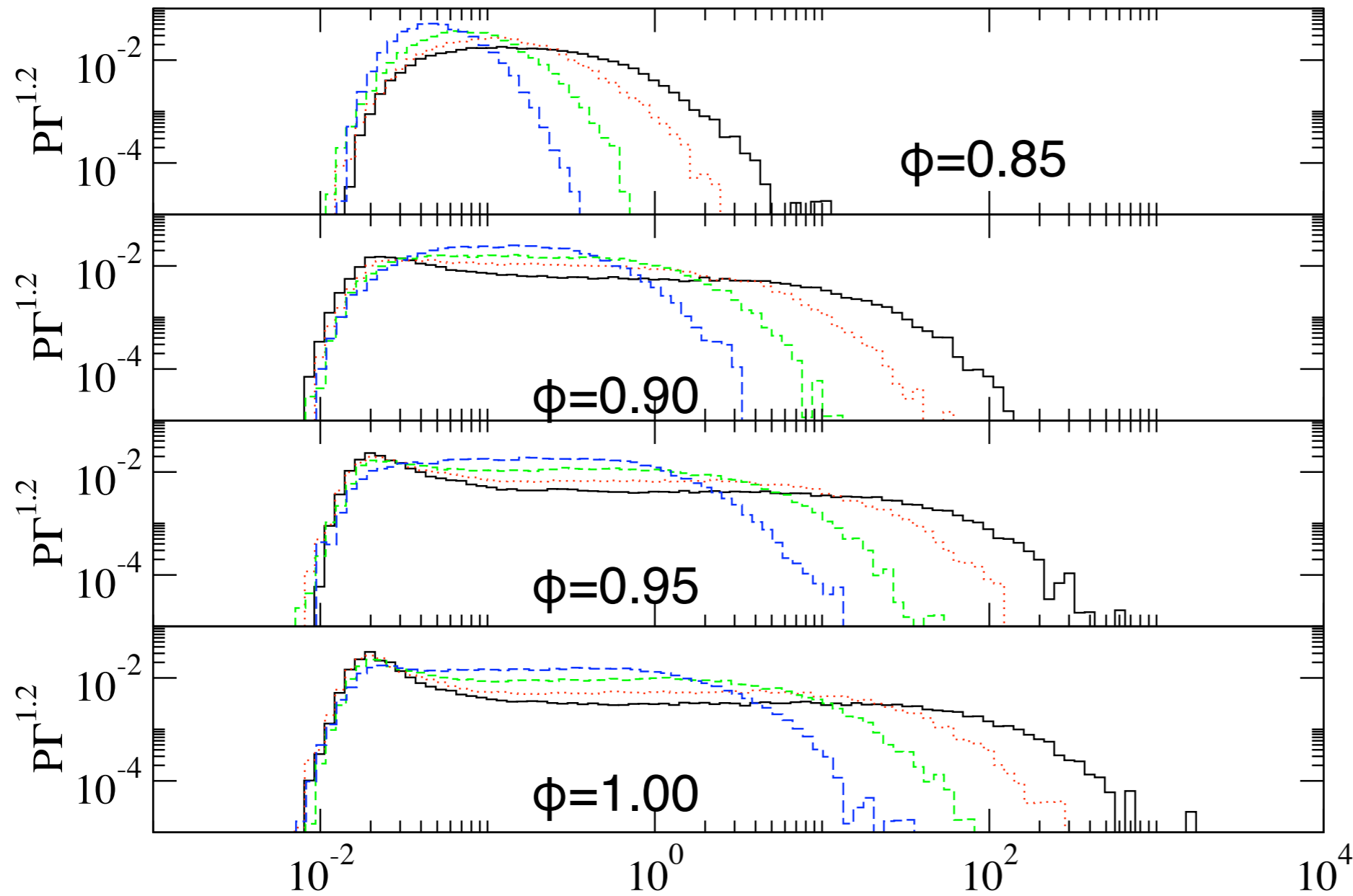
Increasing shear



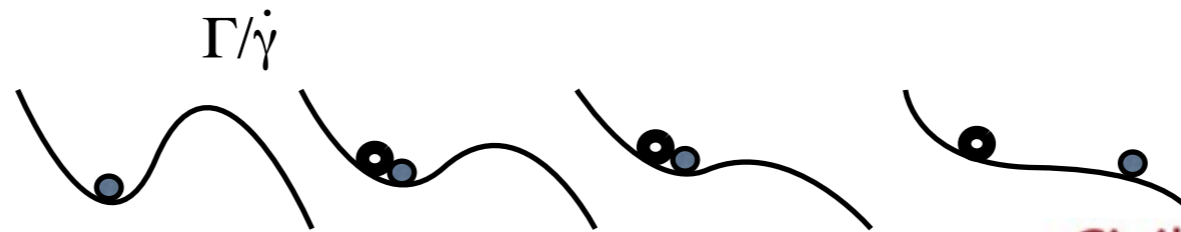
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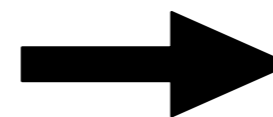
Γ distribution kinematic QS rescaling



• QS scaling:



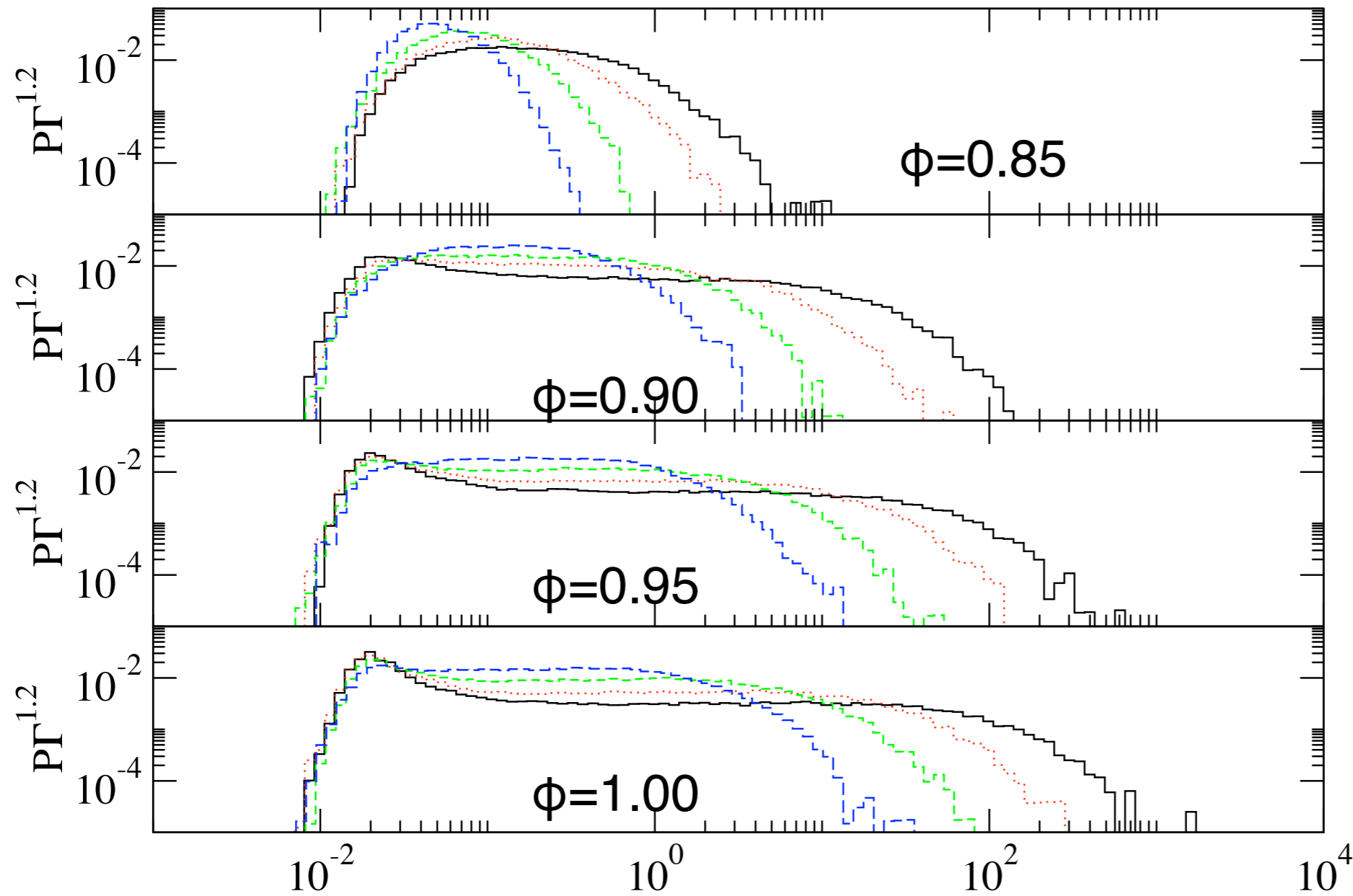
Increasing shear



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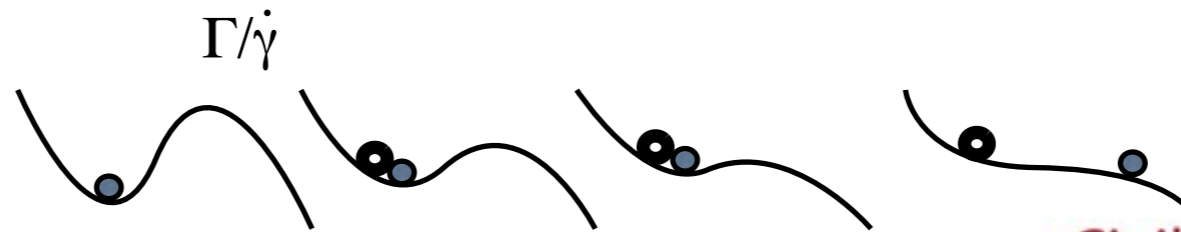
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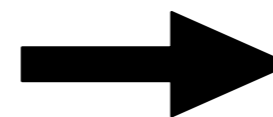


• QS scaling:

$$\Gamma = \frac{D}{\dot{\gamma}} \sum_i \delta v_i^2$$



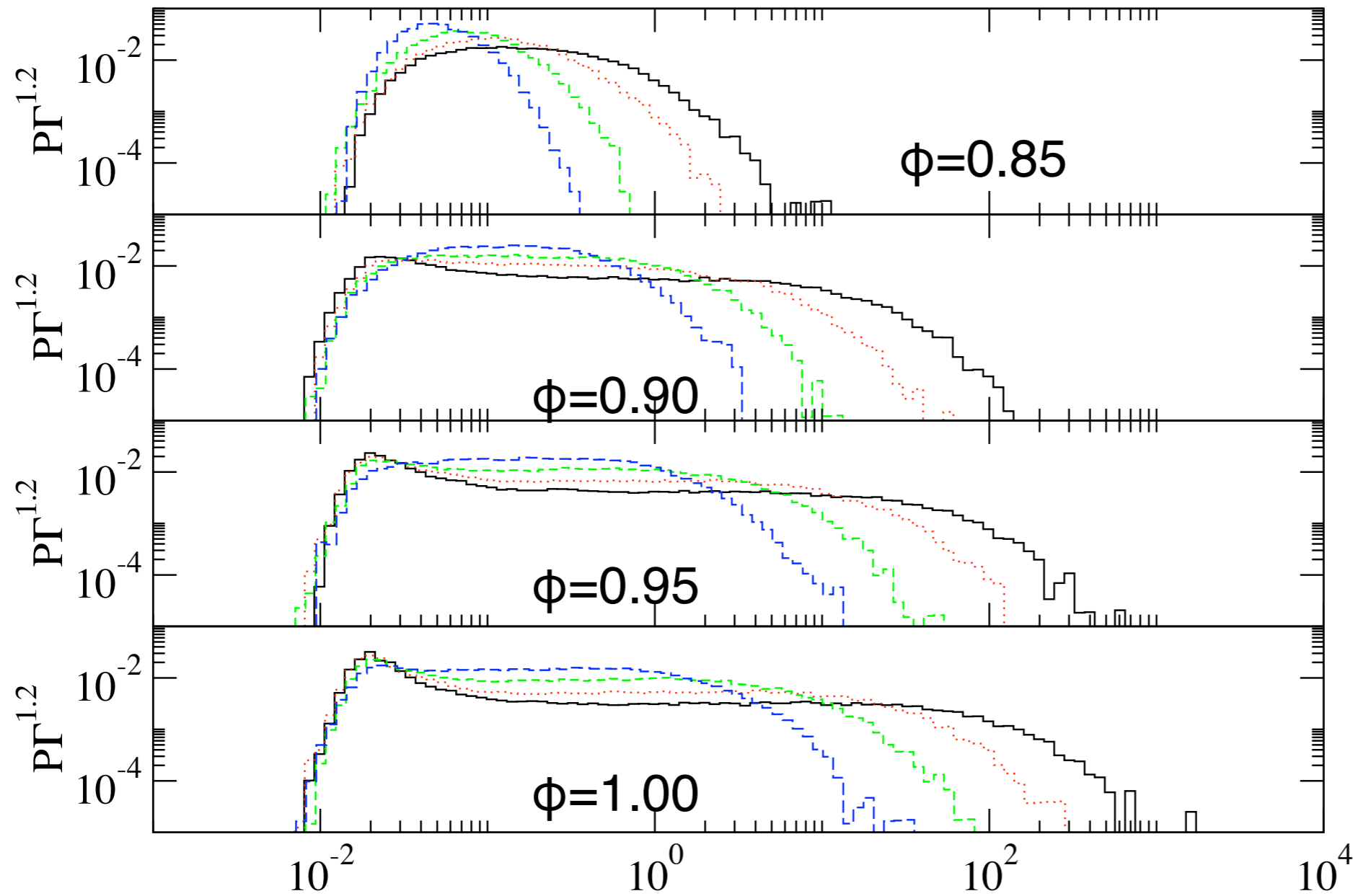
Increasing shear



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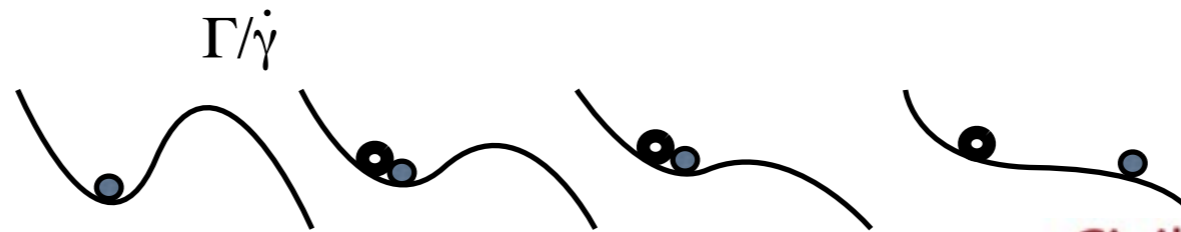
Γ distribution kinematic QS rescaling



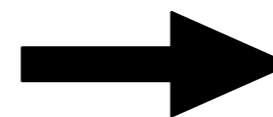
• QS scaling:

$$\Gamma = \frac{D}{\dot{\gamma}} \sum_i \delta v_i^2$$

$$\delta v_i \propto \dot{\gamma}$$



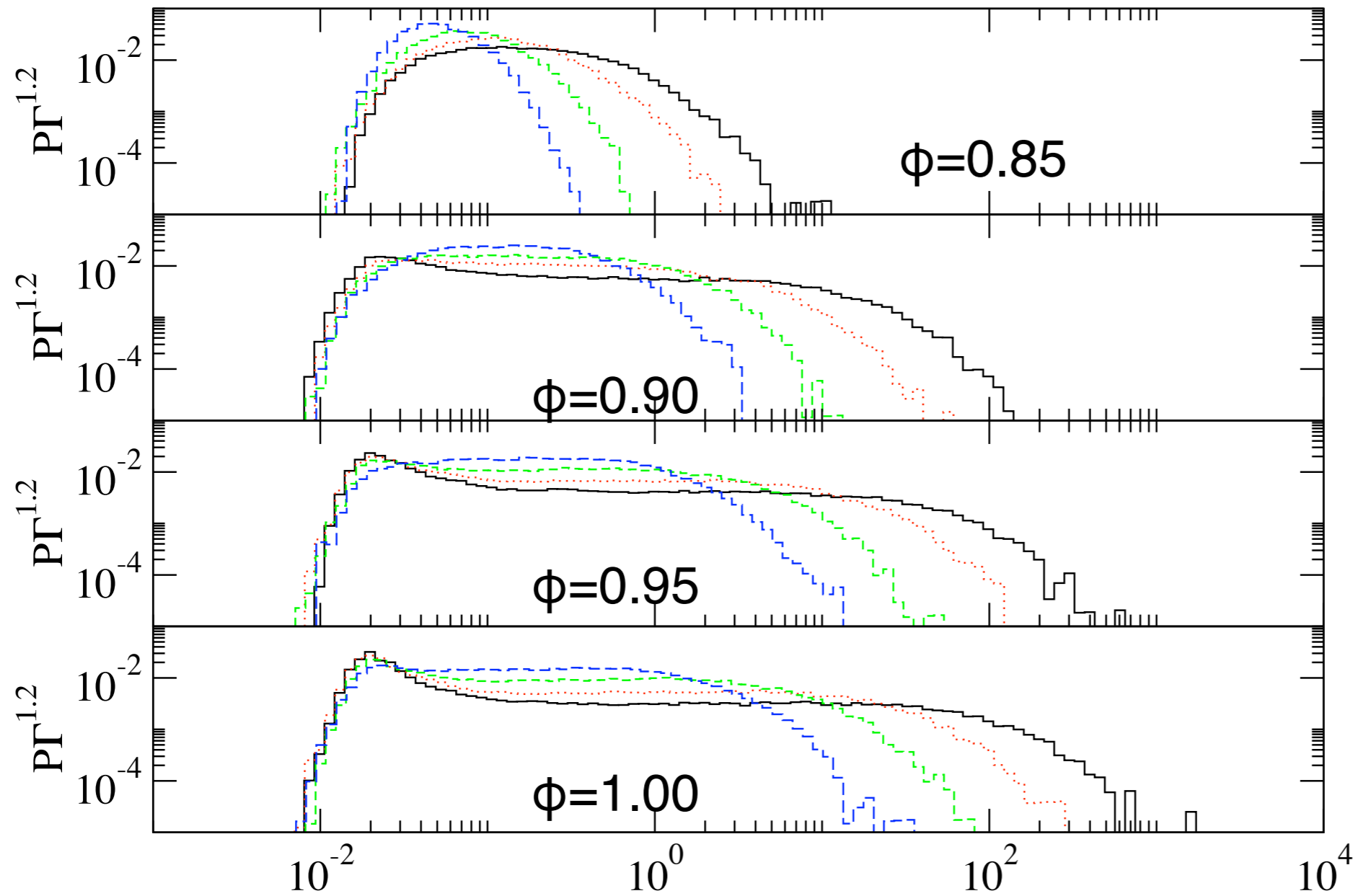
Increasing shear



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Γ distribution kinematic QS rescaling

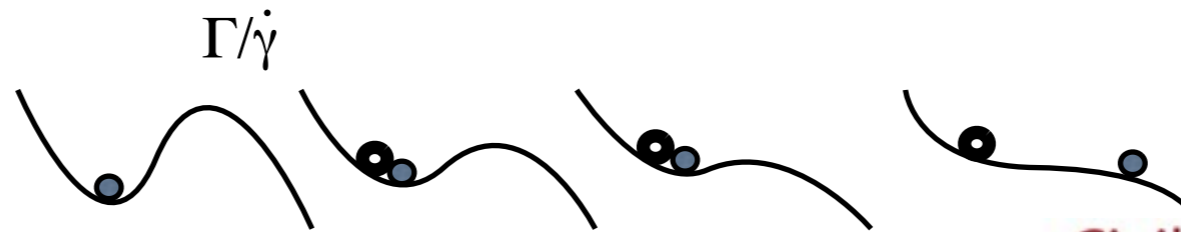


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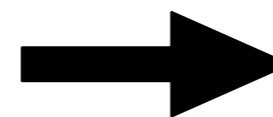
$$\Gamma = \frac{D}{\dot{\gamma}} \sum_i \delta v_i^2$$

$$\delta v_i \propto \dot{\gamma}$$

$$\Gamma \propto \frac{D}{\dot{\gamma}} N \dot{\gamma}^2 = ND \dot{\gamma}$$



Increasing shear



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Conclusion (avalanches/dissipation)

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Conclusion (avalanches/dissipation)

- Instantaneous energy dissipation:

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 - $\phi > \phi_c$, $d\gamma/dt \rightarrow 0$:

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- Questions:
 - Slip line argument predicts $D_{\text{eff}} \sim L$. Can we see it?

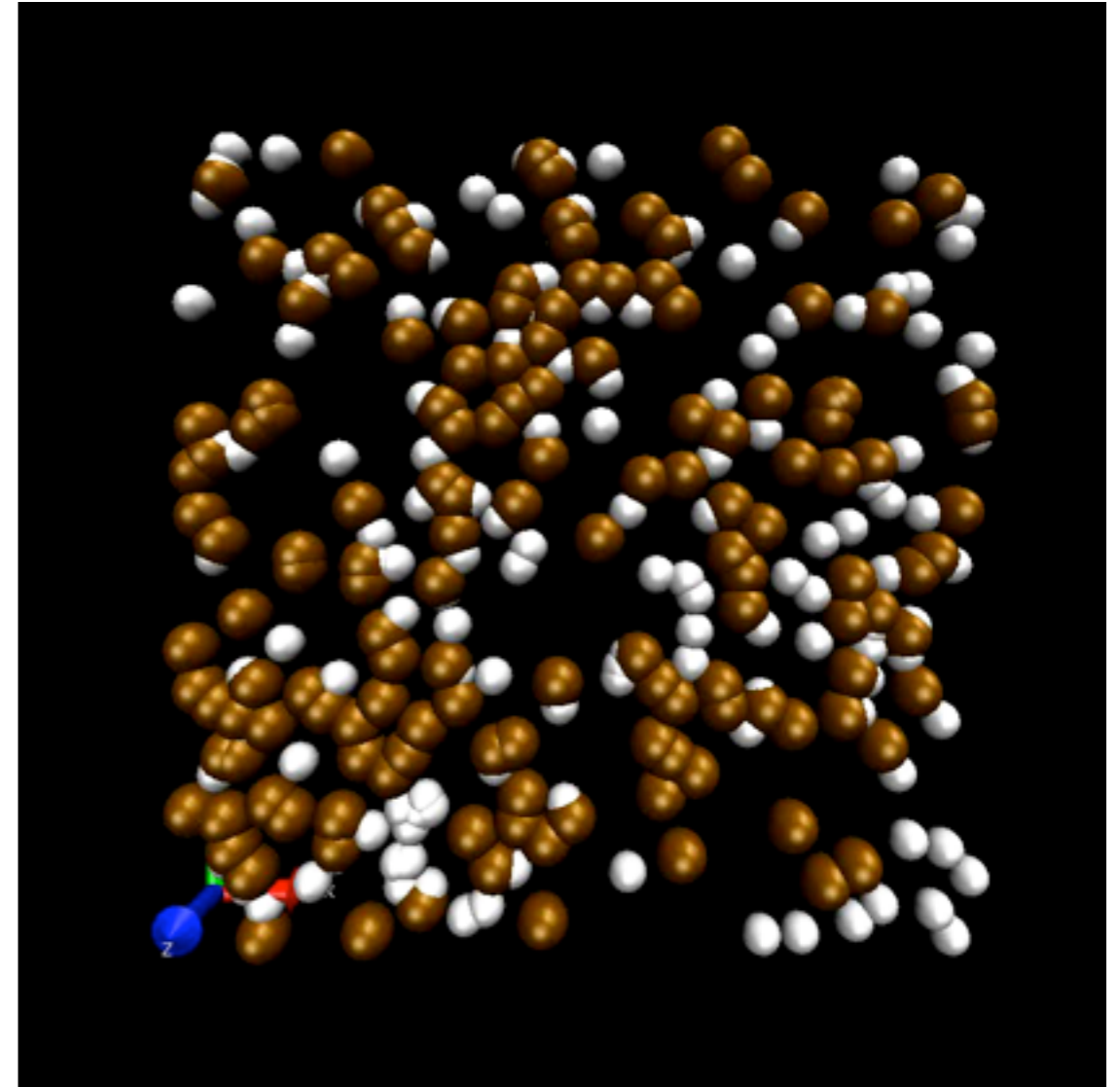
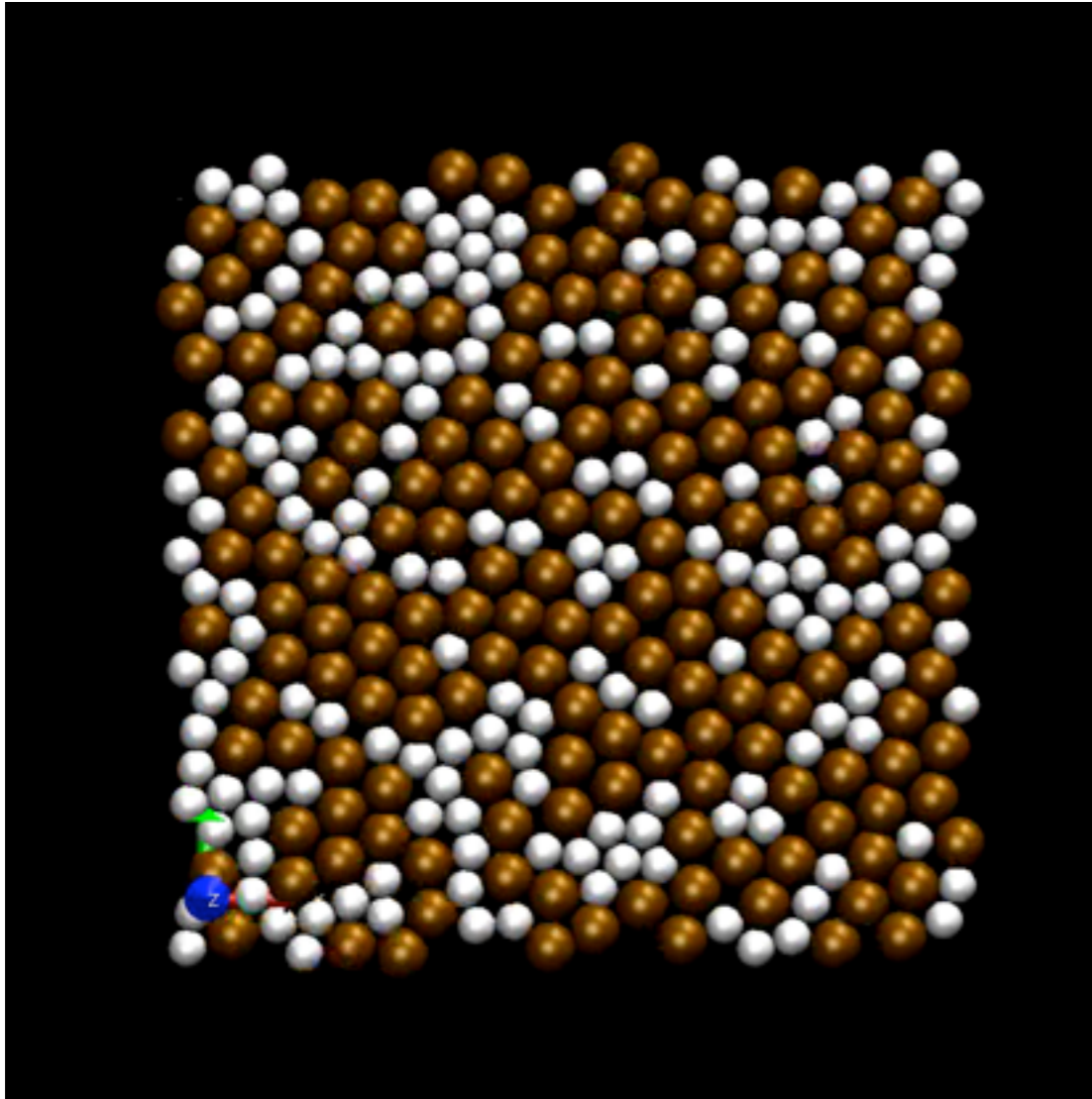
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Conclusion (avalanches/dissipation)

- Instantaneous energy dissipation:
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- Questions:
 - Slip line argument predicts $D_{\text{eff}} \sim L$. Can we see it?
 - How does combined rate/size dictate Fickian cross-over?
 - Is physics the same at the same $\tau_J d\gamma/dt$?

THE END



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Thanks!

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Numerical models / algorithms

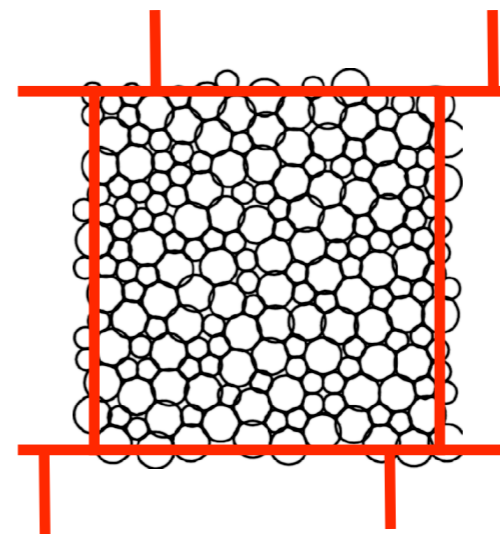
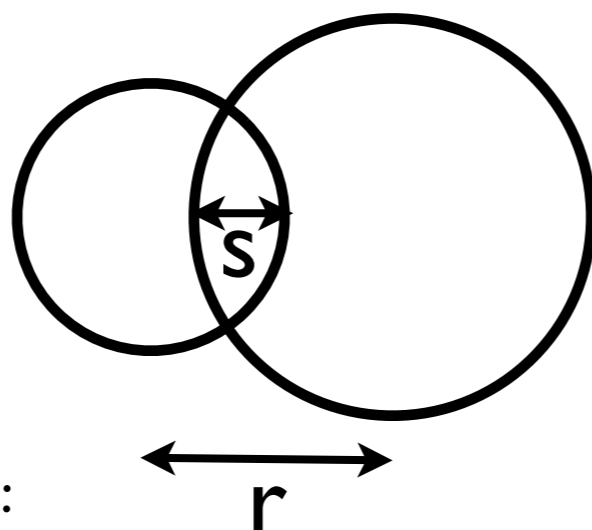
Various interaction potentials:

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

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

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

Binary distribution in 2D



Landscape picture:



(Malandro and Lacks)

Athermal, Quasistatic Procedure:

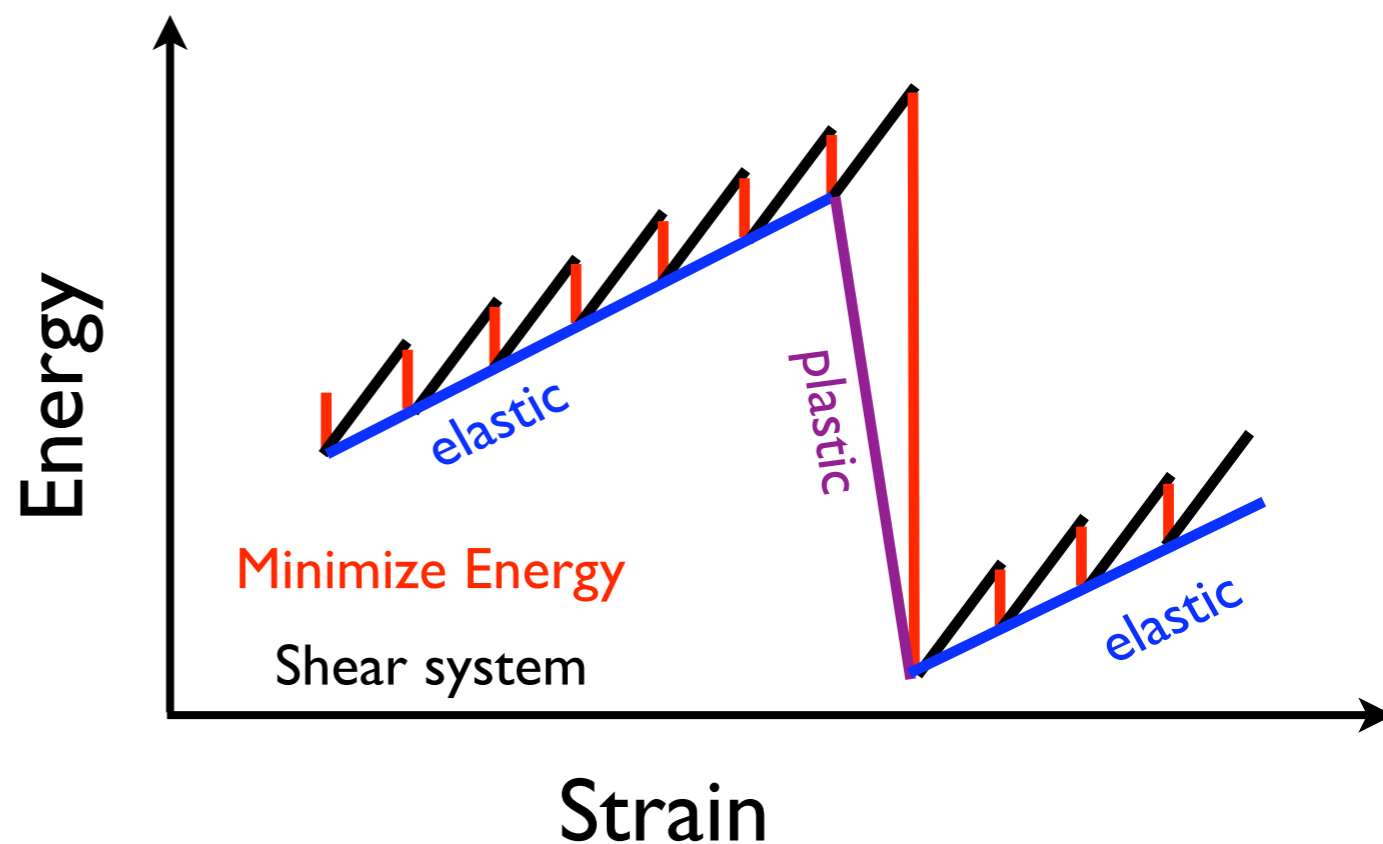
- Minimize potential energy
- Shear boundaries and particles
- Repeat

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

- 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



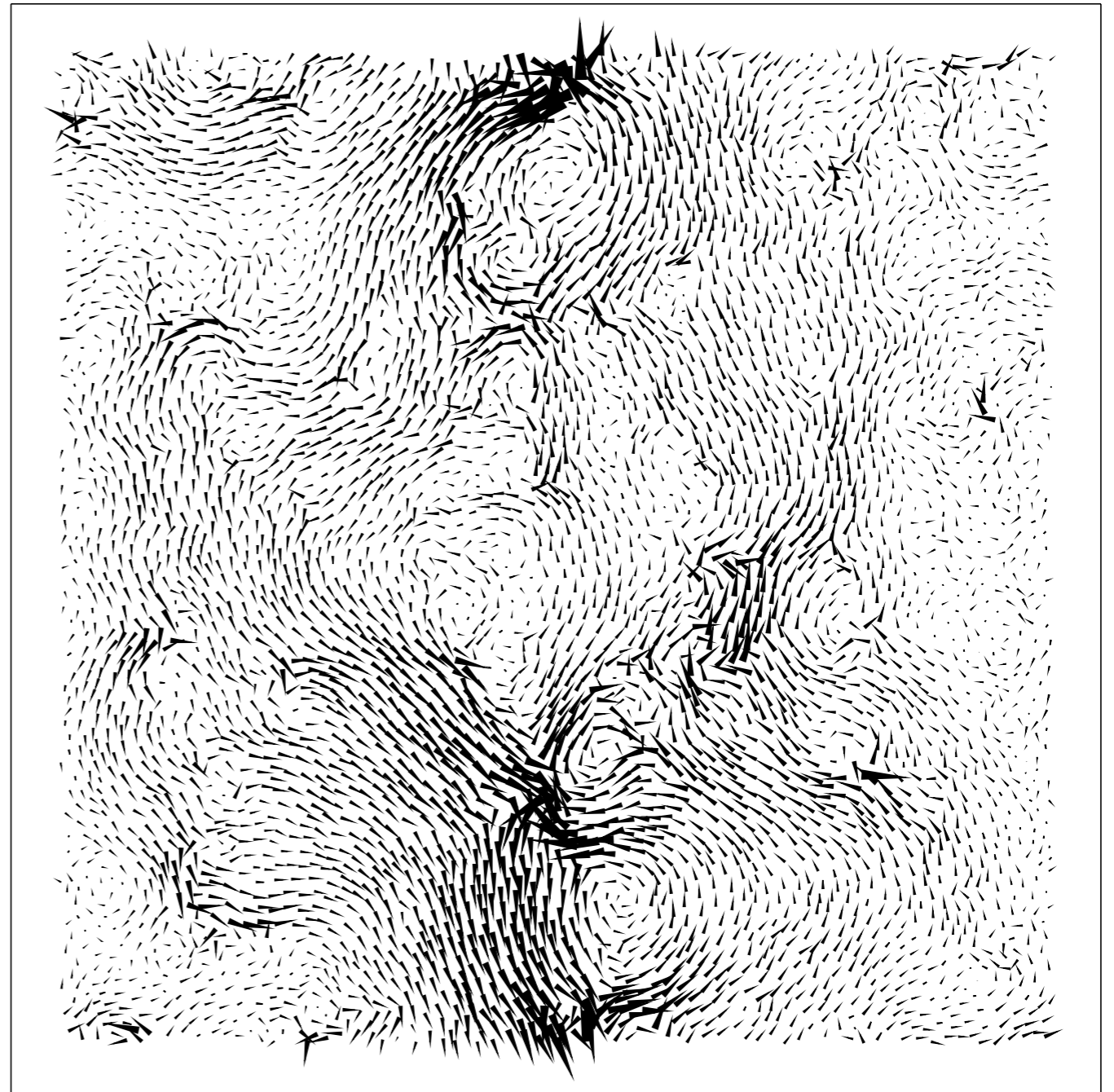
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Linear elastic response (at zero temperature)

- Take a binary Lennard-Jones system
- Quench instantaneously from $T=\infty$ to $T=0$
- Apply infinitesimal shear strain
- Compute deviations from homogeneous shear
- Note vortex-like patterns...
lengthscale?

A. Tanguy et. al. PRB 2002

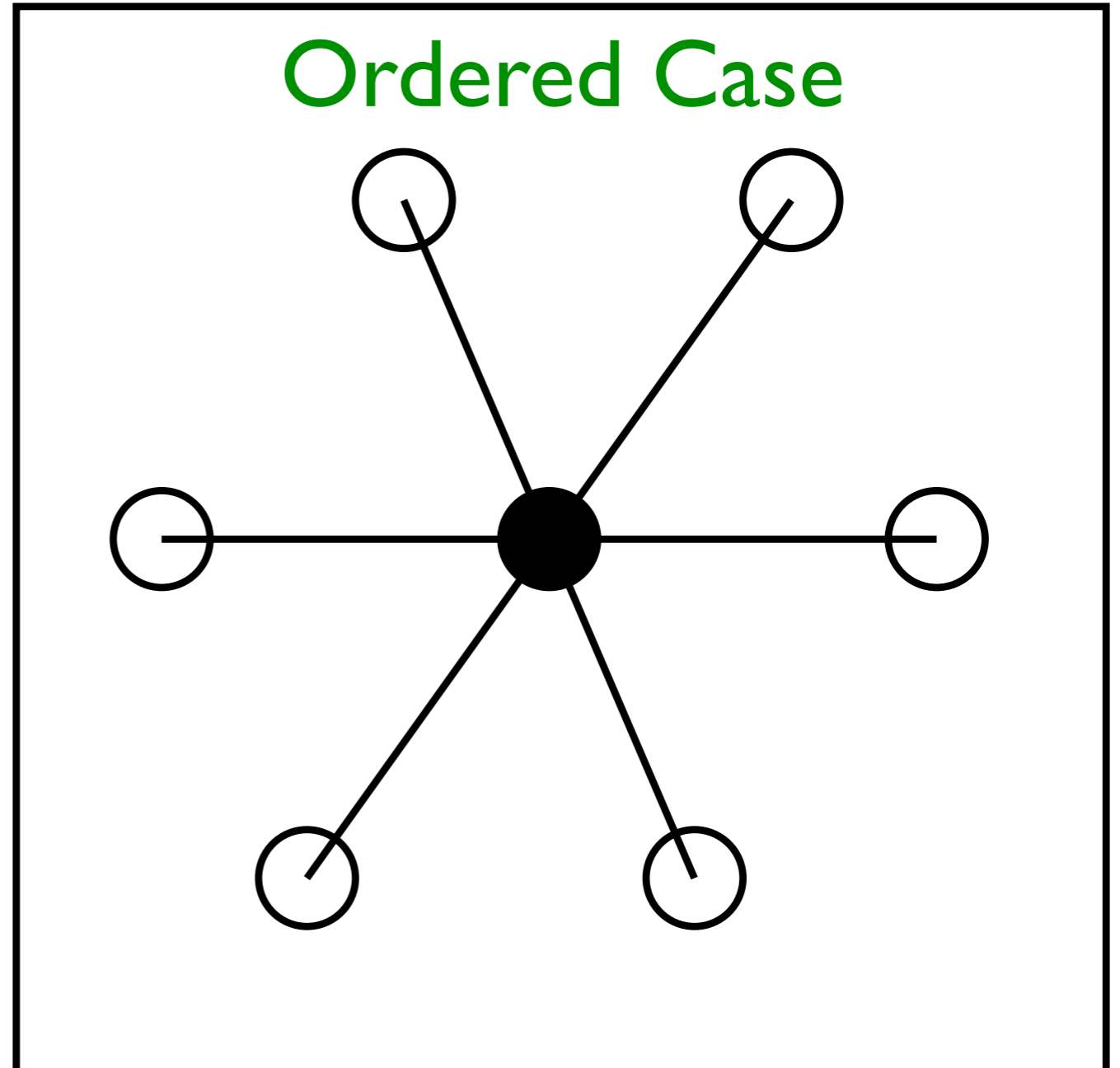


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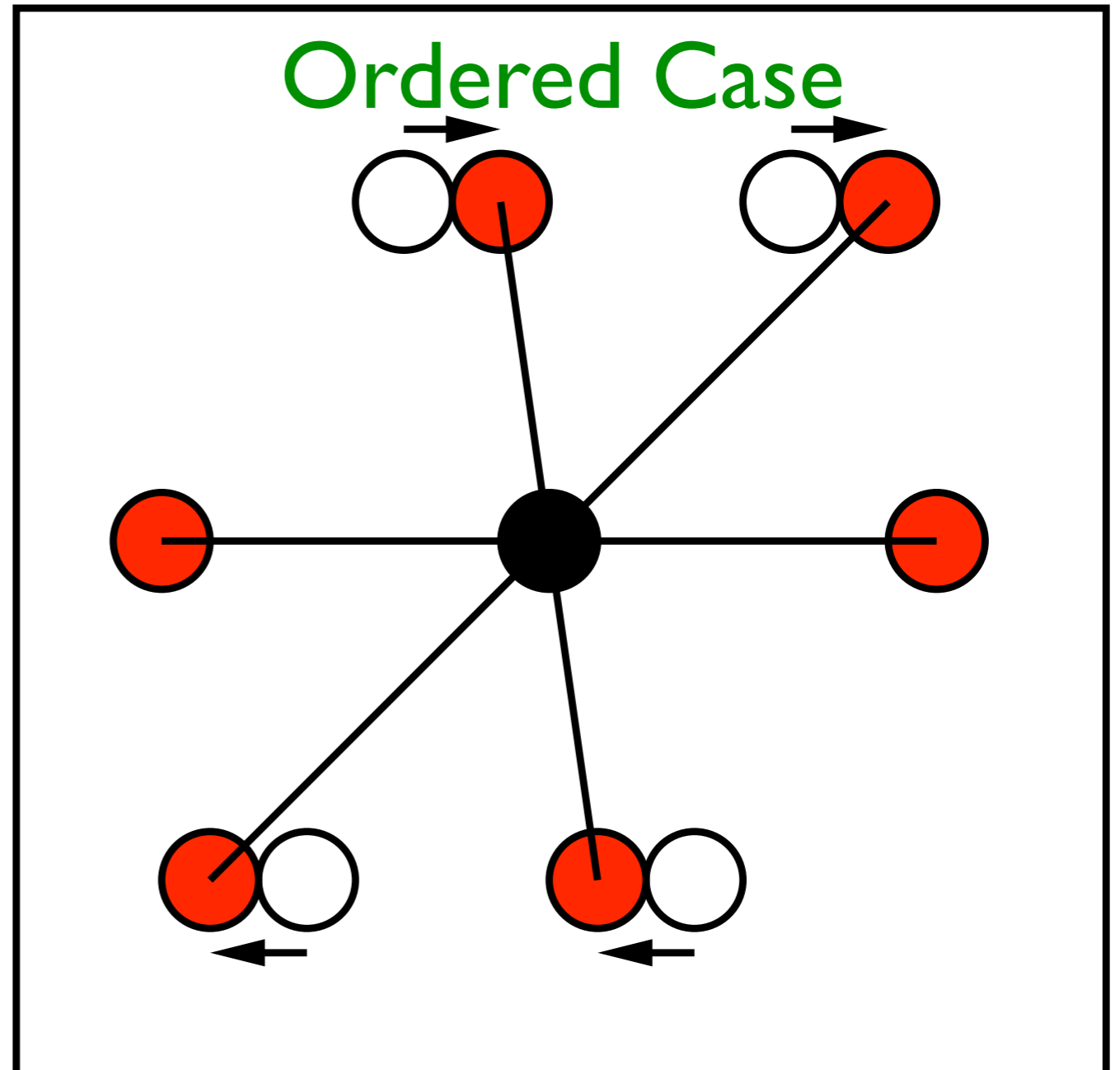
Computing linear response

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



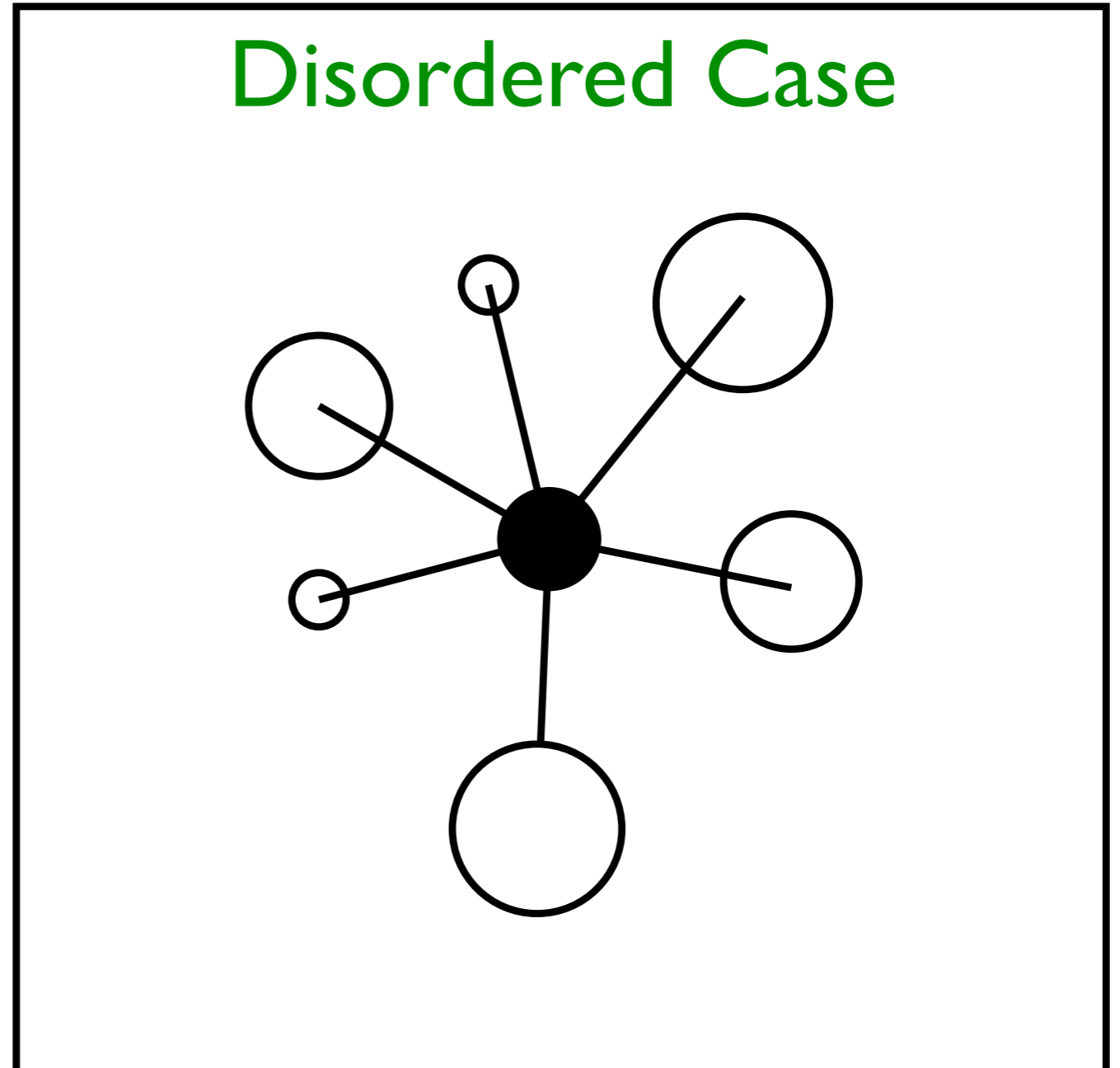
Computing linear response

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



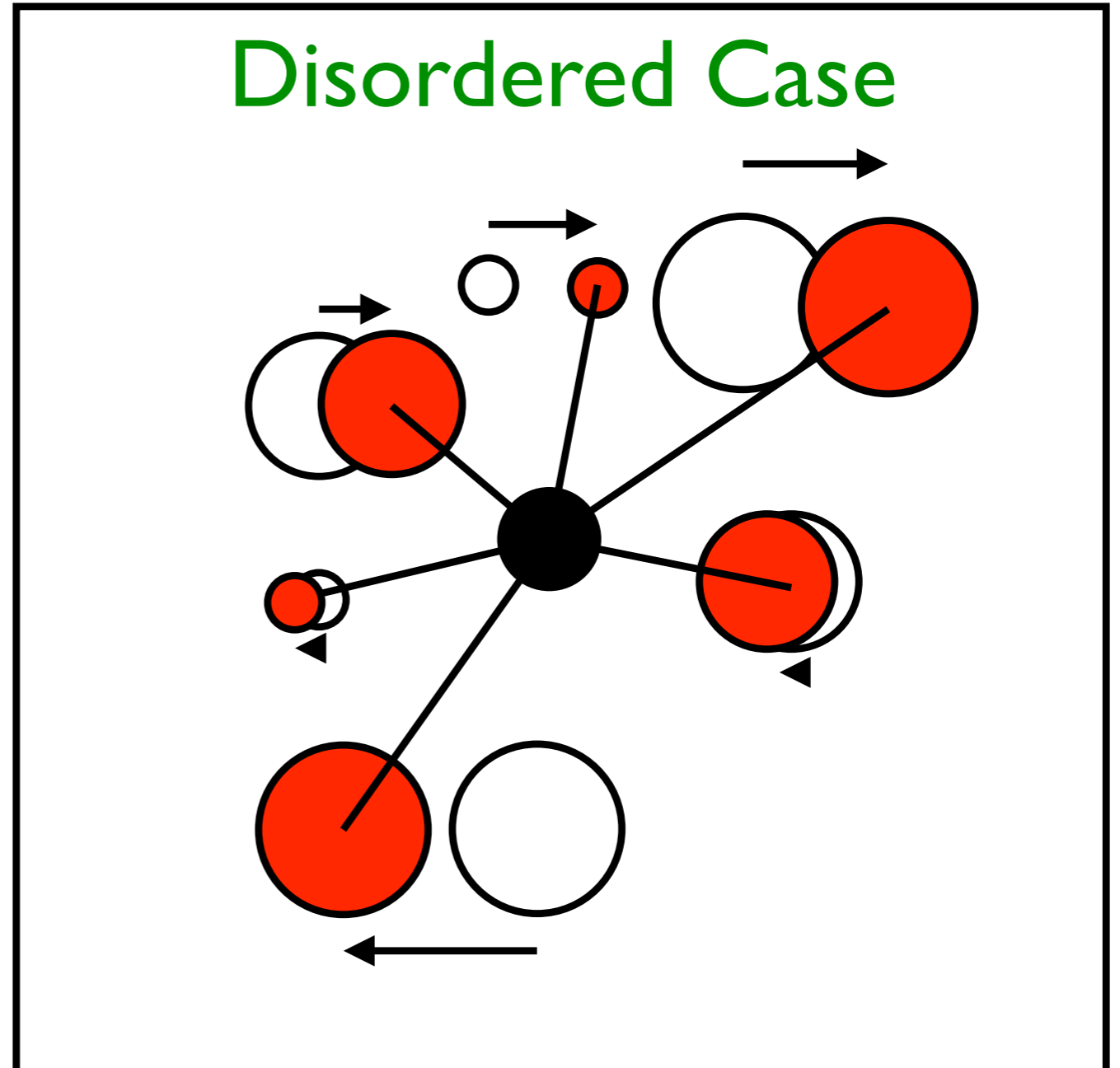
Computing linear response

- Single particle toy problem:
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Computing linear response

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



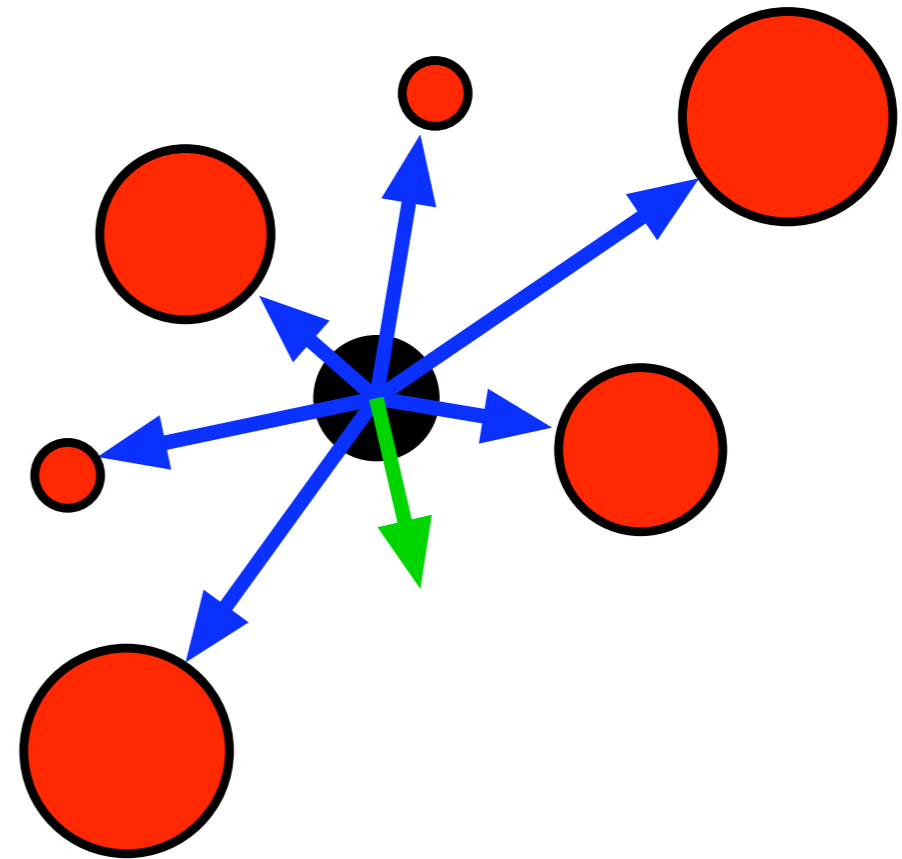
Computing linear response

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

Use Hessian to compute
“Affine force”

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

Disordered Case



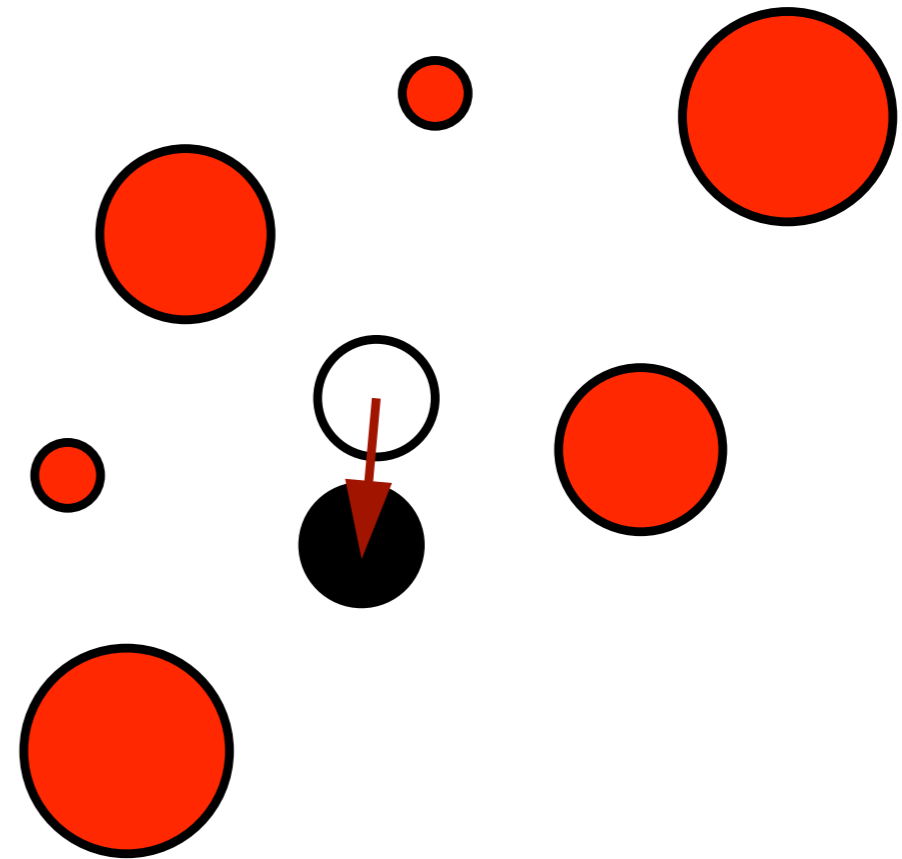
Computing linear response

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

Use Hessian to find position correction

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

Disordered Case

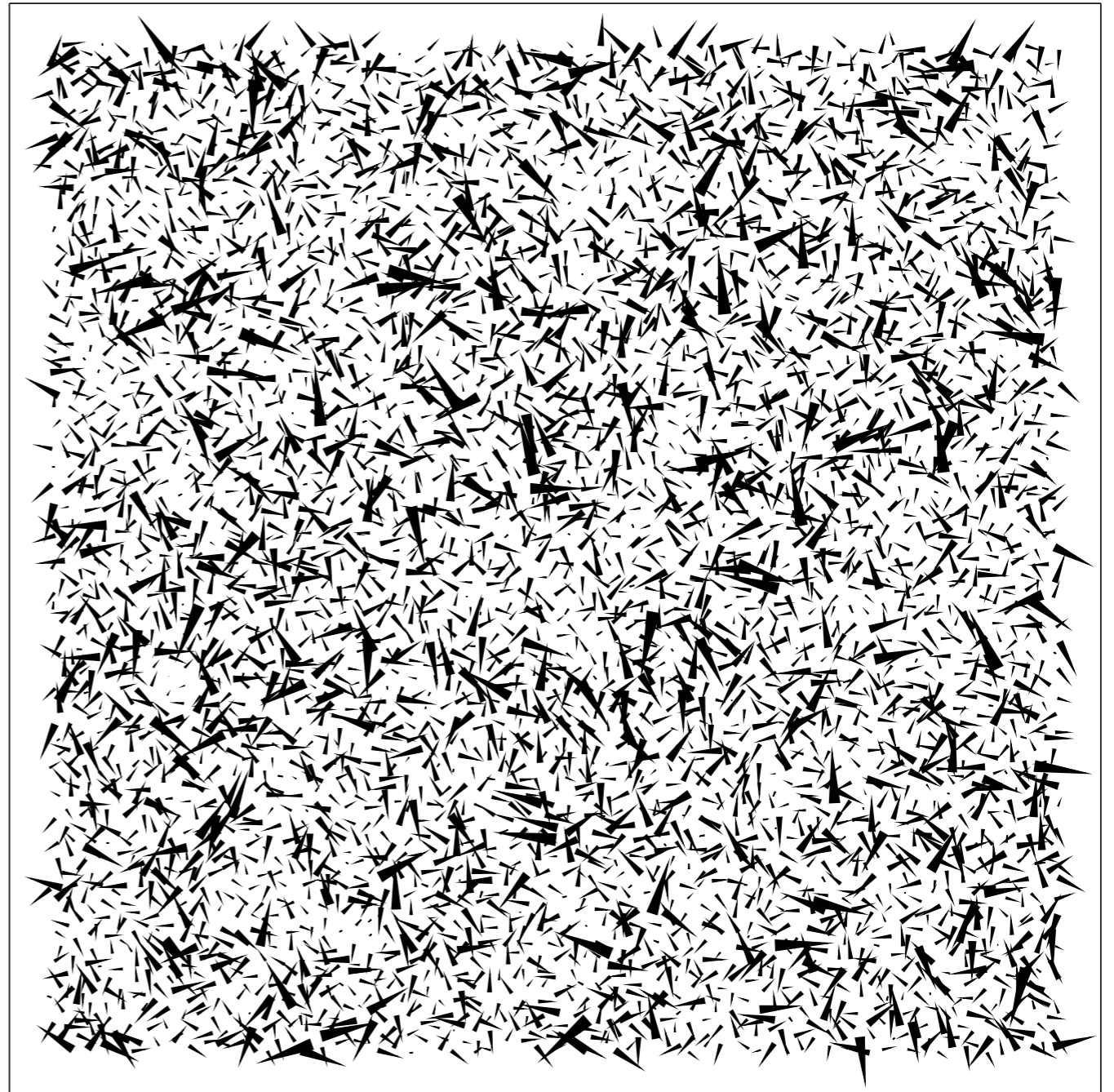


Computing linear response

- Back to full assembly:

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

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



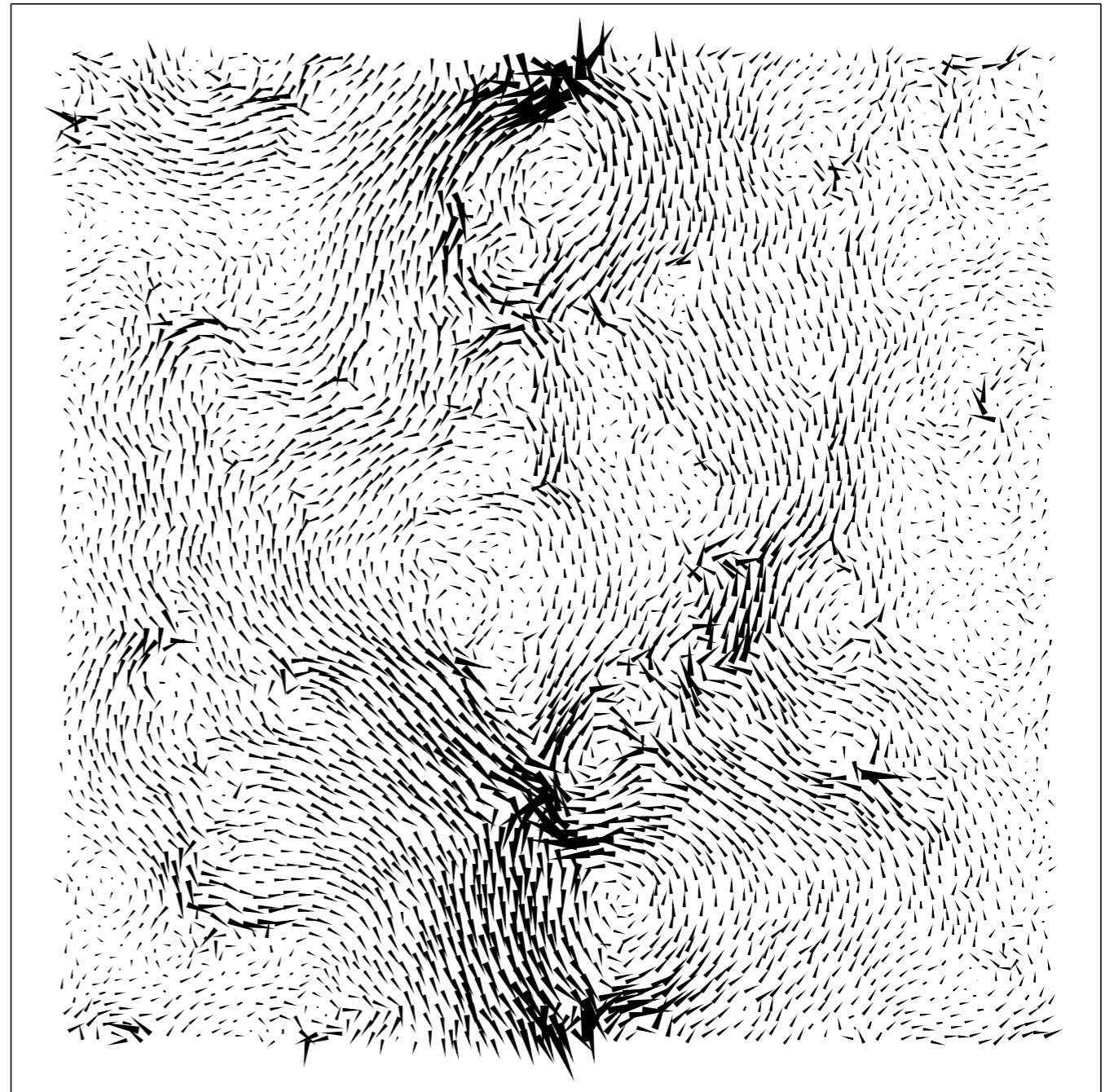
Computing linear response

- Back to full assembly:

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

Force balance:

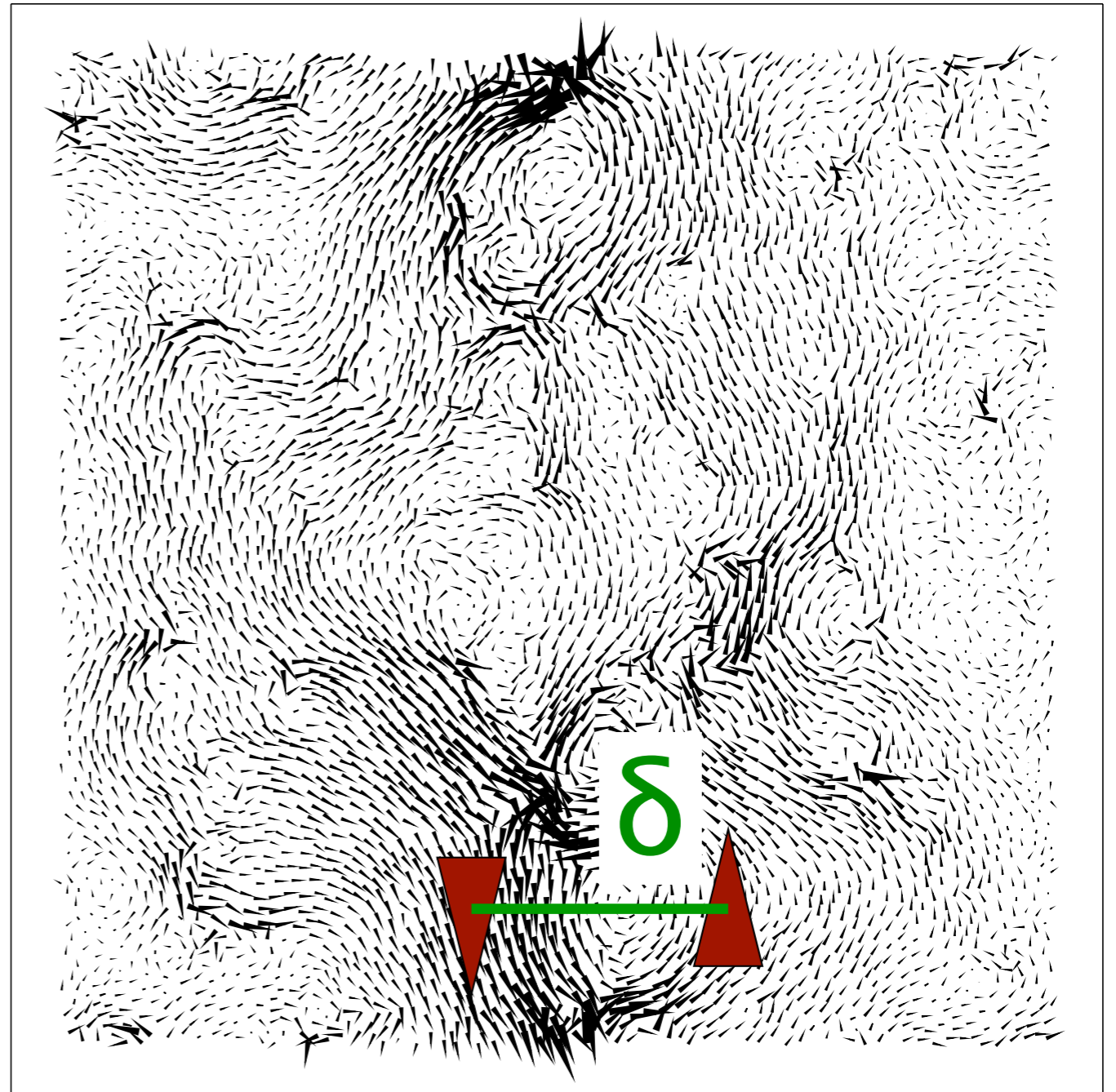
Affine forces, $\vec{\Xi}$, must be balanced by correction forces, $\mathbf{H}^{-1}_{ij} d\mathbf{x}_j$



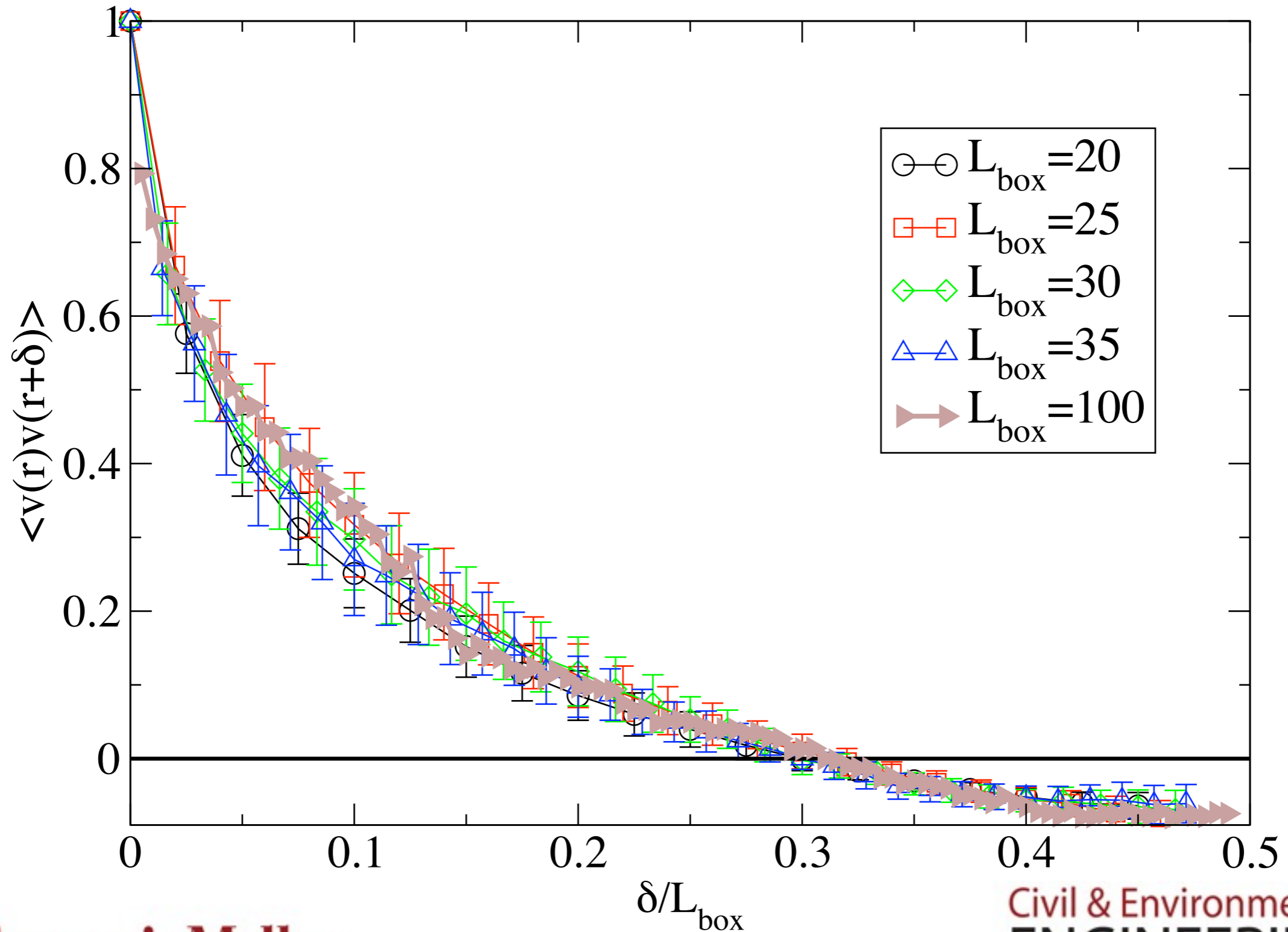
Spatial autocorrelation function $g(\delta)$

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

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



Spatial autocorrelation function $g(\delta)$



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$g(\delta)$: theoretical form

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

$g(\delta)$: theoretical form

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

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

$g(\delta)$: theoretical form

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

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

- Assume:

- Ξ is a random dipole field
- Ψ_p are plane waves
- $\lambda_p = k_p^2$; $\Xi_p = k_p$

$g(\delta)$: theoretical form

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

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

- **Assume:**

- $\vec{\Xi}$ is a random dipole field
- Ψ_p are plane waves
- $\lambda_p = k_p^2$; $\vec{\Xi}_p = k_p$

Approximate dr_i as random sum of plane waves:

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

$g(\delta)$: theoretical form

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

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

- Assume:

- $\vec{\Xi}$ is a random dipole field

- Ψ_p are plane waves

- $\lambda_p = k_p^2$; $\vec{\Xi}_p = k_p$

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

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

Then $g(\delta)$ is:

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

$g(\delta)$: theoretical form

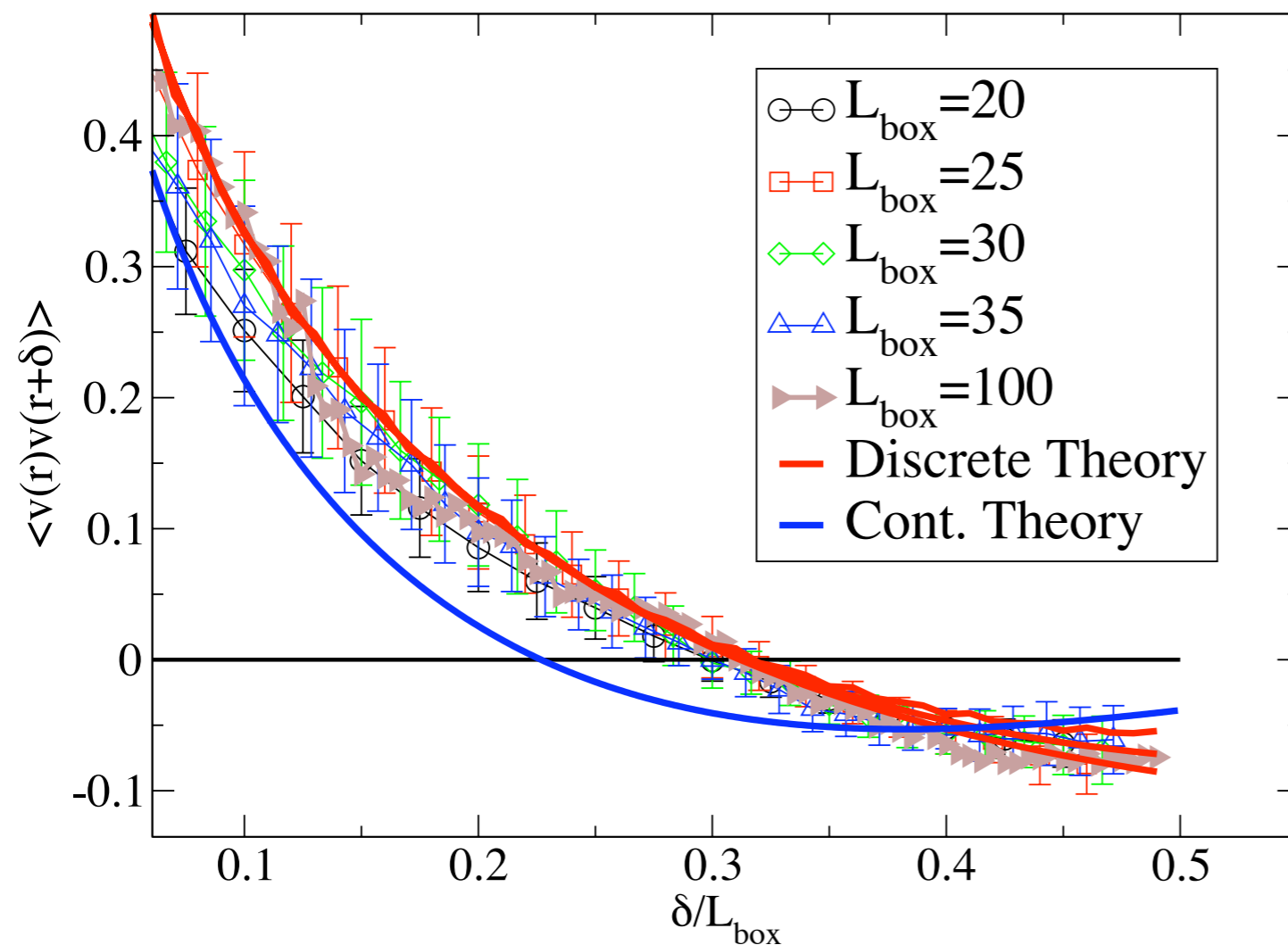
$$g(\vec{\delta}) \sim \sum_{k=(m,n)} \frac{\cos(2\pi \vec{k} \cdot \vec{\delta} / L)}{k^2}$$

Similar to DiDonna
+Lubensky,

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

but:

- Fully discrete derivation



Blue curve:

Semi-continuum

Red curve(s):

Partial sum ($n=40$)

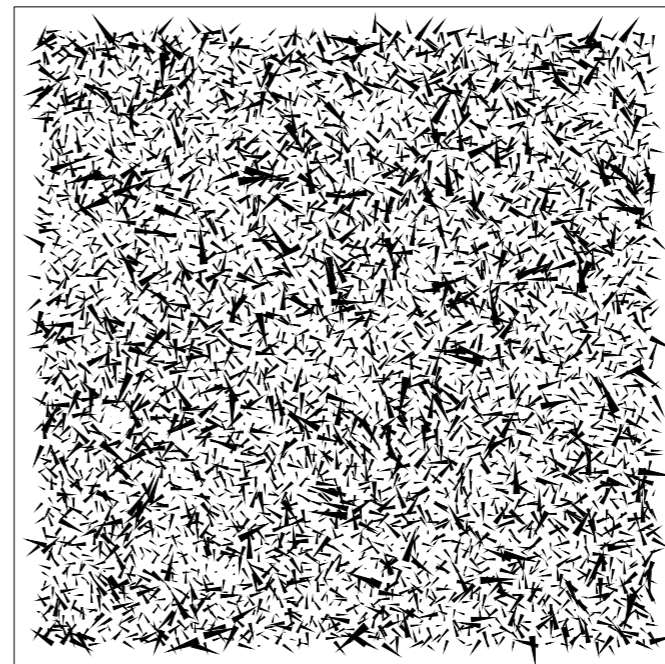
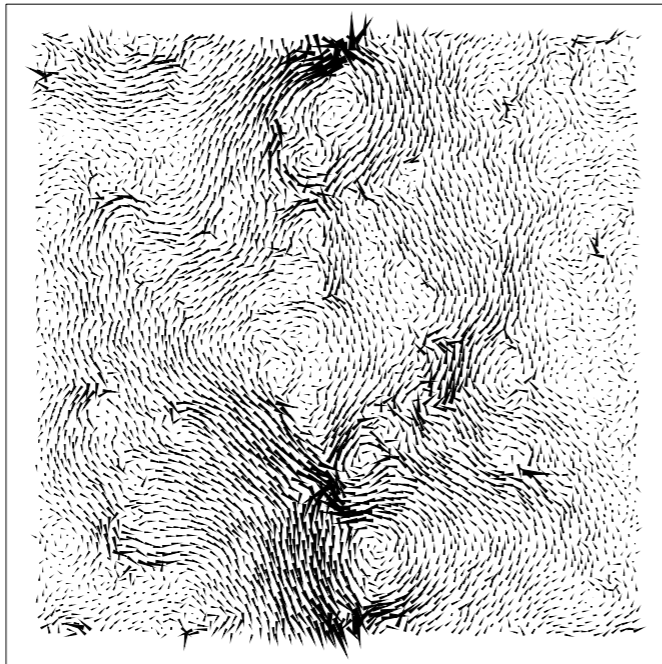
3 different angles

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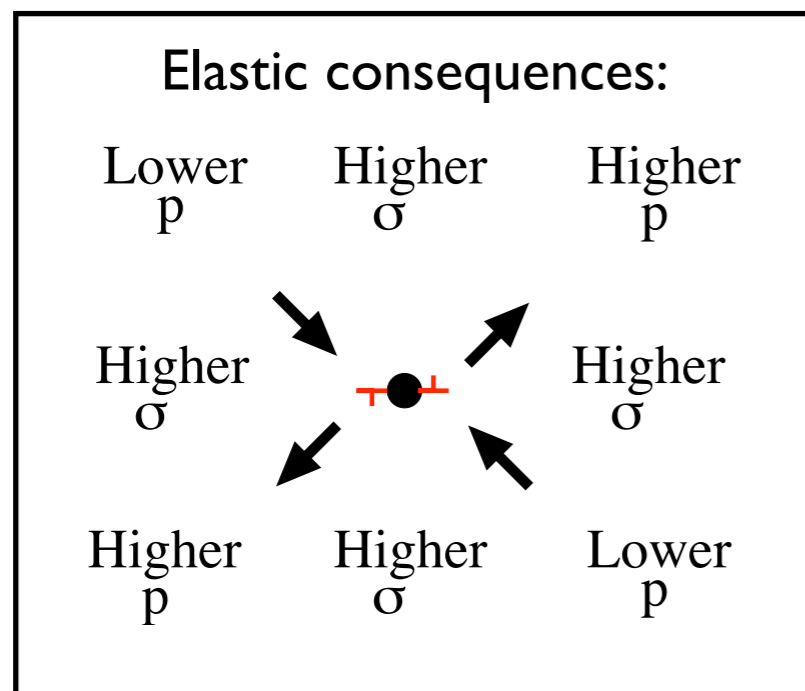
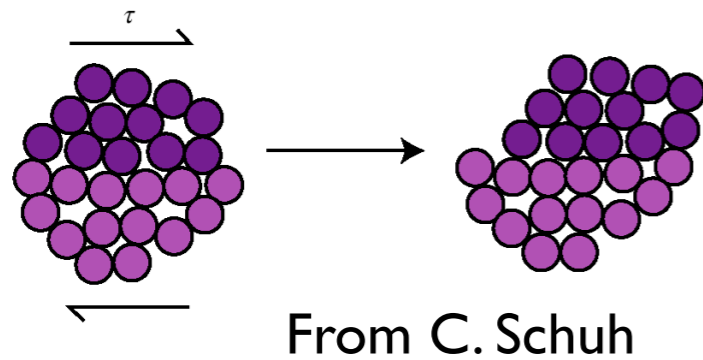
Summary: Elastic response

- Linear elastic (zero temperature) response is inhomogeneous.
- Displacement fluctuations appear as vortices
- Size scales with system size... no characteristic length
- “Affine forces”: a new measure of local disorder.
- Fluctuations derived from approximating eigenmodes as plane waves and affine forces as a random dipoles.

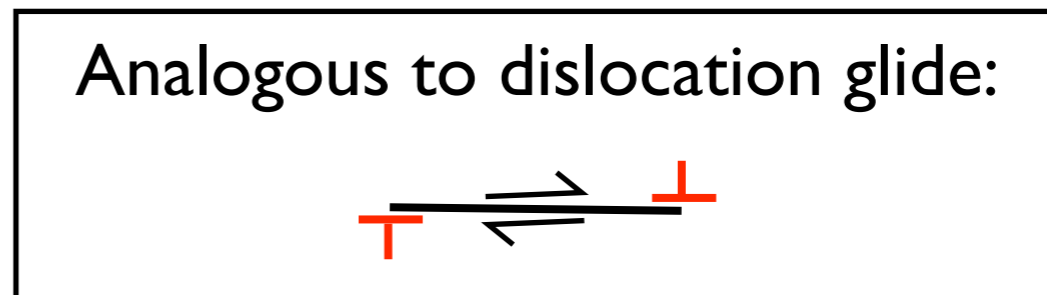
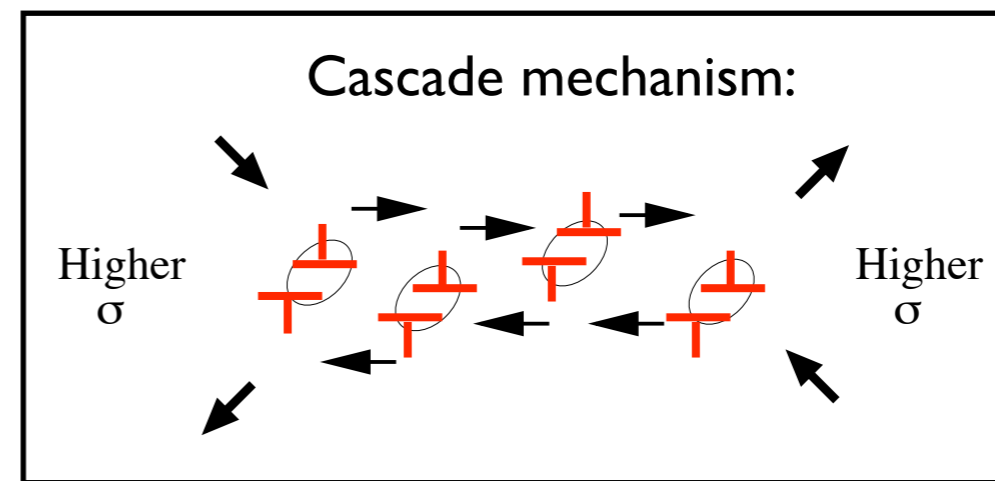


Plastic response (Shear Transformation Zones)

No crystal... so no dislocations...
but then what controls plasticity?

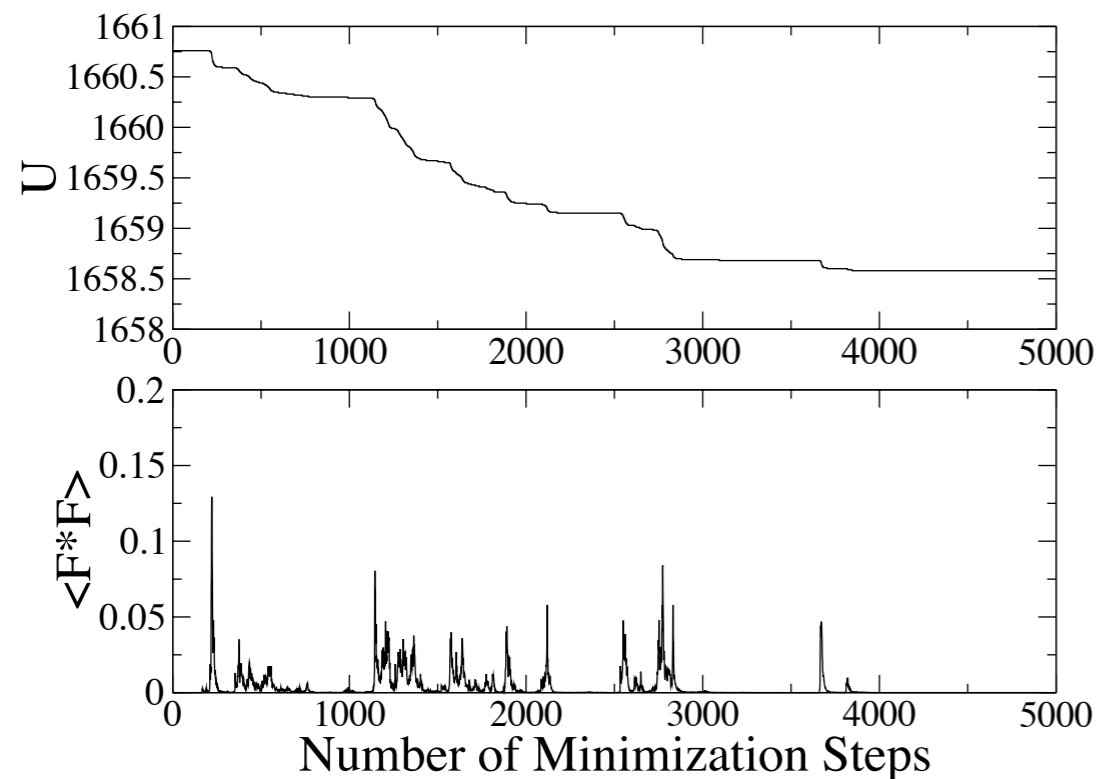
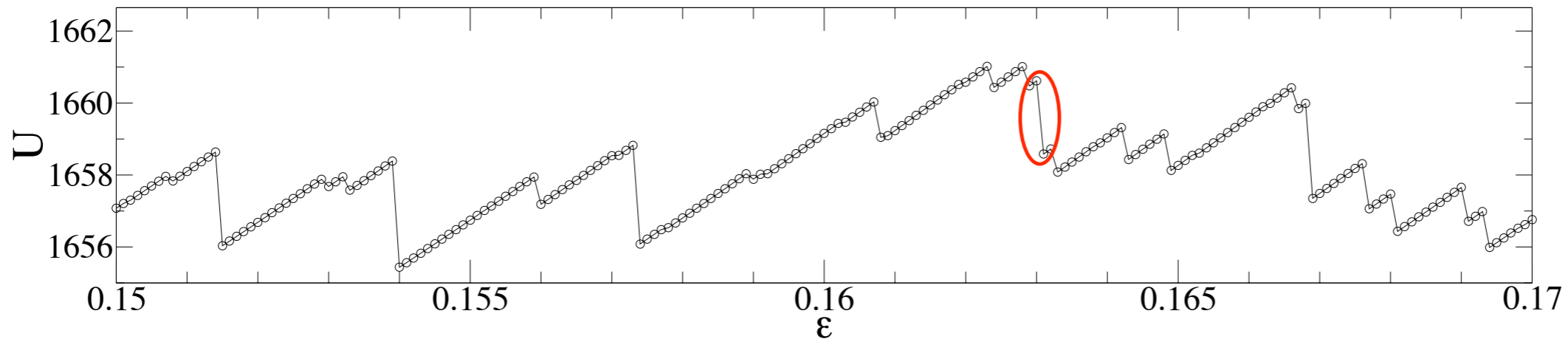


- Shear Transformation Zone (STZ) Mechanism:
 - Argon and Kuo: bubble raft experiments
 - Maeda and Takeuchi: computer simulations
 - Bulatov and Argon: banding mechanism
 - Falk and Langer: mean field theory



What are the consequences of organization of local shear zones?

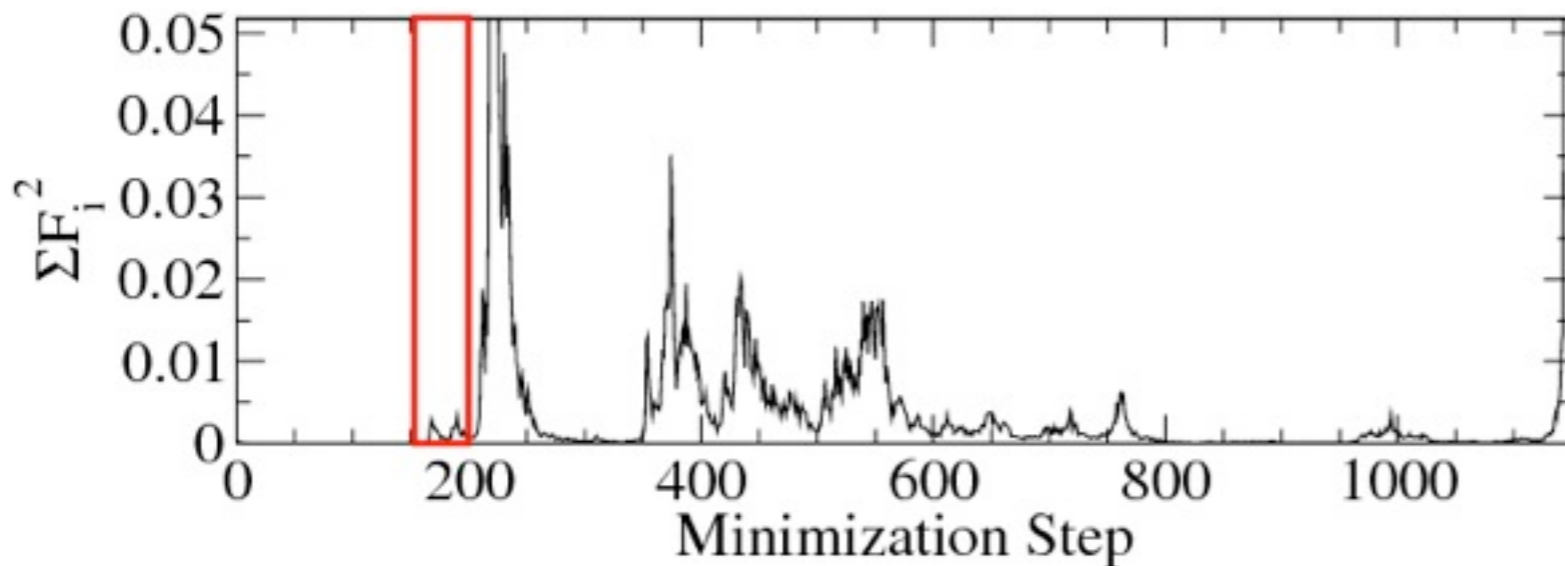
Typical plastic cascade



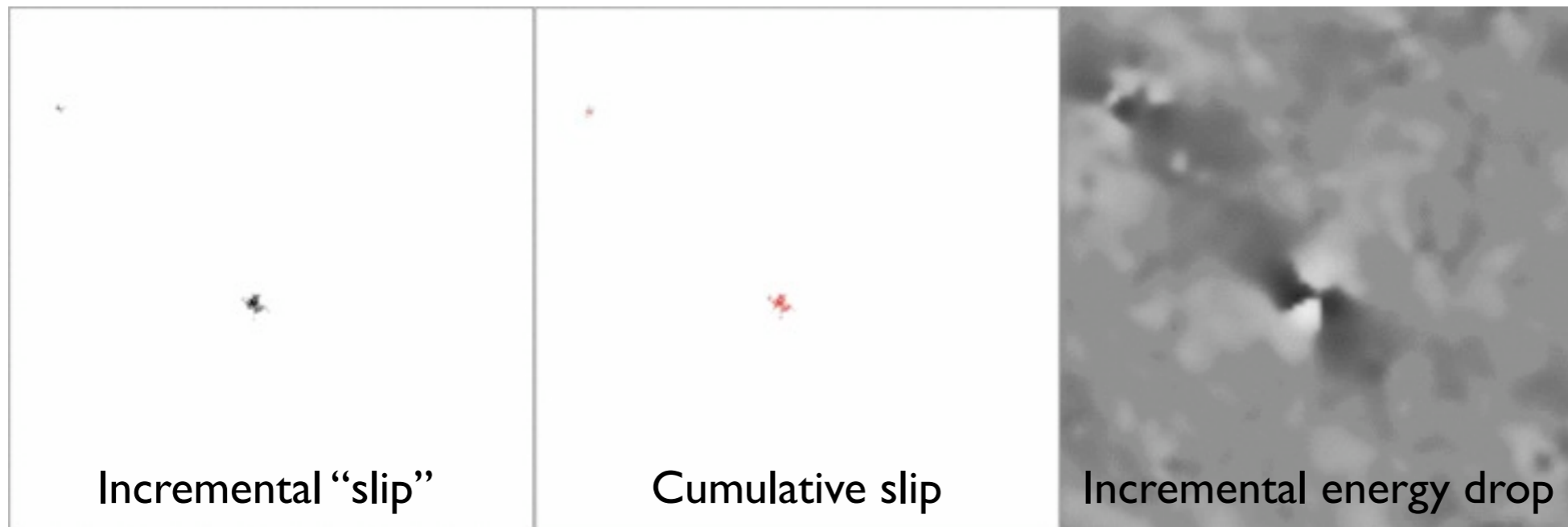
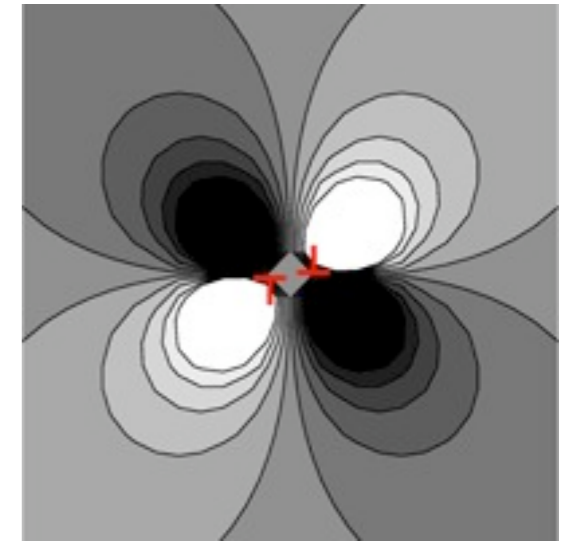
- Protocol: shear, relax...
- Single typical plastic event
- All relaxation at one strain
- “Number of minimization steps” analogous to time
 $\langle F^2 \rangle \sim dU/dt$
- Descent is intermittent...

Typical plastic cascade

Initial portion of descent from previous slide:



Expected energy change after nucleation of localized slip:



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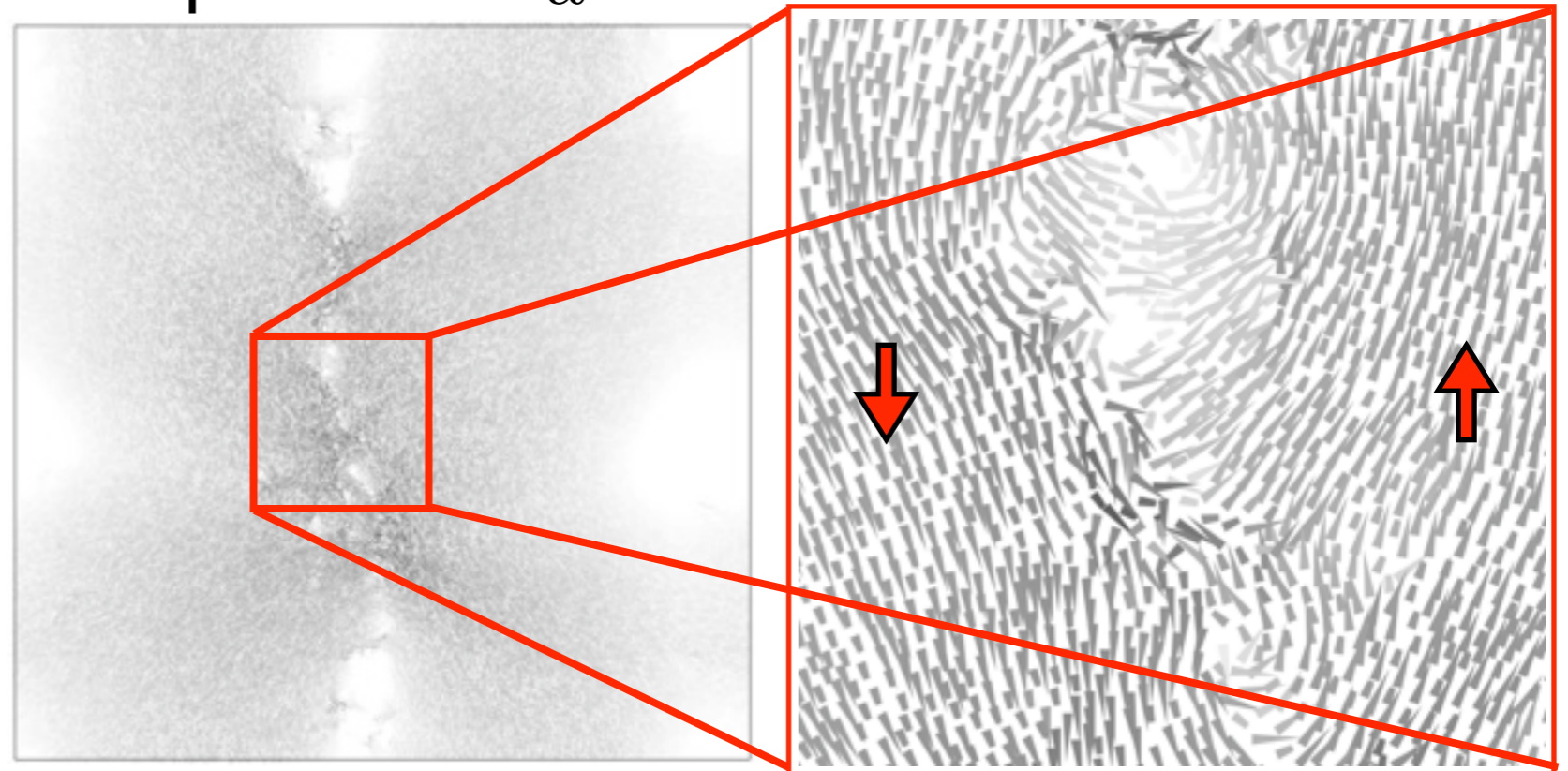
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Typical plastic cascade

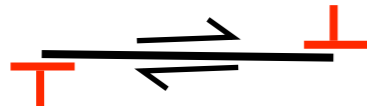
At the end of the whole cascade, we are left with a slip line:

“Slip”: $\vec{u} - \langle \vec{u} \rangle$

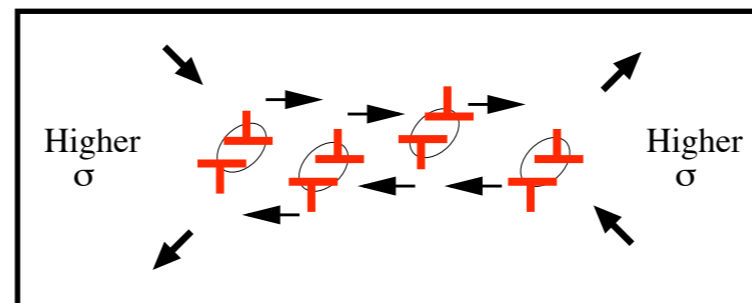
Displacement: \vec{u}



Analogous to dislocation glide:



But with local shearing zones:



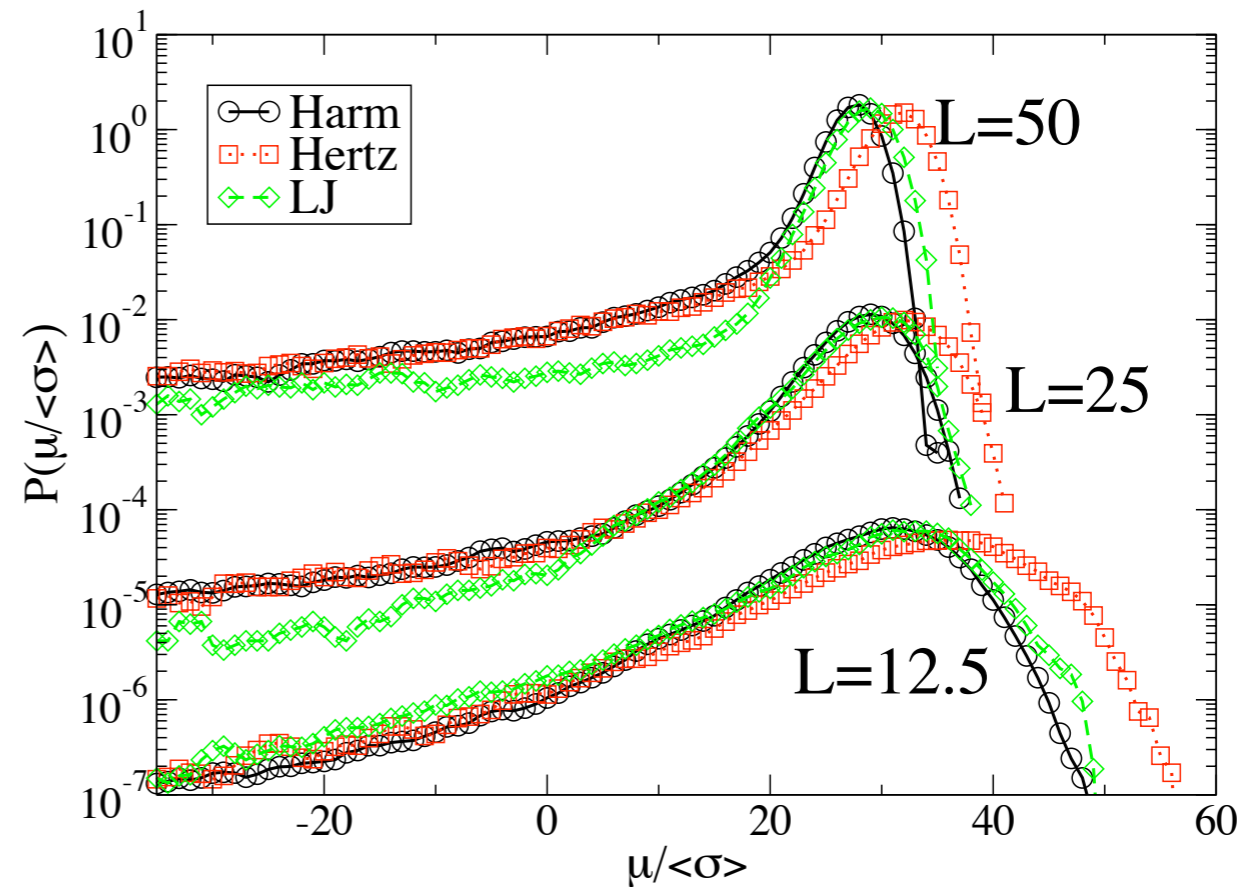
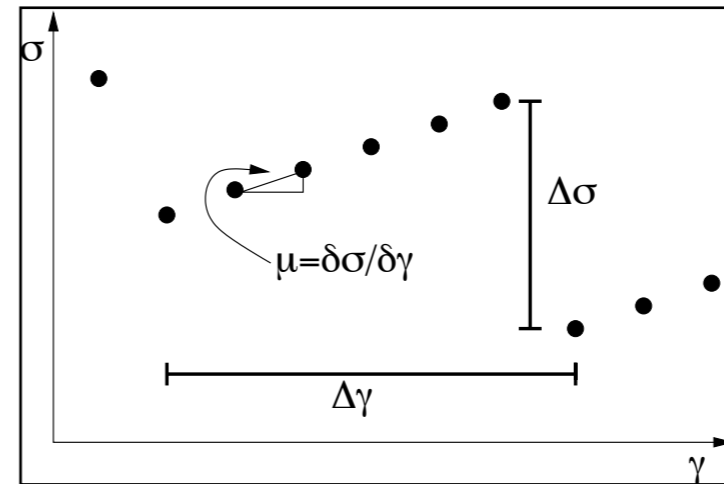
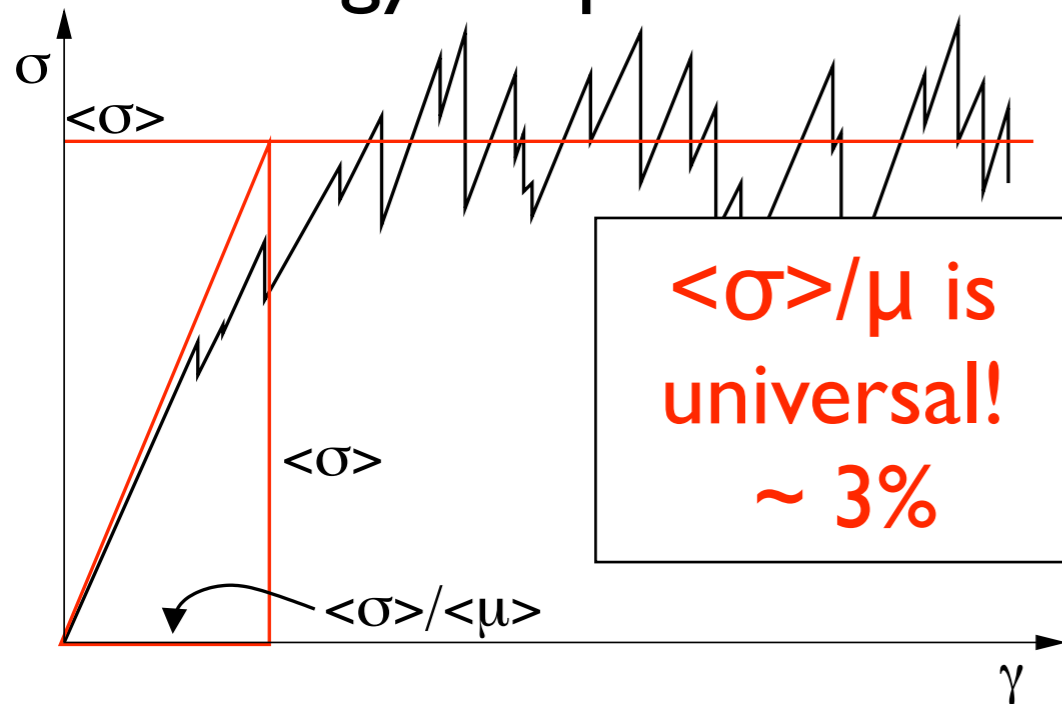
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Statistics and size scaling

Collect statistics for different system size and interaction potentials:

- “Modulus”
- Elastic interval
- Stress drop
- Energy drop



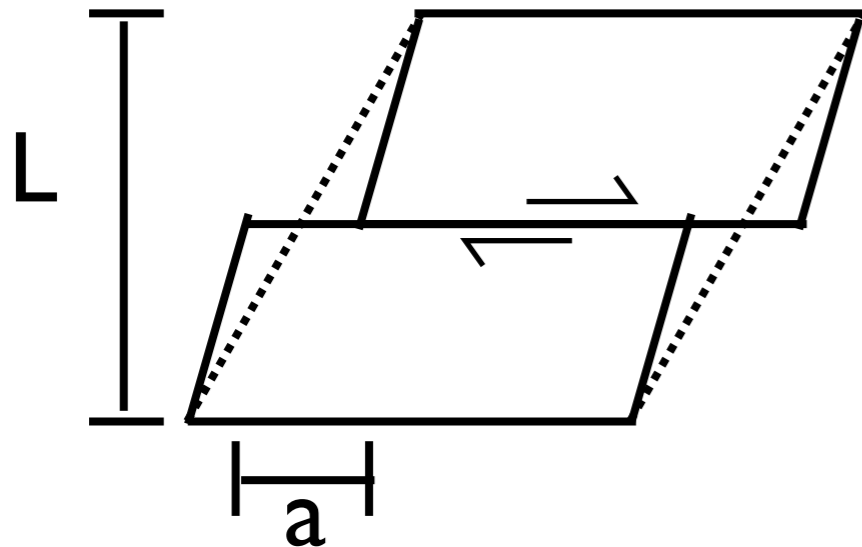
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Statistics and size scaling

Collect statistics for different system size and interaction potentials:

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

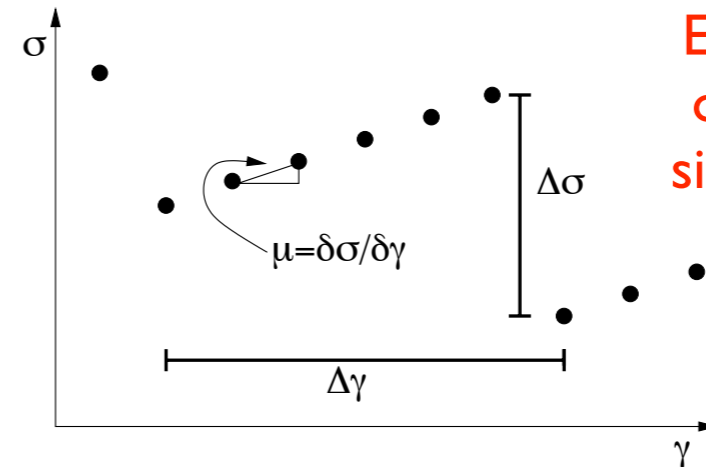


$$\Delta\gamma \sim a/L$$

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

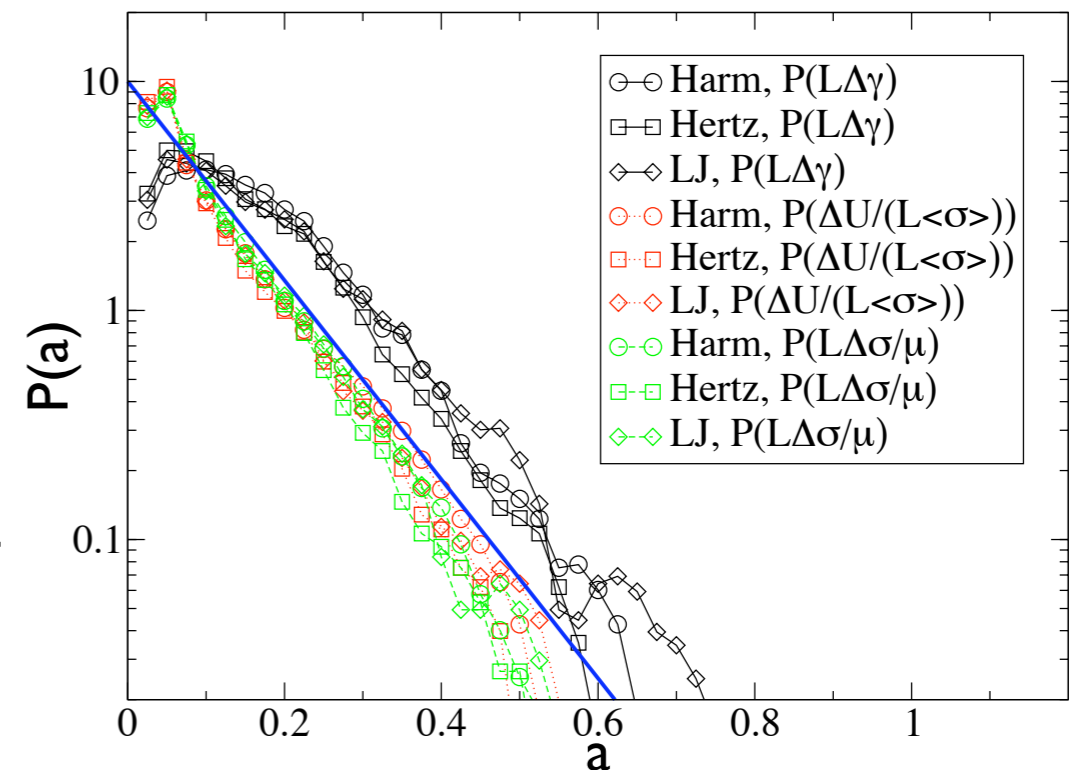
$$\Delta U \sim (L^2/\mu)\langle\sigma\rangle\Delta\sigma \sim aL\langle\sigma\rangle$$

Scaling argument: slip by length “a”



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

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

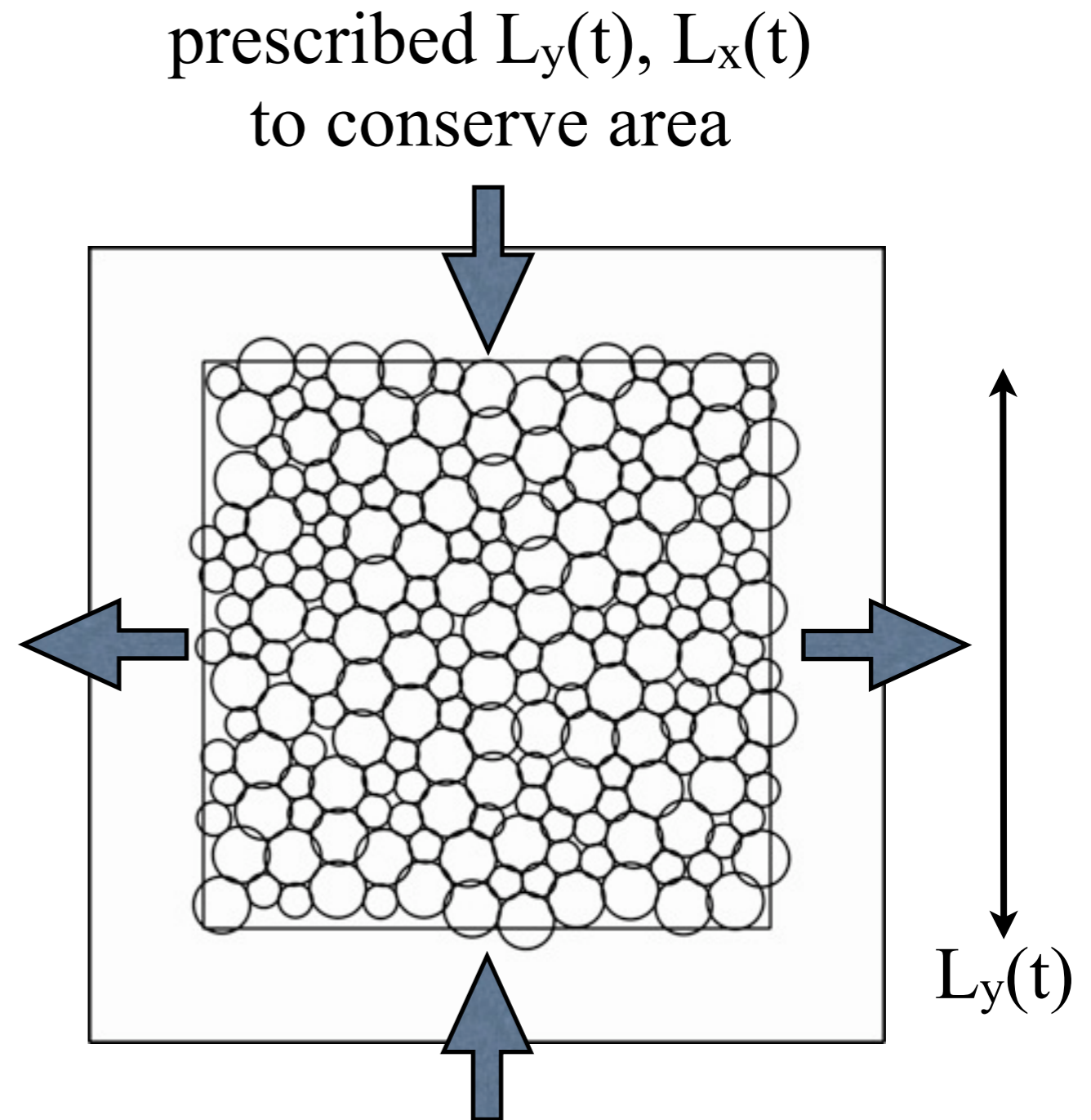


Summary: Plastic response

- Plastic response is intermittent with large, system-spanning events (avalanches)
- Avalanches composed of clusters of local slip (STZs)
- STZs interact elastically
- Universal yield strain $\varepsilon \sim 3\%$... agrees with experiments
- Universal slip amplitude $a \sim .1$ particle diameters... experiments difficult

Zero temperature molecular dynamics

- 2D Molecular Dynamics:
 - binary Lennard-Jones quenched at Pressure=0
 - relative velocity damping (Kelvin/DPD)
 - axial, fixed area strain
 - periodic boundaries
 - system sizes up to 3000x3000 ~ 10M particles
 - Quasi-static limit (about 500 CPU days / run)



Local vorticity, ω

For each triangle:

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

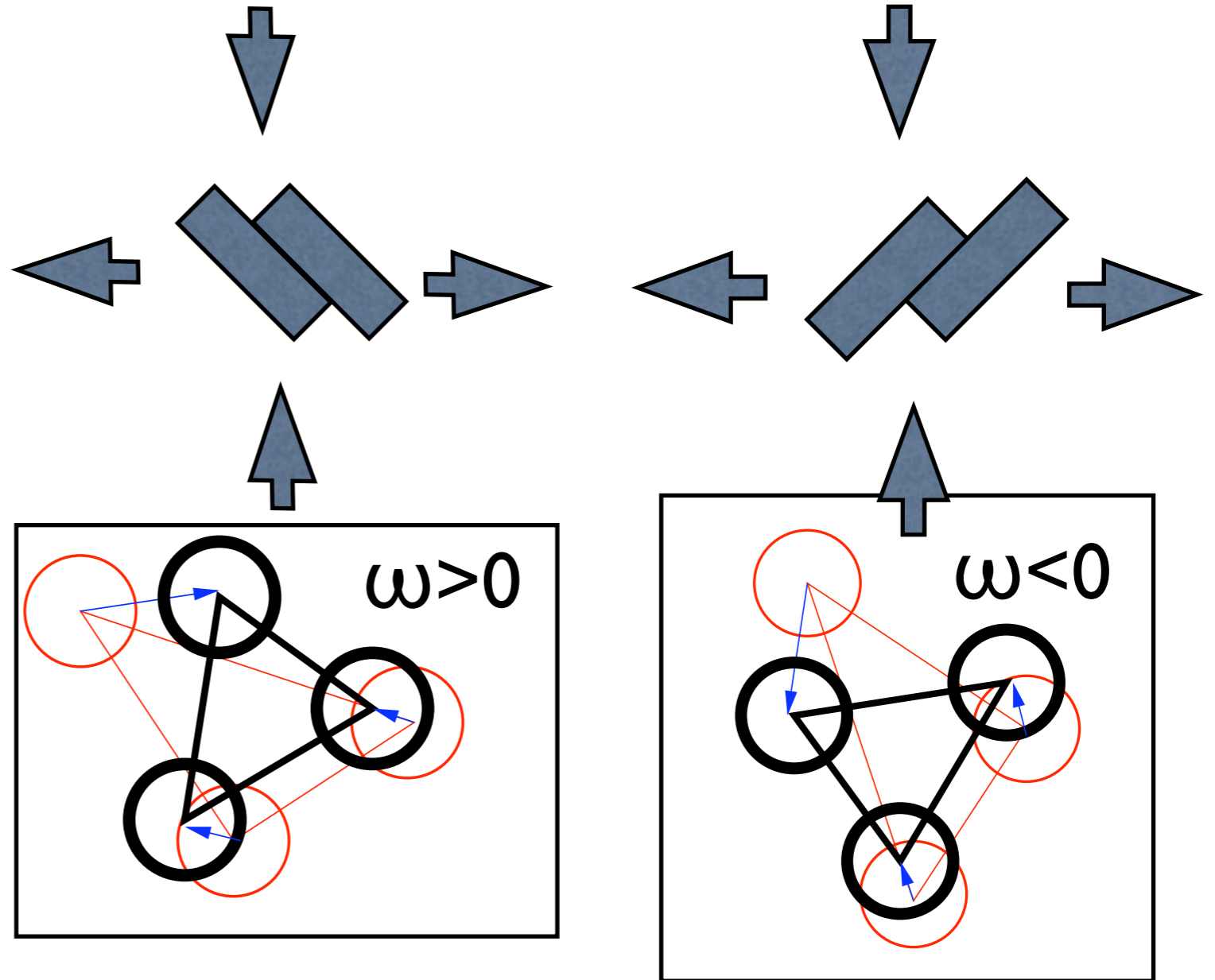
$$\epsilon_1 = \frac{F_{xx} - F_{yy}}{2}$$

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

Invariants:

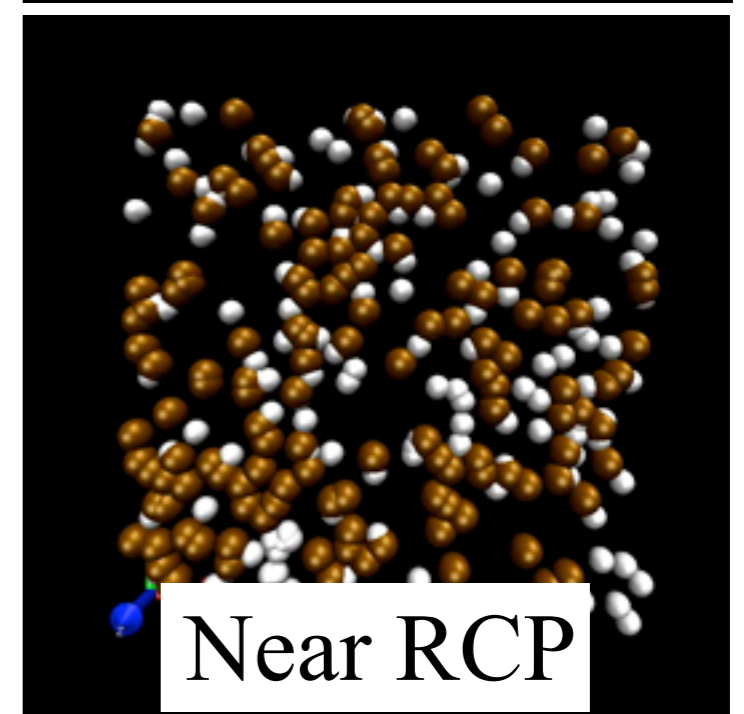
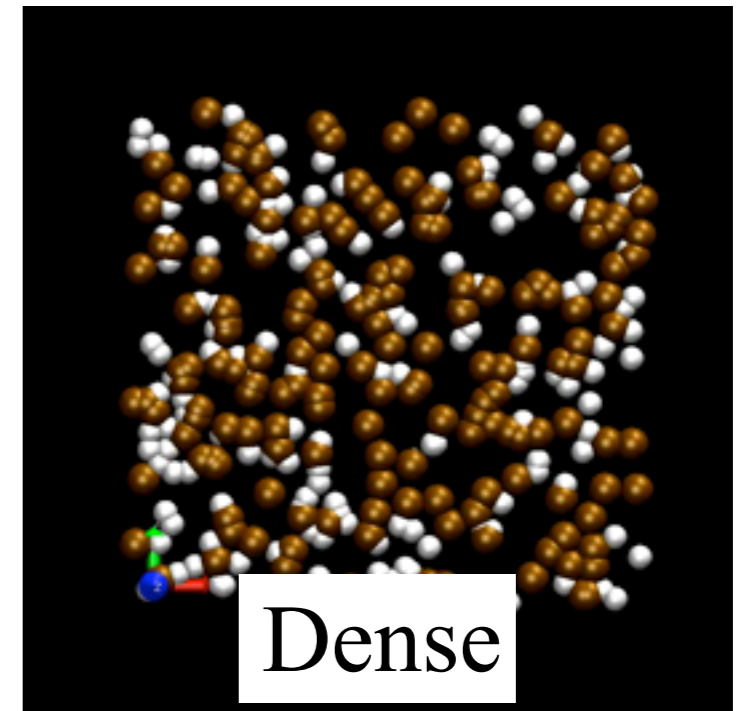
$$\epsilon = \sqrt{\epsilon_1^2 + \epsilon_2^2}$$

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



Future directions

- **Recall:**
 - Differences in elementary physics:
 - Inertial or overdamped?
 - “Real” temperature
 - Dissipation mechanisms / hydrodynamics
 - Coulomb friction
 - Attractive forces / adhesion
- How do microscopic details affect the intermittency, slip avalanches, elasticity, rheology, and yield?
- Currently looking at:
 - densities near random close packing (RCP)
 - massless (mean field bubbles) and massive (frictionless granular DEM) models.



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