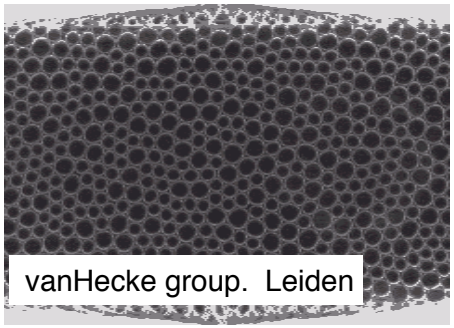
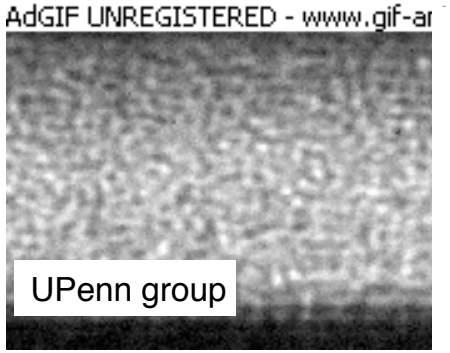
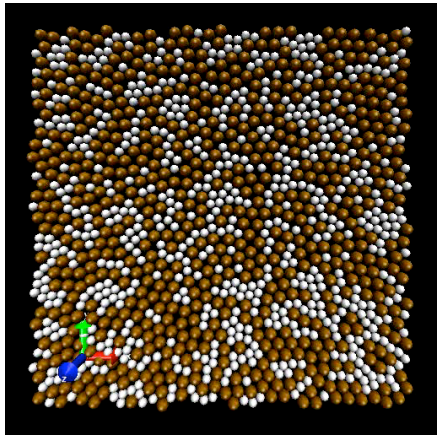
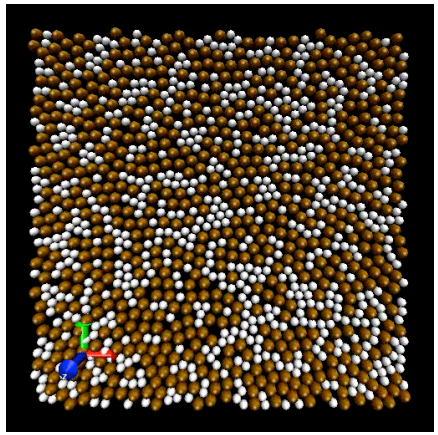
~~Avalanches~~, diffusion, and rheology in soft particle packings









- Robust connection between diffusion and rheology given by organization of plastic strain into “transient slip lines”.
- Qualitative dependence on drag model: “local drag” less rate sensitive than “pair drag”.
- Low rates: Bursty dynamics and transient slip lines span system.
- Intermediate rates: No bursts, but slip lines still span system.
- Higher rates: Slip lines have length ξ which determines diffusion and rheology.
- Highest rates: ξ saturates at particle scale.

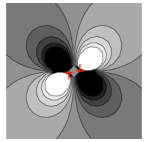
KITP Seminar.

November 2014

Northeastern University

Craig Maloney

Soft and Nanoscale Mechanics



Acknowledgements

- Arka Roy
- Kamran Karimi

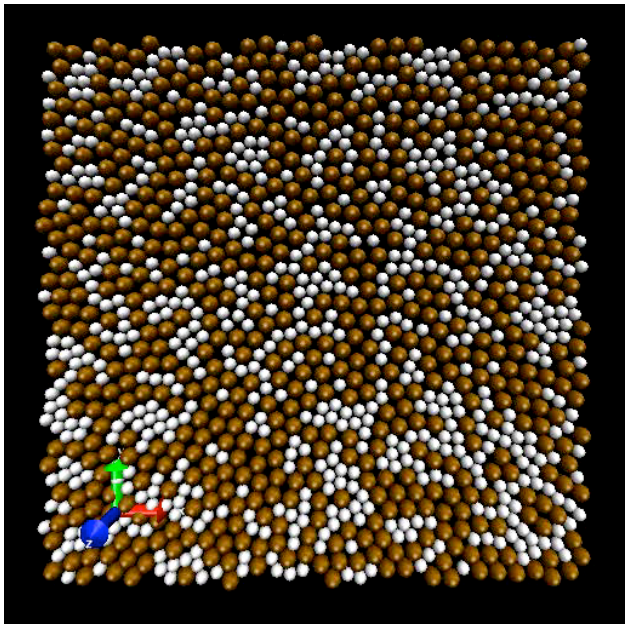
- DMR-1056564
- CMMI-1250199

Outline

- Background and overview
  - Soft particle suspensions
  - Jamming and random close packing
  - Elasticity: Development of shear modulus
  - Plasticity: Development of yield stress
  - Simple models

- Elasticity
  - Scaling laws, (criticality?) and emergent lengthscales
  - Point response
  - Constrained homogeneous deformation
  - Unconstrained homogeneous deformation

- Plasticity:
  - Shear transformations, slip avalanches, and diffusion
  - Short-time intermittency
  - Long time diffusion
  - Plastic strain correlations



Soft glasses

- Particles suspended in liquids can behave like glasses or other conventional amorphous solids.

- Particles can be:
  - solid like in a paste
  - liquid like in an emulsion
  - air like in a foam or mousse

- Technological applications:
  - Device fabrication/assembly
  - Oil / Gas drilling/production
  - Food
  - Personal care
  - Bio/Biomedical

- This work:
  - Athermal
  - Deformable
  - Jammed

Soft sphere rheology

LETTERS
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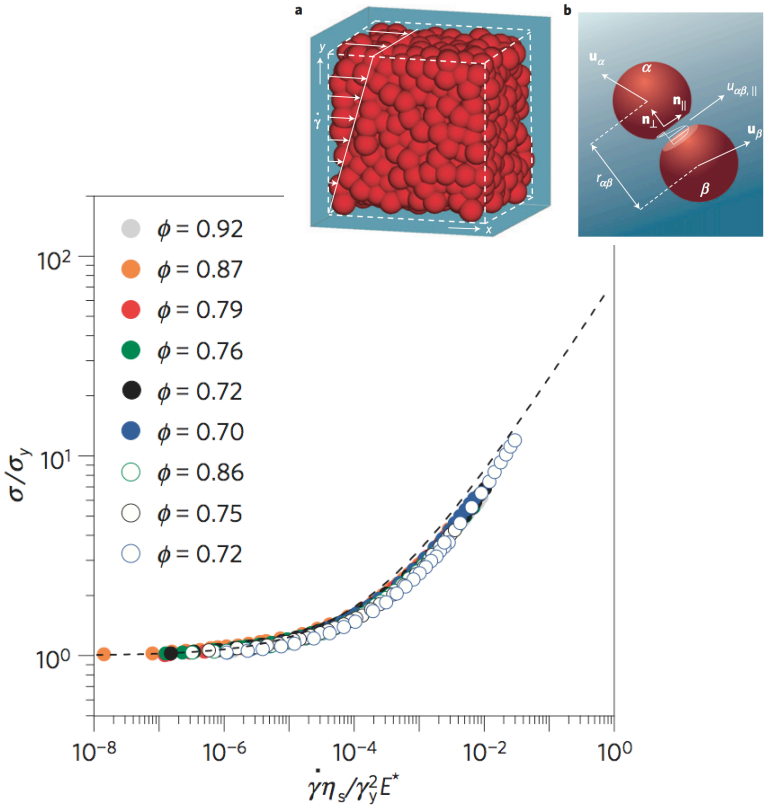
nature materials

A micromechanical model to predict the flow of soft particle glasses

Jyoti R. Seth[1], Lavanya Mohan[1], Clémentine Locatelli-Champagne[2], Michel Cloitre[2]* and Roger T. Bonnecaze[1]



PRL 105, 175701 (2010) PHYSICAL REVIEW LETTERS week ending 22 OCTOBER 2010

Microfluidic Rheology of Soft Colloids above and below Jamming

K. N. Nordstrom,[1] E. Verneuil,[1,2] P. E. Arratia,[1,3] A. Basu,[1] Z. Zhang,[1,2] A. G. Yodh,[1] J. P. Gollub,[1,4] and D. J. Durian[1]
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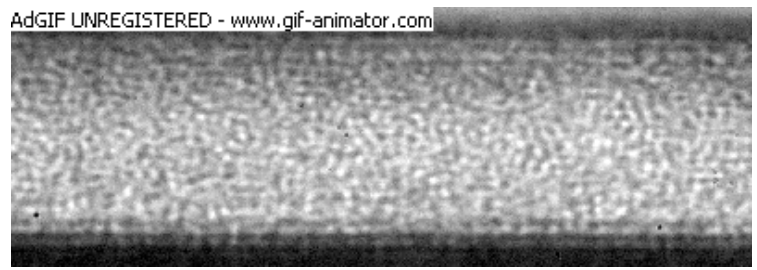
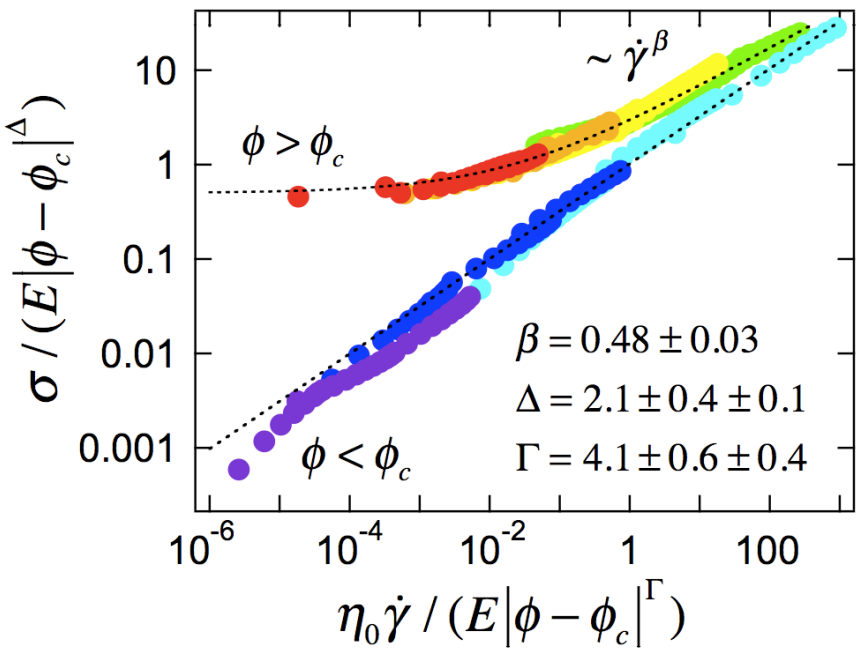
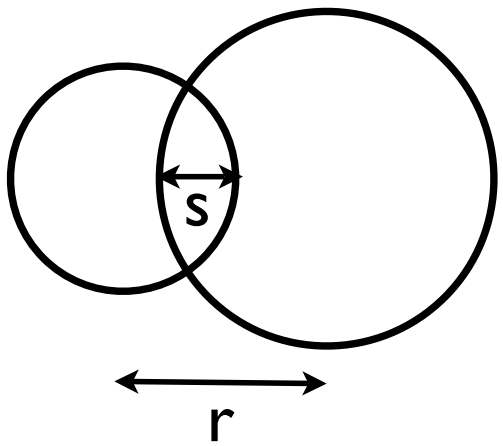
(Received 26 July 2010; published 21 October 2010)

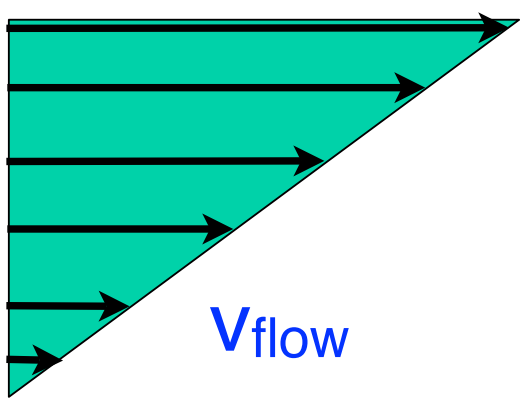




Bubble model (Durian)



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

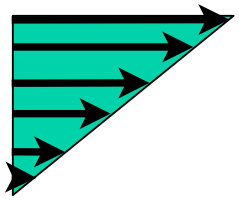


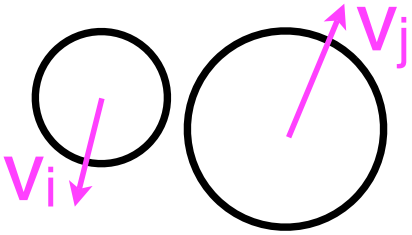
- Repulsion, F_{rep}, linear in overlap, s:
  - $F_{rep}=ks$
  - (could be arbitrary power of s)
- Drag, F_{drag}, w/r/t imposed flow:
  - $F_{drag}=b\ (v_{bubble}-v_{flow})$
- For (massless) bubbles, $F_{rep}=F_{drag}$
  - $v_{bubble}=F_{rep}/b + v_{flow}$
- Single timescale: $\tau_D=bR^4/k$
- Dimensionless shearing rate:
  - $De=(d\gamma/dt)\ \tau_D$
    (Deborah number)

Modified, inertial bubble model(s)

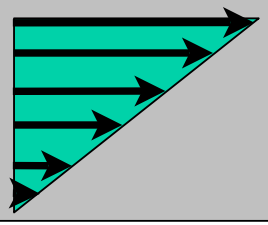
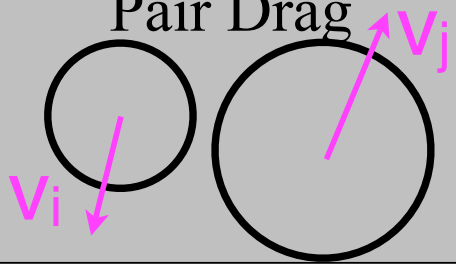
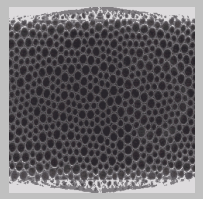
- Modifications:
- F_{drag}, **either** w/r/t imposed flow:
  - $F_{drag}=b\ (v_{bubble}-v_{flow})$

    or
  - $F_{drag\ i\ \alpha} = b\ \Sigma_j\ (v_j-v_i)_\alpha$
- Non-zero mass, Newton's law:
  - $ma_{i\alpha} = F_{rep\ i\ \alpha} + F_{drag\ i\ \alpha}$
- New inertial timescale: $\tau_v=(m/k)^{(1/2)}$
- $\tau_D/\tau_v=b/(km)^{(1/2)}$
- Non-brownian suspension: $\tau_v >> \tau_D$
- Granular material: $\tau_v << \tau_D$



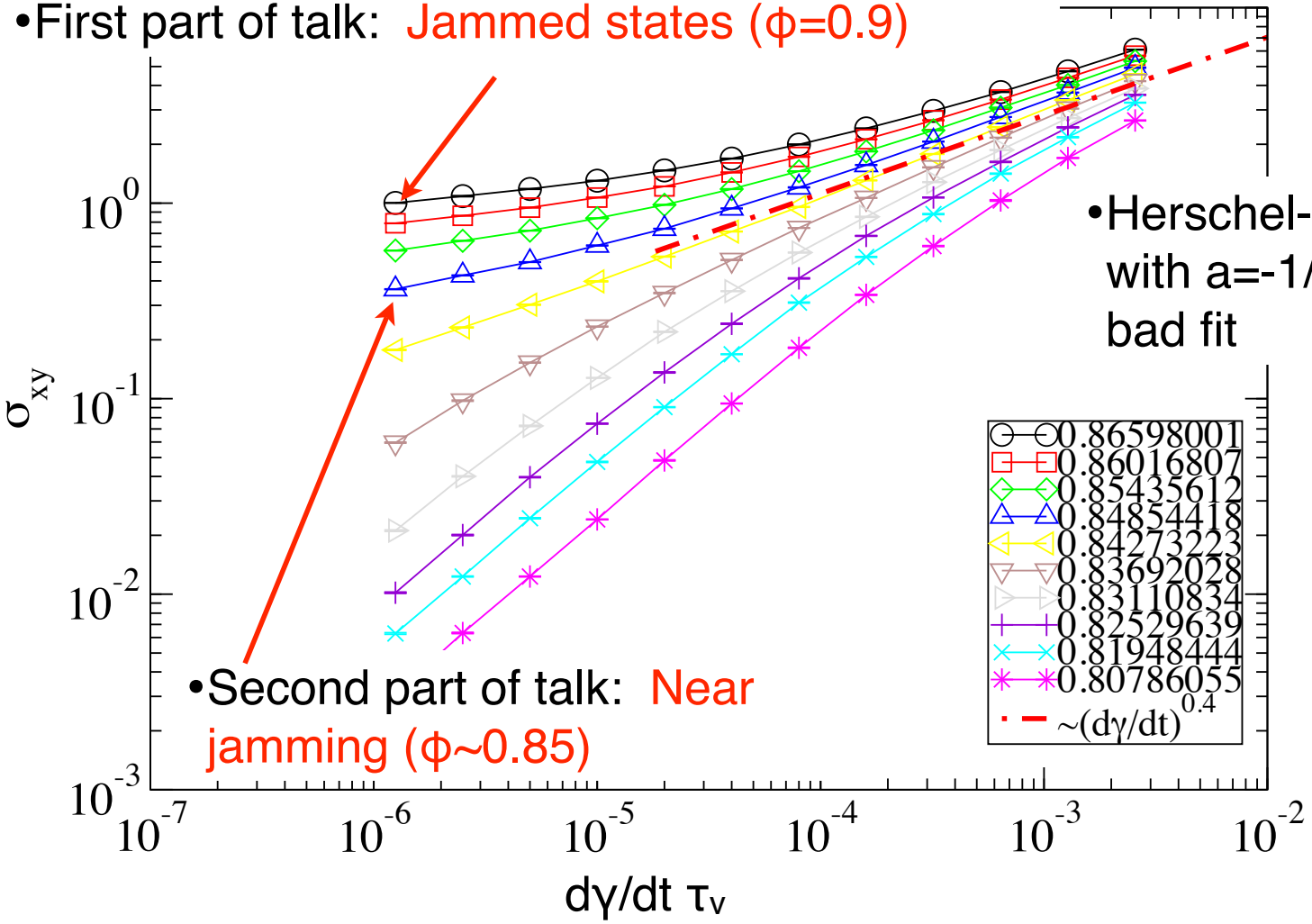


Models

	Mean Drag 	Pair Drag 
Overdamped $\tau_v \ll \tau_D$ 	???	???
Inertial $\tau_v \gg \tau_D$ 	???	Lemaitre and Caroli PRL 2009 $\sigma - \sigma_y = A\sqrt{\dot{\gamma}}$ $< \Delta y^2 > / \Delta\gamma = A(1 - B\dot{\gamma}^{-1/2})$

Flow curves: Pair drag, overdamped, various φ

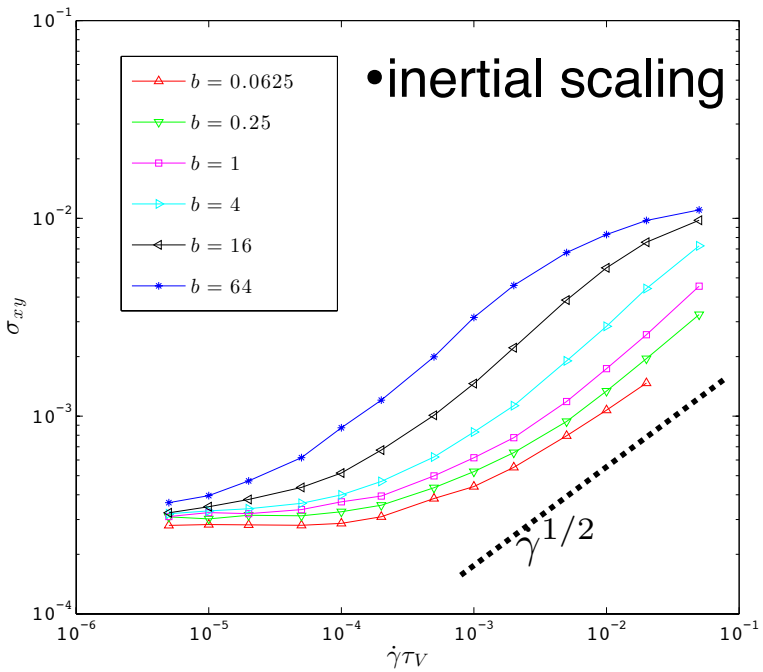
- First part of talk: Jammed states (φ=0.9)

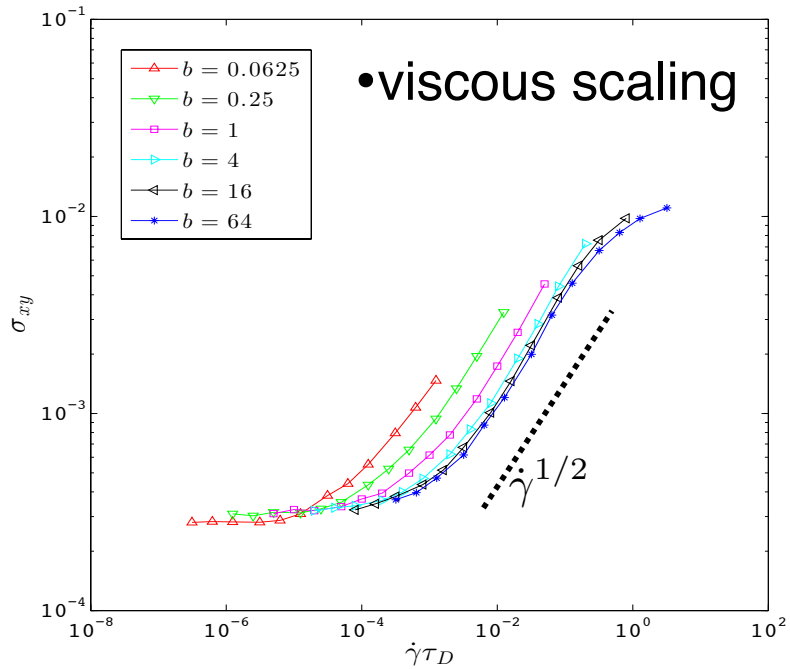


- Herschel-Bulkley with a=-1/2 not a bad fit

- Second part of talk: Near jamming (φ~0.85)

Flow curves: Pair drag various damping, L=20

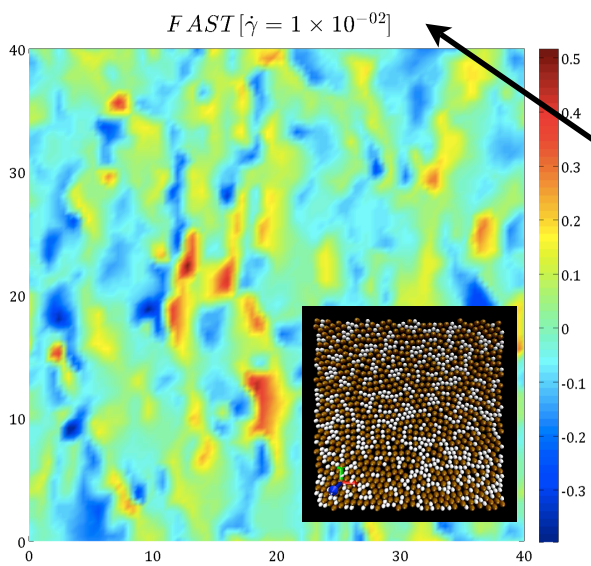


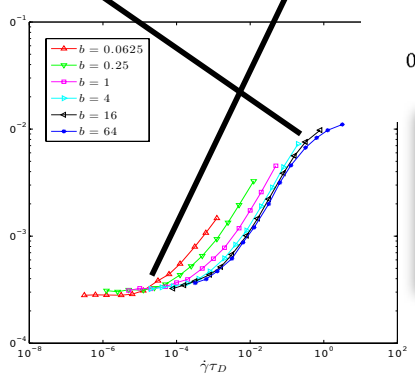


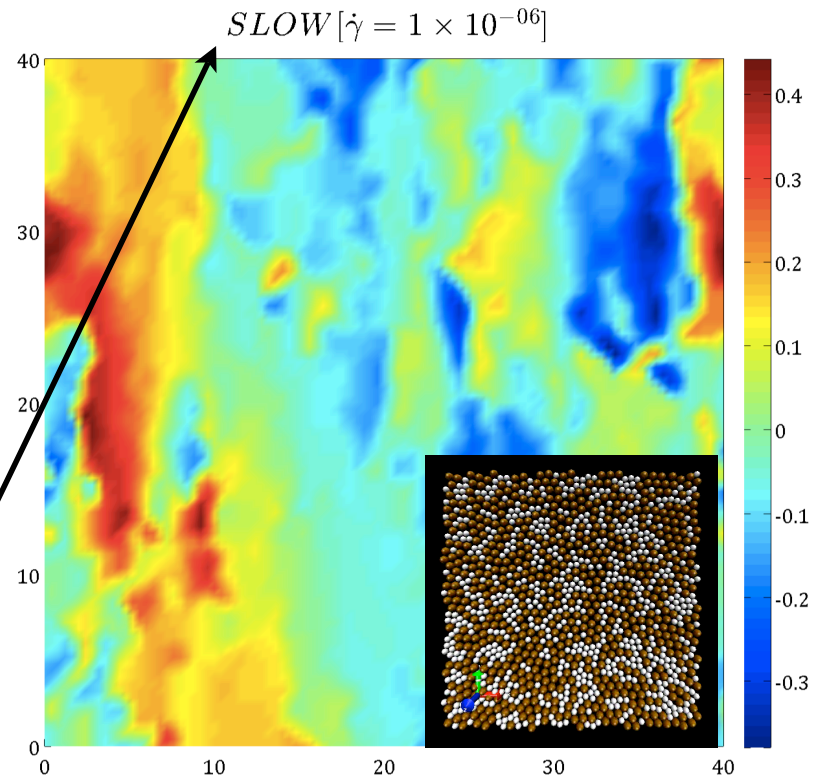
- New result : $\sigma - \sigma_y \sim \dot{\gamma}^{1/2}$
- (Known previously for underdamped case)
- New result: kink at high rate
- Let's look at how things organize in space to try to understand the 1/2 exponent and the kink.

Particle displacements near yield stress and in flow

- Look at vertical displacements
- After velocities de-correlate
- Slow shear:
  - “transient slip line”-like features
  - span the simulation cell
- Fast shear:
  - correlated behavior goes away





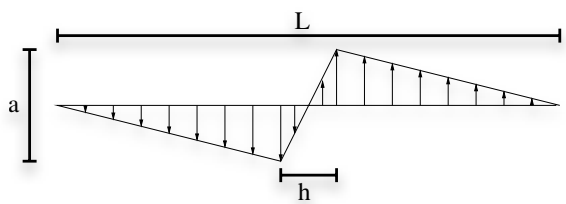


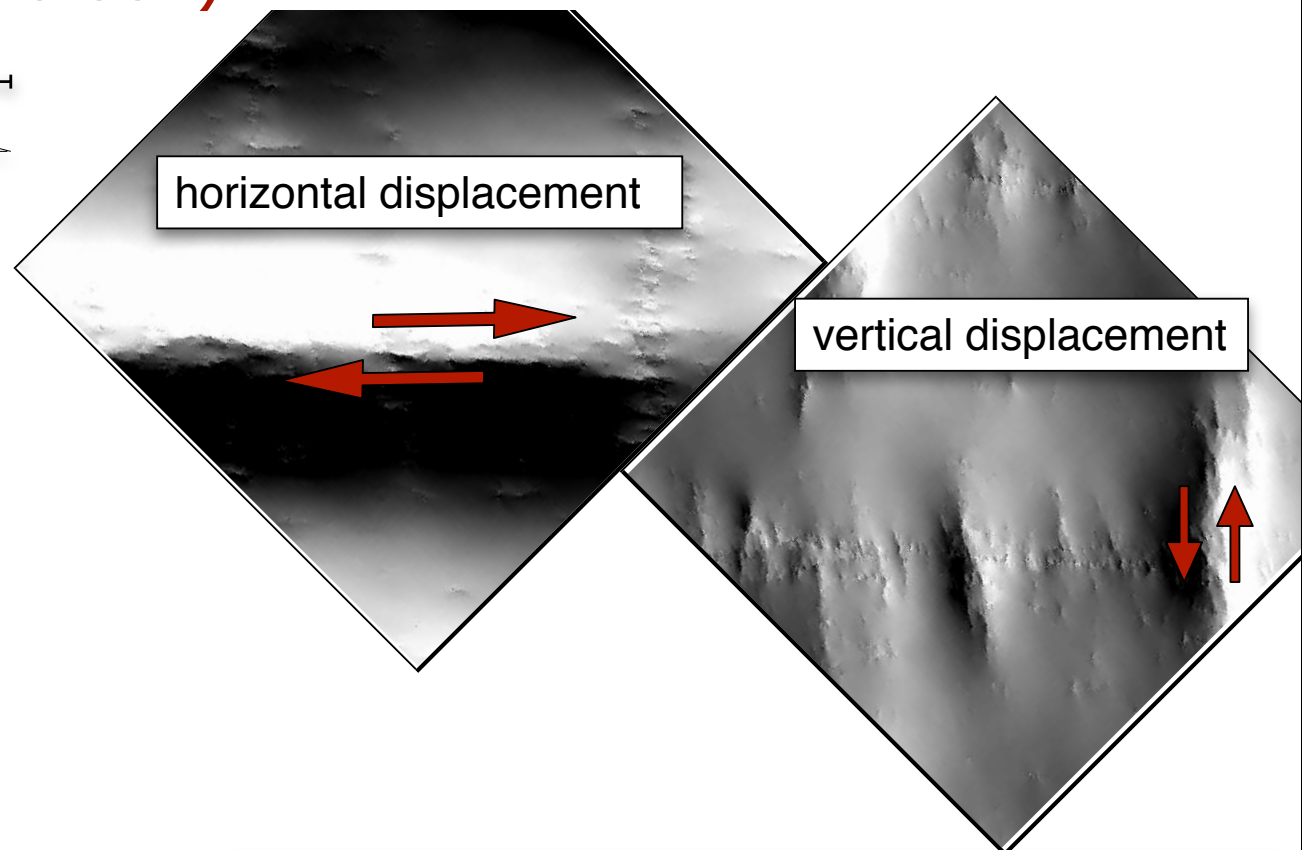
strain relieved ~ a/L ~ 1/40 to 2/40

a~1 to 2 σ_0

Aside: previous work on Lennard-Jones glasses

Typical displacement field (Lennard-Jones), L=1000, ($\Delta\gamma$~0.002)





a~1 to 2 σ_0

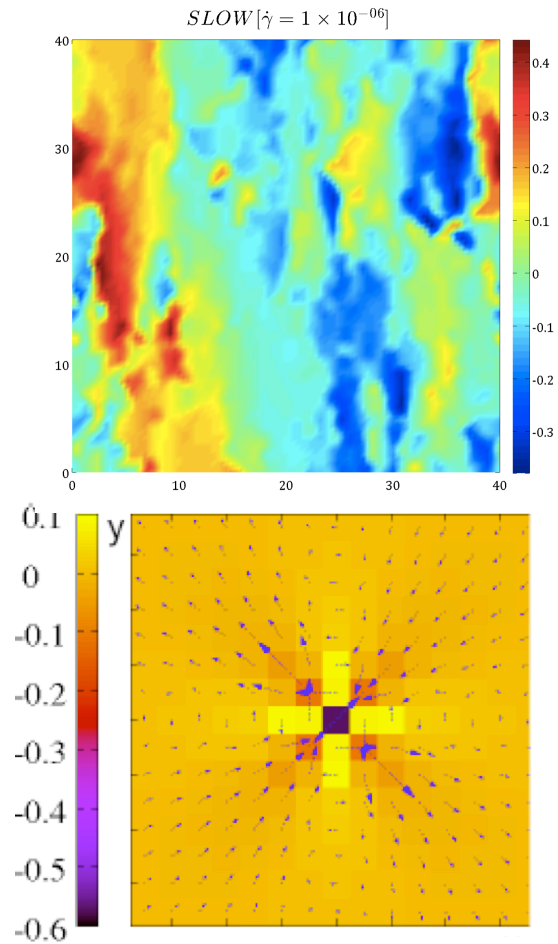
strain in shear zone ~ 2% to 4%

strain relieved ~ a/L ~ 0.002

Maloney and Robbins. J. Phys. Cond. Mat. 2007

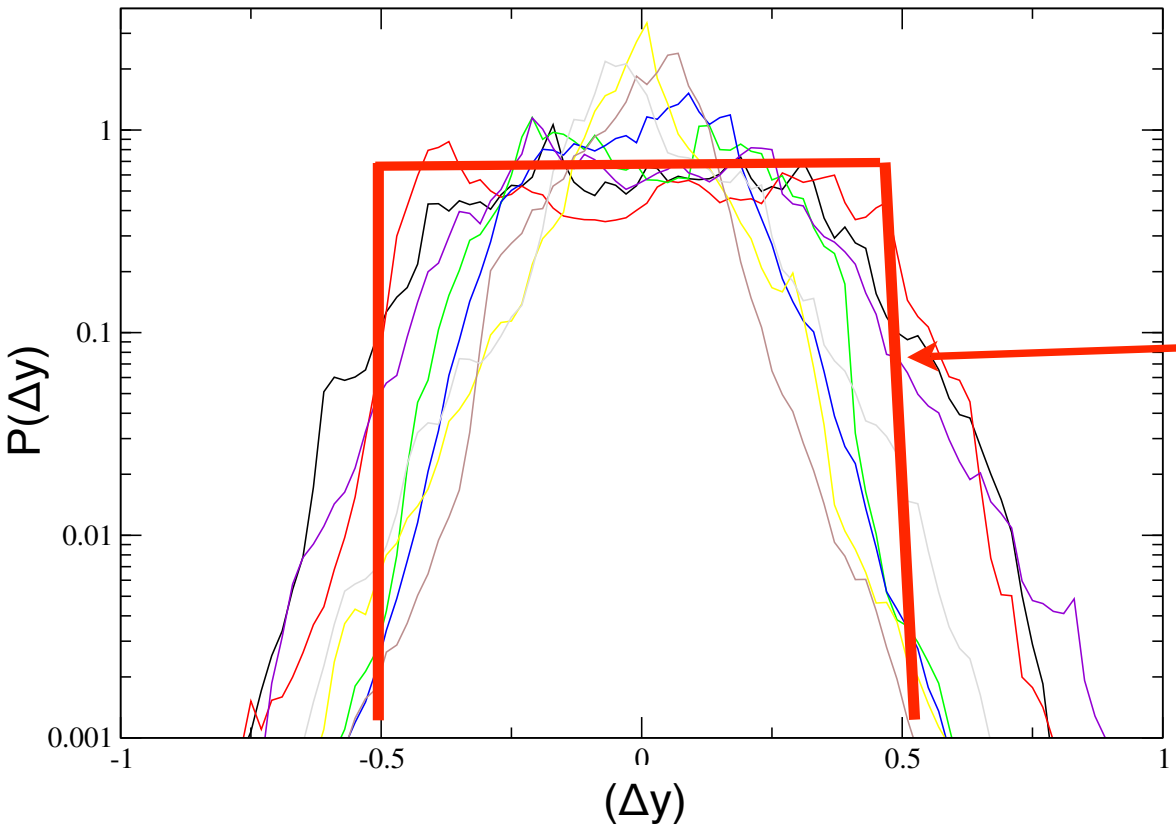
Shear transformation zone (STZ) mechanism

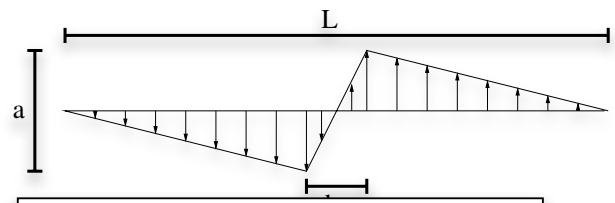
- Local group rearranges (yields)
- Redistributes stresses according to Eshelby
- Mean field description?
- Versions:
  - Bulatov and Argon (1994)
    - kinetic monte carlo
    - rates based on Eshelby
    - yield conditions uniform
  - Vandembroucq, Roux and co-workers
    - extremal quasistatic model (no time)
    - thresholds are stochastic
    - slip amplitudes are fixed
  - Bocquet, Ajdari, Picard, Martens and Barrat
    - dynamical model (can get rheology)
    - thresholds are fixed
    - slip amplitudes are fixed
    - delay times are stochastic



Eshelby Solution (From Barrat)

Ab-initio estimate: quasi-static $D_{eff}=\langle\Delta y^2\rangle/2\Delta\gamma$





active:
P(Δy) flat up to "a"

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

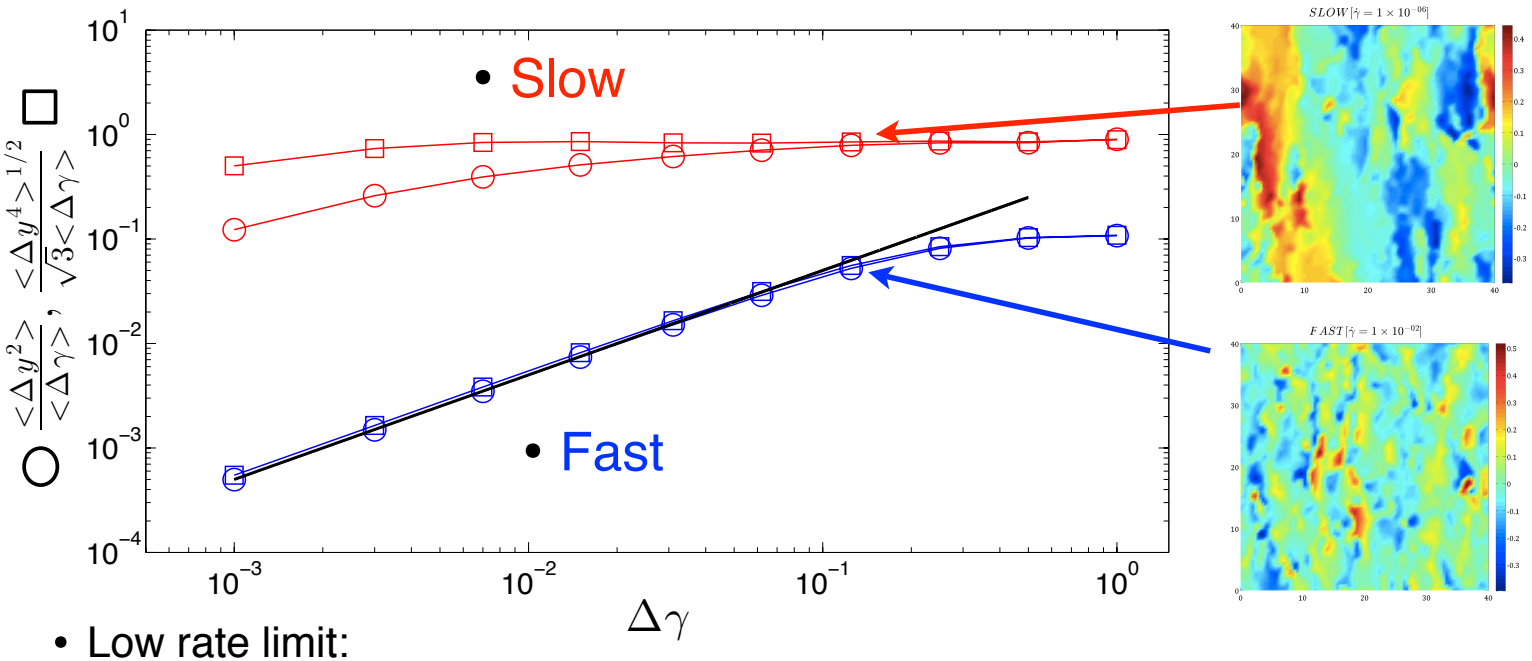
At larger Δγ, these add incoherently

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

Size dependent effective diffusion

(see also, Lemaitre and Caroli)

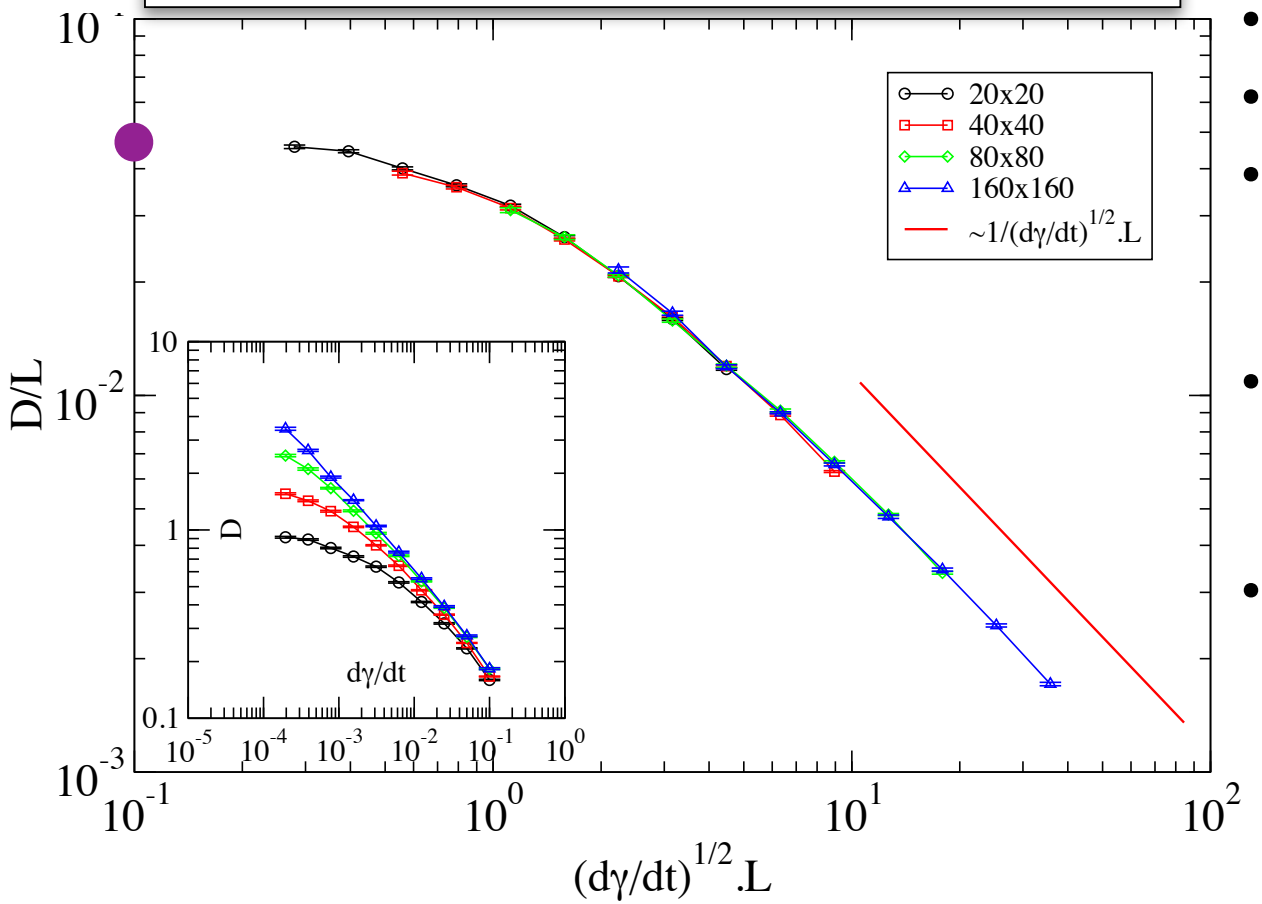
P(Δy) 2nd and 4th moments (Local drag $\tau_d=\tau_v$)



- Low rate limit:
  - P(Δy) non-Gaussian with big tails at early times (kurtosis is power-law)
  - crosses to Gaussian with characteristic D at $\Delta\gamma_c \sim 1/L$
- High rate limit:
  - Gaussian at all times (Maxwell-Boltzmann distribution)
  - ballistic scaling of both moments (solid black line)
  - crossover to diffusive scaling at $\Delta\gamma \sim 1$ independent of rate

Diffusion: pair drag, $\tau_d=\tau_v$, (overdamped) various L.

ab-initio quasi-static: D/L = a/24. a~1 -> D/L ~ 5%

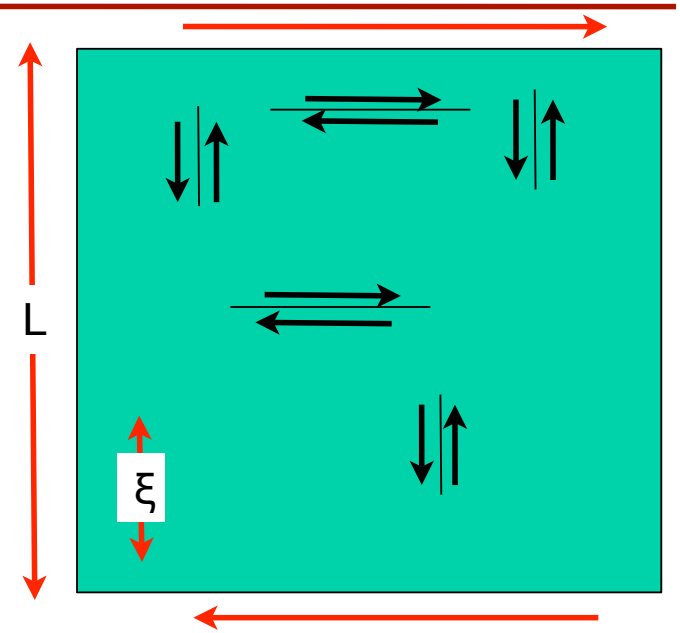


- Define "D" as:
- $D=\langle\Delta y^2\rangle/2\Delta\gamma$
- Should go to plateau if system is "quasi-static"
- L=20 system is at plateau by rate=2×10^{-4}.
- L=160 has no idea about the plateau

- Just like Lemaitre&Caroli result for UNDERDAMPED Lennard-Jones
- Implies $l_{slip}\sim1/\text{rate}^{1/2}$ at high rate away from plateau

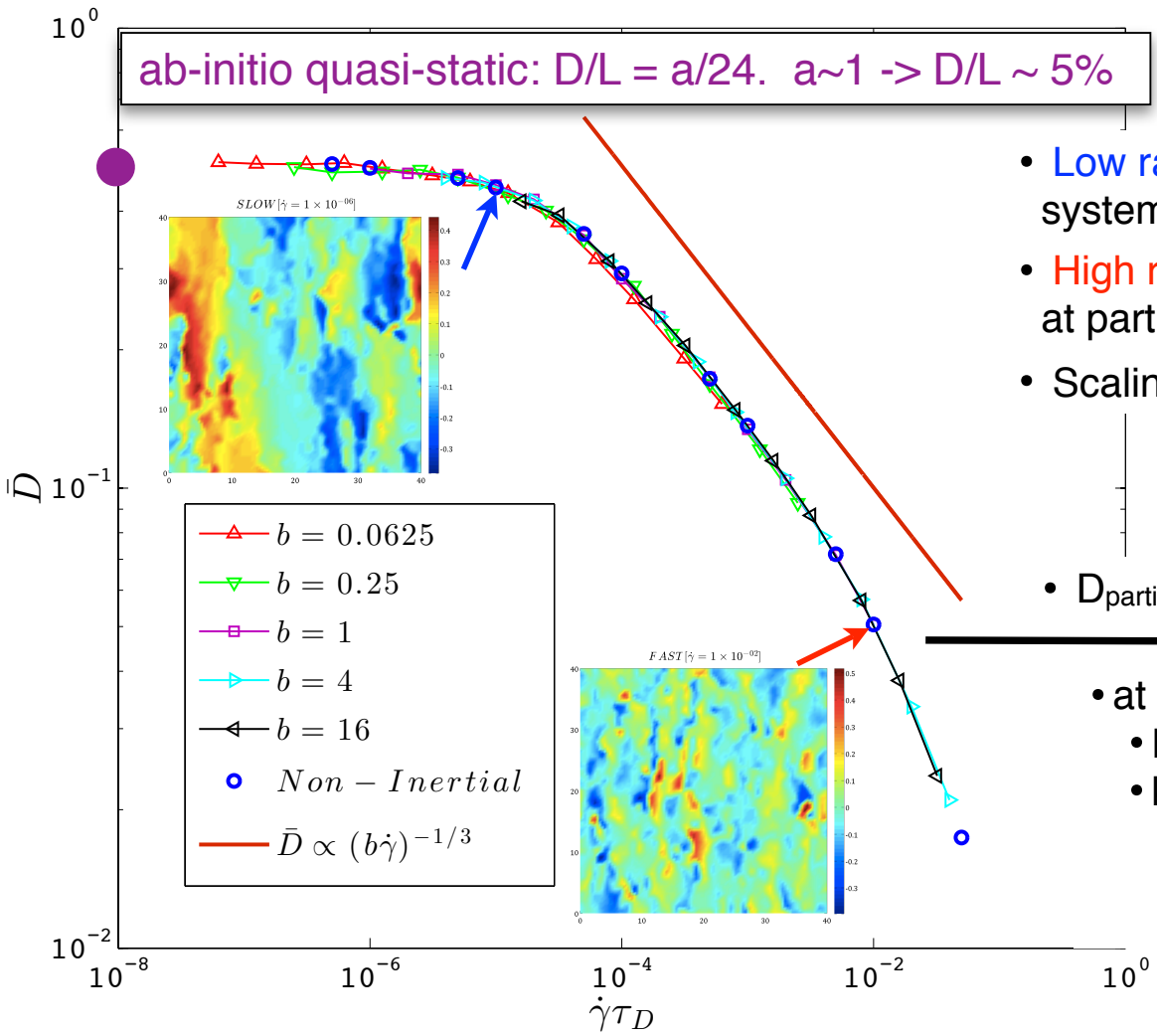
Argument for diffusion/rheology coupling

- Lemaitre and Caroli (PRL 2009):
- Assume: deformation from uncorrelated slip lines of length ξ (assume $\xi \ll L$)
- Linear elasticity gives: $D \sim \xi \ln(L/\xi)$
- Assume: $\sigma - \sigma_y \sim \mu\tau\,(d\gamma/dt)$ where τ is formation time of a slip line
- Suppose $\tau \sim \xi$ (biggest assumption)
- Then: $\sigma - \sigma_y \sim \mu\xi\,(d\gamma/dt) \sim \mu D(d\gamma/dt)$
- For pair drag $D \sim (d\gamma/dt)^{-1/2}$ (at large rate) predicts $\sigma - \sigma_y \sim \mu(d\gamma/dt)^{1/2}$.



- Works for pair drag.
- Already known for inertial (Lennard-Jones)...
- new result here is for overdamped
- What about “local drag”???

Diffusion: local drag, various damping, L=20



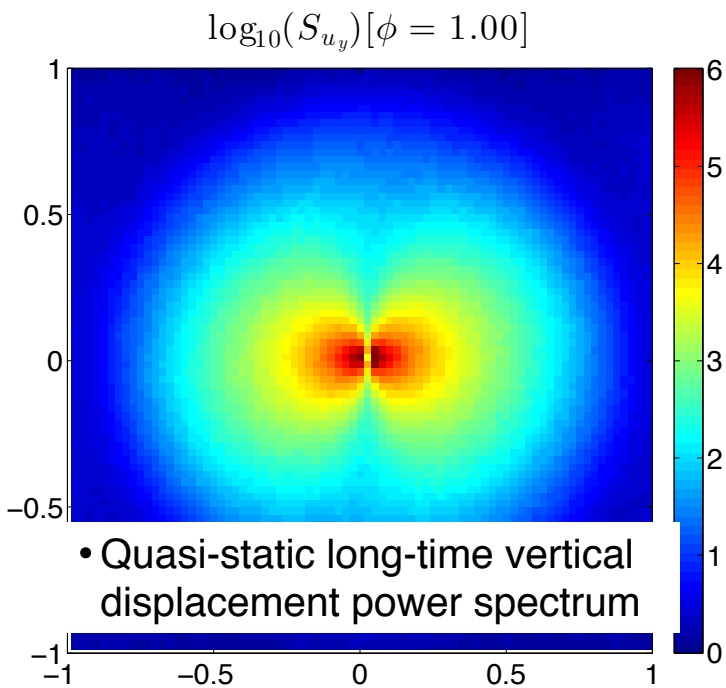
- Low rate: correlations saturate at system size.
- High rate: correlations disappear at particle scale
- Scaling regime: $D/L \sim (d\gamma/dt)^{(-1/3)}$

- $D_{particle\text{-}scale}/D_{quasi\text{-}static} \sim a/L \sim 1/20$

- at "particle scale":
  - $D=0.05\ a^2$
  - kink in BOTH D AND σ (see below)

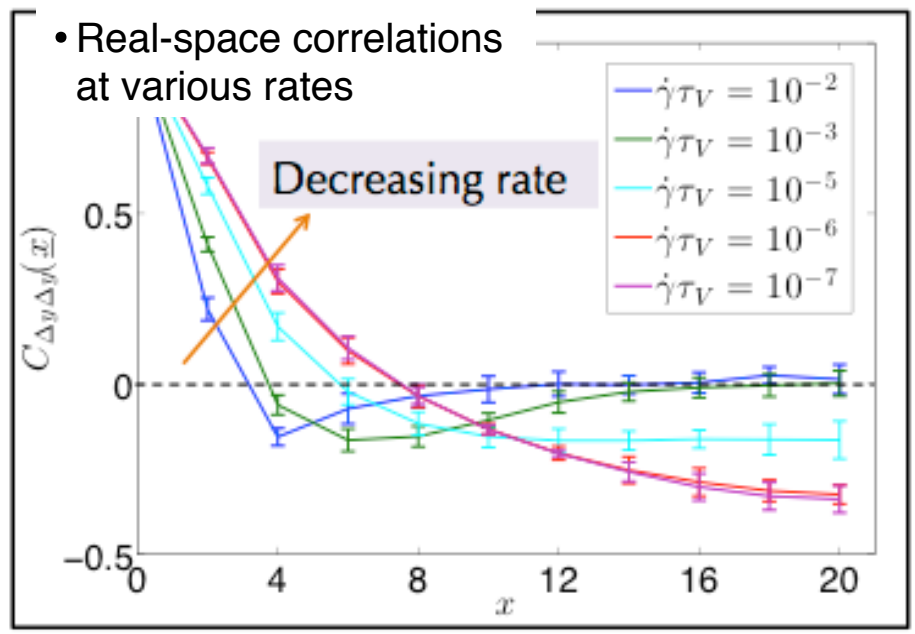
Spatial structure: local drag, overdamped, L=40

- D~(dγ/dt)$^{-1/3}$ implies ξ~ (dγ/dt)$^{-1/3}$. Quantitative agreement?
- Power spectrum of Δy, S(Δy)~q$^{-2.5}$ along x axis.
- Not understood. Should be S~q^{-2} for a "sawtooth" slip line.
- Real space correlations "not inconsistent with" ξ~ (dγ/dt)$^{-1/3}$.



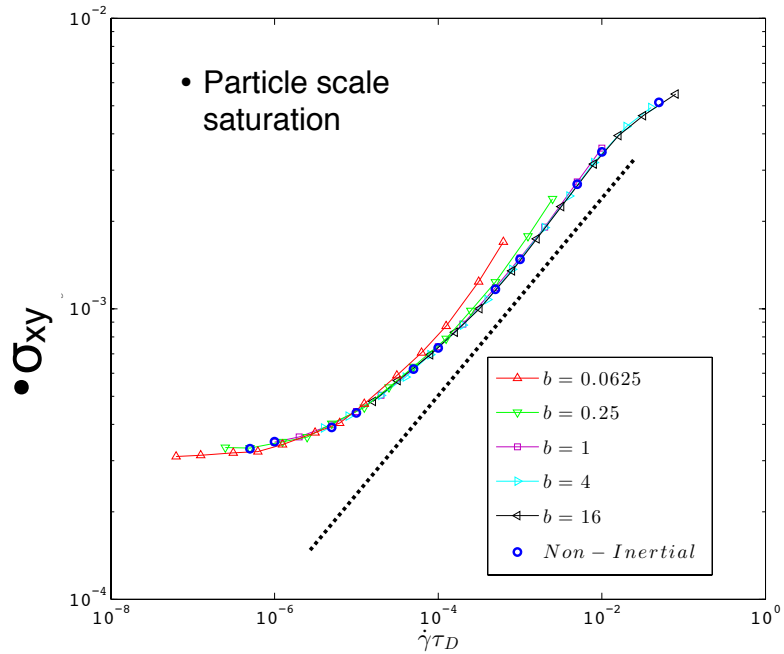
- Quasi-static long-time vertical displacement power spectrum

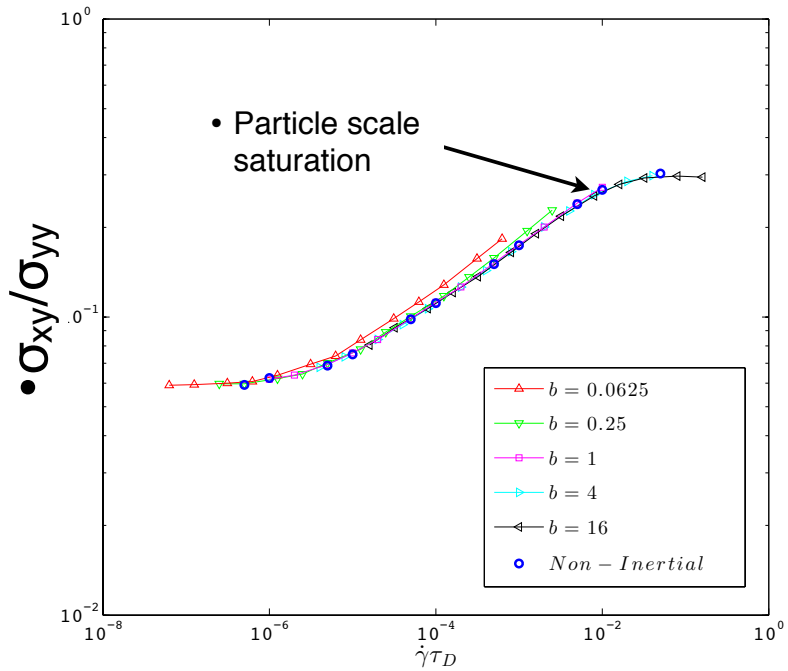
$$C_{\Delta y \Delta y}(\underline{x}) = \frac{\langle \Delta y(\underline{r}) \Delta y(\underline{r} + \underline{x}) \rangle}{\langle \Delta y(\underline{r}) \Delta y(\underline{r}) \rangle}$$



- Real-space correlations at various rates

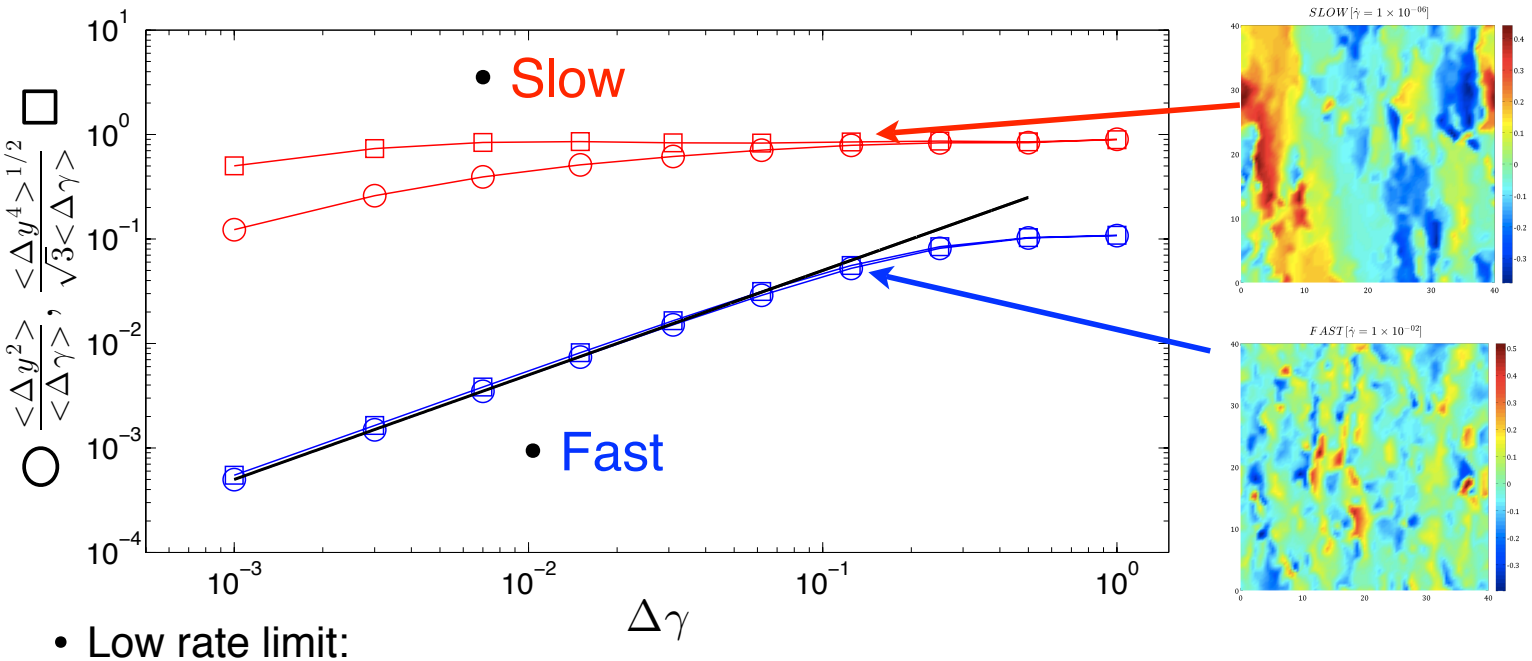
Rheology/friction: Local drag L=20





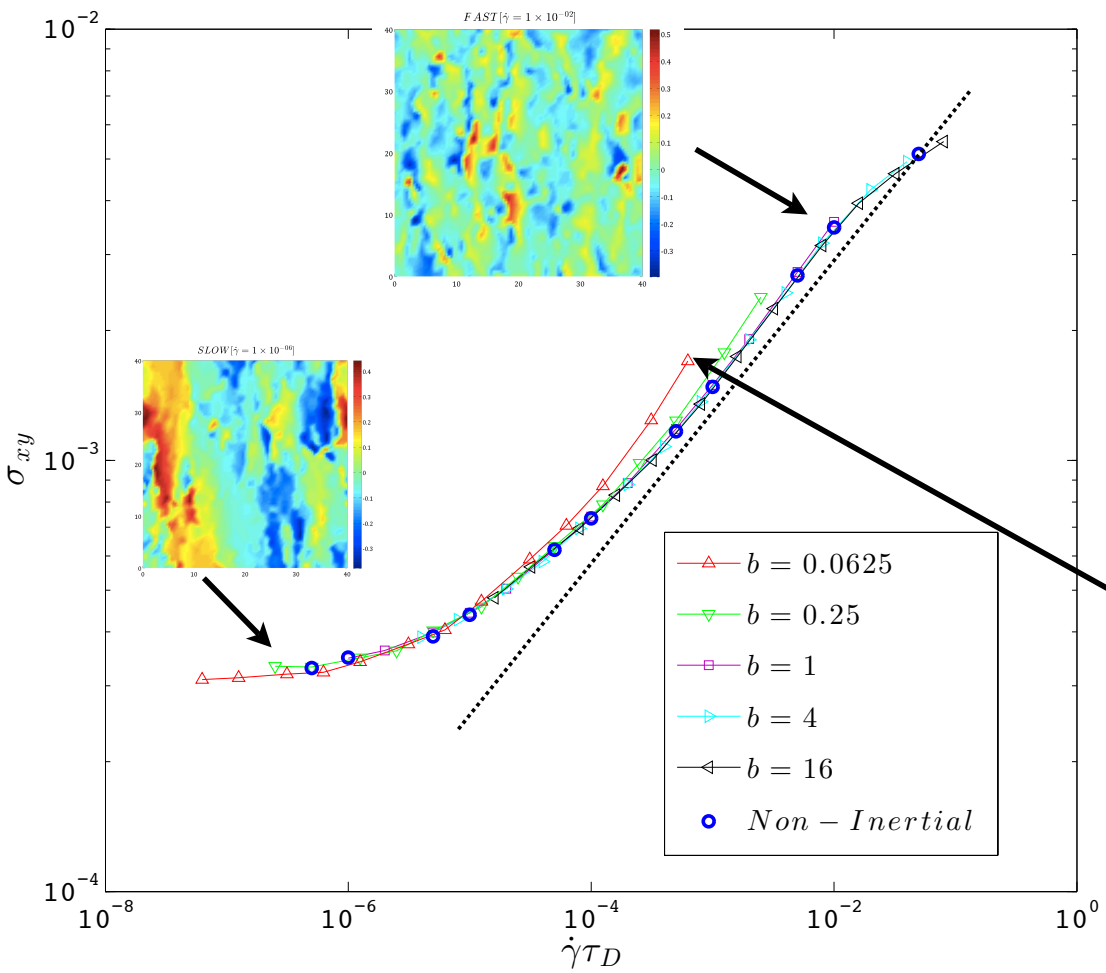
- Hershel Bulkley Rheolgoy exponent same as diffusion, 1/3.
- High rate cross-over more obvious in dynamic friction.
- Above rate = 10^{-2}, spatial correlations are completely absent.

P(Δy) 2nd and 4th moments (Local drag $\tau_d=\tau_v$)



- Low rate limit:
  - P(Δy) non-Gaussian with big tails at early times (kurtosis is power-law)
  - crosses to Gaussian with characteristic D at $\Delta\gamma_c \sim 1/L$
- High rate limit:
  - Gaussian at all times (Maxwell-Boltzmann distribution)
  - ballistic scaling of both moments (solid black line)
  - crossover to diffusive scaling at $\Delta\gamma \sim 1$ independent of rate

Flow curves: Local drag, various damping, L=20



- Low rate: correlations saturate at system size.
- High rate: correlations disappear at particle scale
- τ_d/τ_v=1/16, just starting to inertia at highest shear rate
- HB exponent~1/3.

Dissipation (Intermittency in time)

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

- Energy change under affine deformation = σ
- Identify as input power
- Identify as dissipation rate

- For local drag

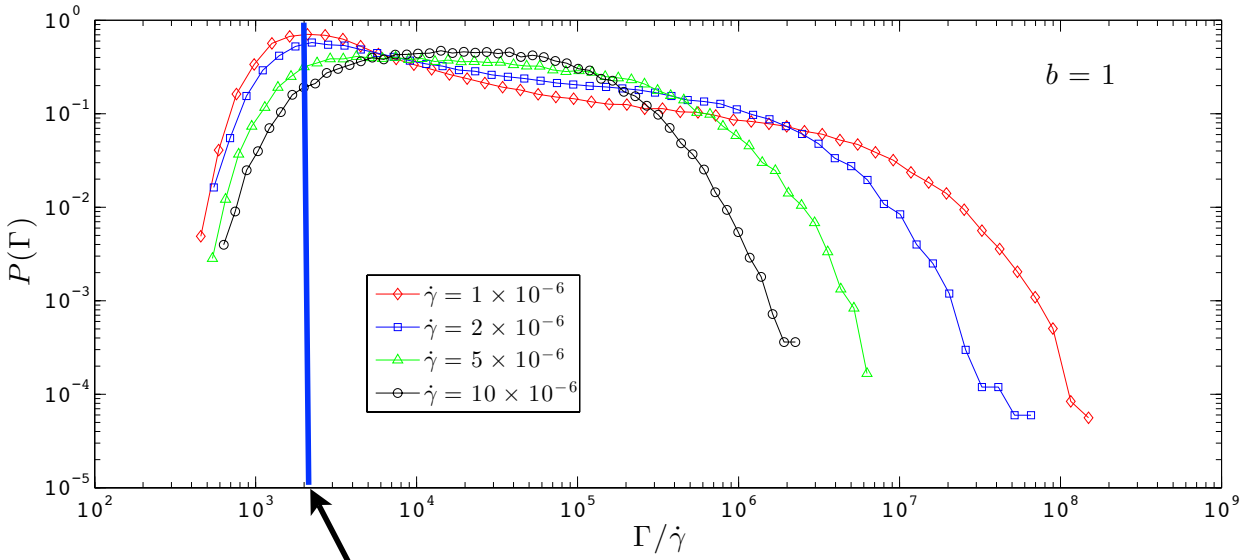
$$\Gamma\dot{\gamma} = \sigma\dot{\gamma} - \frac{dU}{dt} = \sum_i \vec{F}_i \cdot \delta\vec{v}_i = D\sum_i \delta v_i^2$$

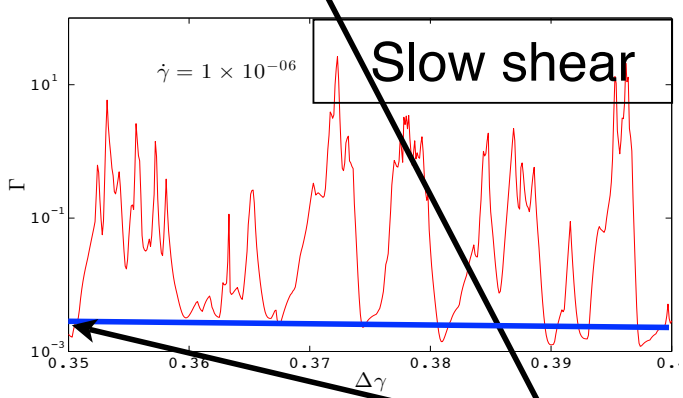
$$\langle\Gamma\rangle = \langle\sigma\rangle = \frac{DN}{\dot{\gamma}}\langle\delta v^2\rangle$$

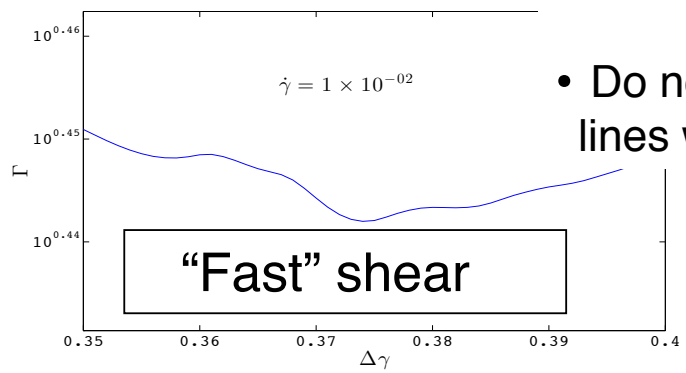
- Ono *et. al. PRE 2003*
- Rheology = fluctuations

- Γ is energy dissipated per unit strain
- Like an instantaneous decorrelation rate

Dissipation spectrum: local drag ($\tau_d=\tau_v$) (L=40)



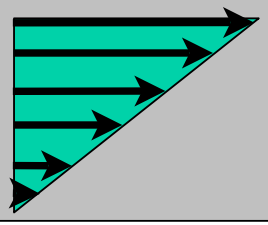
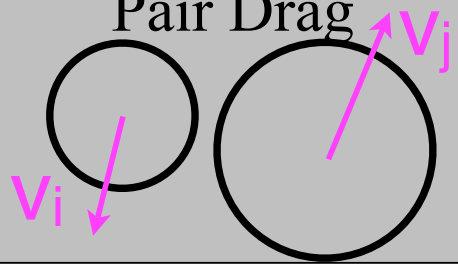
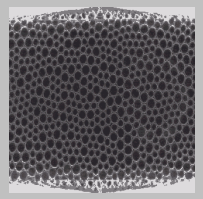




- Slow shear:
  - "Quasi-static Peak" at low Γ
  - Power-law at high Γ
- Fast shear:
  - Gaussian
- Avalanches "go away" while still: $\xi \sim L$ and $D \sim D_{QS}$
- Do not confound slip lines with avalanches!

•QS peak: $v \sim \dot{\gamma} \quad \Gamma \sim \dot{\gamma}$

Conclusions

	Local Drag 	Pair Drag 
Overdamped $\tau_v \ll \tau_D$ 	new result: $\sigma-\sigma_y \sim (d\gamma/dt)^{1/3}$ $D \sim (d\gamma/dt)^{-1/3}$ at high rate	new result: $\sigma-\sigma_y \sim (d\gamma/dt)^{1/2}$ $D \sim (d\gamma/dt)^{-1/2}$ at high rate
Inertial $\tau_v \gg \tau_D$ 	??? looks like exponent is bigger than 1/3, surprisingly difficult to obtain underdamped limit.	like Lemaitre+Caroli: $\sigma-\sigma_y \sim (d\gamma/dt)^{1/2}$ $D \sim (d\gamma/dt)^{-1/2}$ at high rate