

Dense disordered active matter

June 16 and 17
Disorder in complex
systems summer school
Institut Pascal

Lisa Manning
Syracuse University

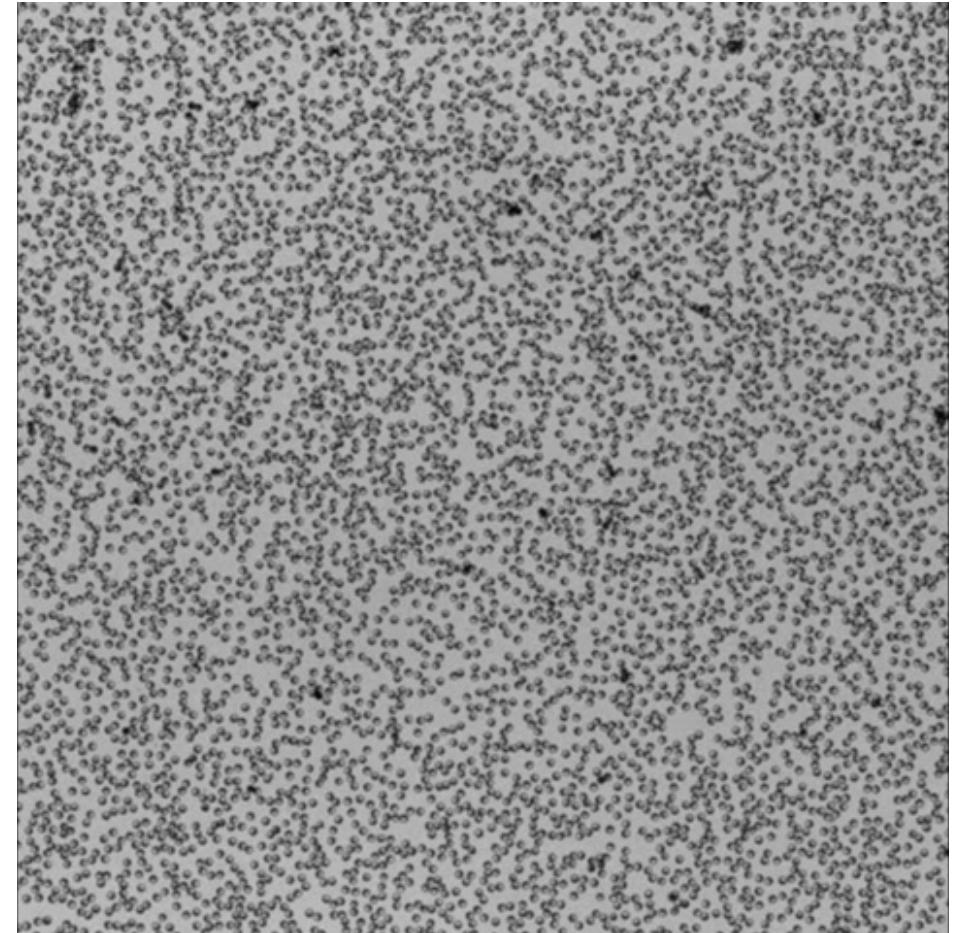


Motivation: Would like a theory of active matter

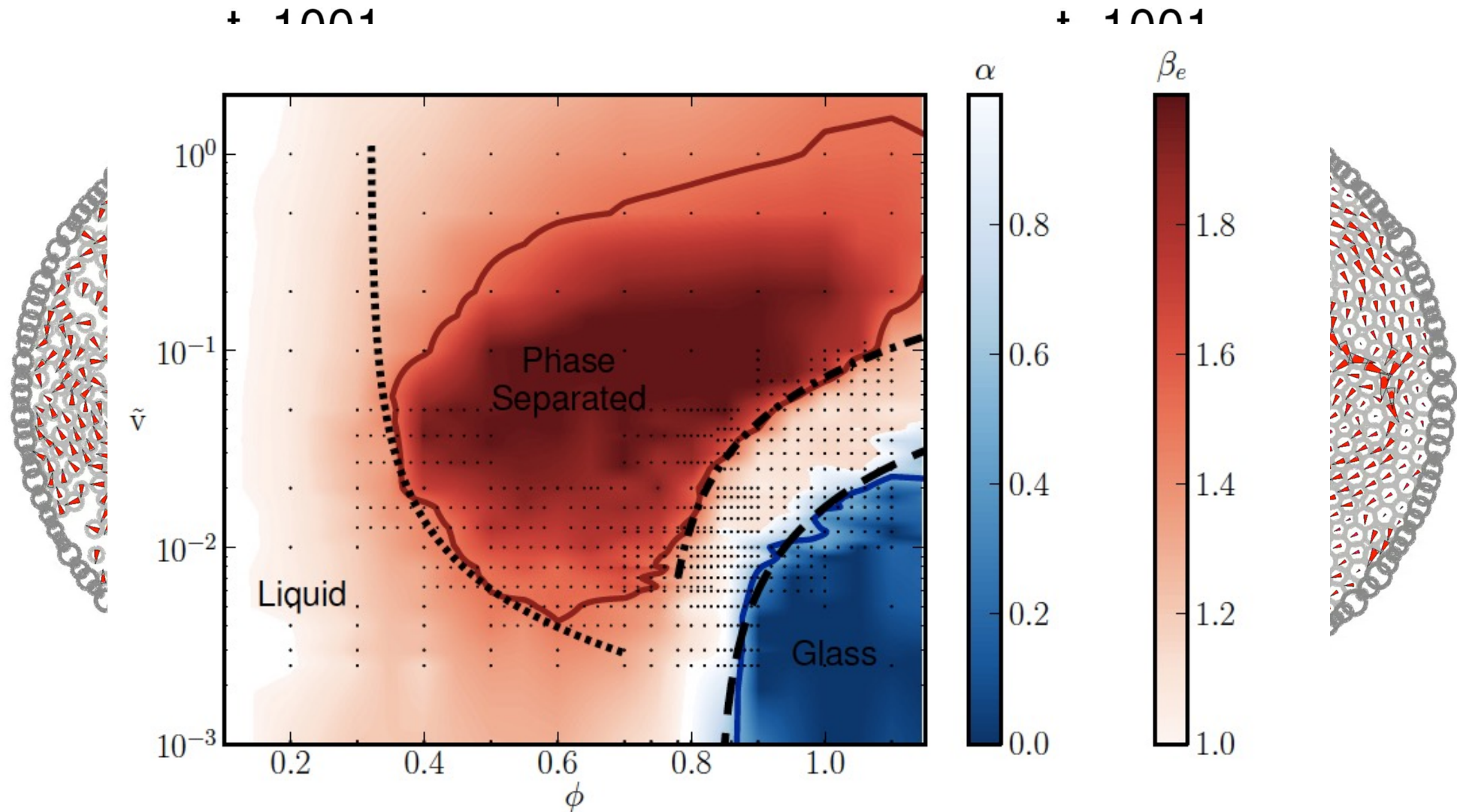


From talk by Julien Tailleur

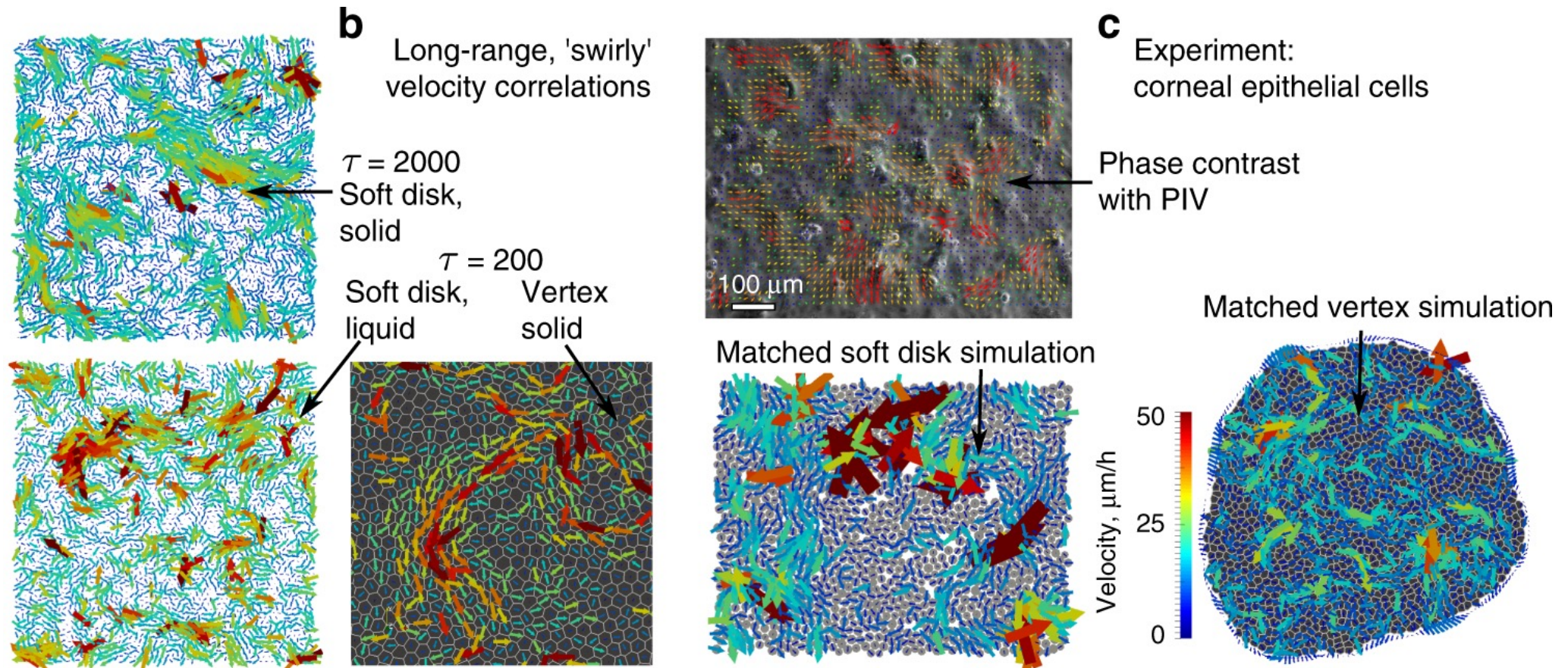
- breaking time-reversal invariance generates beautiful new types of behavior:
 - Giant number fluctuations
 - Motility induced phase separation



At high densities, dynamics change

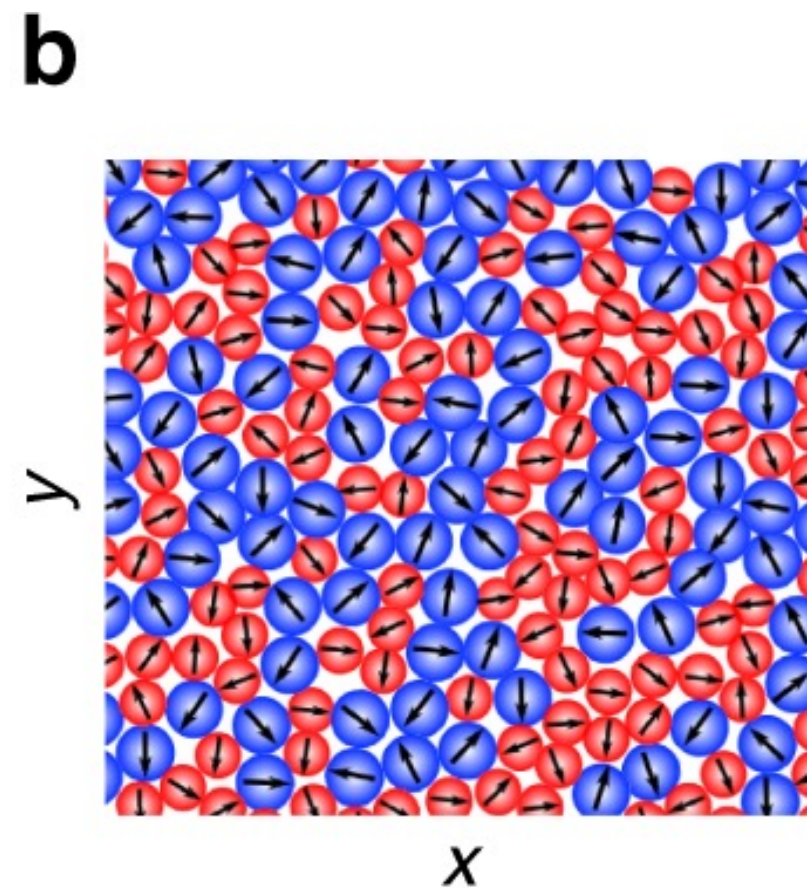
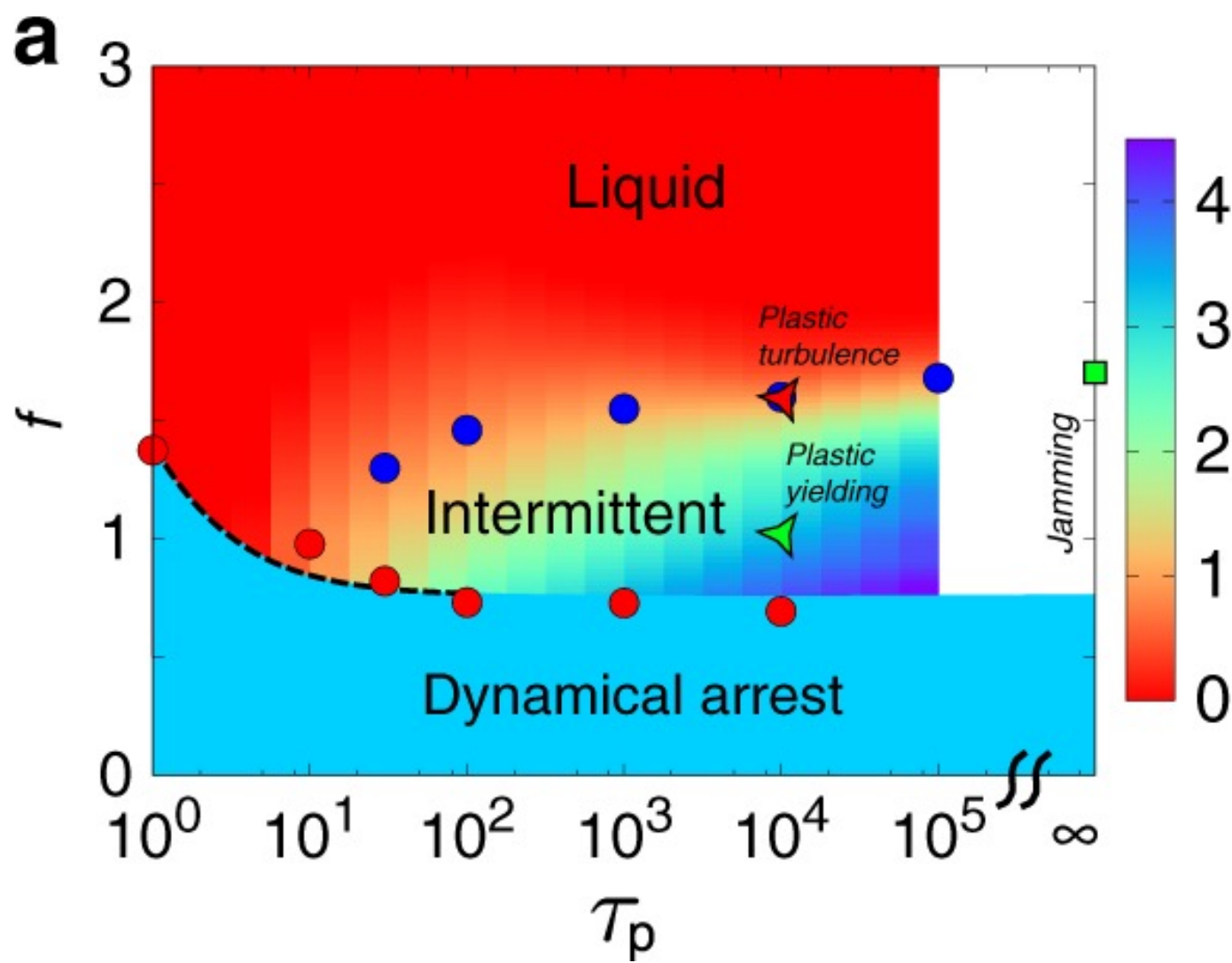


The dynamics become “swirly”: long-range velocity correlations

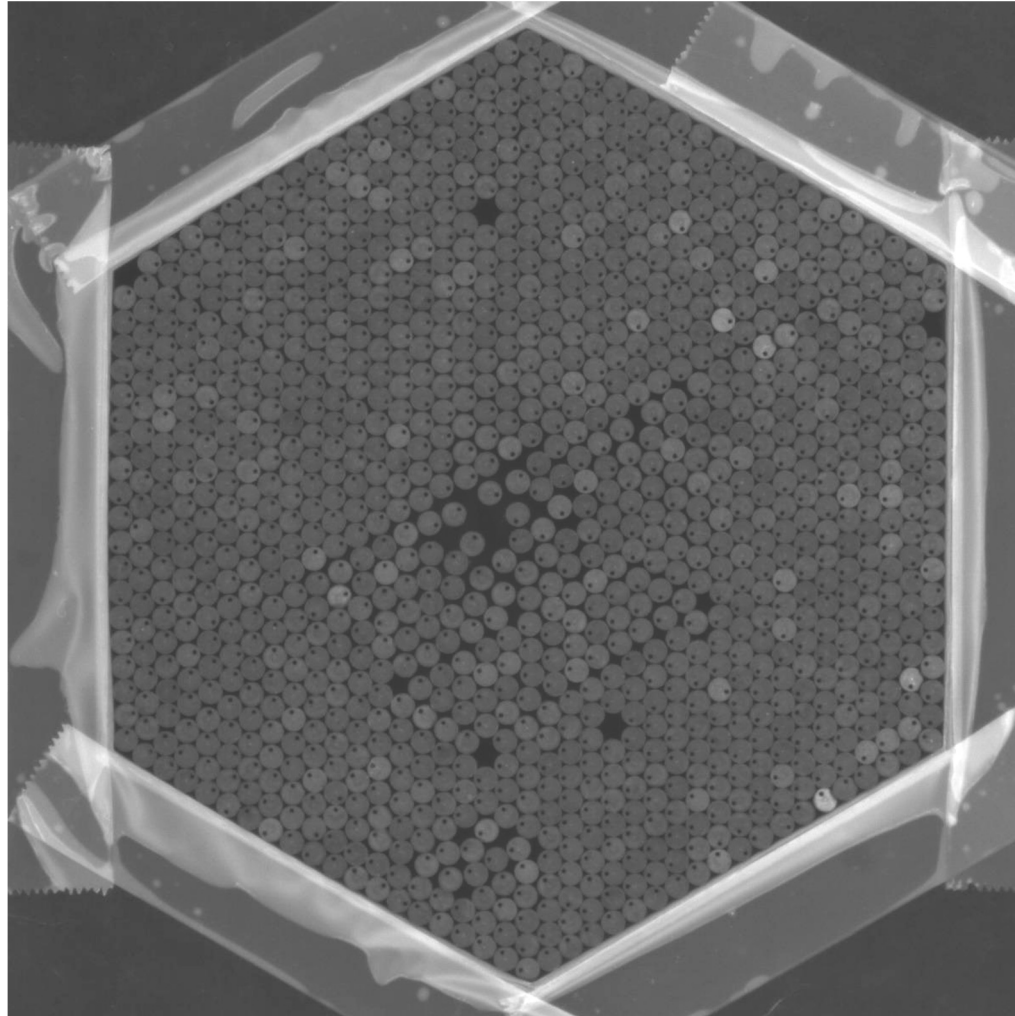


Henkes et al Nature communications (2020)

dynamics share some features with fluids, some with solids (c.f. fluid turbulence talks last week)



Displacements clearly related to underlying solid-like structure, looks “self-shearing”



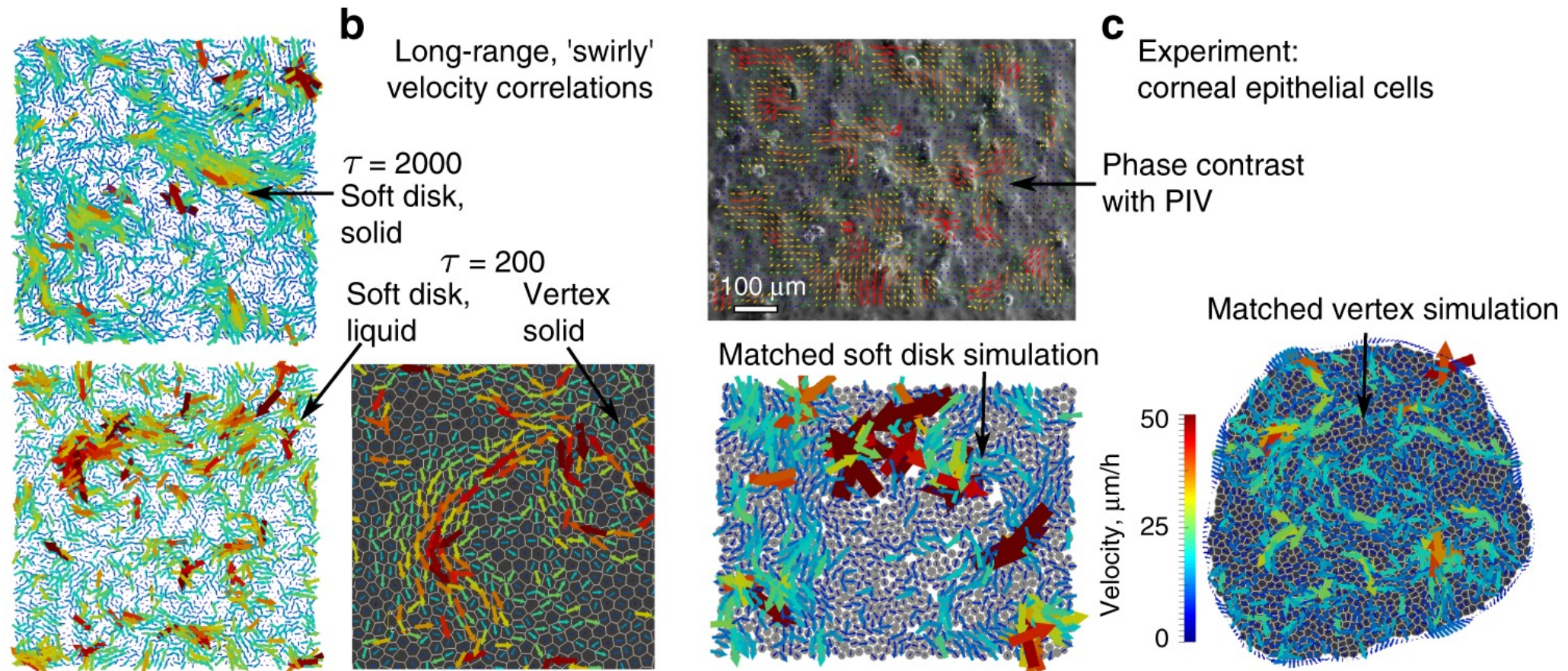
In ordered systems, one can design function using defects:

In this video, an optimized embedded cluster of variable-diameter particles (yellow) is shown undergoing multiple swelling/shrinking cycles. Defects are created and then move, producing shear slip along a single crystal plane.

Today: long-range velocity correlations
Tomorrow: intermittency and avalanches

These are images from simulations that are “solid-like” in the passive state

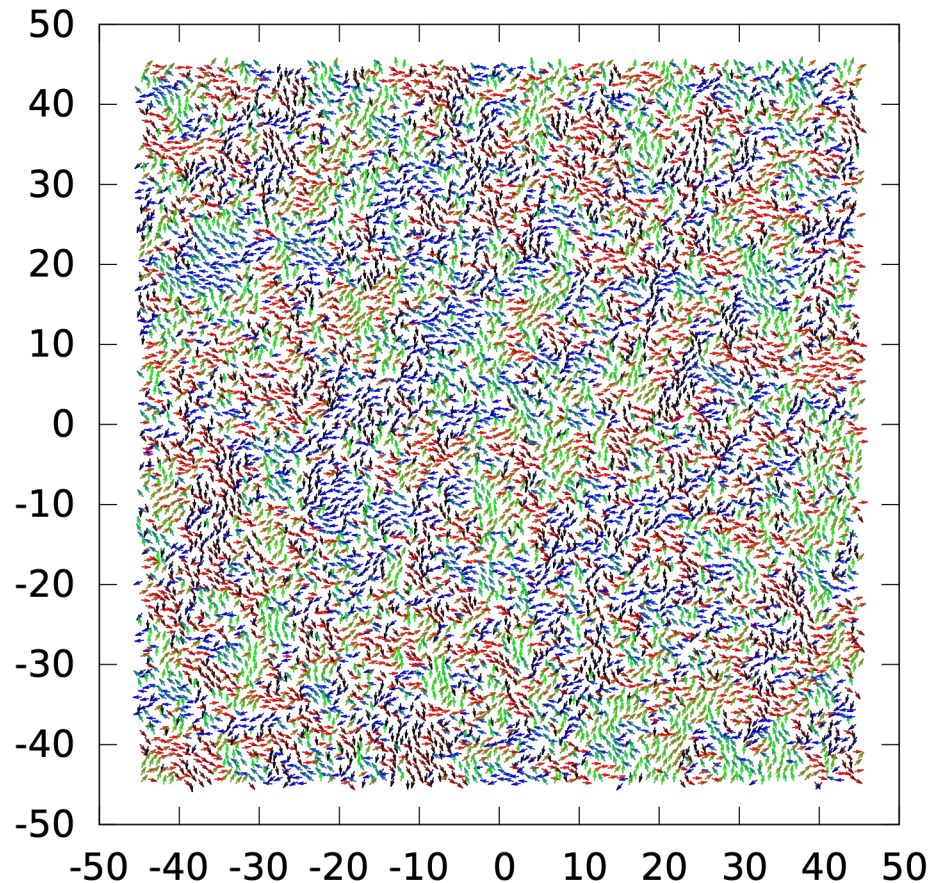
soft discs with packing fraction above jamming or vertex model with shape index below rigidity



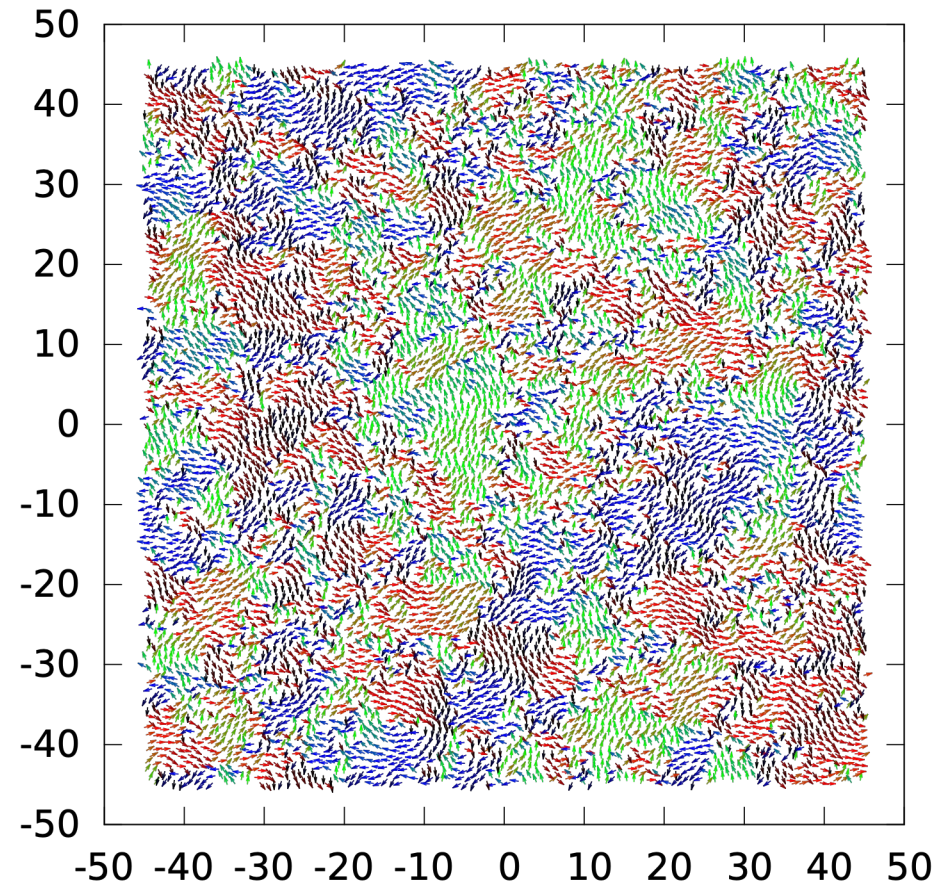
Dense Fluid Systems

Increasing velocity correlation with increasing persistence time.

Longitudinal $\rightarrow \omega_{\parallel}(q) = \frac{1}{N} \langle |\hat{\mathbf{q}} \cdot \mathbf{v}(\mathbf{q})|^2 \rangle$
 $\tau = 0.14$



$\omega_{\perp}(q) = \frac{1}{N} \langle |\mathbf{v}(\mathbf{q}) - \hat{\mathbf{q}}(\hat{\mathbf{q}} \cdot \mathbf{v}(\mathbf{q}))|^2 \rangle \rightarrow$ Transverse
 $\tau = 10$



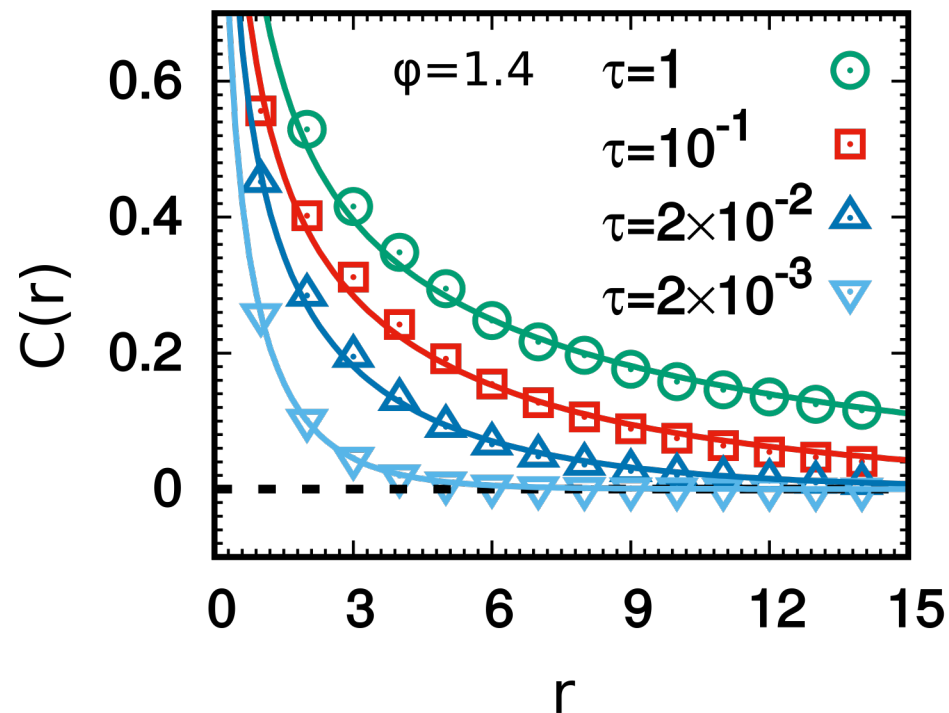
Velocity Correlations: solid-like starting point

Equal time velocity correlation length increases with increasing persistence time.

Arrested active systems.

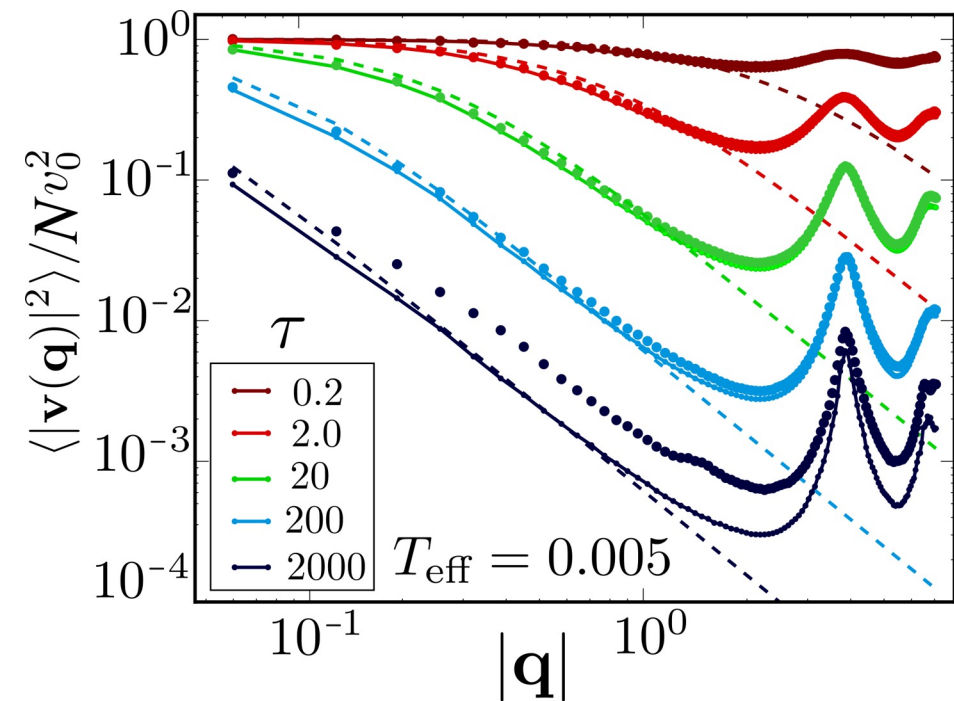
Lines are theoretical calculations.

Theory assumes vibrations around average positions.



Caprini *et al.* Phys. Rev. Res., **2**, 023321 (2020).

Theory approximates system as an amorphous elastic solid.



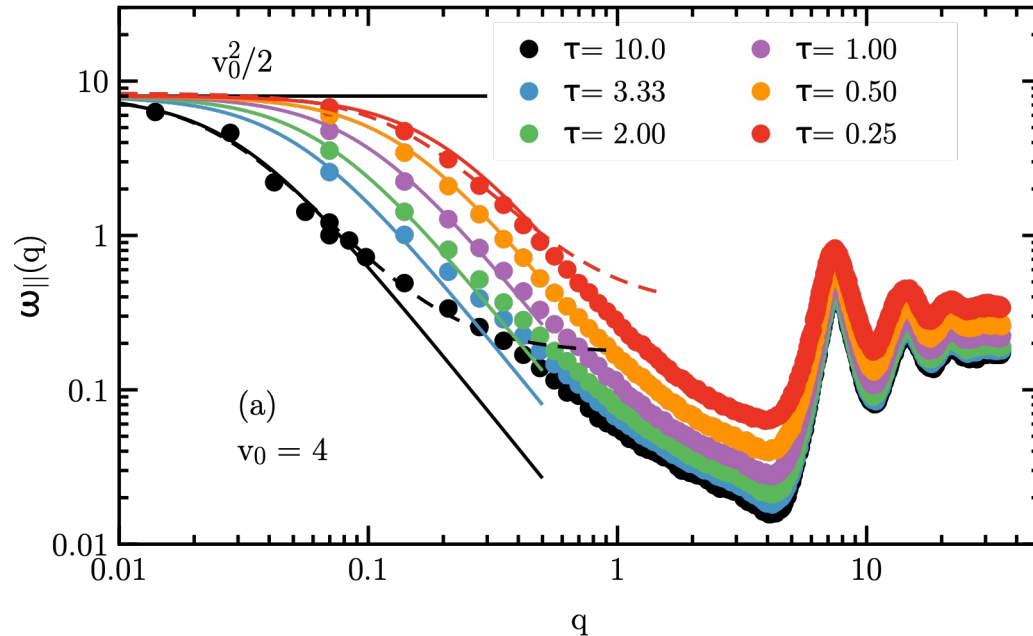
Henkes *et al.*, Nat. Commun., **11**, 1 (2020).

Velocity Correlations: liquid-like starting point

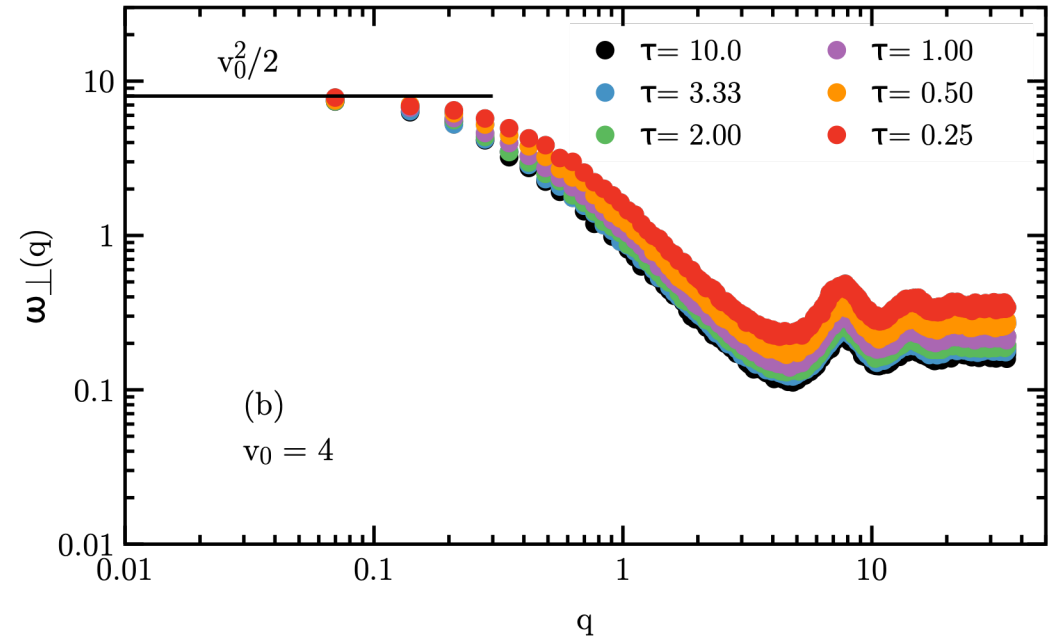
Equal time velocity correlations grow with increasing persistence time.

Dashed lines are numerical fits.

Solid lines are predictions of an approximate theory for longitudinal correlations.



$$\omega_{\parallel}(q) = \frac{1}{N} \langle |\hat{\mathbf{q}} \cdot \mathbf{v}(\mathbf{q})|^2 \rangle$$

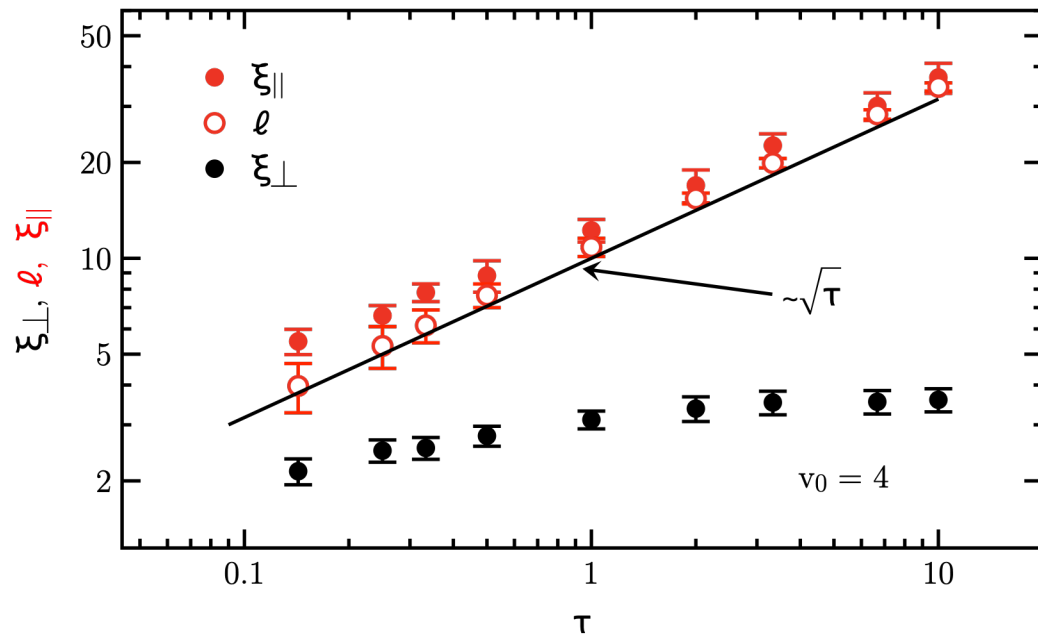


$$\omega_{\perp}(q) = \frac{1}{N} \langle |\mathbf{v}(\mathbf{q}) - \hat{\mathbf{q}}(\hat{\mathbf{q}} \cdot \mathbf{v}(\mathbf{q}))|^2 \rangle$$

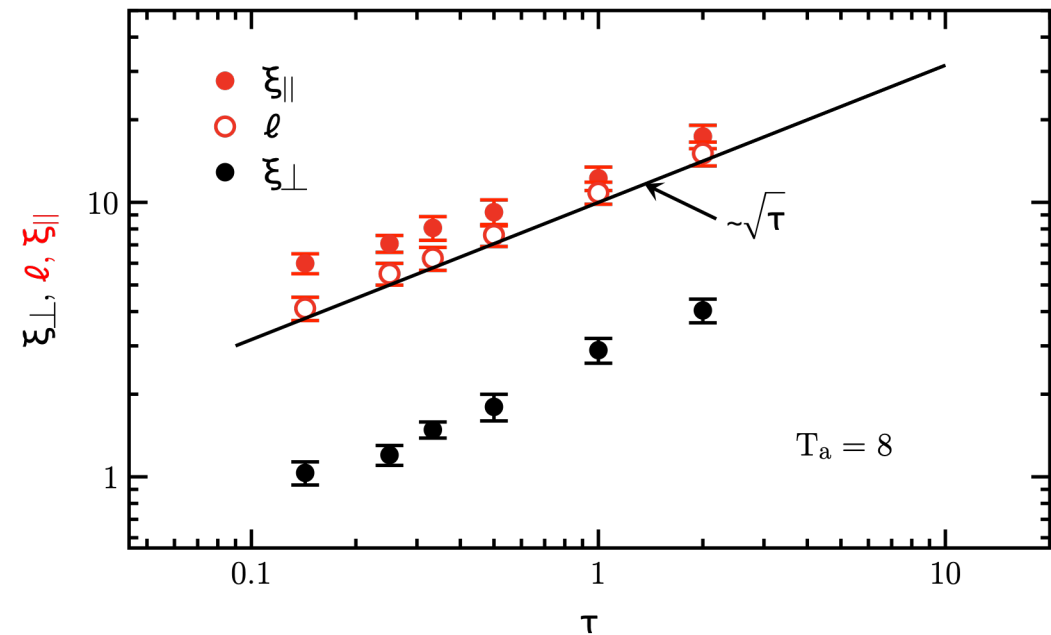
Comparison of scaling prediction with simulations

$$\ell = \sqrt{\tau B_v / (\gamma \rho)}$$

$\xi_{||}$ and ξ_{\perp} obtained from fits to $\omega_{||}(q)$ and $\omega_{\perp}(q)$.
Open symbols are results of the theory.



Fixed magnitude of the velocity.



Fixed active temperature.

References for derivations today:

- Henkes, S. Kostanjevec, K., Collinson, J.M, Sknepnek, R and Bertin, E., Nat. Commun., **11**, 1 (2020).
 - see also Henkes, Fily, Marchetti PRE 2011
 - Bi, Yang, Marchetti, Manning PRX 2016
- Grzegorz Szamel and Elijah Flenner, EPL 133, 60002 (2021)

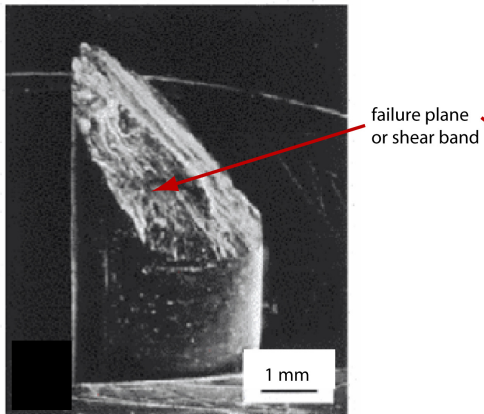
Day 2

Review: response of materials under shear

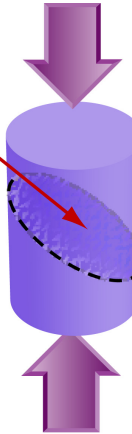
here, focus on zero temperature, limit of infinitely slow driving

Sheared disordered materials are well-studied

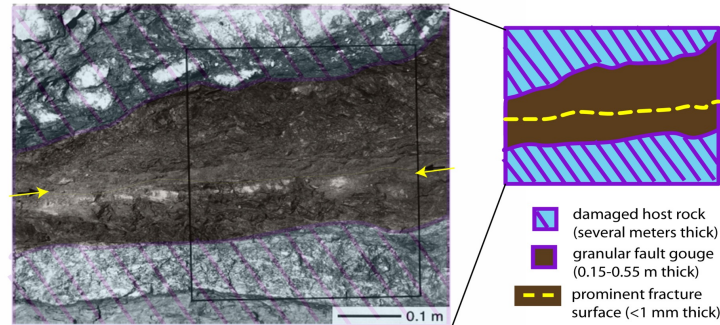
bulk metallic glasses



W. Johnson Group, Caltech

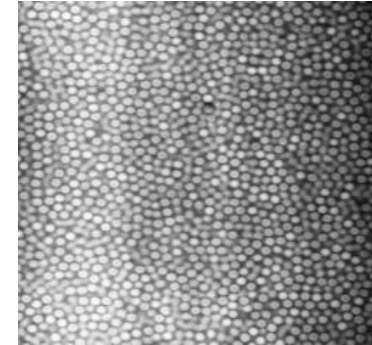


granular fault gouge



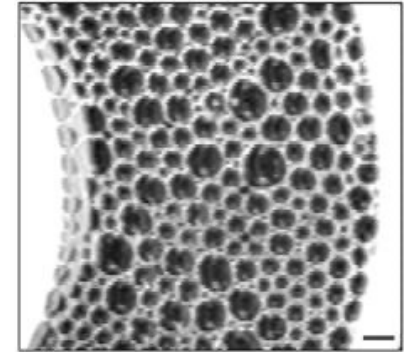
F. M. Chester and J. S. Chester, *Tectonophys.*
295, 1998.

colloids



Amann et al 2013

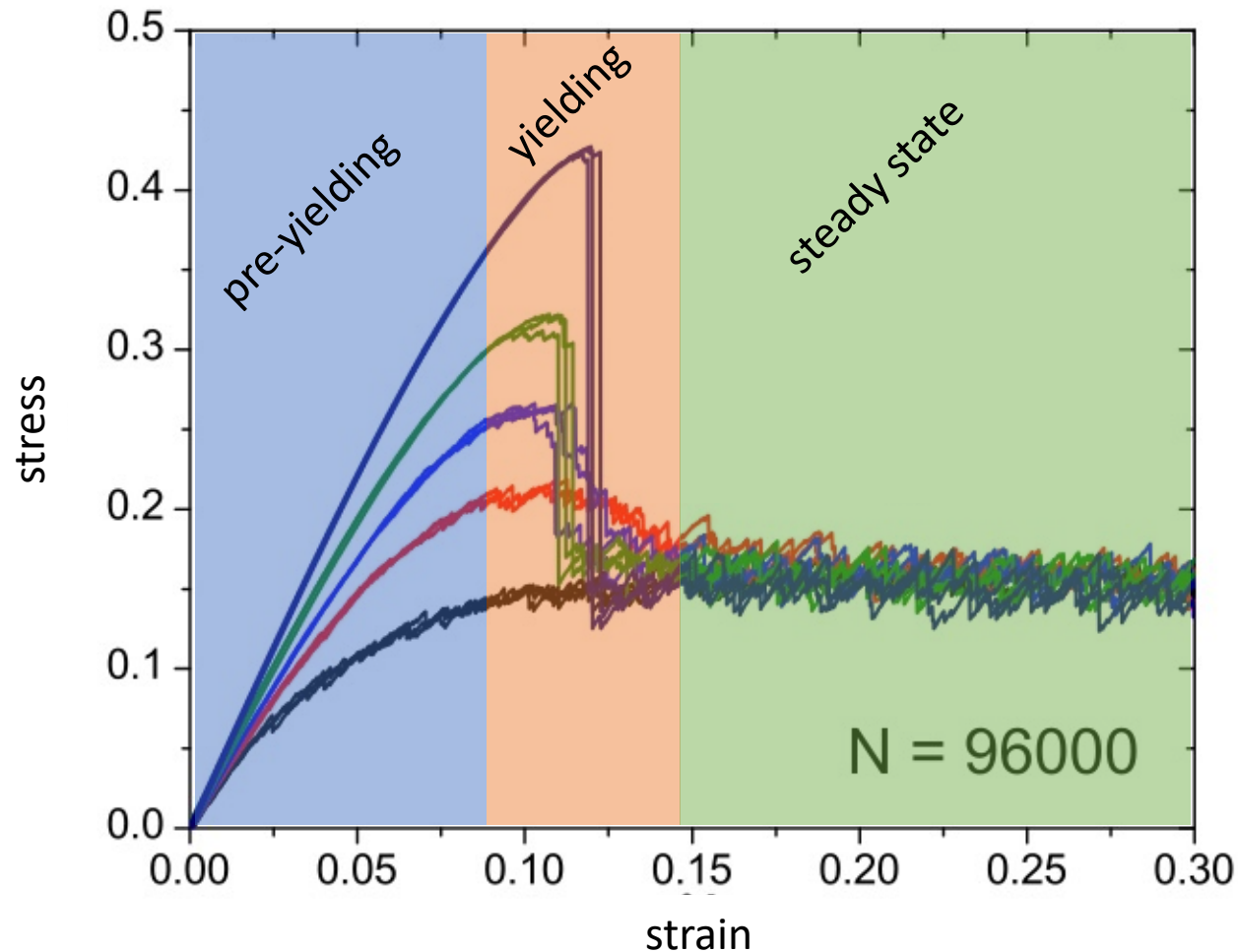
foams



Lauridsen et al 2002

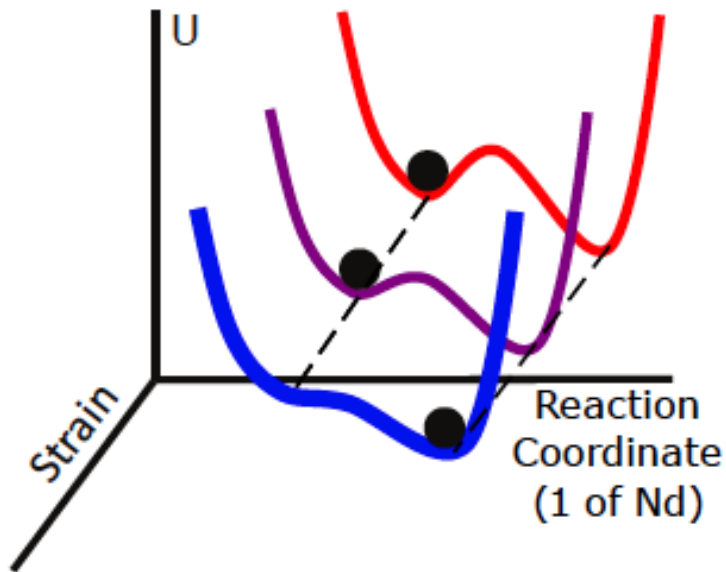
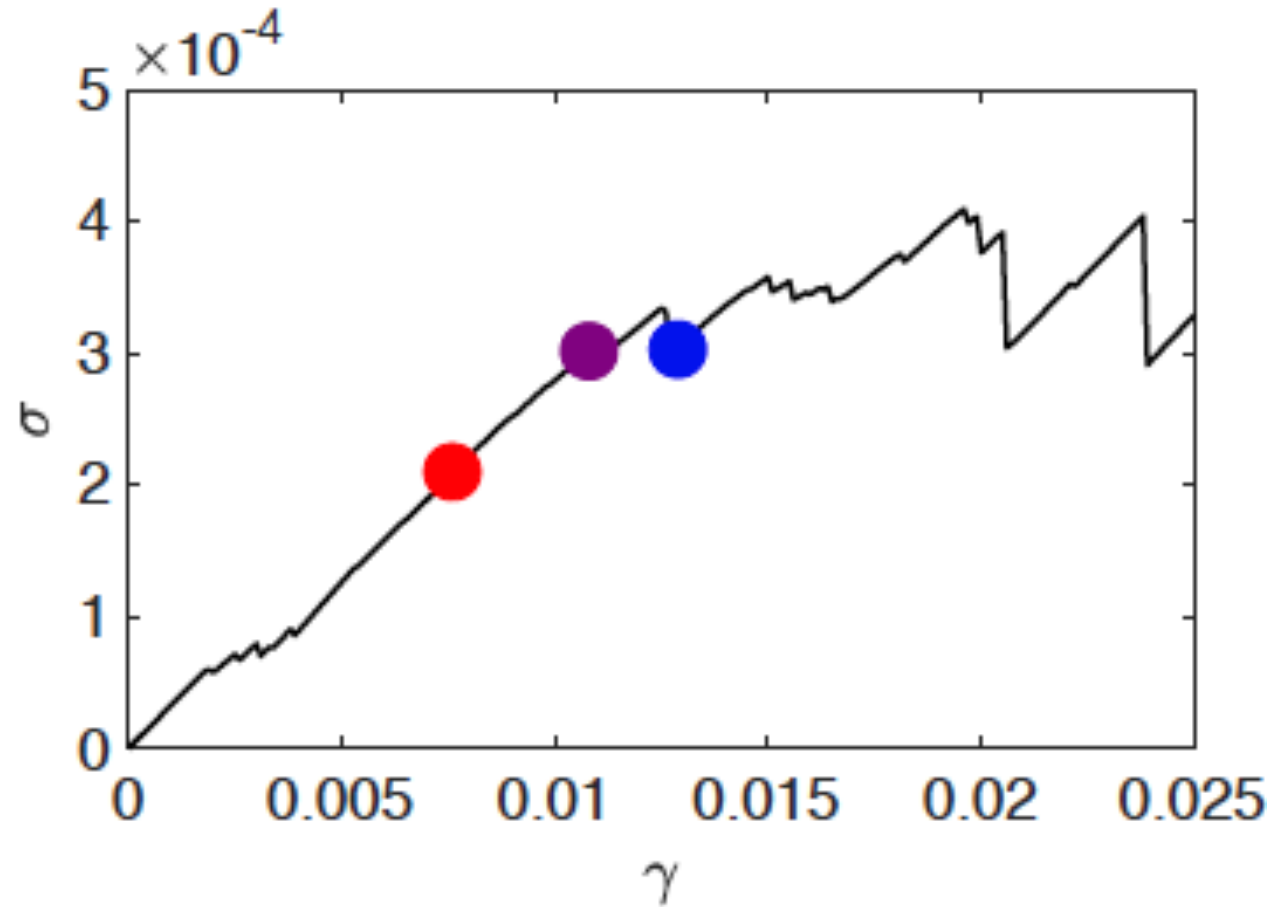
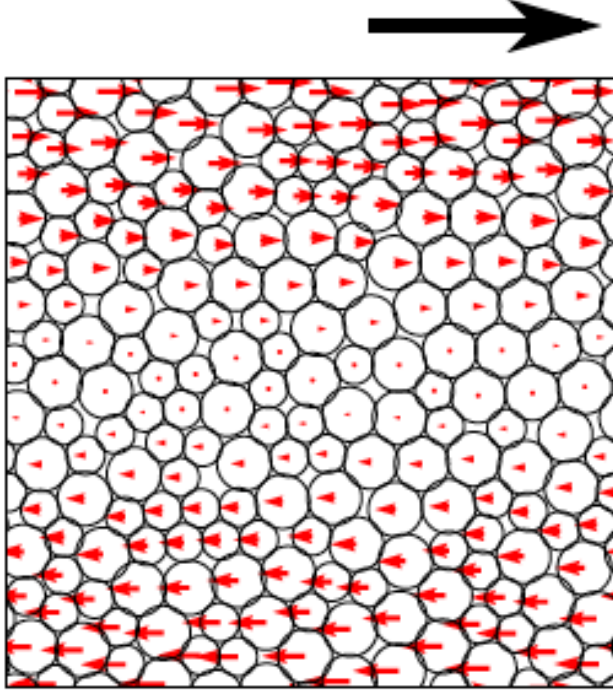
Though perhaps still not well understood.

Plastic rearrangements and avalanches are well-studied in three regimes:



c.f. talk by Kirsten
Martens yesterday

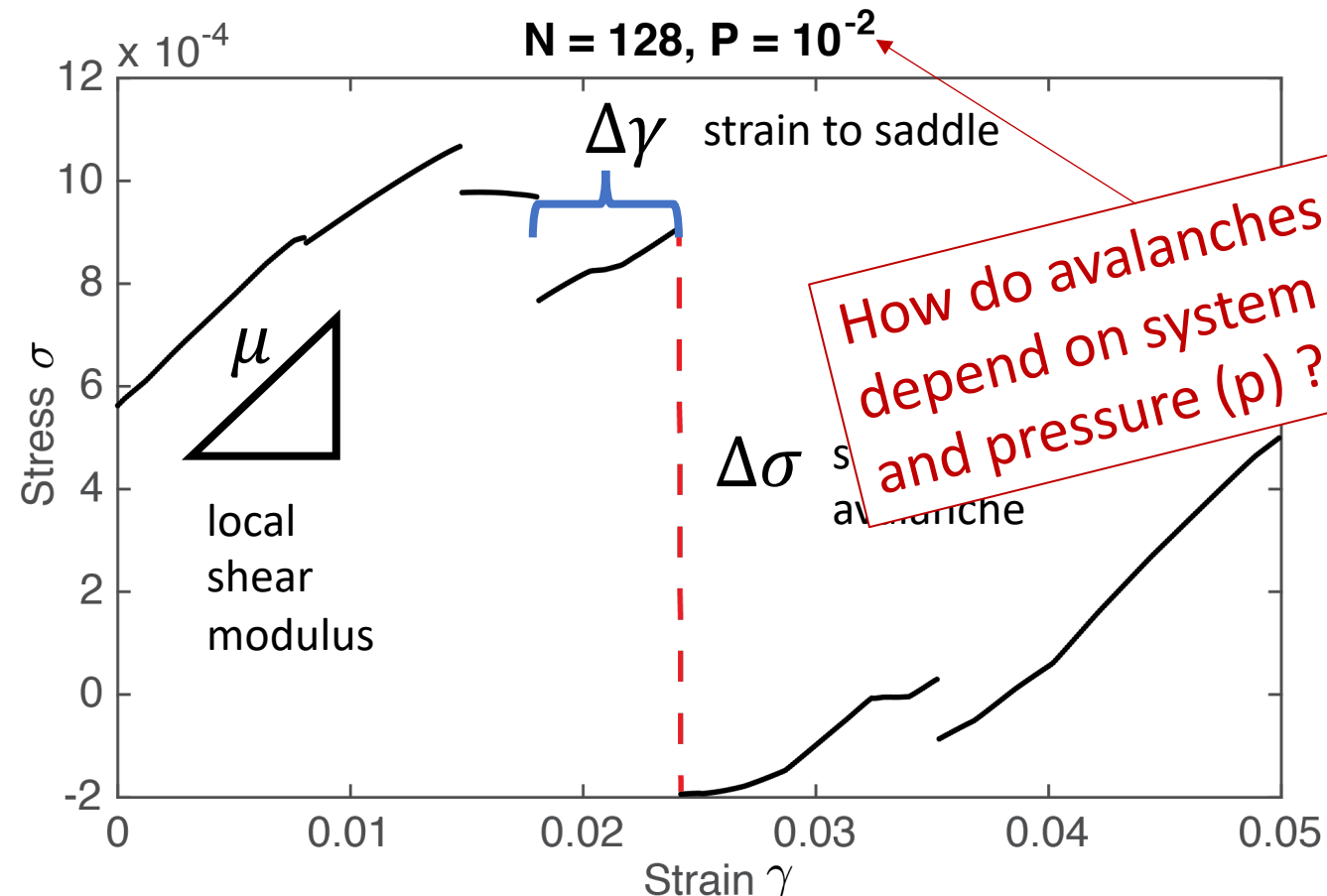
Athermal, Quasistatic Shear (AQS)



Quantifying linear response and avalanches in the **pre-yielding** regime

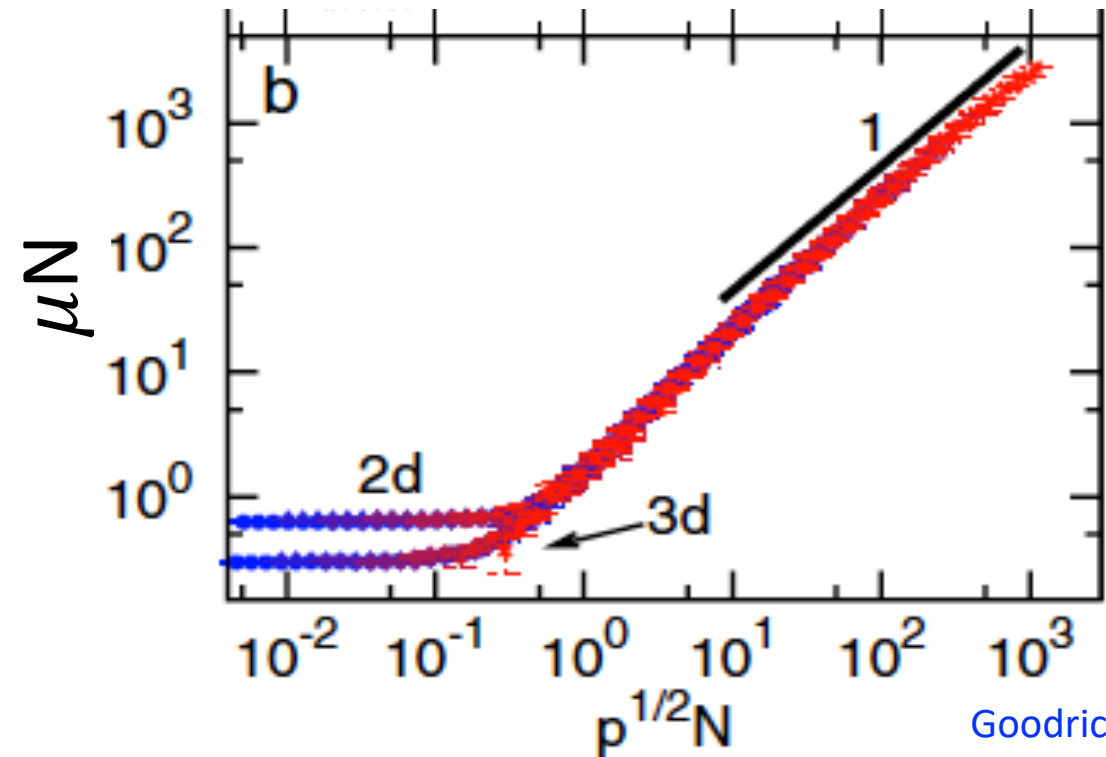
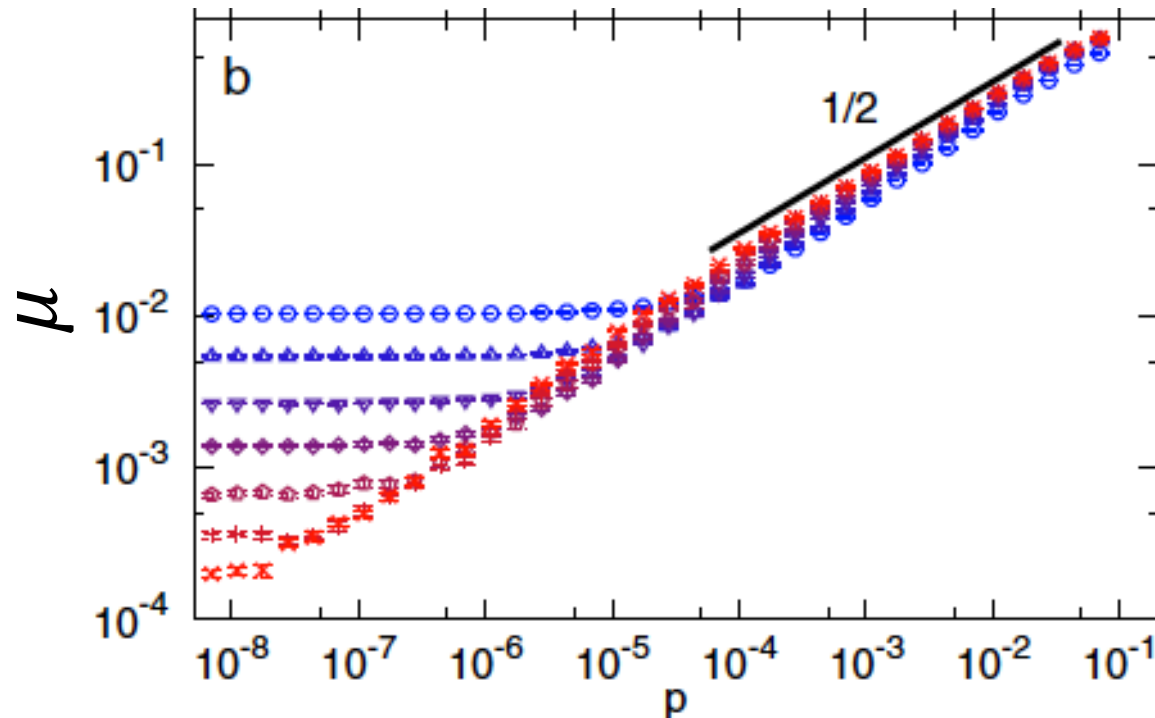


Peter Morse



Shear modulus

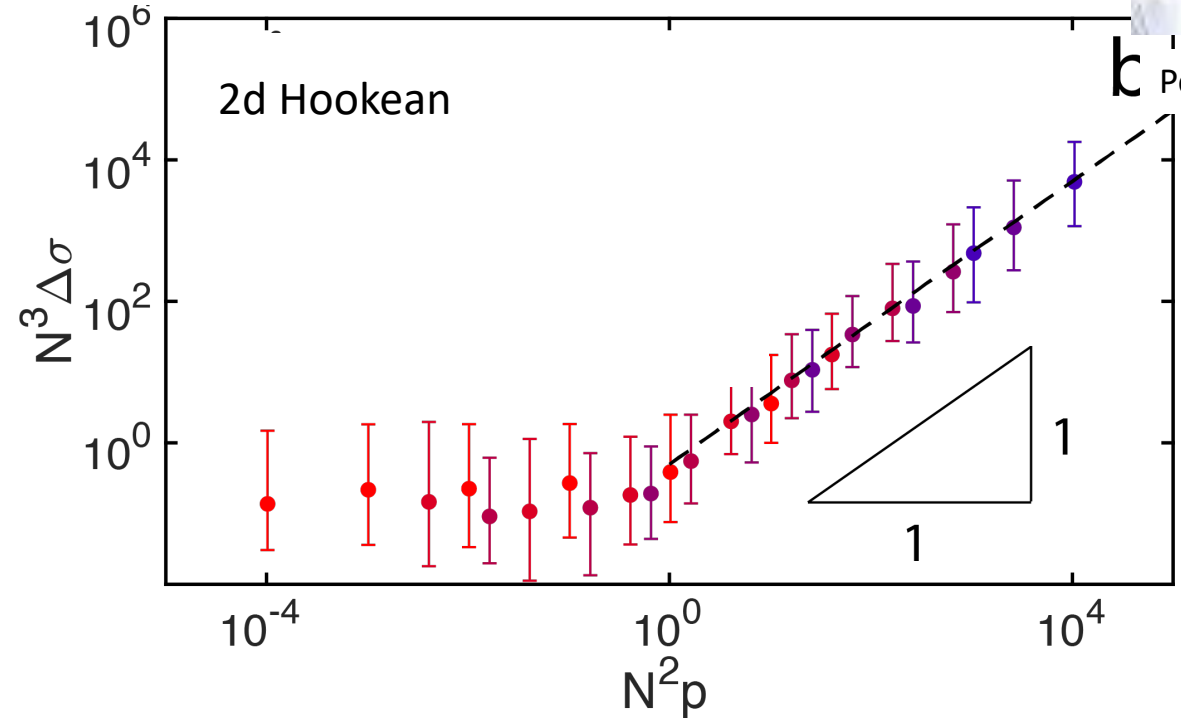
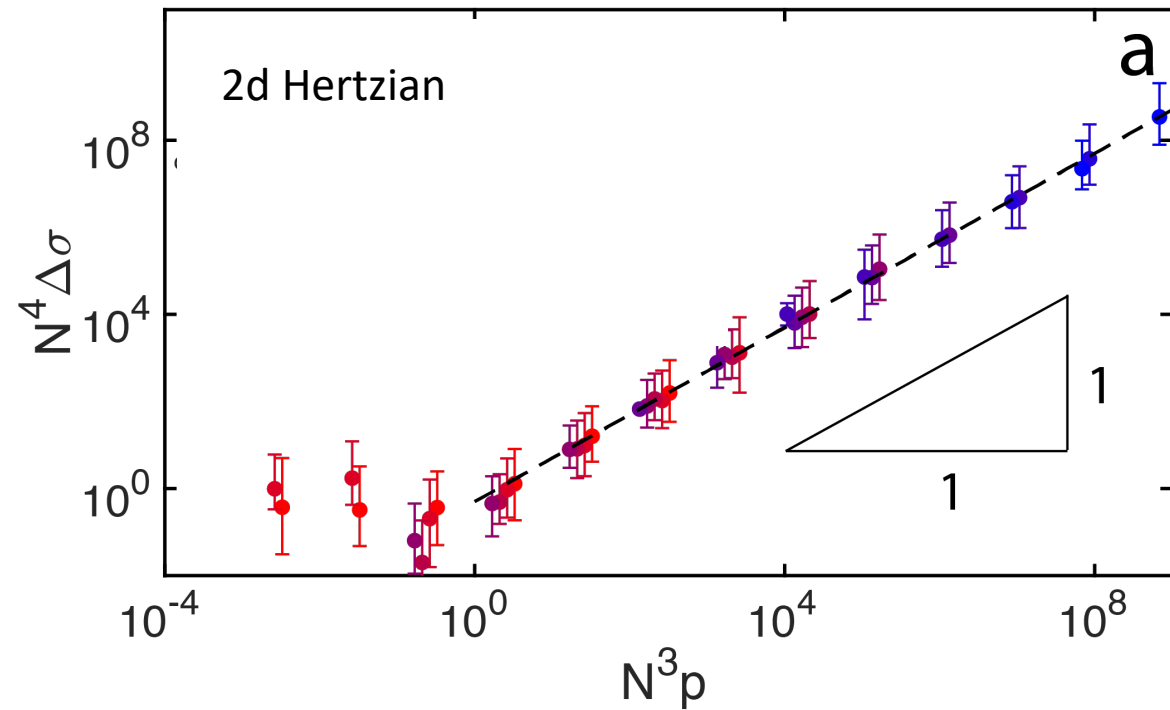
- Calculated directly from dynamical matrix (curvatures of landscape)
- Observe finite-size scaling: $\mu = N^y F(p^\eta N)$, $y = -1$; $\eta = 1/2$
- Isostatic system is singular in linear response, while at any finite pressure the system is analytic around $p \rightarrow 0^+$ (hard sphere limit)



Nonlinear stress drops show same finite-size scaling as shear modulus(!)



Peter Morse

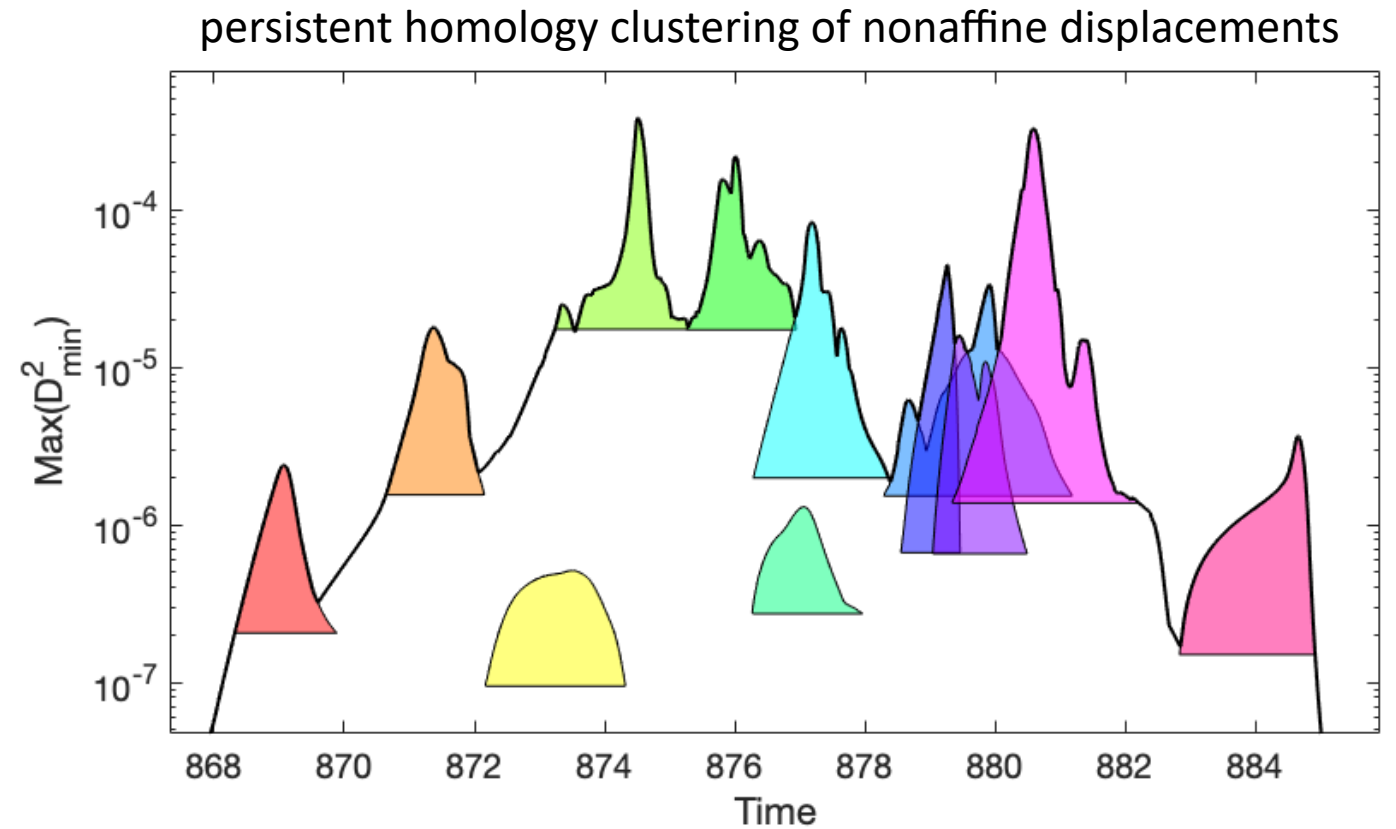
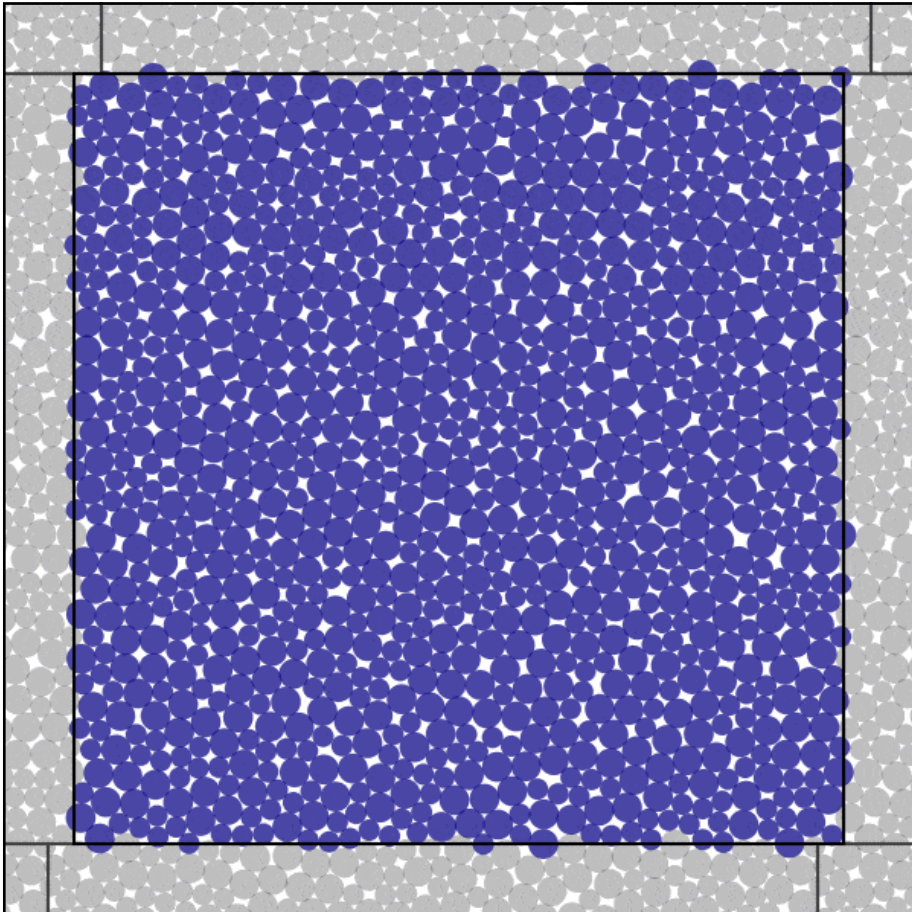


- Extend scaling argument: $z - z_{iso} = N^\gamma W(N^\beta p)$; $\beta = 2(\alpha - 1)$
 - $\alpha=5/2$ for Hertzian and $\alpha=2$ for Hookean [O'Hern PRL 2002](#), [Goodrich PRL 2012](#)
- For systems in the high N and p regime: $\langle \Delta\sigma \rangle \sim \frac{p}{N}$

Stress drops associated with bursts of localized deformation

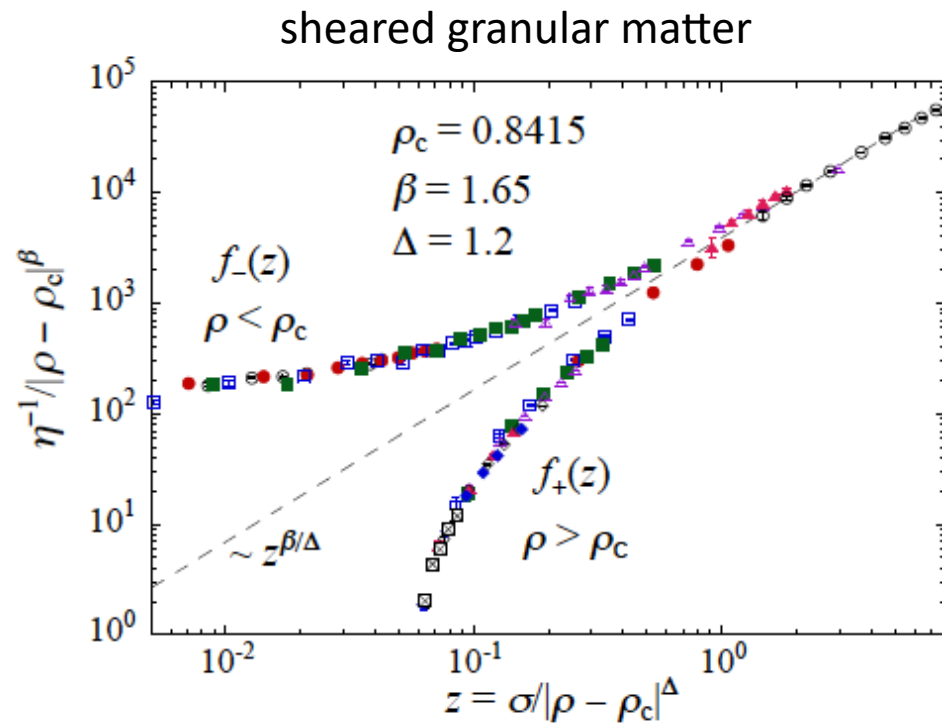


Ethan Stanifer

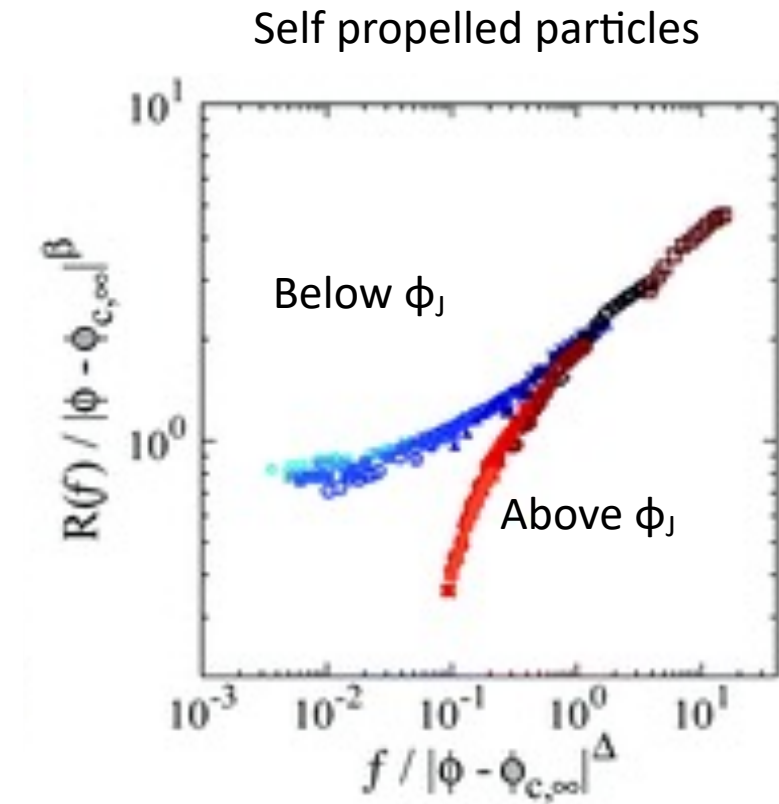


What happens in active matter?

Lots of suggestive results at finite rates of driving

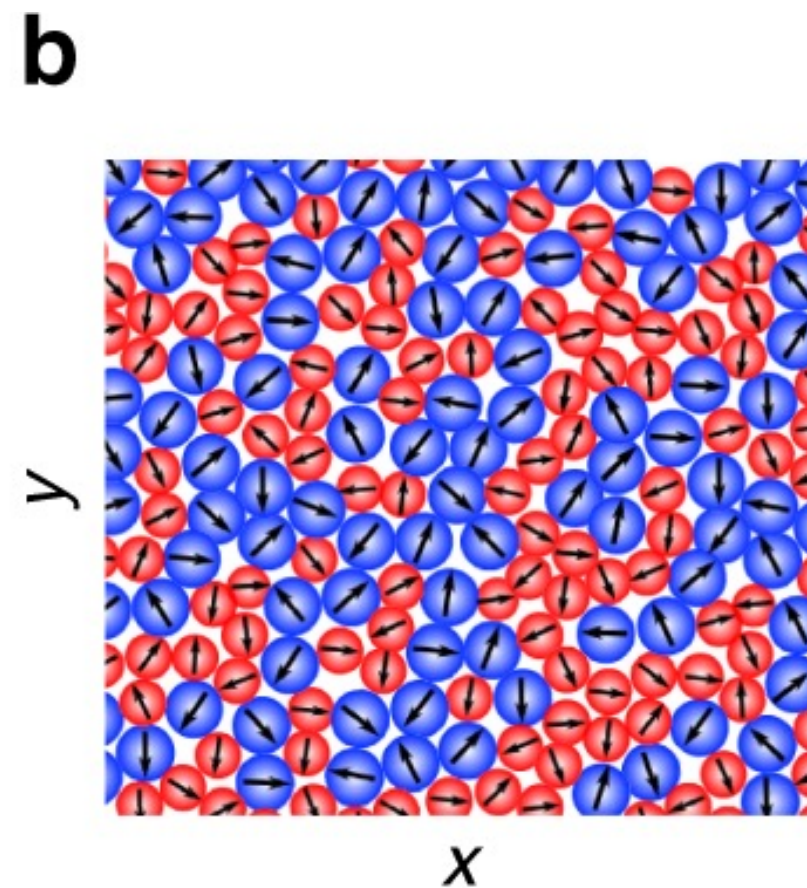
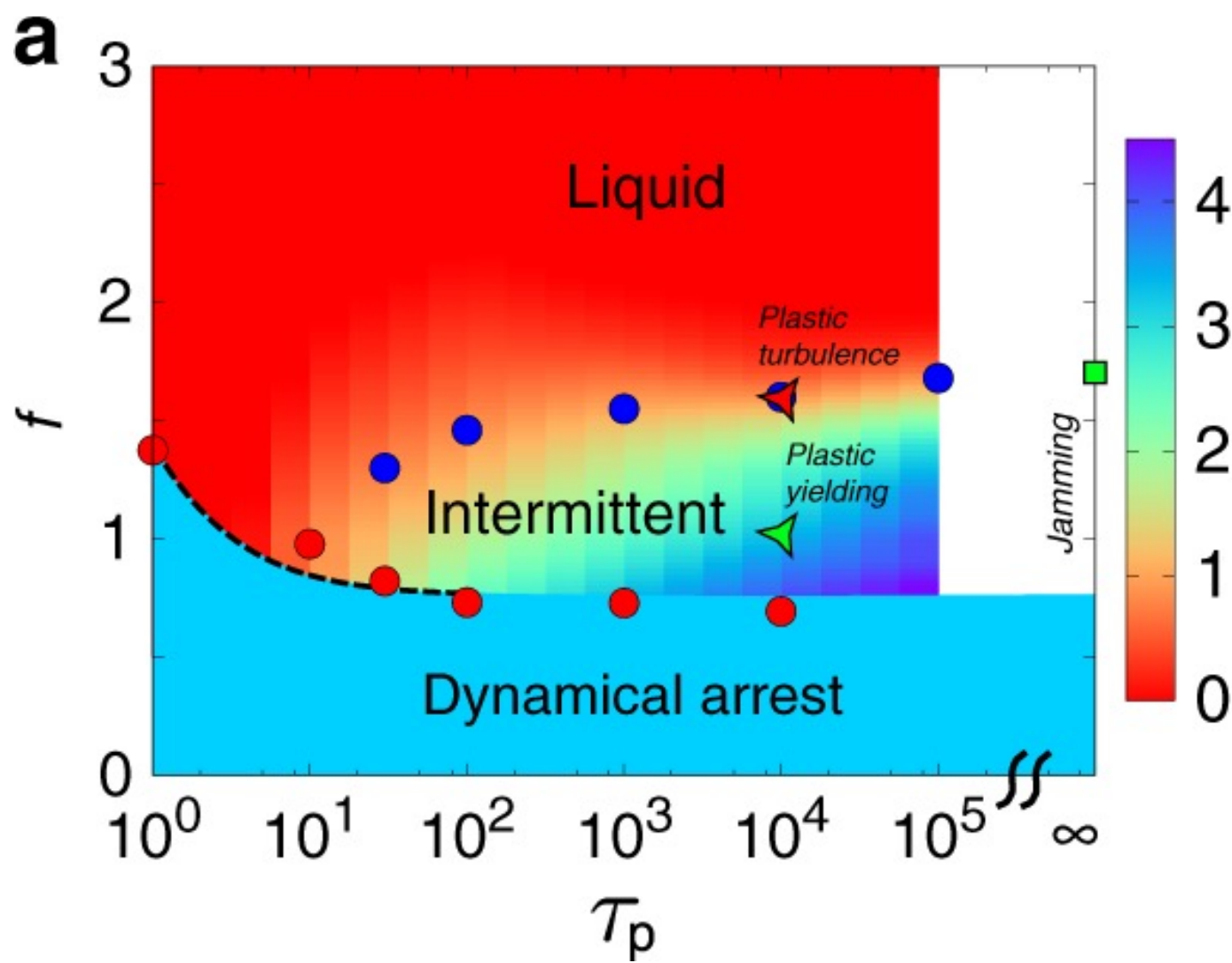


Olsson, Teitel, PRL (2007)



Liao, Xu, Soft Matter (2018)

dynamics share some features with fluids, some with solids (c.f. fluid turbulence talks last week)



What happens in active matter?

Lots of suggestive results at finite rates of driving

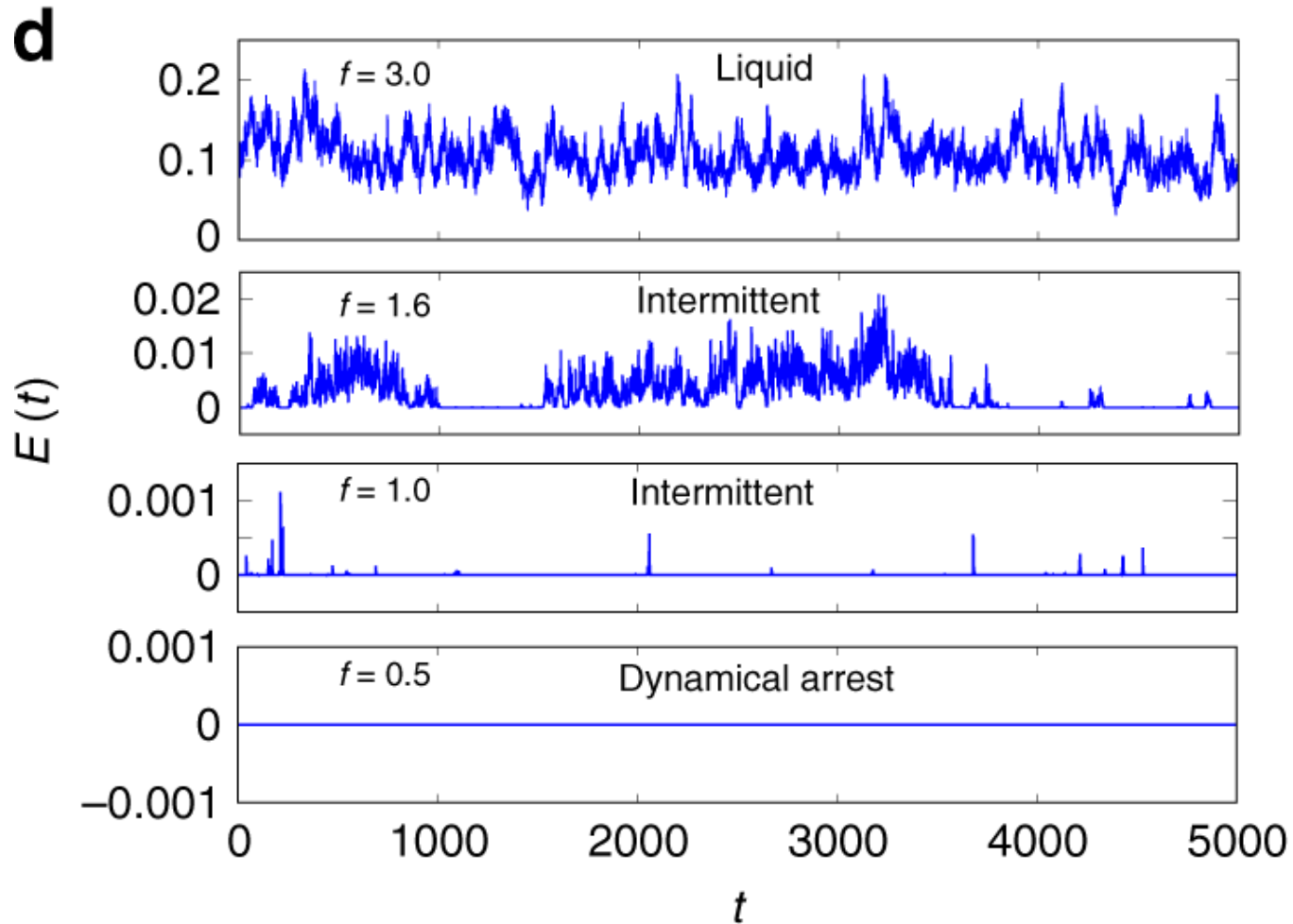
Plus additional work by:

Nandi and Gov (Nandi EPJE 2018, 2019)

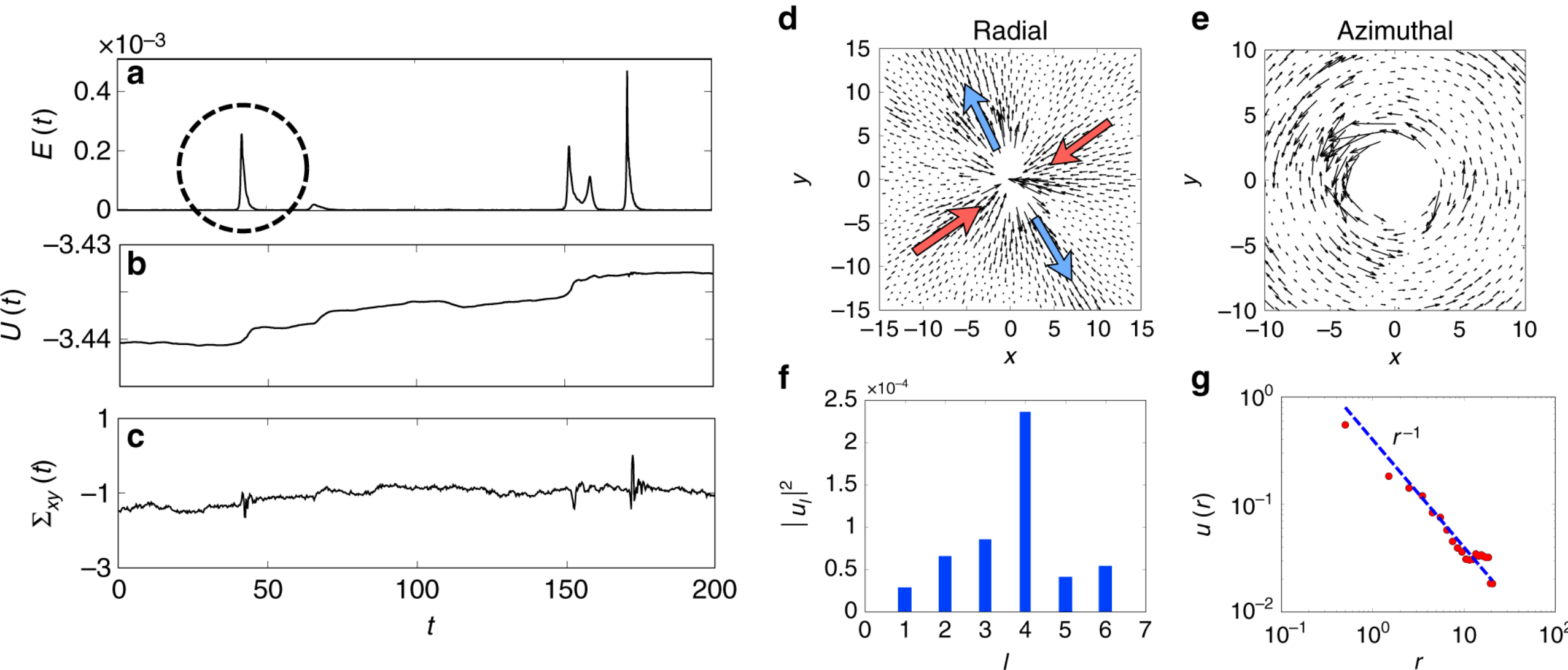
Mandal and Sollich (arXiv:1911.04558, 2020)

Silke Henkes and co-workers (Nature Communications, 2020)

At low forces and large persistence times, dynamics becomes highly intermittent



Intermittency driven by local plastic rearrangements



What happens in active matter?

Let's try to first look at the analogous limit to AQS:

zero temperature, in the limit that driving is infinitely persistent and
infinitely slow

focus on initial response (pre-yielding regime)



Peter Morse



Sudeshna Roy



Elisabeth
Agoritsas

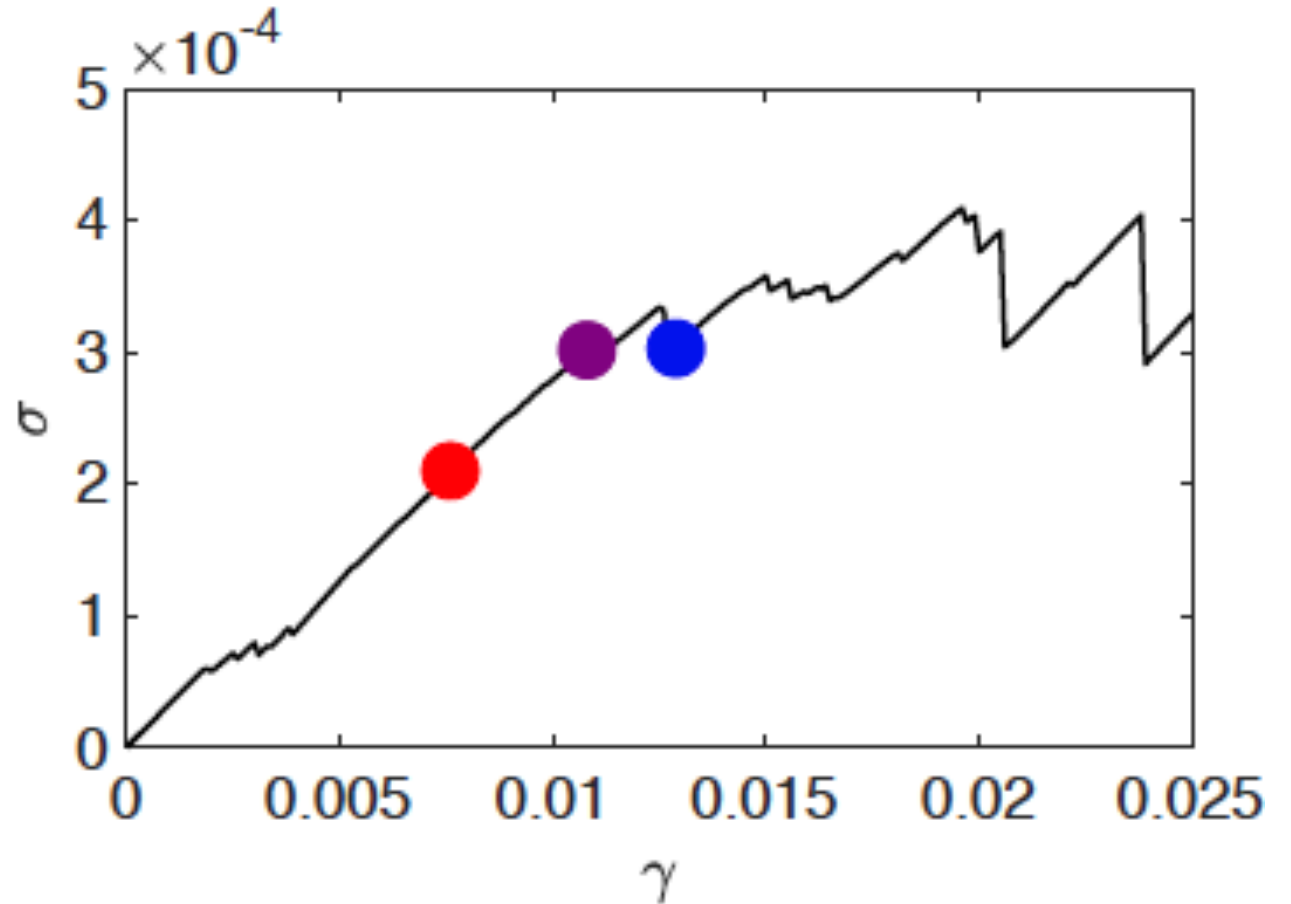
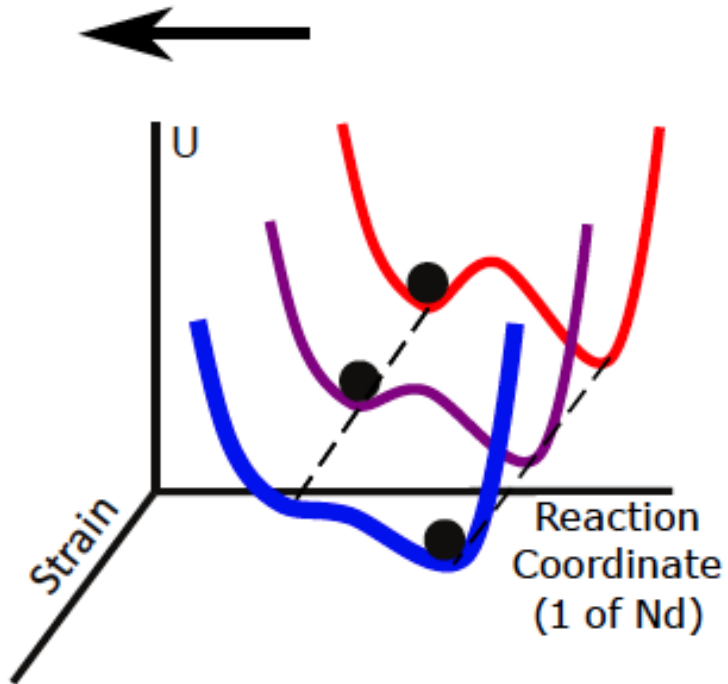
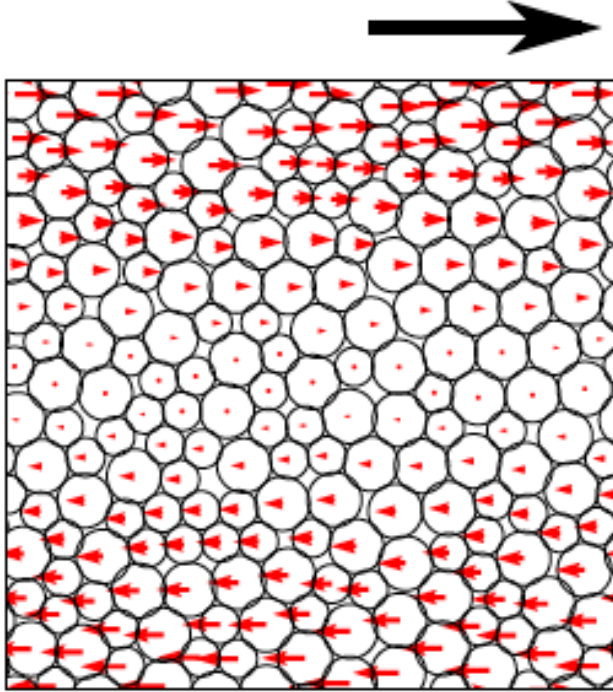


Ethan Stanifer

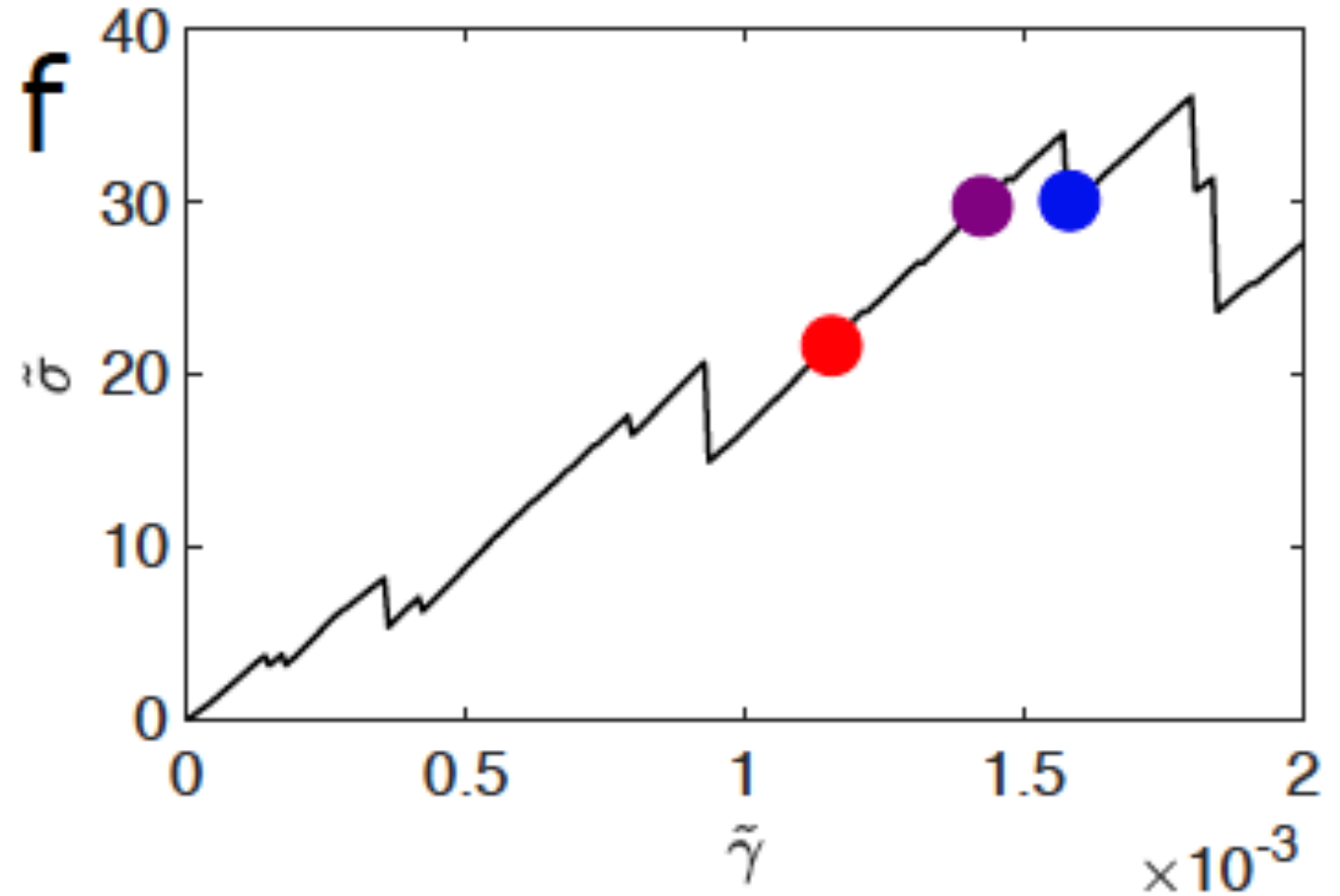
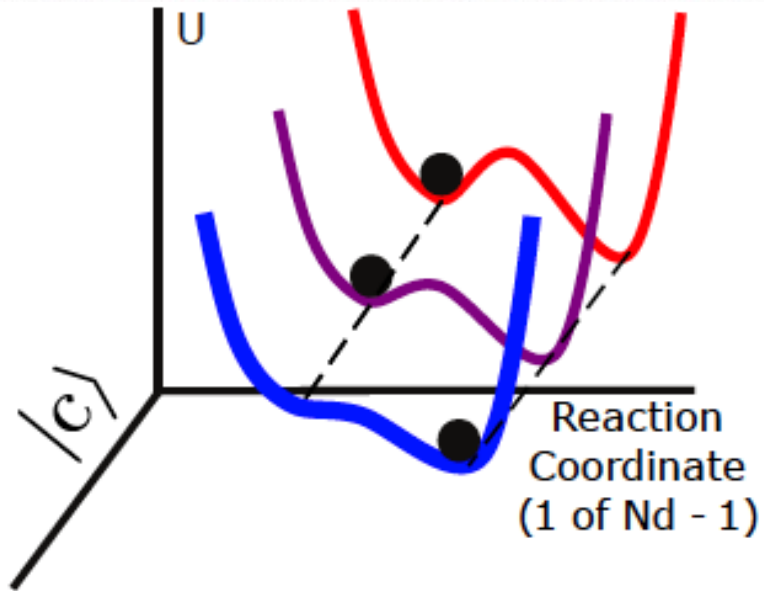
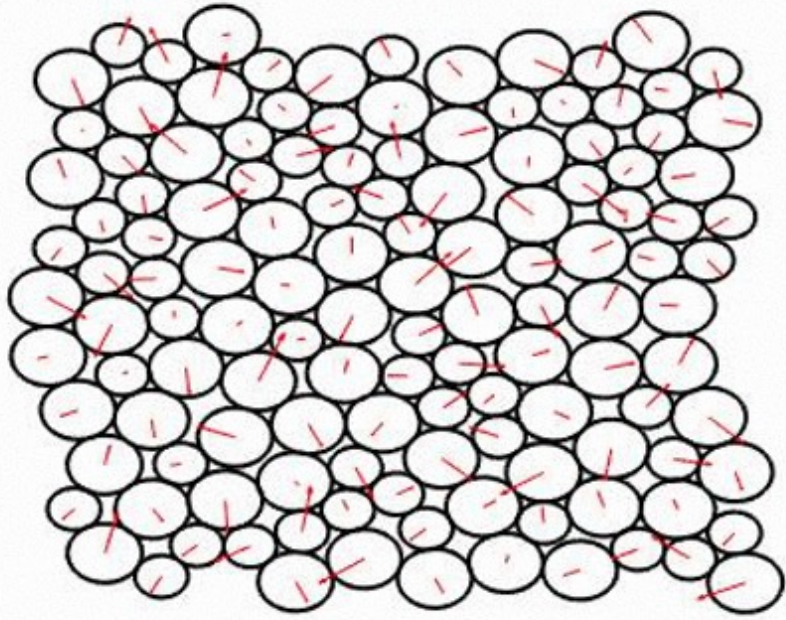


Eric Corwin

Recall: Athermal, Quasistatic Shear (AQS)



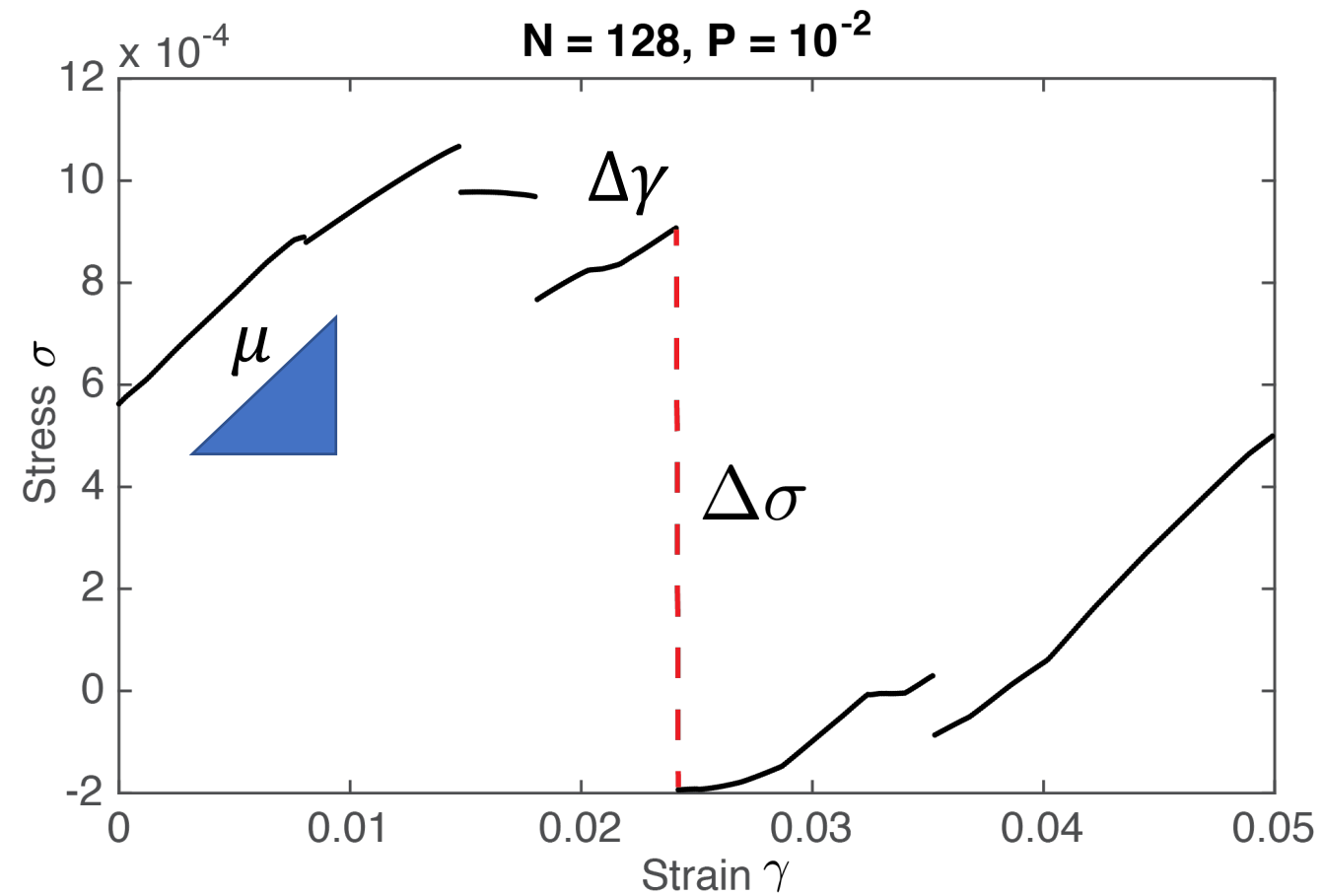
Athermal, Quasistatic Random Displacement (AQRD)



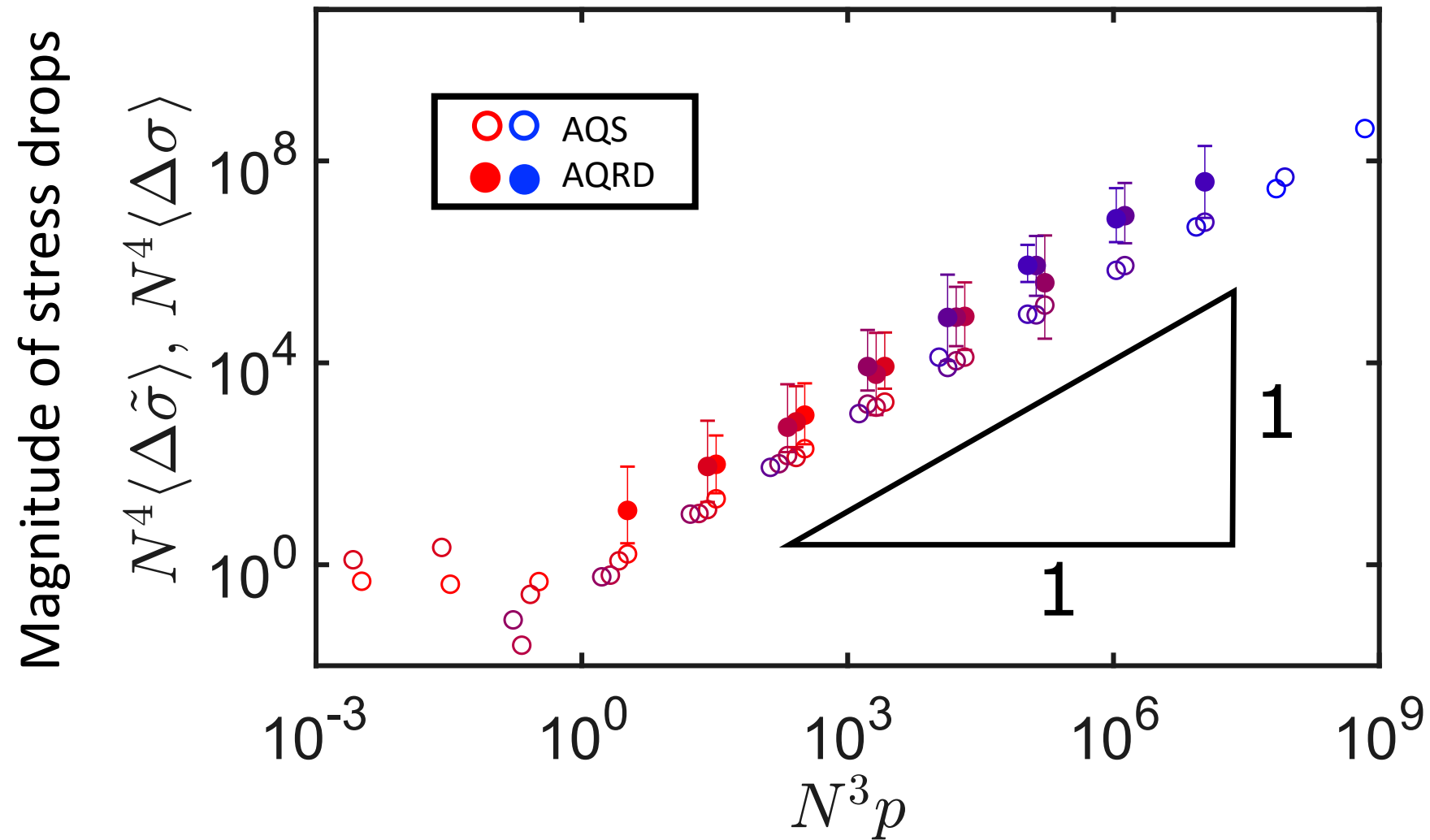
Fix the displacement (fixed strain experiment), not the force (creep experiment)

Morse et al, PNAS, 2021

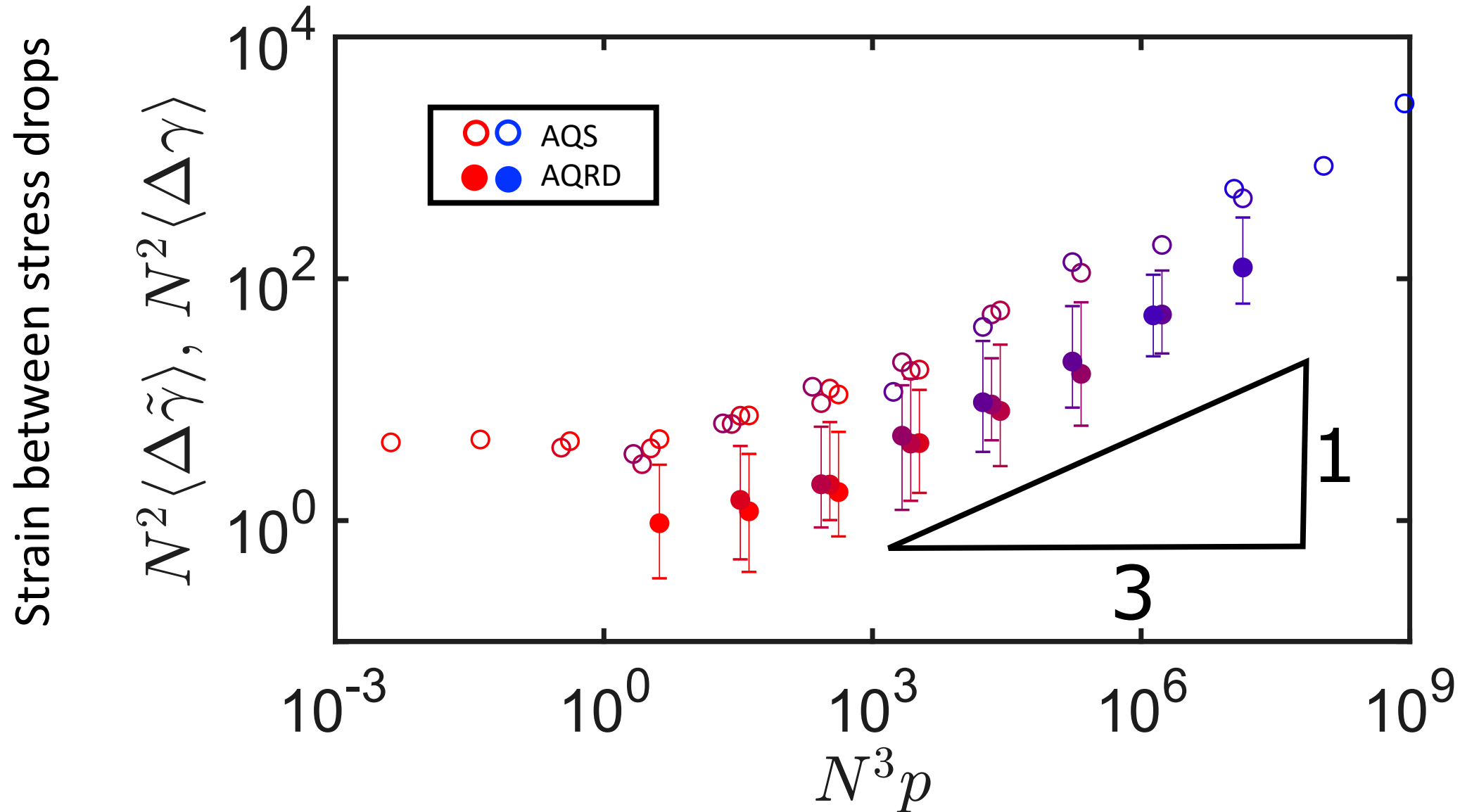
Recall: linear, nonlinear response



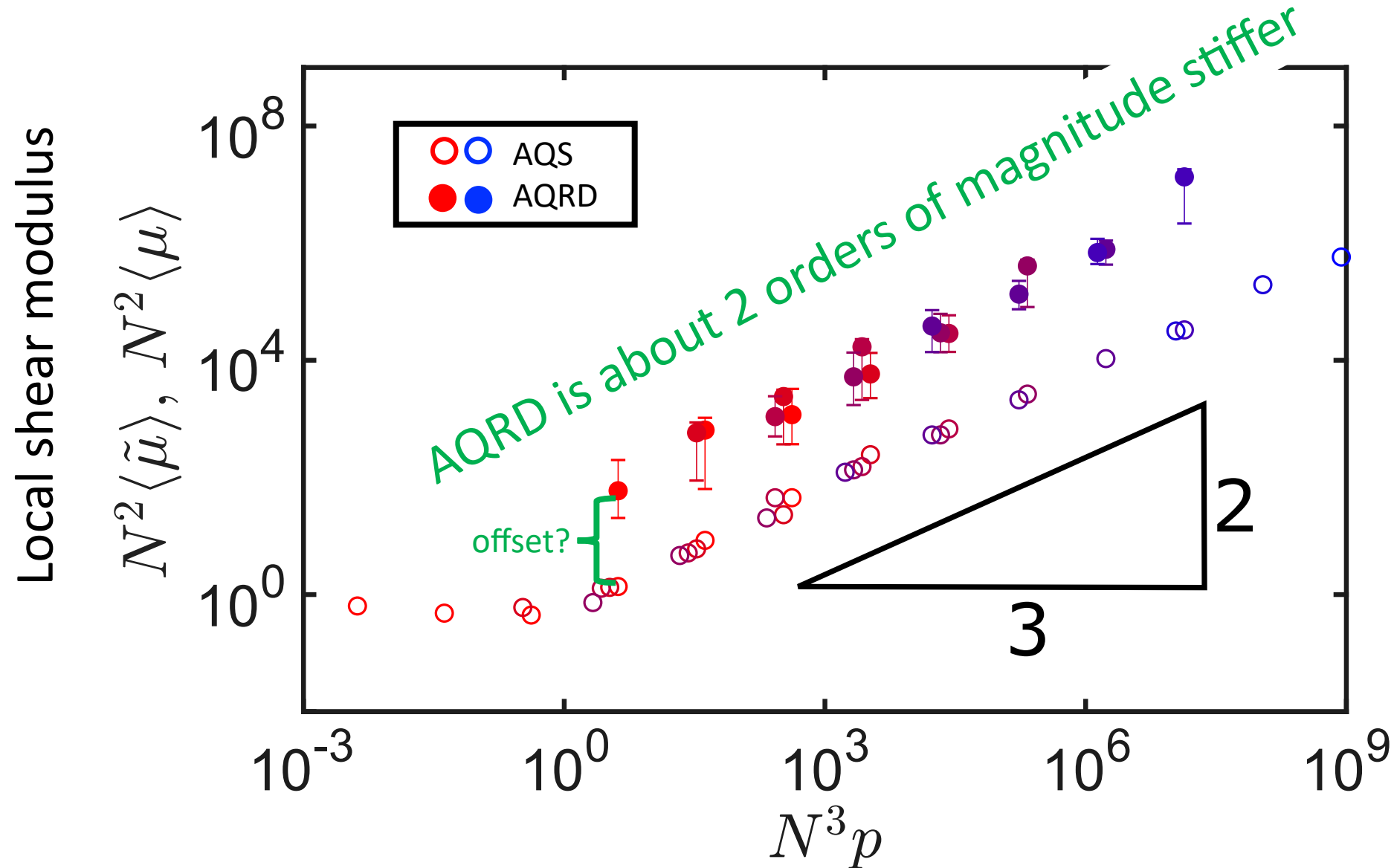
AQRD and AQS exhibit exactly the same scaling with N,p



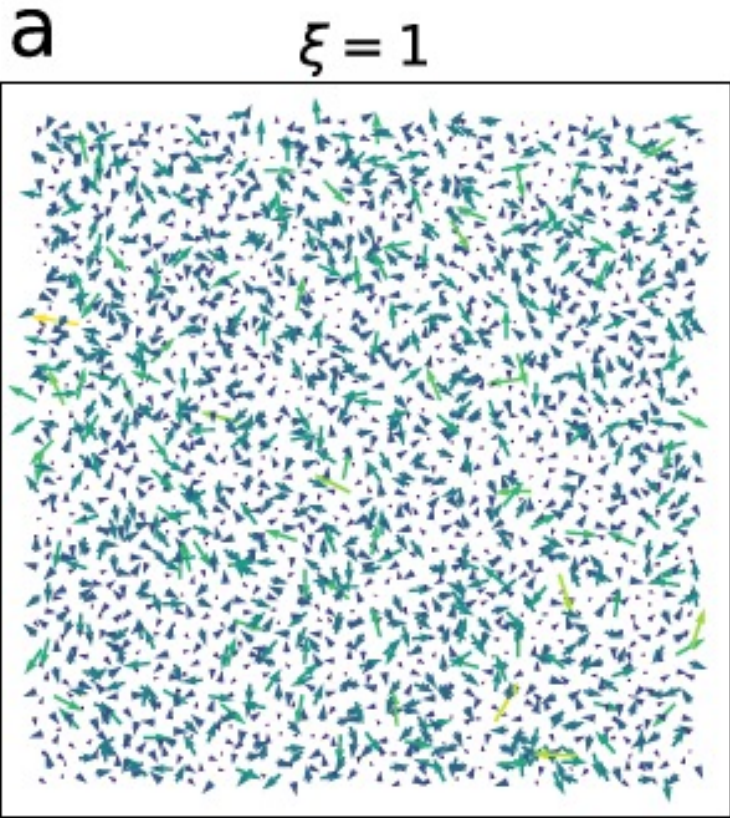
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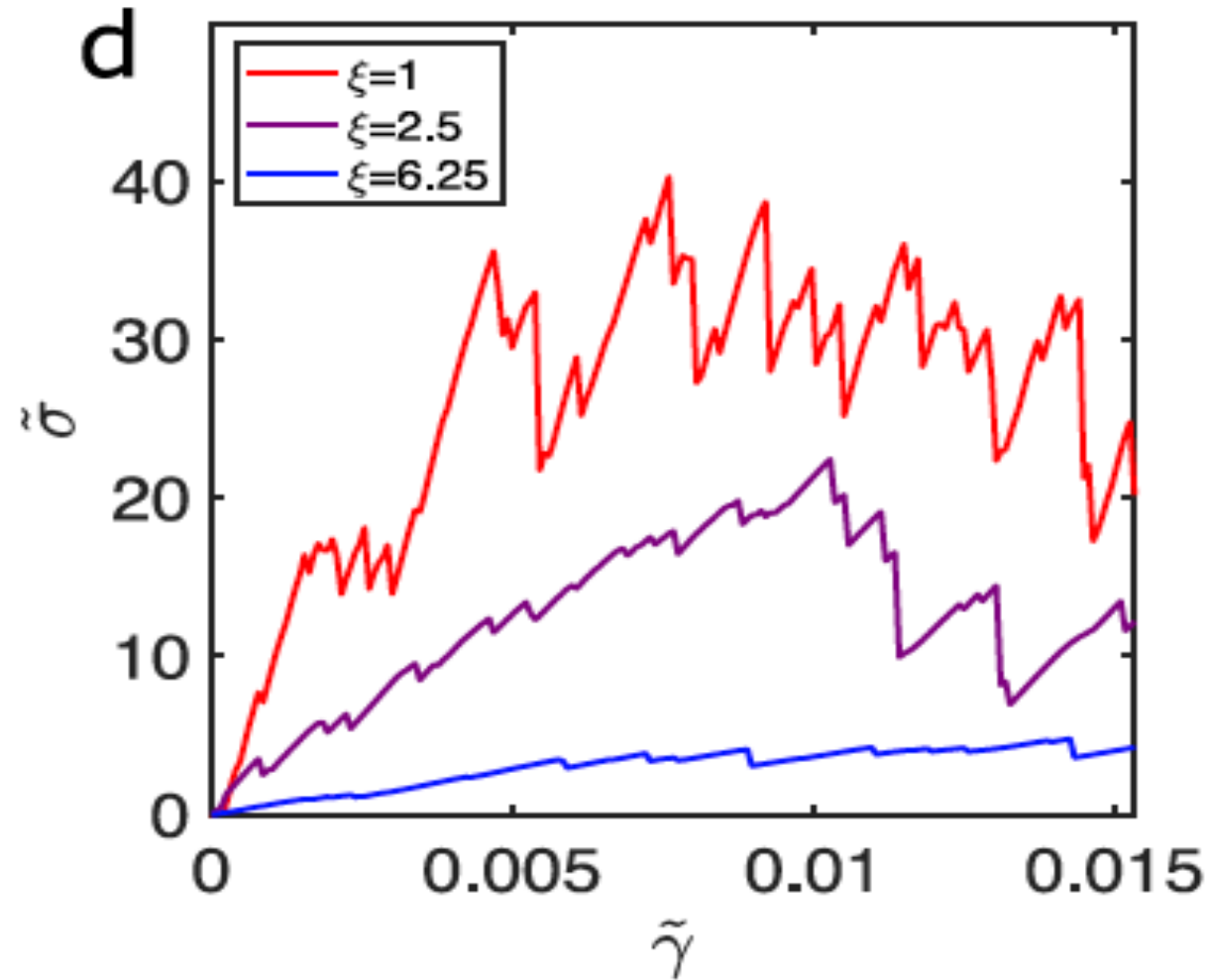
AQRD and AQS exhibit exactly the same scaling with N,p



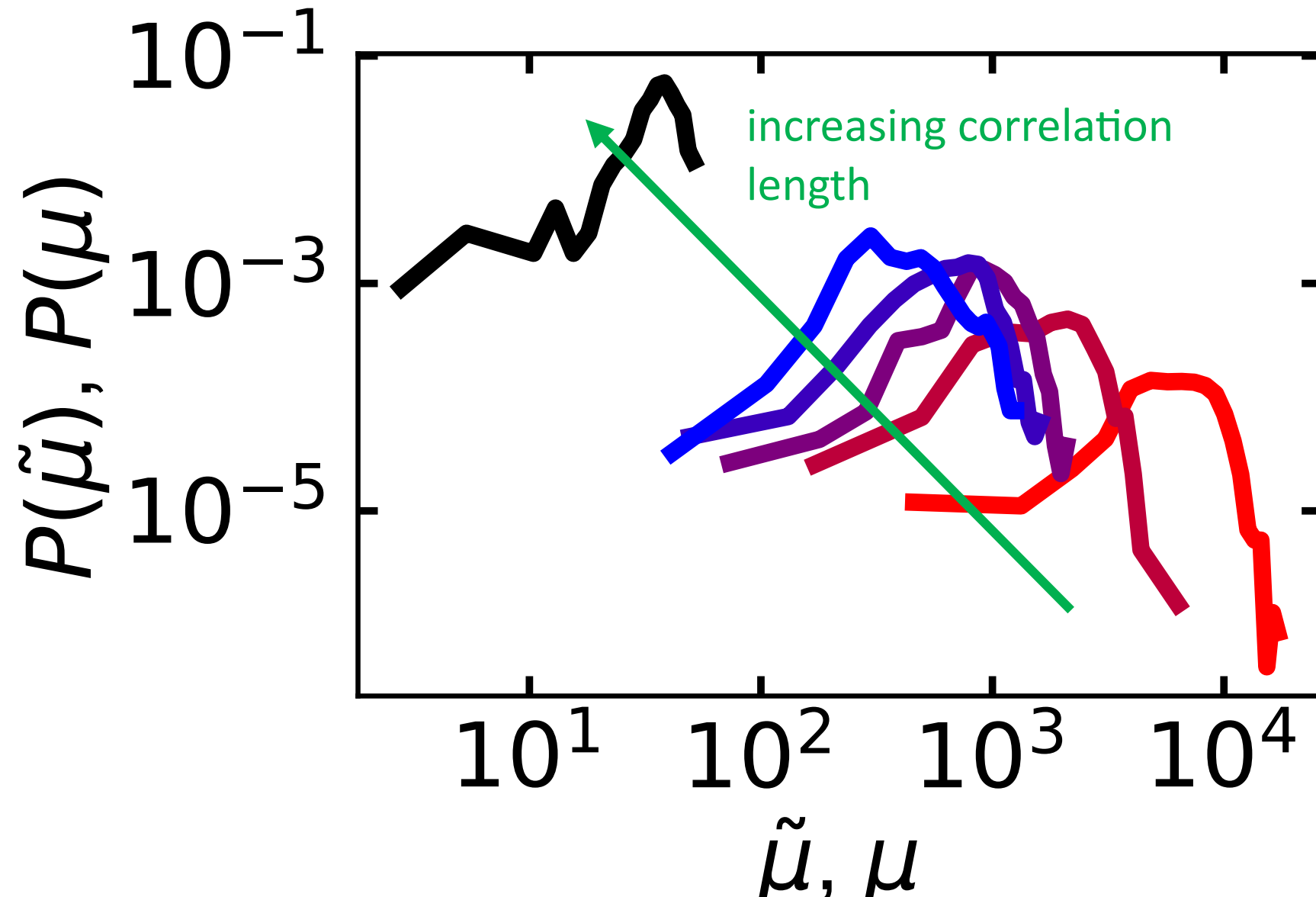
Random Gaussian displacement fields



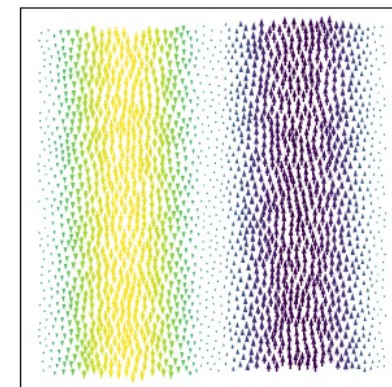
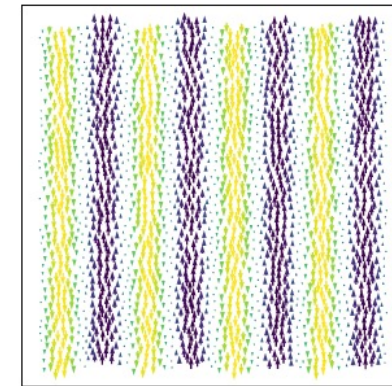
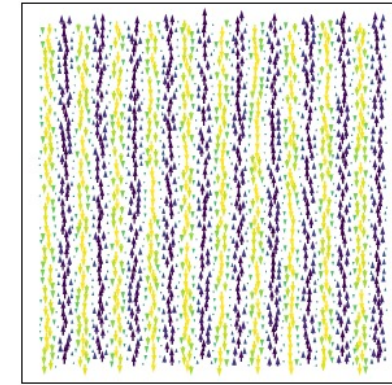
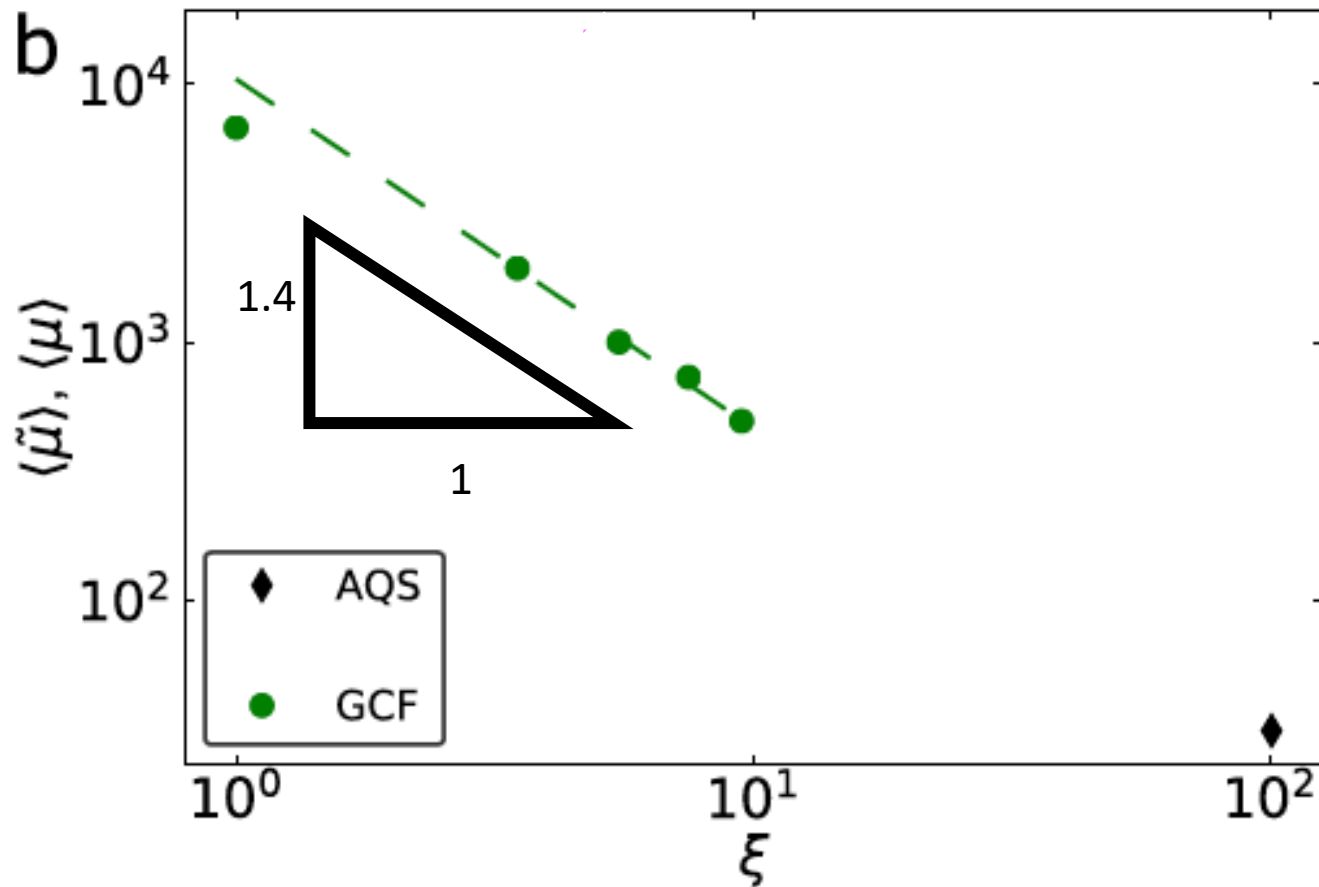
Stiffness changes with correlation length



Stiffness changes with correlation length



The shear modulus appears to be a power law function of the correlation length



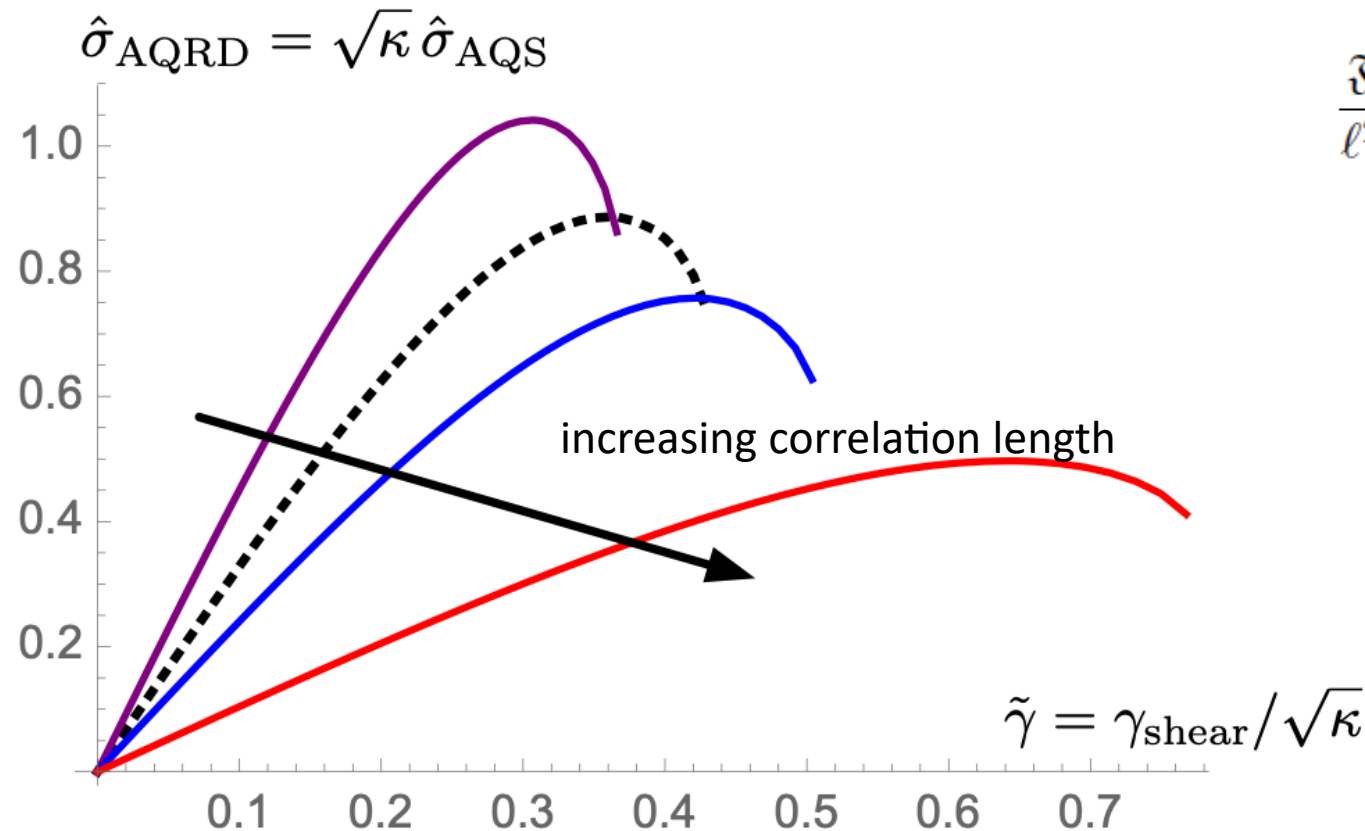
Why?

I will work a tiny bit of this out on the board: prediction for infinite-dimensional solution for AQRD dynamics



Elisabeth Agoritsas

$$\kappa \equiv \frac{\mu_{\text{AQRD}}}{\mu_{\text{AQS}}} = \frac{\mathfrak{F}}{\ell^2}, \quad \gamma_{\text{shear}} = \tilde{\gamma} \sqrt{\kappa}, \quad \sigma_{\text{AQS}} = \sigma_{\text{AQRD}}(\tilde{\gamma}) / \sqrt{\kappa}.$$

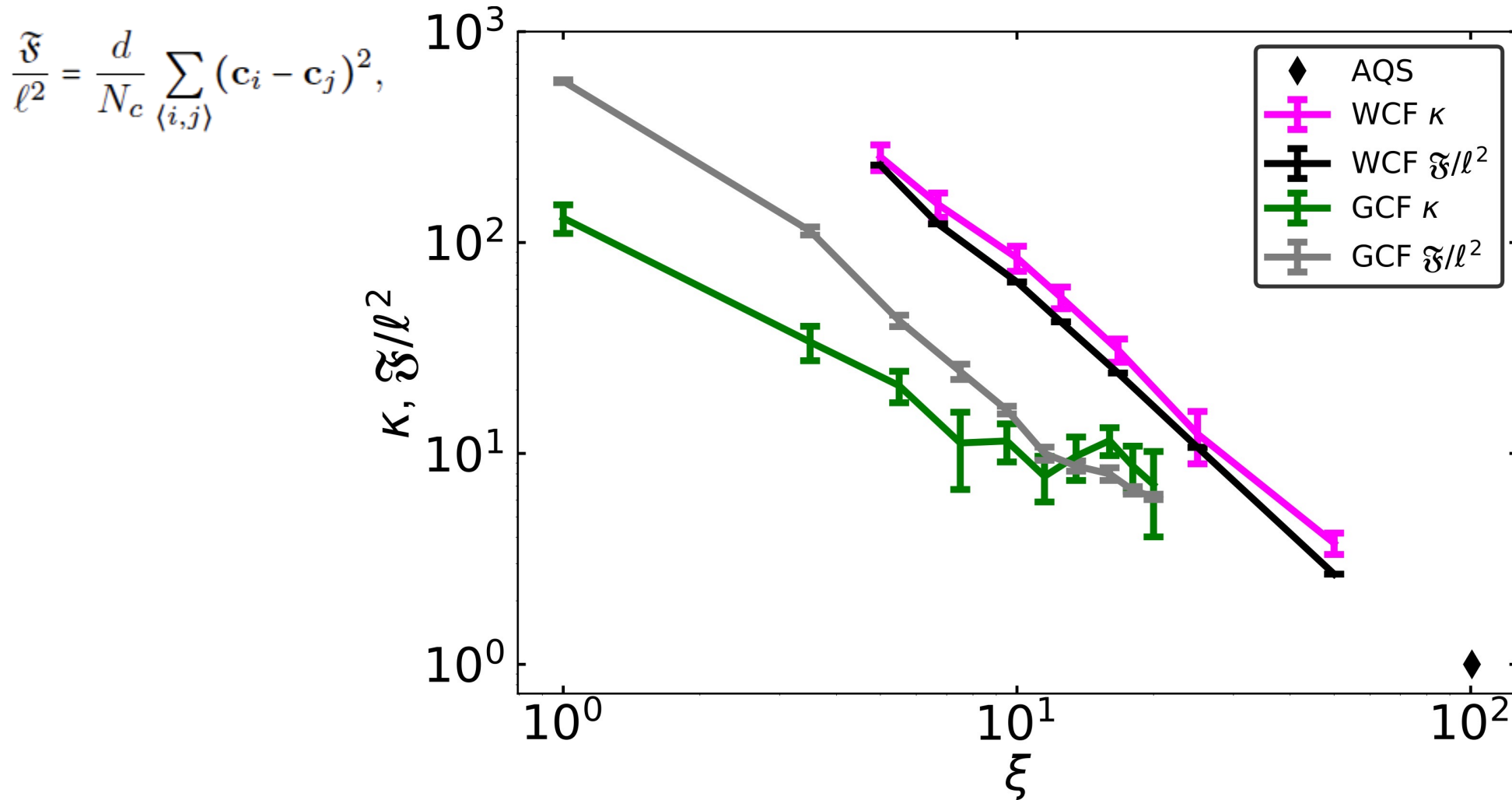


$$\frac{\mathfrak{F}}{\ell^2} = \frac{d}{N_c} \sum_{\langle i,j \rangle} (\mathbf{c}_i - \mathbf{c}_j)^2,$$

local strain induced by active displacement field $|\mathbf{c}\rangle$

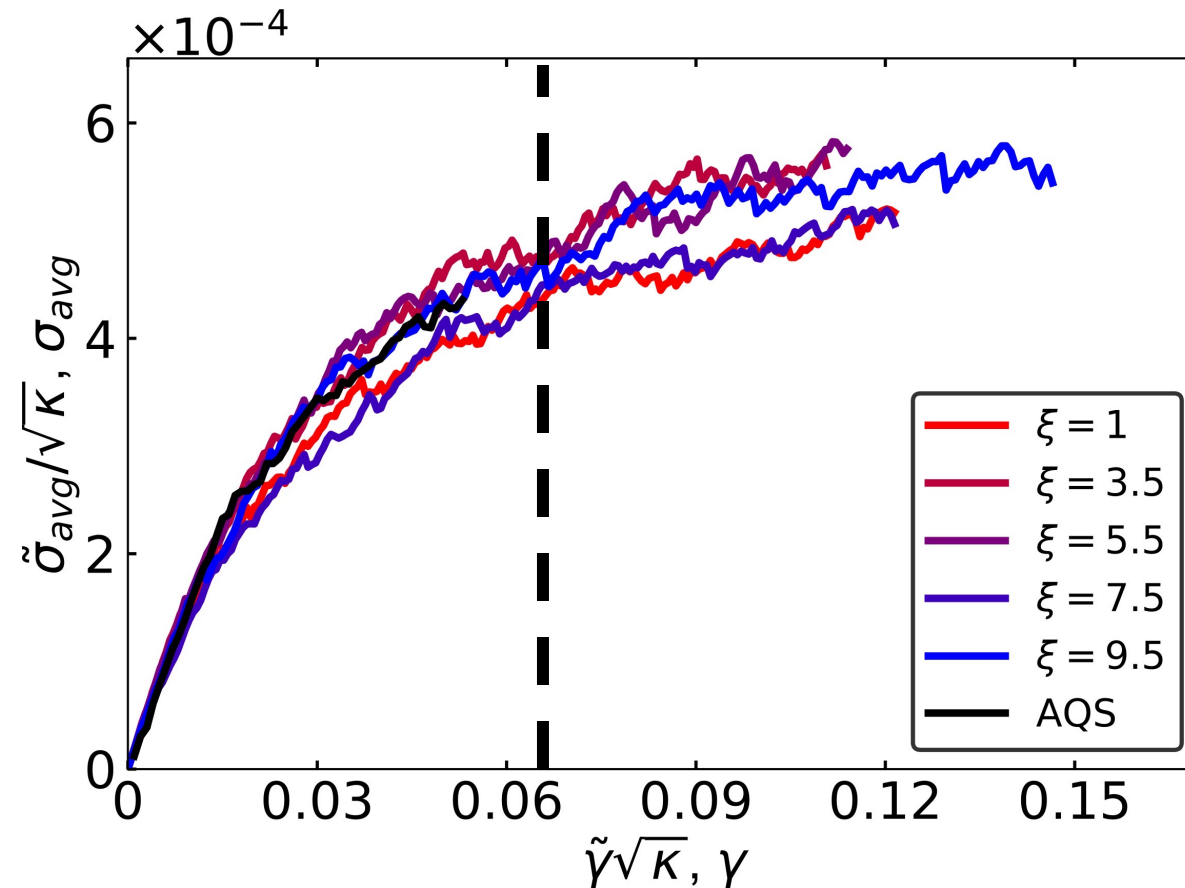
Test: calculate MF expression for $\frac{\mathfrak{F}}{\ell^2}$, compare $\kappa \equiv \frac{\mu_{\text{AQRD}}}{\mu_{\text{AQS}}}$

Neglects all higher order correlations between particles displacements in lower dimensions.



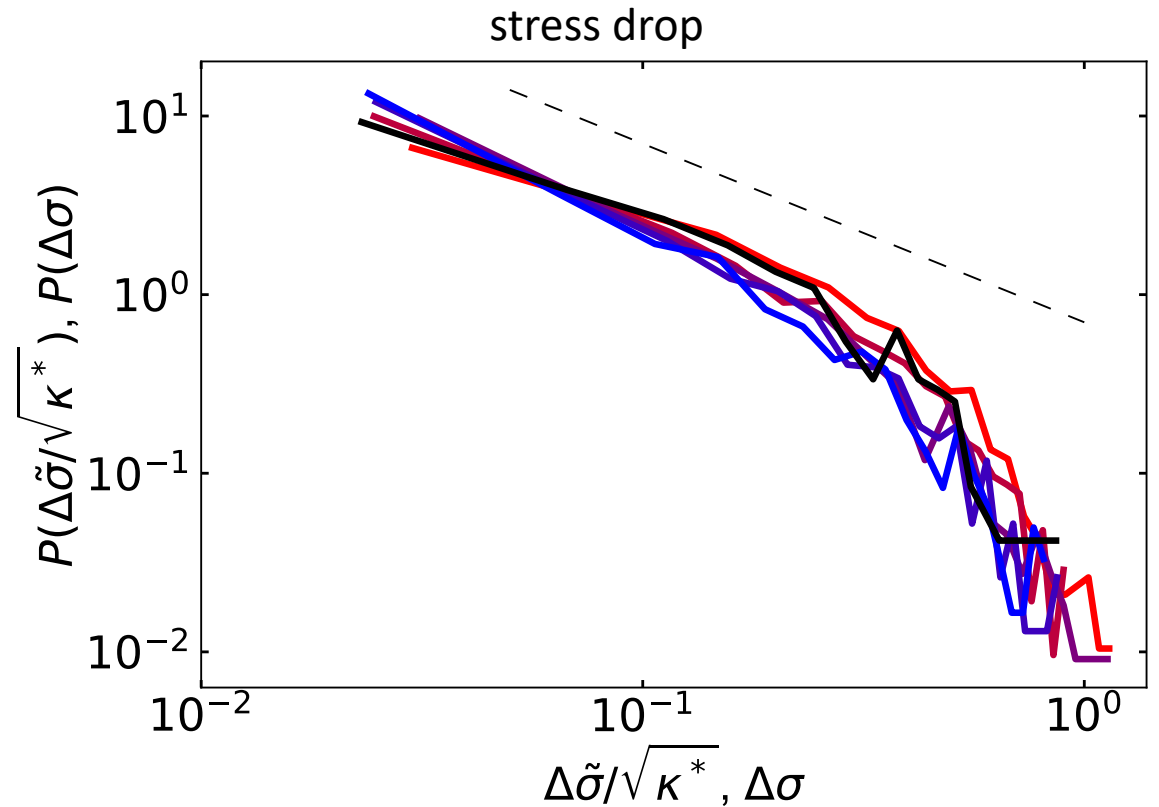
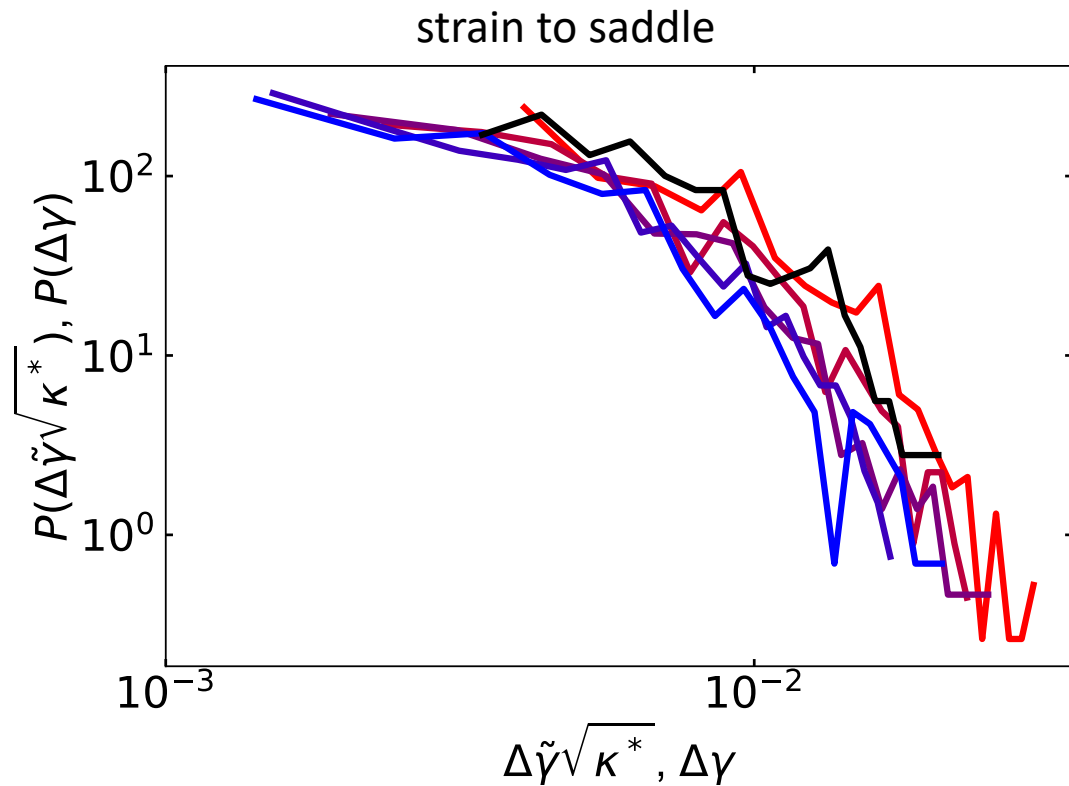
Let's treat $\kappa \equiv \frac{\mu_{\text{AQRD}}}{\mu_{\text{AQS}}}$ as the rescaling parameter in low d:

$$\gamma_{\text{shear}} = \tilde{\gamma}\sqrt{\kappa}, \quad \sigma_{\text{AQS}} = \sigma_{\text{AQRD}}(\tilde{\gamma})/\sqrt{\kappa}.$$

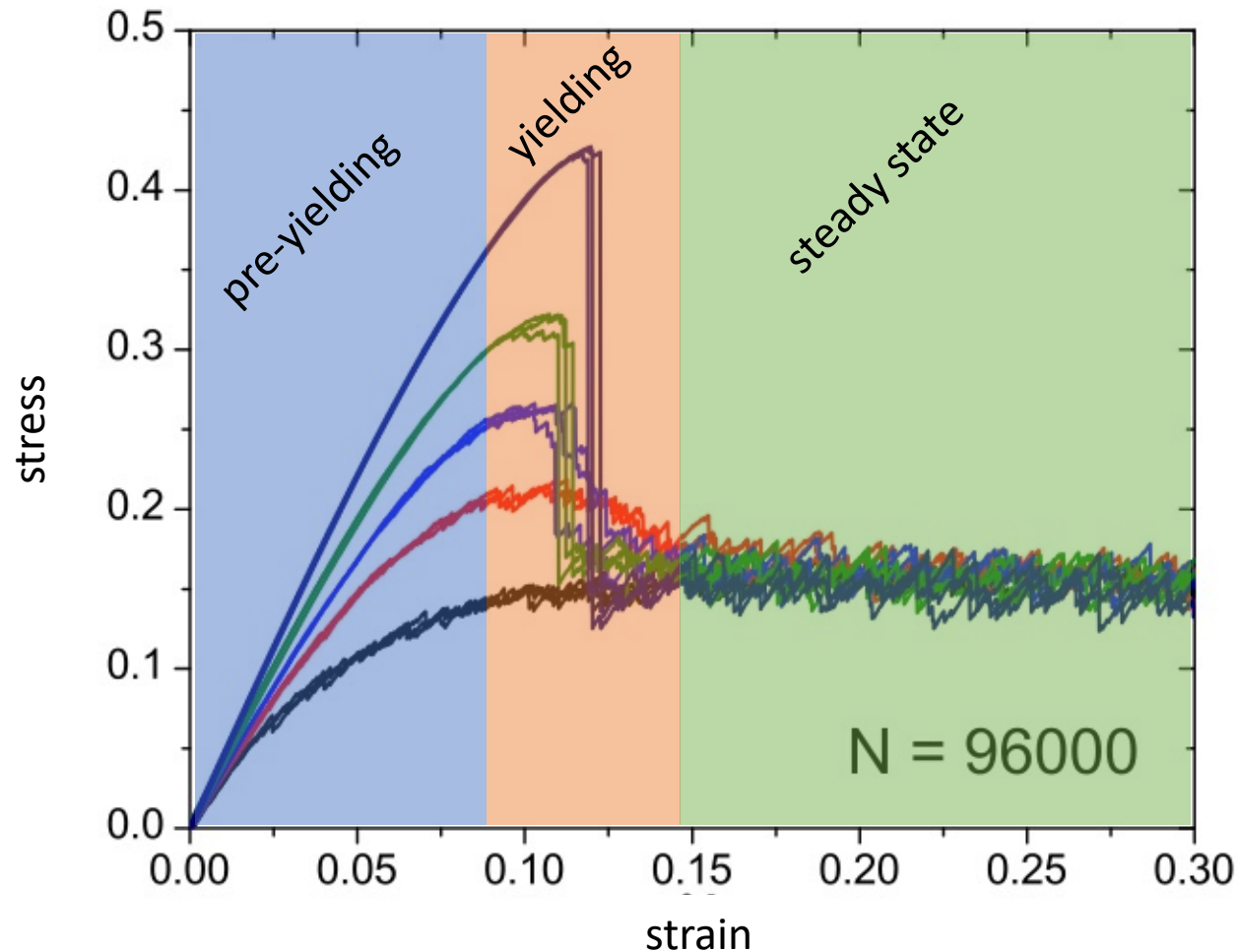


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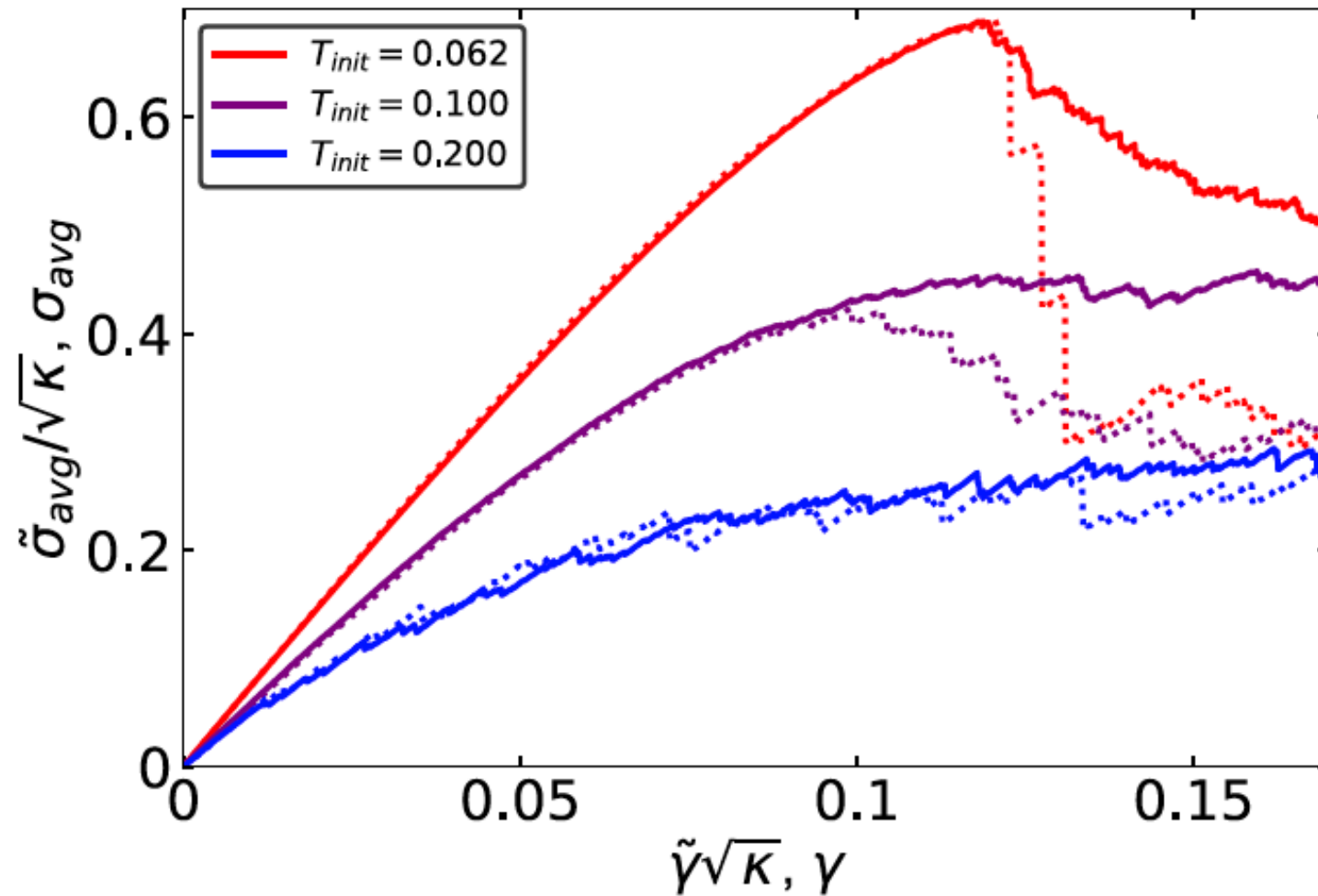


What about beyond “pre-yielding” regime



c.f. talk by Kirsten
Martens yesterday

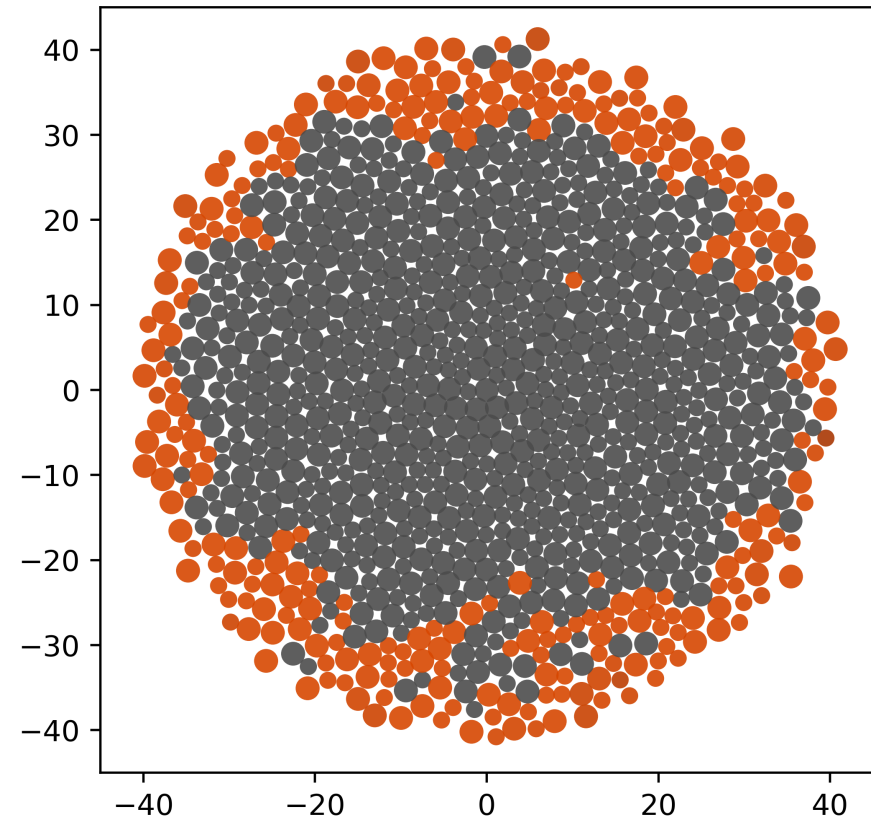
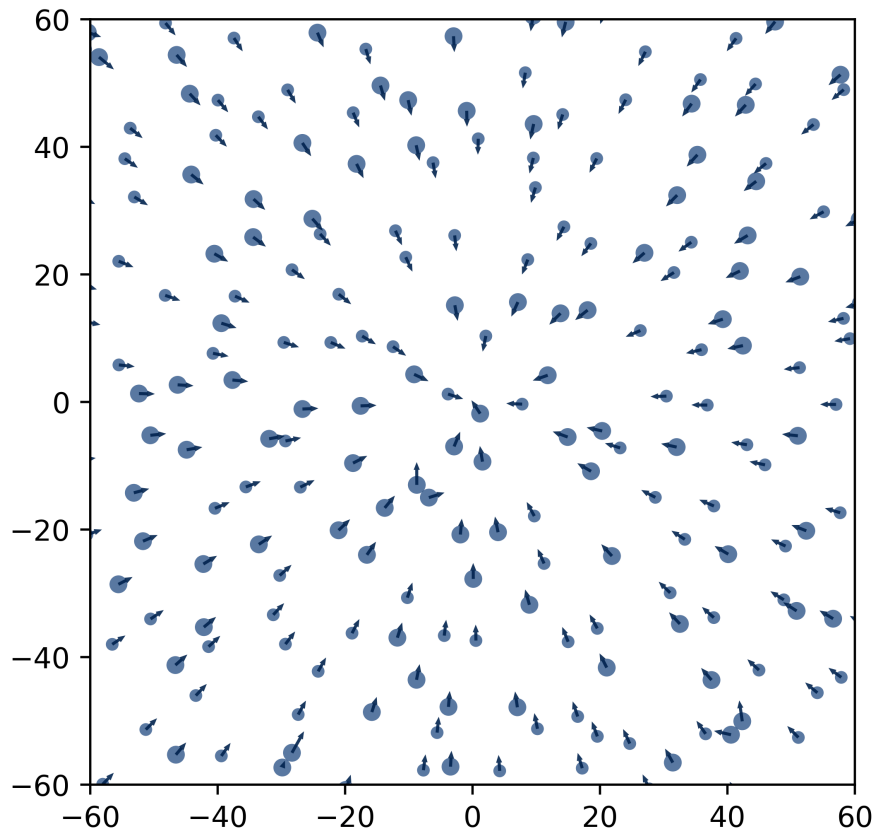
Outlook: changing material stability:



Can we break this direct link between shear and active matter?



Julia Giannini



Not so different from real crowds with dangerous crushing events



Conclusions and Outlook

- In the limit of slow driving, shear strain is simply a special case of infinitely persistent active driving.
 - The linear (shear modulus) and nonlinear (stress drop, strain to saddle) response in the pre-yielding regime possess identical scaling.
 - All the data can be collapsed using the effective parameter $\kappa \equiv \frac{\mu_{\text{AQRD}}}{\mu_{\text{AQS}}}$ as predicted by mean-field
 - The mean-field prediction for the exact value of $\kappa \equiv \frac{\mu_{\text{AQRD}}}{\mu_{\text{AQS}}} = \frac{\tilde{\mathfrak{F}}}{\ell^2}$ is close, but not quite right.
 - The macroscopic shear modulus and stress overshoot changes with material stability as expected, though the nature of the yielding transition may change.
- What happens to shear bands in brittle materials? Are the same defects excited?
- What happens at finite strain rates, persistence times? (c.f. Kirsten Martens)

Infinite-dimensional solution for AQRD dynamics



Elisabeth
Agoritsas

Global shear

$$\mathbf{x}_i(t) = \underbrace{\mathbf{x}_i(0) + \gamma(t) x_{i,2}(0) \hat{\mathbf{x}}_1}_{\text{distance between pairs}} + \mathbf{u}_i(t)$$

$$\mathbf{r}_{ij}(t) = \underbrace{\mathbf{r}_{ij}(0) + \gamma(t) r_{ij,2}(0) \hat{\mathbf{x}}_1}_{\text{gap between pairs}} + \mathbf{w}_{ij}(t)$$

Random local forcing

$$\mathbf{x}_i(t) = \underbrace{\mathbf{x}_i(0) + \gamma(t) \mathbf{c}_i}_{\text{non-affine motion}} + \mathbf{u}_i(t)$$

$$\mathbf{r}_{ij}(t) = \underbrace{\mathbf{r}_{ij}(0) + \gamma(t) (\mathbf{c}_i - \mathbf{c}_j)}_{\text{non-affine motion}} + \mathbf{w}_{ij}(t)$$

distance between pairs

$$r_{ij}(t) = \ell \left(1 + \frac{h_{ij}(t)}{d} \right)$$

gap between pairs

non-affine motion

Infinite-dimensional solution for AQRD dynamics



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Global shear

$$\mathbf{x}_i(t) = \underbrace{\mathbf{x}_i(0) + \gamma(t) x_{i,2}(0) \hat{\mathbf{x}}_1}_{\text{shear}} + \mathbf{u}_i(t)$$

$$\mathbf{r}_{ij}(t) = \underbrace{\mathbf{r}_{ij}(0) + \gamma(t) r_{ij,2}(0) \hat{\mathbf{x}}_1}_{\text{shear}} + \mathbf{w}_{ij}(t)$$

Random local forcing

$$\mathbf{x}_i(t) = \underbrace{\mathbf{x}_i(0) + \gamma(t) \mathbf{c}_i}_{\text{local forcing}} + \mathbf{u}_i(t)$$

$$\mathbf{r}_{ij}(t) = \underbrace{\mathbf{r}_{ij}(0) + \gamma(t) (\mathbf{c}_i - \mathbf{c}_j)}_{\text{local forcing}} + \mathbf{w}_{ij}(t)$$

$$\mathbf{c}_{ij} = \mathbf{c}_i - \mathbf{c}_j$$

In infinite dimensions, global shear is a special case of random local forcing: $\mathbf{c}_i = x_{i,2}(0) \hat{\mathbf{x}}_1$ $\mathbf{c}_{ij} = r_{ij,2}(0) \hat{\mathbf{x}}_1$

Generally then:

$$\mathbf{c}_i = \mathcal{C}(\mathbf{x}_i(0))$$

$$\overline{\mathcal{C}(\mathbf{x})} = 0$$

$$\overline{\mathcal{C}(\mathbf{x}) \cdot \mathcal{C}(\mathbf{x}')} = \ell^2 \underbrace{\Xi f_\xi(|\mathbf{x} - \mathbf{x}'|)}_{\text{(unitless)}}$$

$$f_\xi(x) = \frac{e^{-x^2/(2\xi^2)}}{\sqrt{2\pi}\xi}$$

For relative local displacements: $\overline{\mathbf{c}_{ij}} = 0$

$$d \overline{\mathbf{c}_{ij} \cdot \mathbf{c}_{i'j'}} \xrightarrow{(d \rightarrow \infty)} 0 : (ij) \neq (i'j')$$

$$d \overline{\mathbf{c}_{ij}^2} \xrightarrow{(d \rightarrow \infty)} = 2\ell^2 \Xi [f_\xi(0) - f_\xi(\ell)] \equiv \mathfrak{F}(\Xi, \ell, \xi)$$

For individual local displacements: $\overline{\mathbf{c}_i} = 0$

$$\overline{\mathbf{c}_i \cdot \mathbf{c}_j} = \ell^2 \Xi f_\xi(r_{ij}(0))$$

Infinite-dimensional solution for AQRD dynamics



Elisabeth Agoritsas

Global shear

$$\mathbf{x}_i(t) = \underbrace{\mathbf{x}_i(0) + \gamma(t) x_{i,2}(0) \hat{\mathbf{x}}_1}_{\text{shear}} + \mathbf{u}_i(t)$$

$$\mathbf{r}_{ij}(t) = \underbrace{\mathbf{r}_{ij}(0) + \gamma(t) r_{ij,2}(0) \hat{\mathbf{x}}_1}_{\text{shear}} + \mathbf{w}_{ij}(t)$$

Random local forcing

$$\mathbf{x}_i(t) = \underbrace{\mathbf{x}_i(0) + \gamma(t) \mathbf{c}_i}_{\text{forcing}} + \mathbf{u}_i(t)$$

$$\mathbf{r}_{ij}(t) = \underbrace{\mathbf{r}_{ij}(0) + \gamma(t) (\mathbf{c}_i - \mathbf{c}_j)}_{\text{forcing}} + \mathbf{w}_{ij}(t)$$

Many-body dynamics: $\zeta [\dot{\mathbf{x}}_i(t) - \dot{\gamma}(t) \mathbf{c}_i] = \mathbf{F}_i(t) + \boldsymbol{\xi}_i(t)$, with $\mathbf{F}_i(t) = - \sum_{j(\neq i)} \nabla v(|\mathbf{x}_i(t) - \mathbf{x}_j(t)|)$

Large-dimension assumptions:

$$|\mathbf{u}_i(t)| \sim \mathcal{O}(1/d), \quad |\mathbf{w}_{ij}(t)| \sim \mathcal{O}(1/d)$$

\Rightarrow Self-consistent scalar stochastic process for the gap, with three kernels:

$$r_{ij}(t) = \ell \left(1 + \frac{h_{ij}(t)}{d} \right)$$

$$\begin{aligned} k^{\mu\nu}(t) &\sim \langle \nabla_\mu \nabla_\nu v \rangle, \\ M_C^{\mu\nu}(t, s) &\sim \langle \nabla_\mu v \nabla_\nu v \rangle \\ M_R^{\mu\nu}(t, s) &\sim \delta \langle \nabla_\mu v \rangle / \delta P_\nu \end{aligned}$$

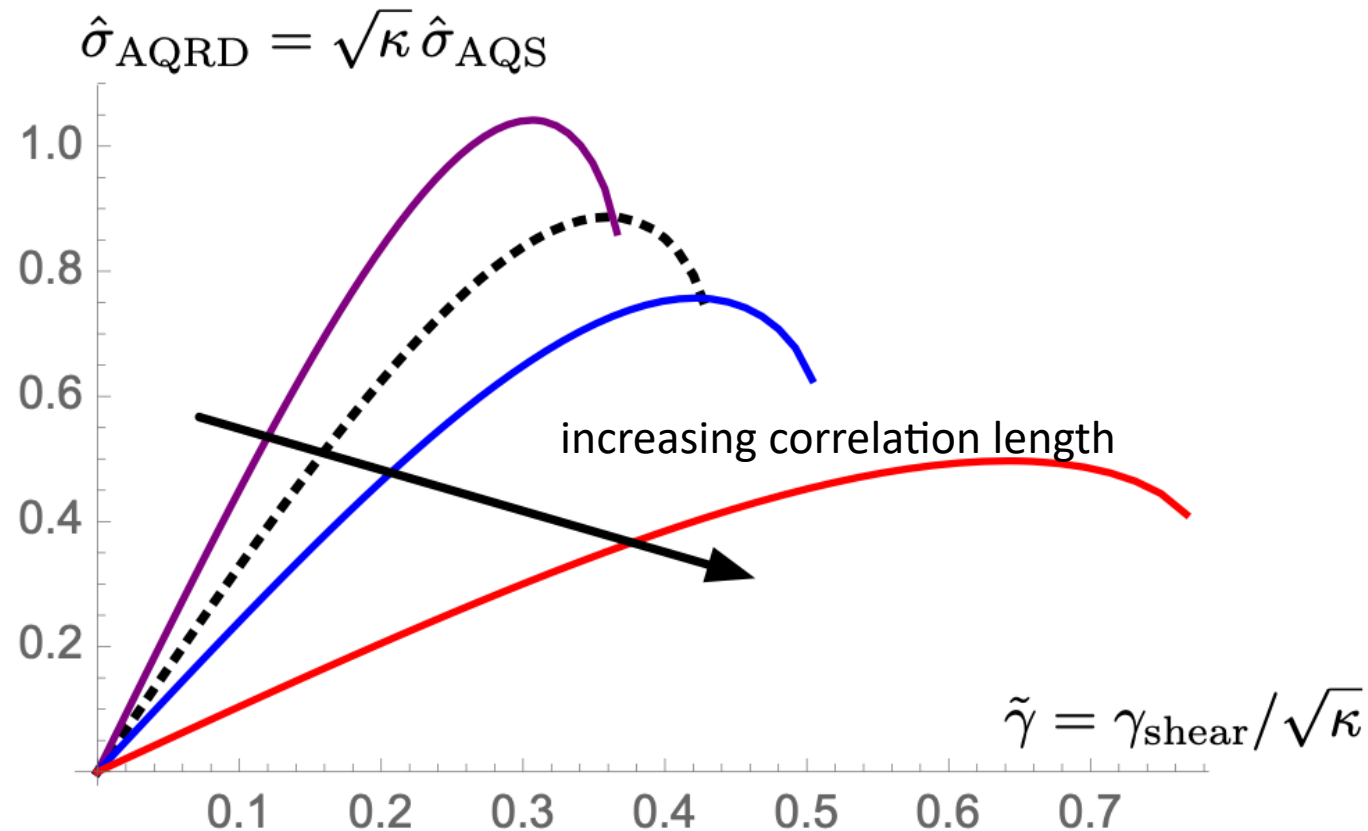
Infinite-dimensional solution for AQRD dynamics



Elisabeth
Agoritsas

$$\mathfrak{F}(\Xi, \ell, \xi) = d\overline{\mathbf{c}_{ij}^2} = 2\ell^2\Xi [f_\xi(0) - f_\xi(\ell)]$$

$$\kappa \equiv \frac{\mu_{\text{AQRD}}}{\mu_{\text{AQS}}} = \frac{\mathfrak{F}}{\ell^2}, \quad \gamma_{\text{shear}} = \tilde{\gamma}\sqrt{\kappa}, \quad \sigma_{\text{AQS}} = \sigma_{\text{AQRD}}(\tilde{\gamma})/\sqrt{\kappa}.$$



Extra slides

2D Active Brownian Particles

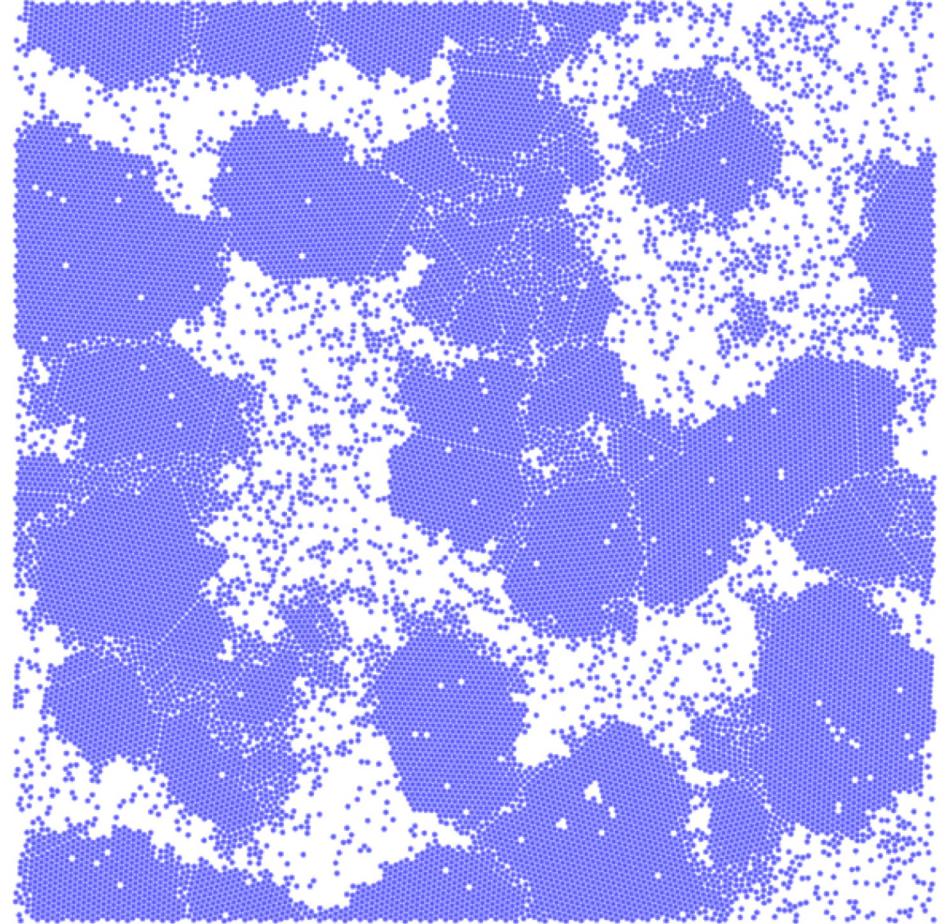
$$\dot{\mathbf{r}}_i = -\nabla \sum_j V(r_{ij}) + \gamma v_0 \mathbf{n}_i$$

$$\dot{\phi} = \eta_i$$

$$\mathbf{n}_i = (\cos(\phi_i), \sin(\phi_i))$$

$$\langle \eta_i(t) \eta_j(t') \rangle = 2D_r \delta_{ij} \delta(t - t')$$

- Persistence time $\tau = 1/D_r$.
- Long time MSD of an isolated particle grows as $2v_0^2 t / D_r$.
- Define an active temperature $T_a = v_0^2 \gamma / (2D_r)$.



Approximate Theory

Start from the equation of motion.

$$\gamma \dot{\mathbf{r}}_i = -\nabla_i \sum_j V(r_{ij}) + \gamma v_0 \mathbf{n}_i$$

Derive an expression relating velocity polarization and force fields.

$$\gamma \mathbf{v}(\mathbf{q}; t) = \sum_j \sum_{k \neq j} \mathbf{F}_{jk} e^{-i\mathbf{q} \cdot \mathbf{r}_j} + \gamma v_0 \mathbf{n}(\mathbf{q}; t)$$

$$\mathbf{v}(\mathbf{q}; t) = \sum_j \dot{\mathbf{r}}_j e^{-i\mathbf{q} \cdot \mathbf{r}_j(t)} \quad \mathbf{n}(\mathbf{q}; t) = \sum_j \mathbf{n}_j e^{-i\mathbf{q} \cdot \mathbf{r}_j(t)}$$

Rewrite first term on the right hand side.

$$i\mathbf{q} \cdot \sum_j \sum_{k \neq j} \mathbf{r}_{jk} \frac{\mathbf{r}_{jk}}{2r_{jk}} V'(r_{jk}) \left[\frac{e^{i\mathbf{q} \cdot \mathbf{r}_{jk}} - 1}{i\mathbf{q} \cdot \mathbf{r}_{jk}} \right] e^{-i\mathbf{q} \cdot \mathbf{r}_j} = -i\mathbf{q} \cdot \mathbf{\Pi}_v(\mathbf{q}; t)$$



Interaction part of the pressure tensor.

Approximate Theory

Assume in direct space $\Pi_v(\mathbf{r}; t)$ can be expressed in terms of the deviation of the microscopic density ρ .

$$\Pi_v(\mathbf{r}; t) \approx \langle \Pi_v(\mathbf{r}; t) \rangle + \mathbf{I}(\partial_\rho P_v)(\rho(\mathbf{r}; t) - \rho)$$

After some manipulations we arrive at the following expression.

$$\langle |\hat{\mathbf{q}} \cdot \mathbf{v}(\mathbf{q})|^2 \rangle = \frac{N v_0^2}{2} \frac{1}{1 + q^2 \tau B_v / (\gamma \rho)}$$

$B_v = \rho \partial_\rho P_v$ is the interaction part of the bulk modulus.

We can identify a longitudinal correlation length.

$$\ell = \sqrt{\tau B_v / (\gamma \rho)}$$

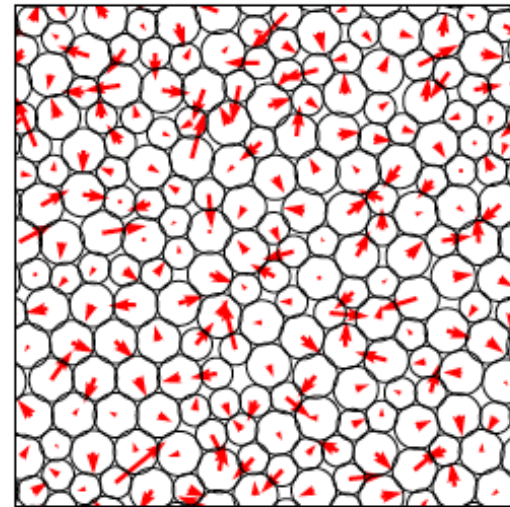
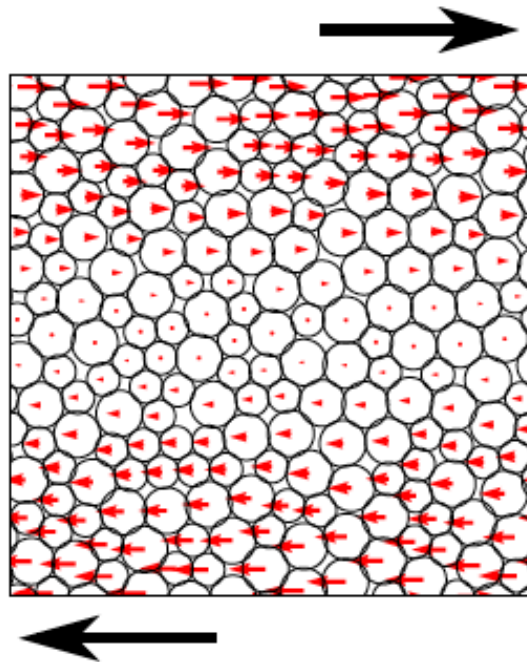
Difference between strain and unit vector in coordinate space

$$u_i^\alpha = \gamma \delta^{\alpha x} (y_i - L_y/2)$$

$$|u(\gamma)| = \gamma \left[\sum_i (y_i - L_y/2)^2 \right]^{1/2}$$

$$|u(\gamma)| \approx \gamma L_y \sqrt{N/12}$$

$$\tilde{\gamma} = \frac{\tilde{u}}{L_y \sqrt{\frac{N}{12}}}$$



Algorithm for AQRD

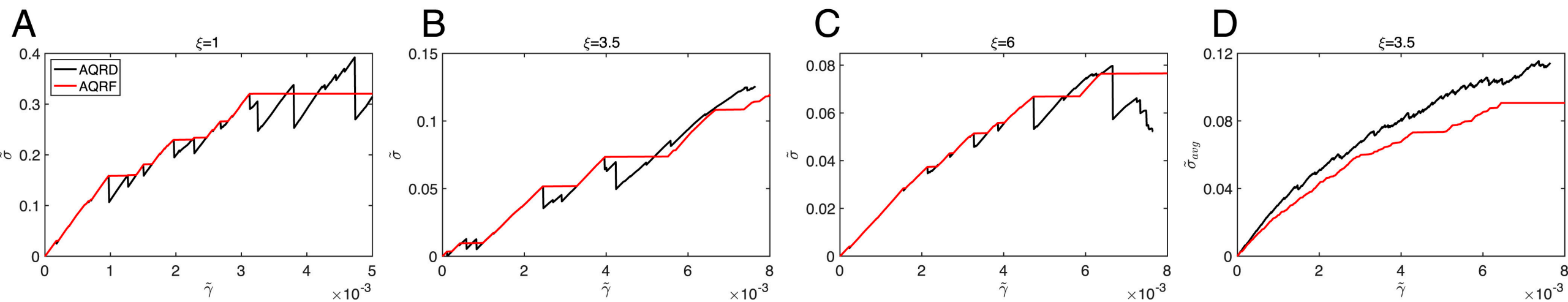
$$|x\rangle = |x^{min}\rangle + \tilde{u} |c\rangle$$

$$|F^{ext}\rangle = -\lambda |c\rangle \quad |F\rangle - \langle c|F\rangle |c\rangle$$

$$\tilde{\sigma} = \frac{dU}{d\tilde{\gamma}} = \sum_{i=1}^N \left(\frac{\partial U}{\partial x_i^{\parallel}} \frac{dx_i^{\parallel}}{d\tilde{\gamma}} + \frac{\partial U}{\partial x_i^{\perp}} \frac{dx_i^{\perp}}{d\tilde{\gamma}} \right)$$

$$\tilde{\sigma} = - \sum_{i=1}^N \mathbf{F}_i \cdot \mathbf{c}_i L_y \sqrt{\frac{N}{12}} = - \langle F|c\rangle L_y \sqrt{\frac{N}{12}}$$

Random displacement vs. Random force



Generating Gaussian random field

$$\tilde{\psi}(\mathbf{k}_{nm}) = A(\mathbf{k}) \exp\{ (iB(\mathbf{k})) \} \quad \mathbf{k}_{nm} = \left(\frac{2\pi n}{L_x}, \frac{2\pi n}{L_x} \right)$$

$$\tilde{f}(|\mathbf{k}|) = \exp\left[\left(-\frac{|\mathbf{k}|^2 \xi^2}{8} \right) \right]$$

$$\tilde{\Psi}(\bar{\mathbf{k}}) = \tilde{f}(|\mathbf{k}|) \tilde{\psi}(\mathbf{k})$$



$$\Psi(\mathbf{x}) = \sum_{n,m=1}^Q A_{nm} e^{-|\mathbf{k}_{nm}|^2 \xi^2 / 8} \cos(B_{nm} + \mathbf{k}_{nm} \cdot \mathbf{x})$$

$$\mathbf{c}_i = \Psi(\mathbf{x}_i)$$