

# (ガラスの)破壊現象が示す 非平衡臨界性

ゆらぎと応答のスケール分離？

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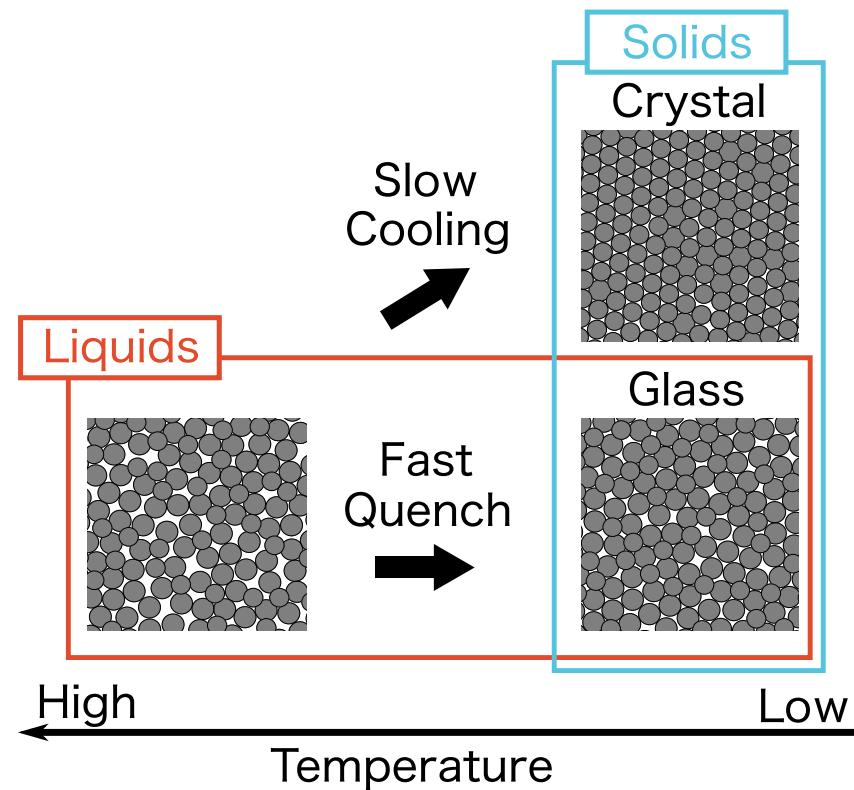
# Agenda

- Introduction (general topics)  
What are glasses? Marginal stability?
- Glasses under External Field  
Non-eq. criticality governing structural failure
- Effect of Structural Failure: Mechanical Aspect  
Structural origin of a universal rheological law
- Effect of Structural Failure: Dynamical Aspect  
Governed by a distinct correlation length?

# Introduction

# Glass Transition

- Emergence of universal "phase" of matters -



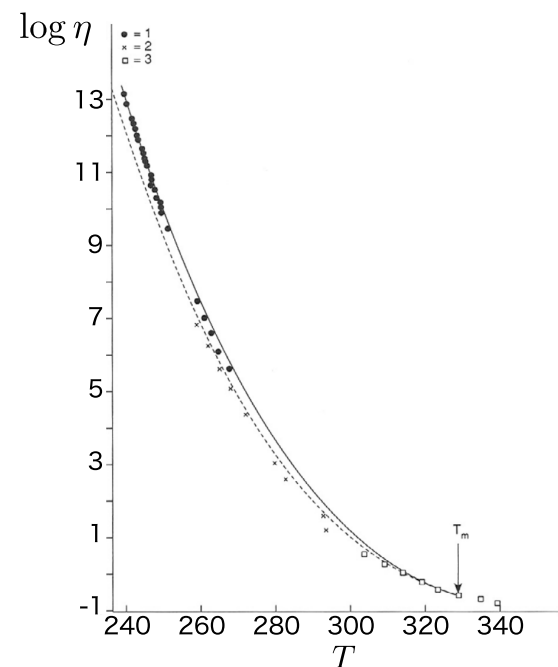
- ▶ Found in various soft matter systems universally
- ▶ Self-generated randomness: no randomness in Hamiltonian (simple liquids, alloys, colloids, polymer, emulsion, suspension, etc.)
- ▶ Glass "transition" = phase transition?
- ▶ **Extremely viscous liquid?** Solid with random structure?



# Structures vs. Dynamics

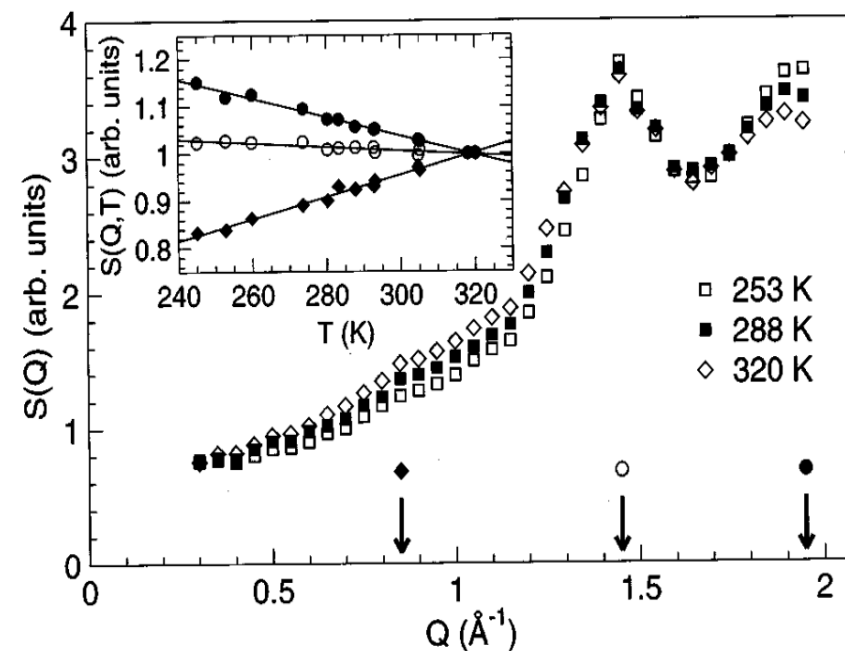
- Which is "the" essential factors of glass physics? -

## Viscosity vs. temperature



[1] Alcoutlabi, J. Phys.: Condens. Matter (2005)

## Static structure factor



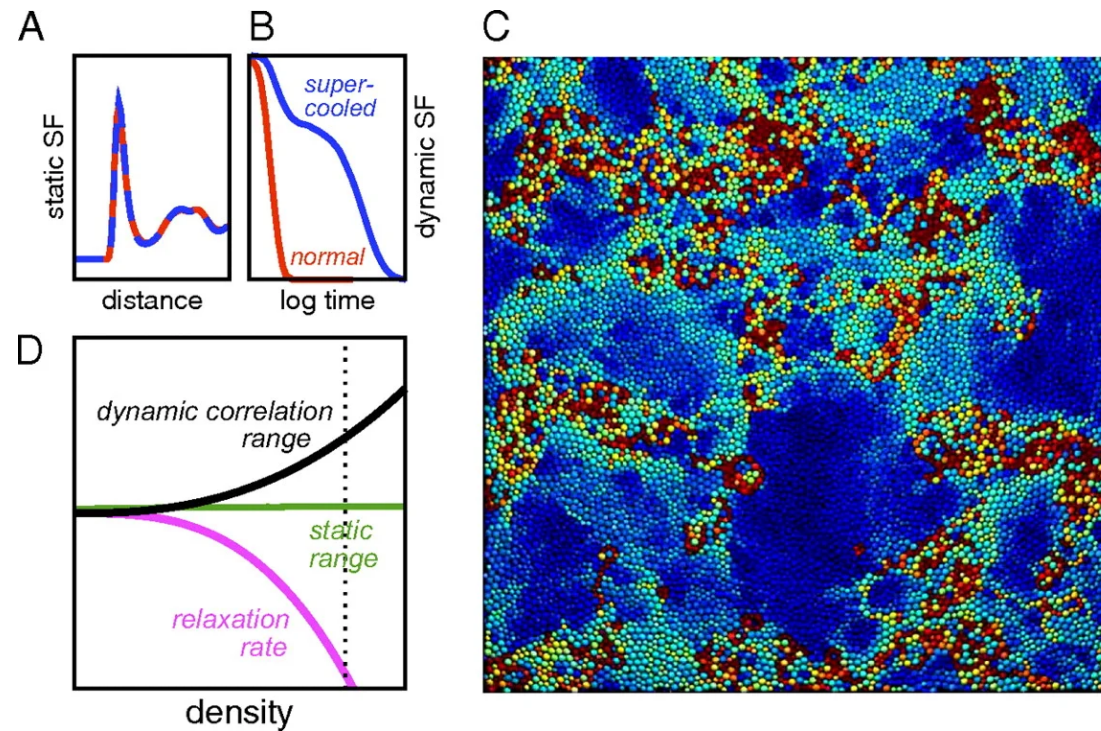
[2] Tölle, Phys. Rev. E (1997)

- ▶ Viscosity changes by more than 10 orders between **250 – 320K**
- ▶ Static structure barely changes between these temperatures

# Structures vs. Dynamics

- Which is "the" essential factors of glass physics? -

## Dynamic heterogeneity



Garrahan, PNAS (2011)

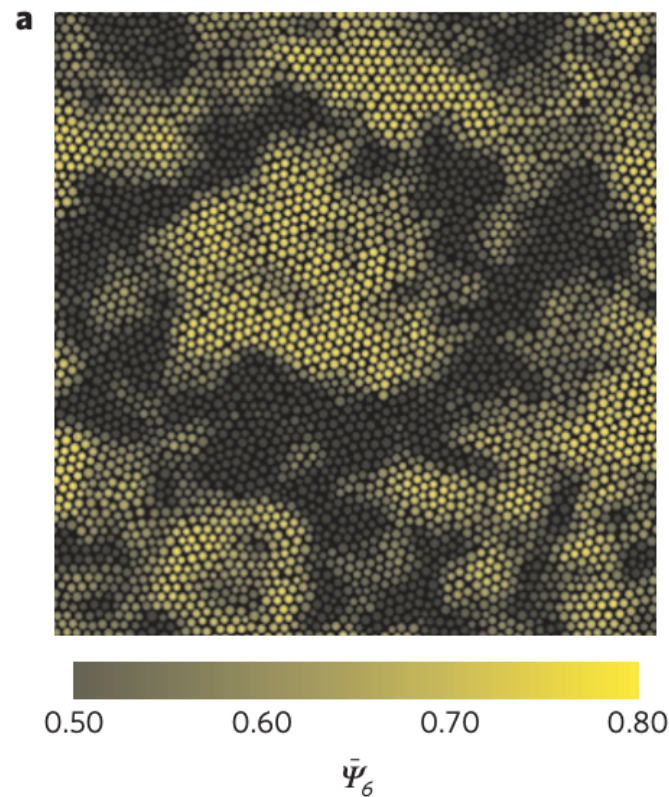
- ▶ Heterogeneous dynamics exhibit "correlated structures"
- ▶ Dynamic correlation length grows as temperature decreases
- ▶ Relaxation time: critical phenomenon-like scaling

Karmakar et al, PNAS 106(10), 3675 (2009)

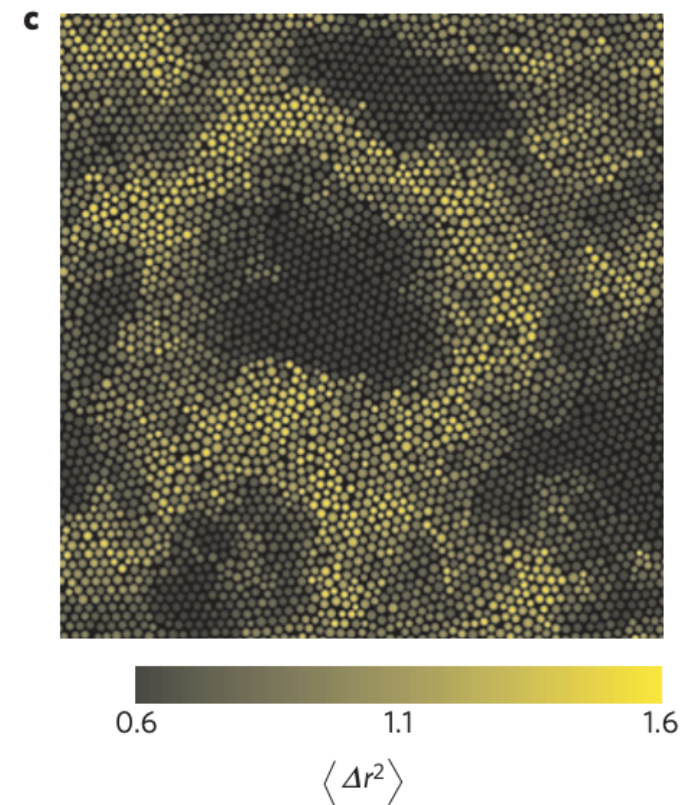
# Structural Order Parameters

- System dependent, tailor-made indicators -

Structural indicator



Dynamics



Tanaka, Nature Materials (2010)

- ▶ Structural "order" strongly correlated with dynamics
- ▶ Initially, heuristic finding in a tailor-made manner
- ▶ Machine learning approaches to find universal one

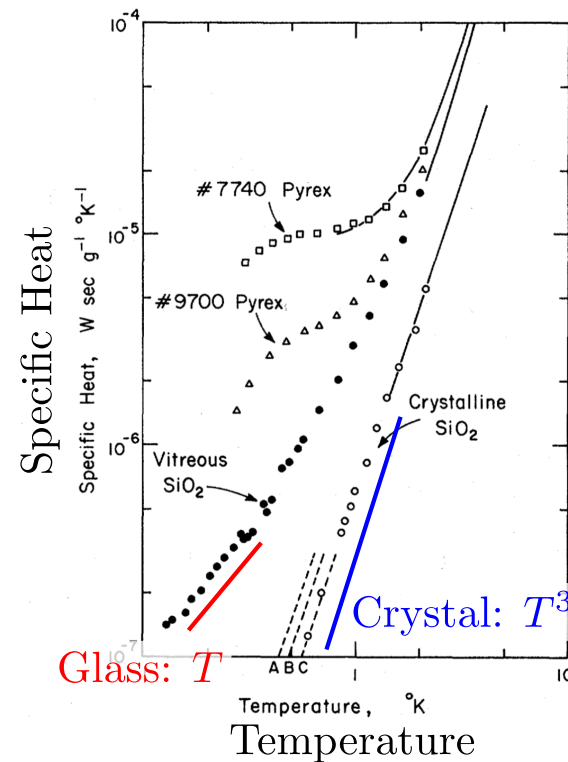
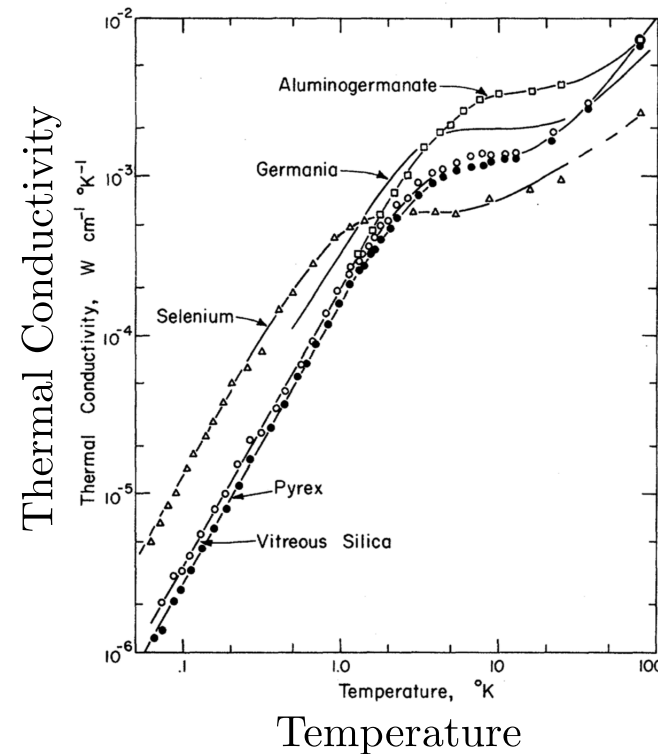
Bapst, Nat. Phys. (2020), Boattini, Nat. Commun. (2020), Shiba, J. Chem. Phys. (2023), Oyama, Front. Phys. (2023) etc.

# Glasses As...

- ▶ "Liquids" with extremely high viscosity?  
(divergence of viscosity, dynamic heterogeneity etc.)
- ▶ "Solids" with random structures?

# Low-Temperature Behavior

- Crystal vs. glasses, universal scaling for glasses -



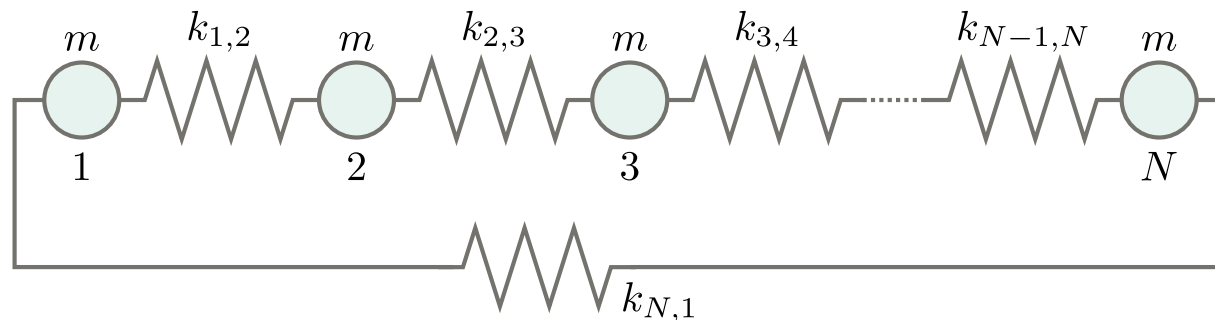
Zeller and Pohl, Phys. Rev. E 4, 2029 (1971)

- ▶ Different glasses obey the same scaling law
  - ▶ Amorphous and crystal obey different scaling laws
  - ▶ Glasses: not dominated by phonon?: Not "solids"?
- (Low-temperature: dominated by low-frequency "modes")

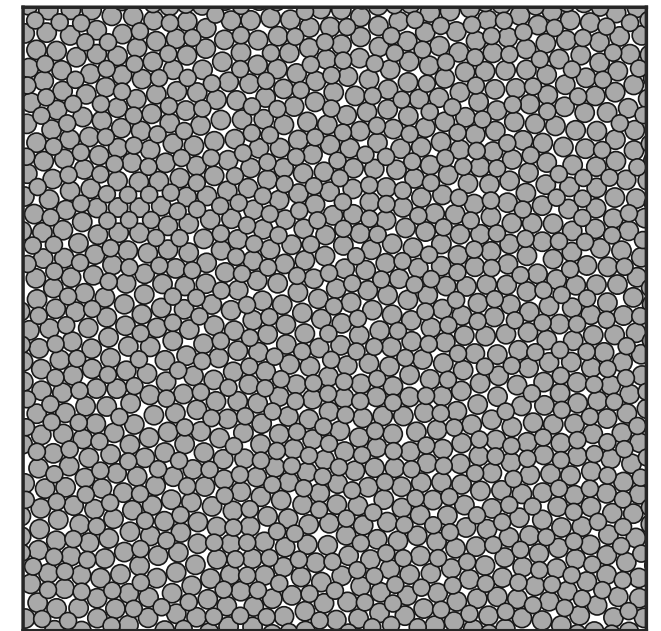


# Glasses As Coupled Oscillators

## N-body coupled harmonic oscillators



## A glass sample



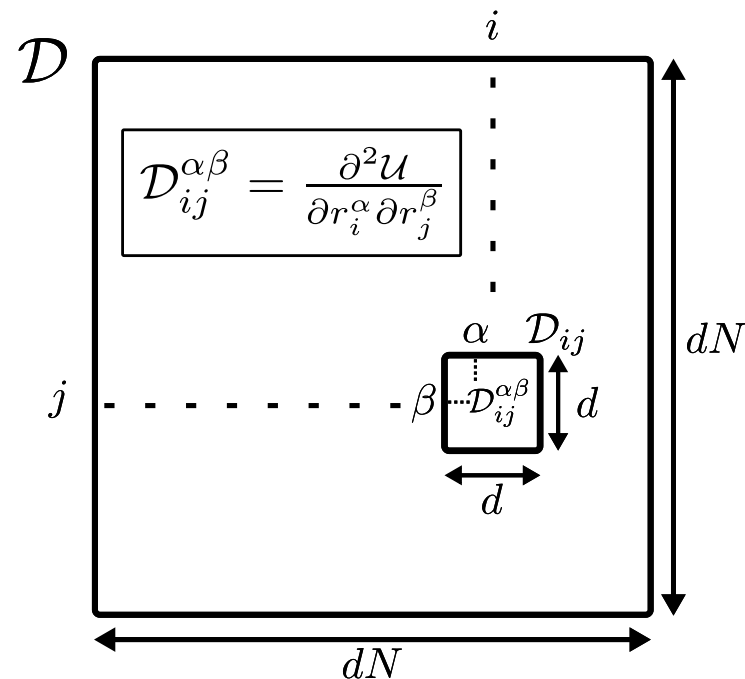
$$\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \vdots \\ \ddot{x}_i \\ \vdots \\ \ddot{x}_N \end{bmatrix} = - \begin{bmatrix} (k_{N,1} + k_{1,2}) & -k_{1,2} & 0 & \cdots & 0 & -k_{N,1} \\ -k_{1,2} & (k_{1,2} + k_{2,3}) & -k_{2,3} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & 0 & -k_{i-1,i} & (k_{i-1,i} + k_{i,i+1}) & k_{i,i+1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -k_{N,1} & 0 & \cdots & 0 & -k_{N-1,N} & (k_{N-1,N}, k_{N,1}) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_i \\ \vdots \\ x_N \end{bmatrix}$$

## Complexities of glasses

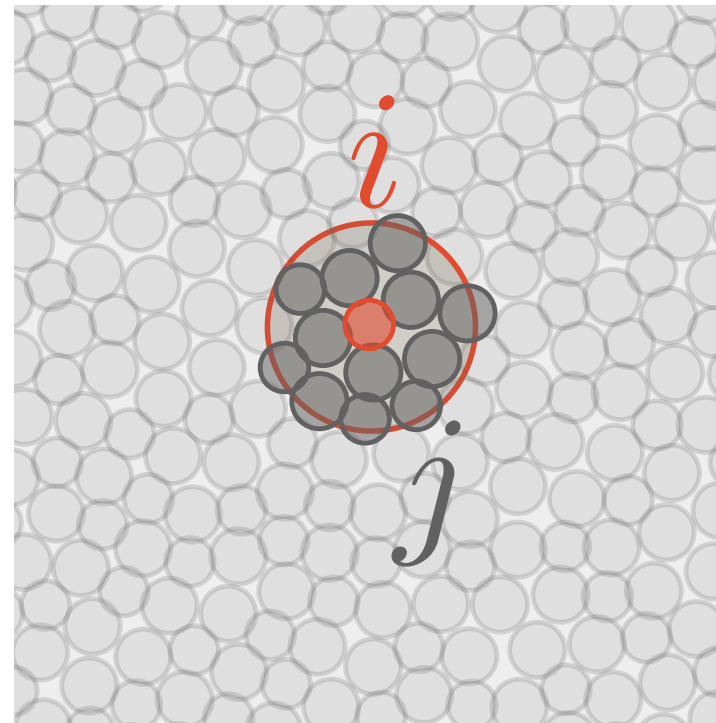
- Complicated "random" structures
  - Non-harmonic potentials (e.g.,  $V_{LJ}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$ )
- Matrix representation with harmonic approximation for small perturbations (equivalent approximation to ones employed in Debye's theory)

# Normal Mode Analysis

## Dynamical Matrix



## Particles interaction

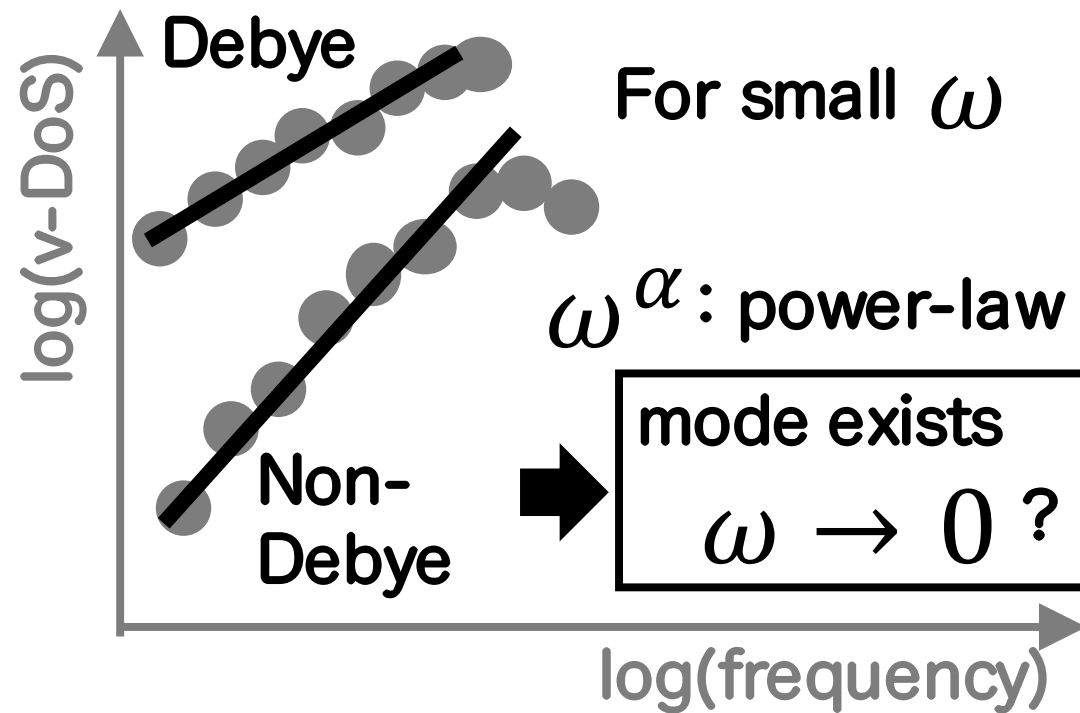


- ▶ Mechanical equilibrium state is assumed (zero temperature)
- ▶ Total potential  $\mathcal{U} = \sum_{ij} V_{ij}(r_{ij})$
- ▶ Obtained by the Euler-Lagrange eq. with harmonic approximation
- ▶ Eigenvalues  $\lambda_k$ : "Spring constants" to small perturbations
- ▶  $\omega_k \equiv \sqrt{\lambda_k}$  gives the eigen-frequency of  $k$ -th eigenmode

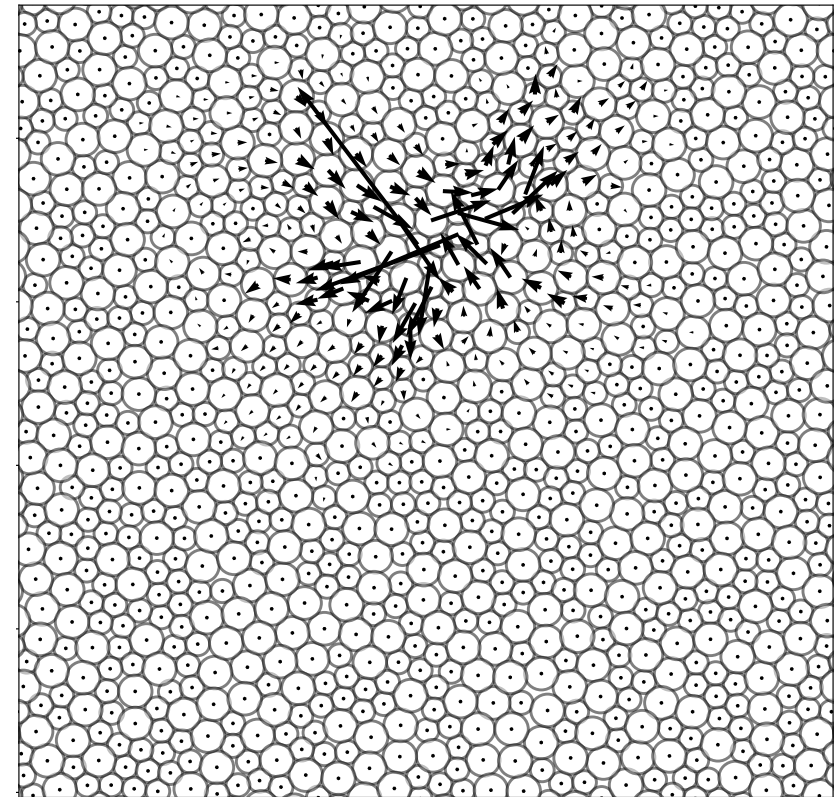
# Low-Frequency Modes in Glasses

- Low frequency anomalous properties -

Vibrational density of states (v-DoS)



Low-frequency plastic modes



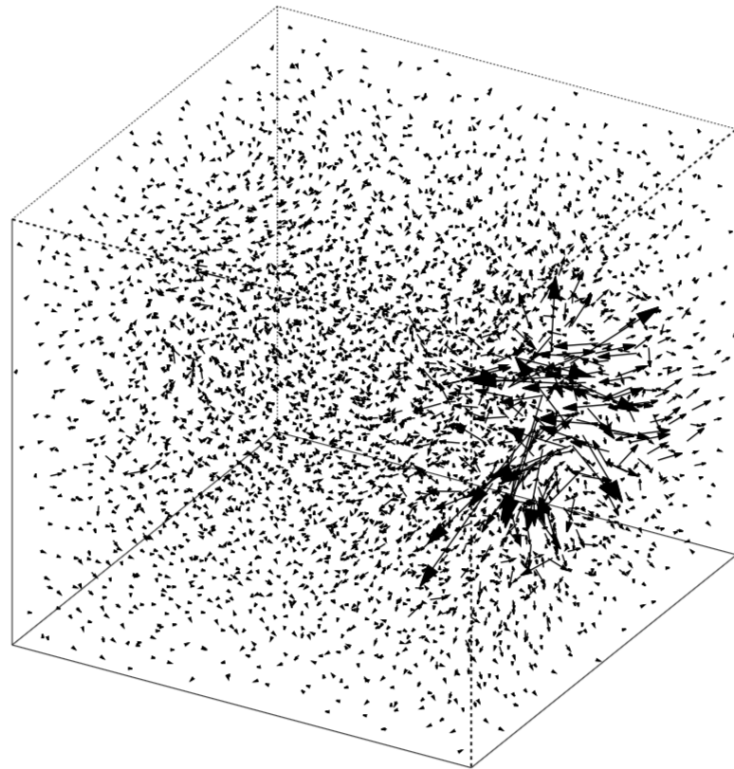
- ▶ "Quasi-localized Vibrational Modes (QLVs)" appear
- ▶ QLV modes are "plasticity-inducing" pattern
- ▶ Infinitesimal perturbation can destabilize the system in  $N \rightarrow \infty$



# QLV vs. Phonon Modes

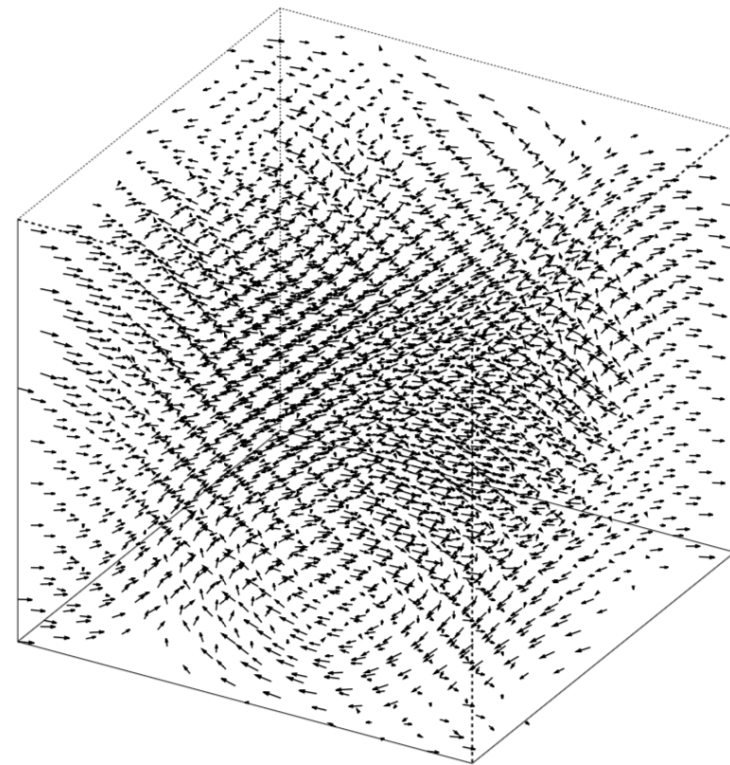
- Difference between low-frequency modes -

Quasi-localized mode



(a) Glass.

Phonon mode



(b) Crystal.

Mizuno and Ikeda, Private Communication

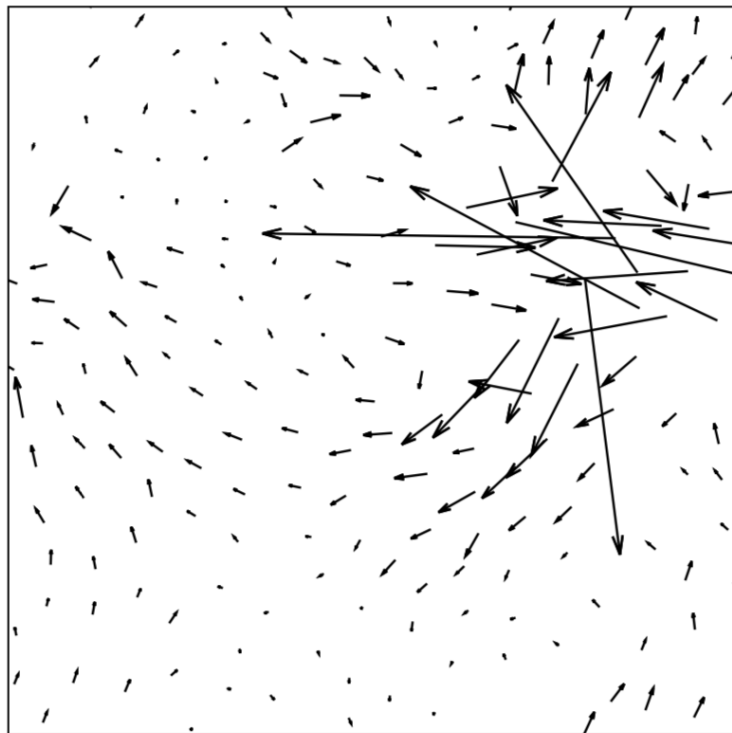
► **Universally observed in various amorphous systems**

Lerner PRL (2016), Mizuno PNAS (2017), Kapteijns PRL (2018), Wang Nat. Commun. (2019), Richard PRL (2020) etc.

# QLV vs. Phonon Modes

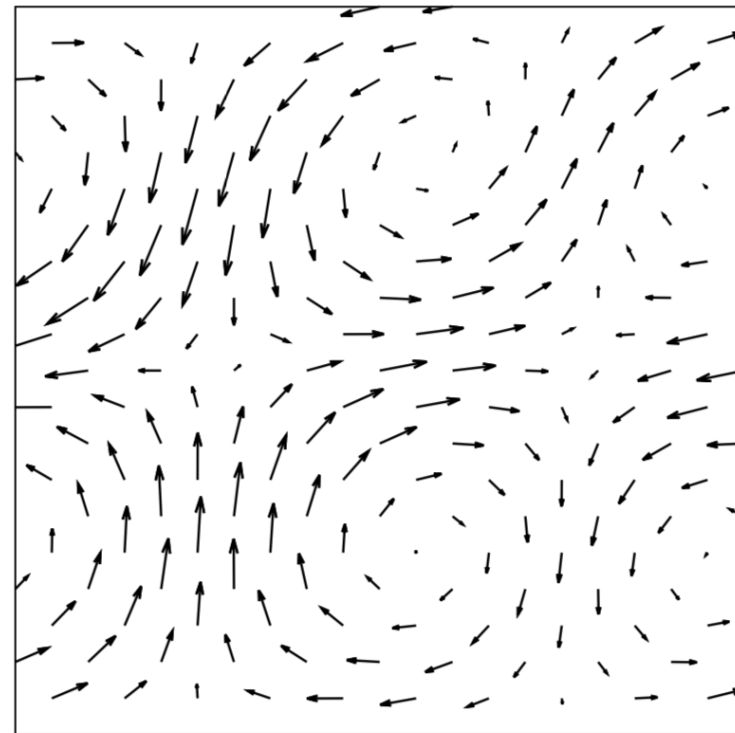
- Difference between low-frequency modes -

Quasi-localized mode



(c) Glass.

Phonon mode



(d) Crystal.

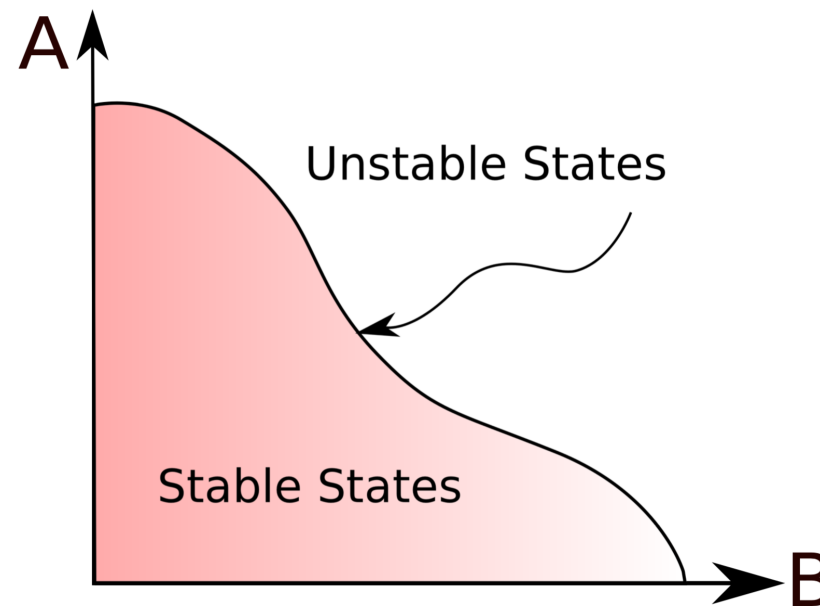
Mizuno and Ikeda, Private Communication

► **Universally observed in various amorphous systems**

Lerner PRL (2016), Mizuno PNAS (2017), Kapteijns PRL (2018), Wang Nat. Commun. (2019), Richard PRL (2020) etc.

# Marginal Stability (MS)

- Candidate for the KEY concept -



Müller, and Wyart, *Annu. Rev. Condens. Matter Phys.* **6**, 177(2015)

- ▶ Theoretical predictions are available  
(e.g.  $\infty$  dimensional mean-field model)

Parisi, Urbani, and Zamponi, "Theory of Simple Glasses", Cambridge University Press (2020)

Franz et al., *PNAS* **112**, 14539 (2015), Biroli and Urbani, *Nat. Phys.* **12**, 1130 (2016)

- ▶ Glasses: extremely vulnerable solids?

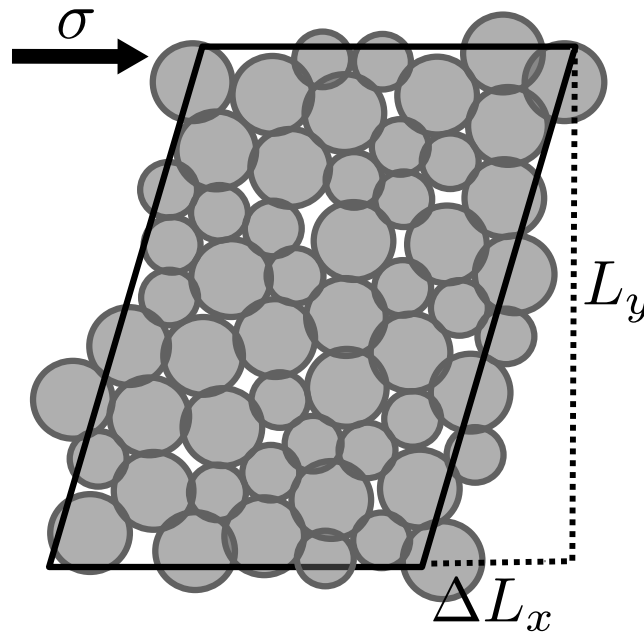
# Glasses under External Field

- Non-eq. criticality governing structural failure -

Oyama, Mizuno, and Ikeda, Phys. Rev. E **104**, 015002 (2021), arXiv:2109.08849

# Prep: (Shear) Strain and Stress

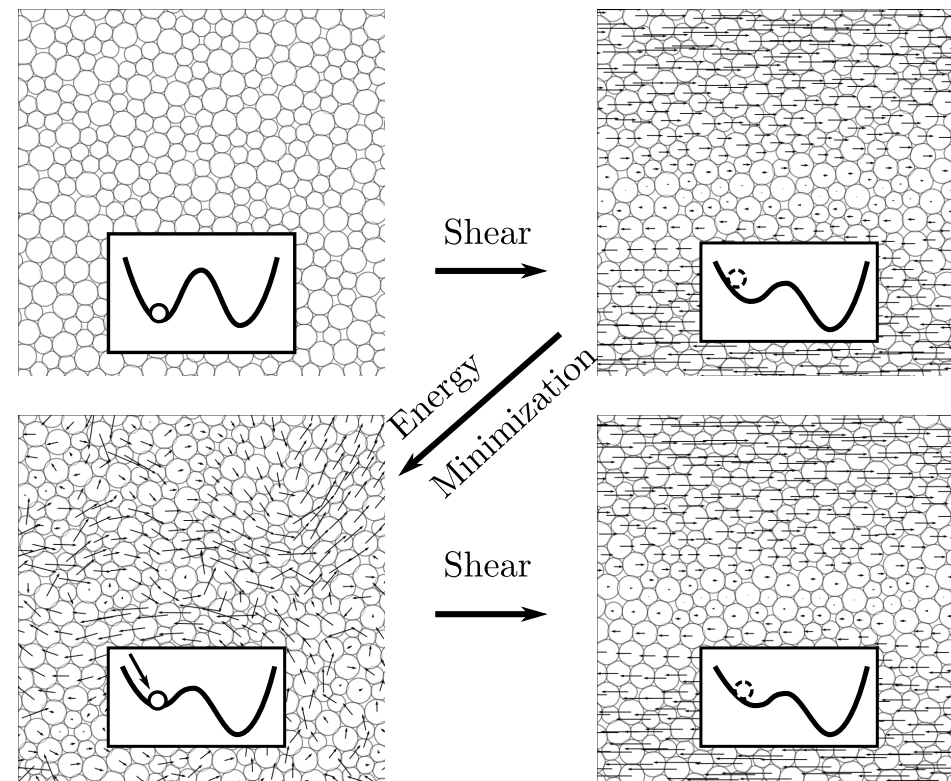
- Fundamental observables for rheology -



- ▶ Strain:  $\gamma = \Delta L_x / L_y$  (dimensionless)
- ▶ Stress:  $\sigma = -\frac{1}{V} \sum_{ij} (r_x^{ij} f_y^{ij} + r_y^{ij} f_x^{ij})$   
(dimension of pressure)
- ▶ Strain  $\gamma$  (or  $\dot{\gamma}$ ) is controlled in this study  
(stress  $\sigma$  can be treated as the response)

# MD Simulation under Athermal Quasistatic Drive

- Method to access purely athermal events -

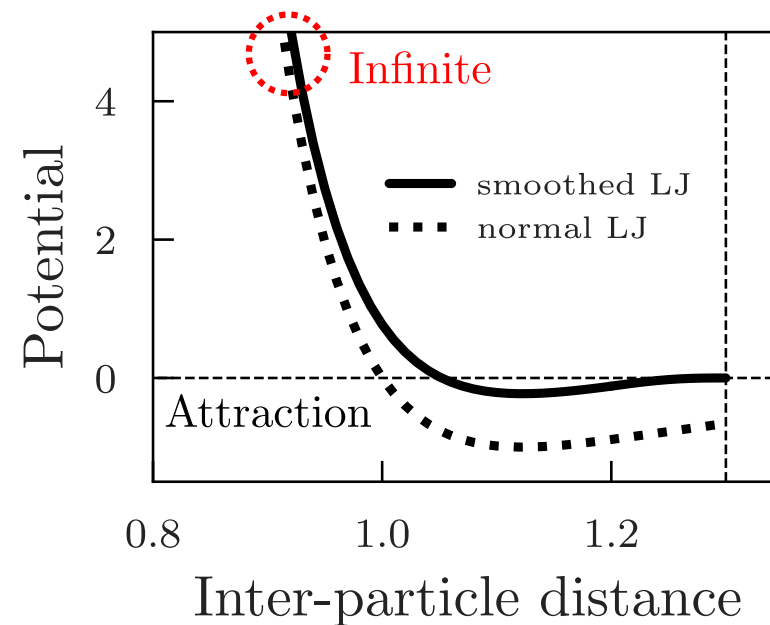


- ▶ Corresponding to  $\dot{\gamma} = 0$
- ▶  $\Delta\gamma = 5 \times 10^{-7} - 5 \times 10^{-6}$  (depending on  $N$ )
- ▶ Only the steady-state data ( $\gamma > 0.25$ ) is utilized

# Inter-particle potentials

- Athermal glass system -

## Smoothed Lennard-Jones potential



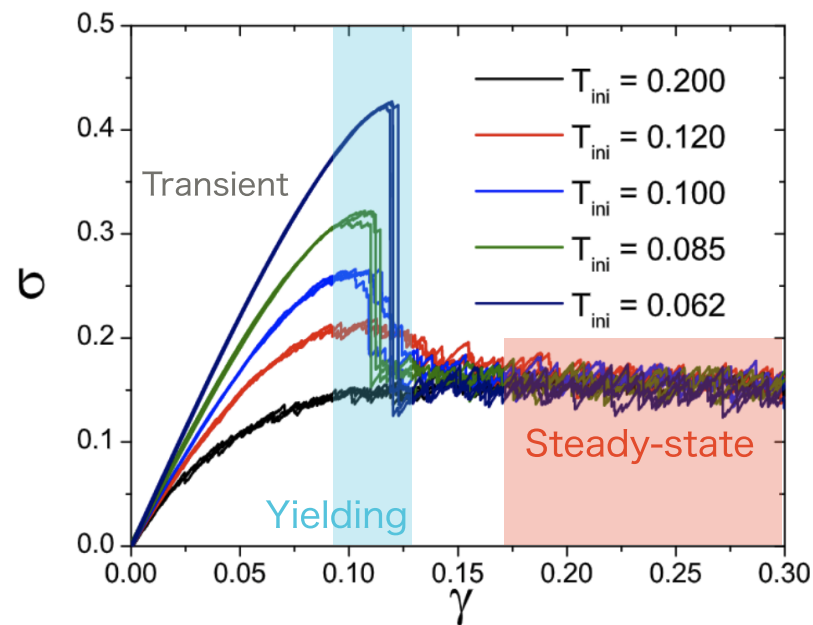
Salerno et al., PRL **109**, 105703 (2012)

- ▶ Attraction & excluded volume effect → dense: glasses
- ▶ Binary mixture (1:1.4 size ratio, 50:50 number ratio)
- ▶ 2D,  $\rho = 1.09$ ,  $N = 512 - 32768$  particles

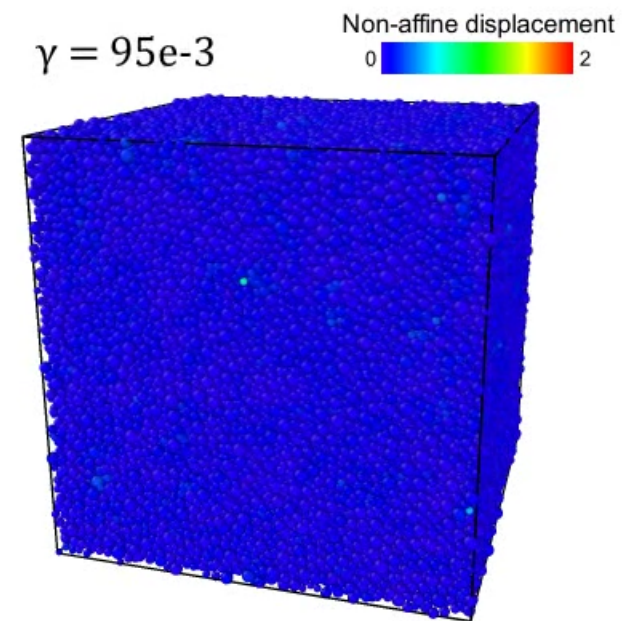
# Response under Athermal Quasistatic Shear

- Yielding transition and ... -

## Stress-strain curve



## Yielding regime movie



Ozawa et al., PNAS 115, 6656 (2018)

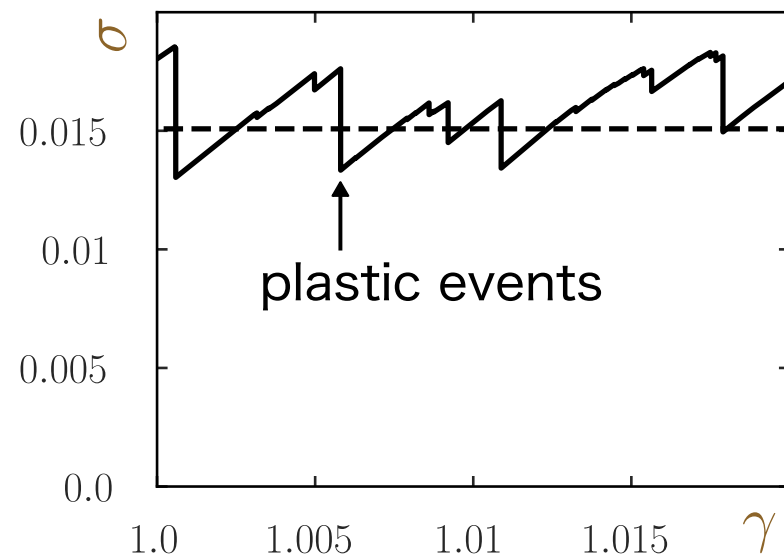
- ▶ Behavior under athermal quasistatic shear
- ▶ Yielding singularity at around  $\gamma = 0.1$
- ▶ Curves **self-organize** into single one after singularity



# Response under Athermal Quasistatic Shear

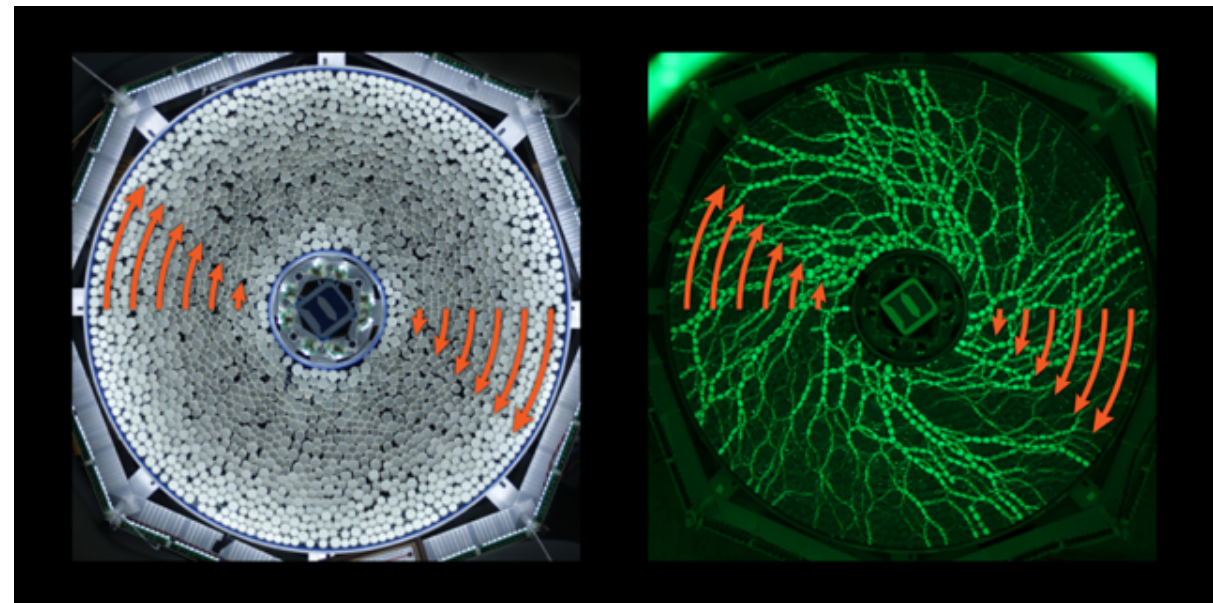
- Steady-state regime -

## Stress-strain curve



Our result

## Experiment (Granular flow)



Yiqiu Zhao(Duke University)/ Luding, Physics, **12**, 109 (2019)

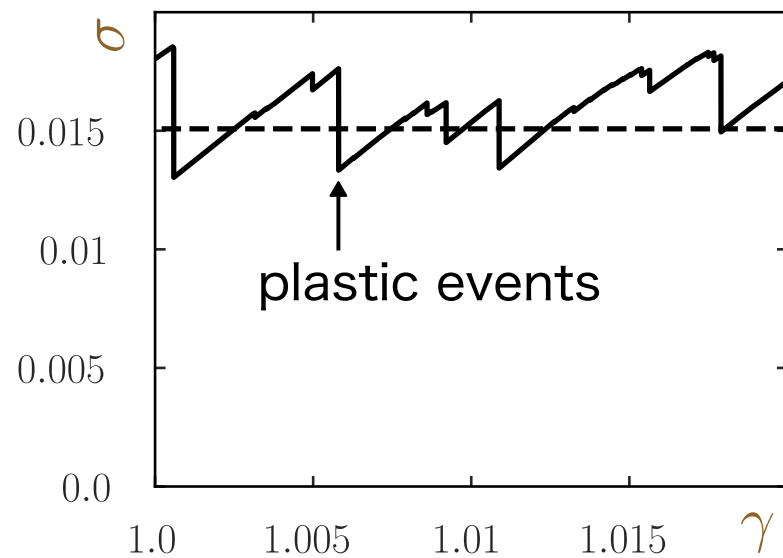
- ▶ Focus on steady-state regime hereafter
- ▶ Can be viewed as a **critical phenomenon?**

Dahmen et al., Nat. Phys. **7**, 554 (2011), Lin et al., PNAS **111**, 14382 (2014)

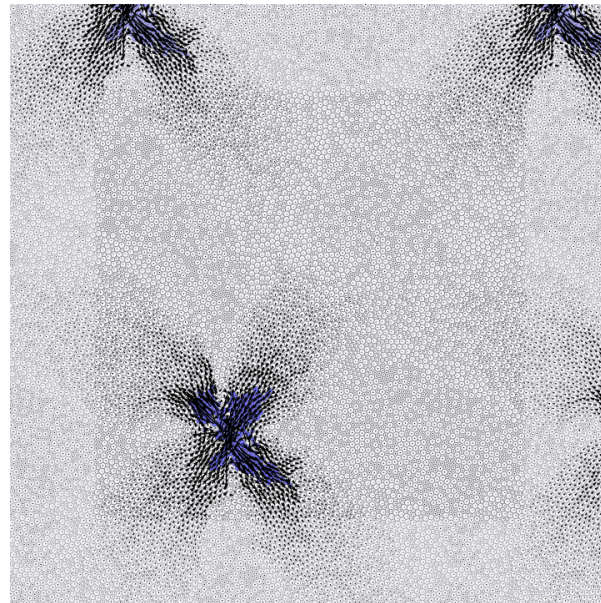
# Steady-state Behavior

- Elastic and plastic = elastoplastic response? -

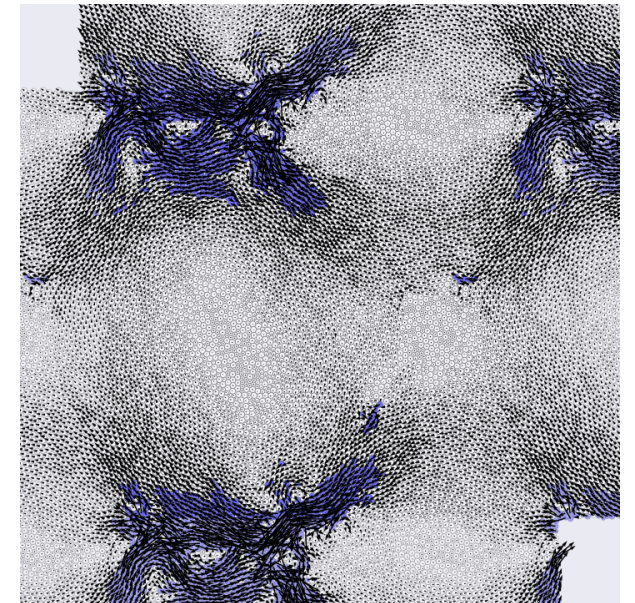
Stress-strain curve



Single ST



Avalanche of STs



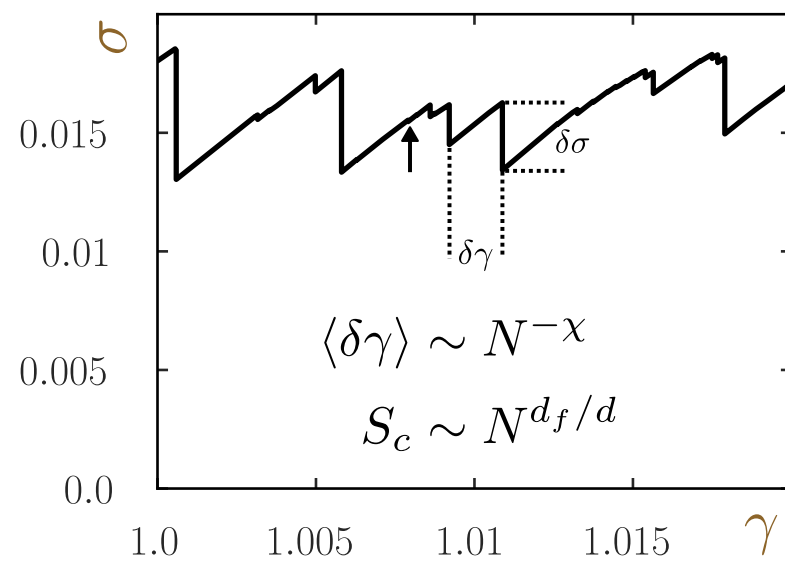
- ▶ Elastic behavior is punctuated by intermittent plastic events
- ▶ Elementary process of plasticity is shear transformation (ST)  
(characterized by quadrupolar strain field)
- ▶ Sometimes organized into avalanches  
(energy released by a ST can trigger other STs)



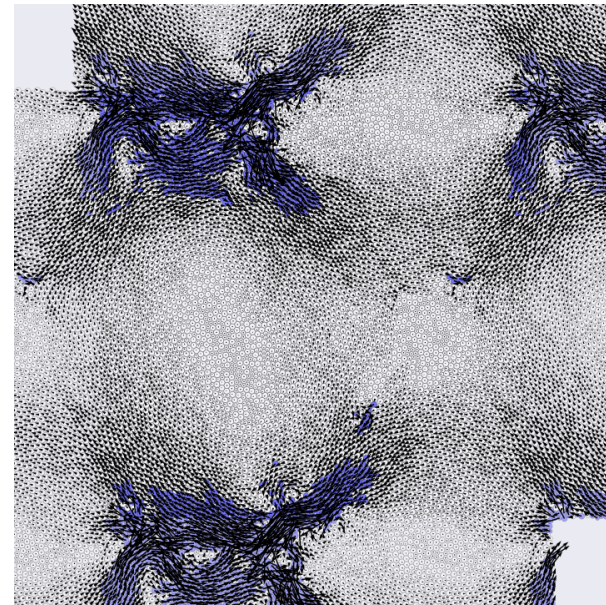
# Statistics of "Avalanches" in Steady State

- One example of avalanche criticalities -

## Definitions and scaling laws



## Avalanche of STs

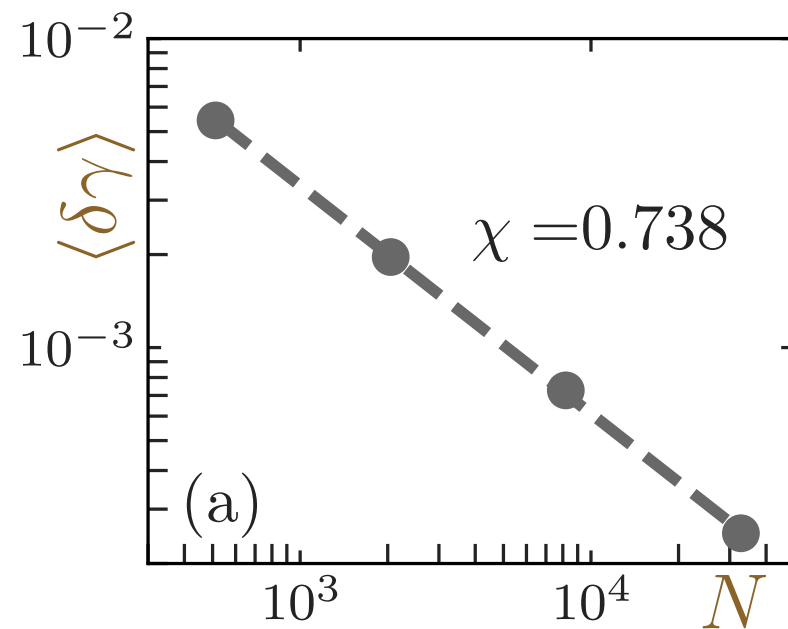


- ▶ Avalanche size  $S \equiv N\delta\sigma$  (unit of energy  $\propto$  volume)
- ▶ "Maximum" avalanche size for system with linear dimension  $L$   
 $S_c(L) \equiv \langle S^2 \rangle / \langle S \rangle$  (assuming  $P(S) = S^{-\tau} f(S/S_c)$ )

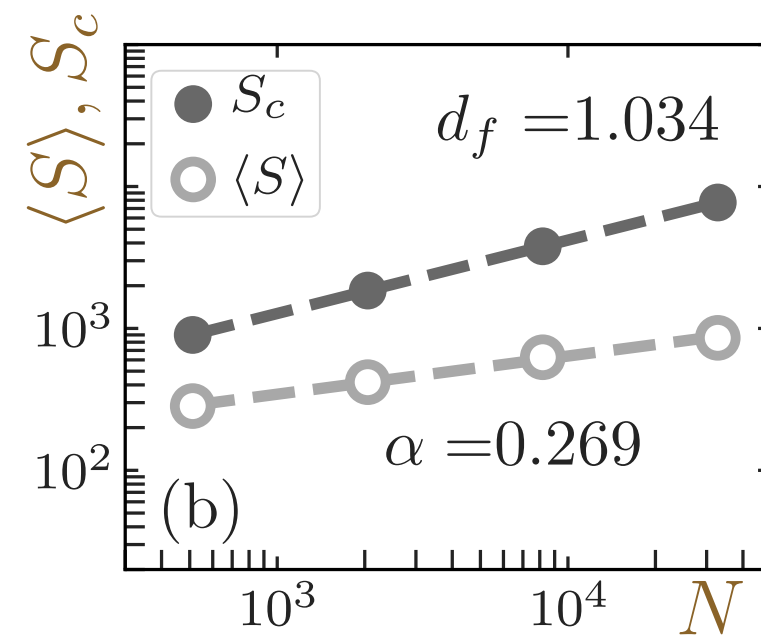
# Typical Avalanching Scaling Laws

- System-size-dependence of avg. strain interval and cutoff avalanche size -

Avg. strain interval



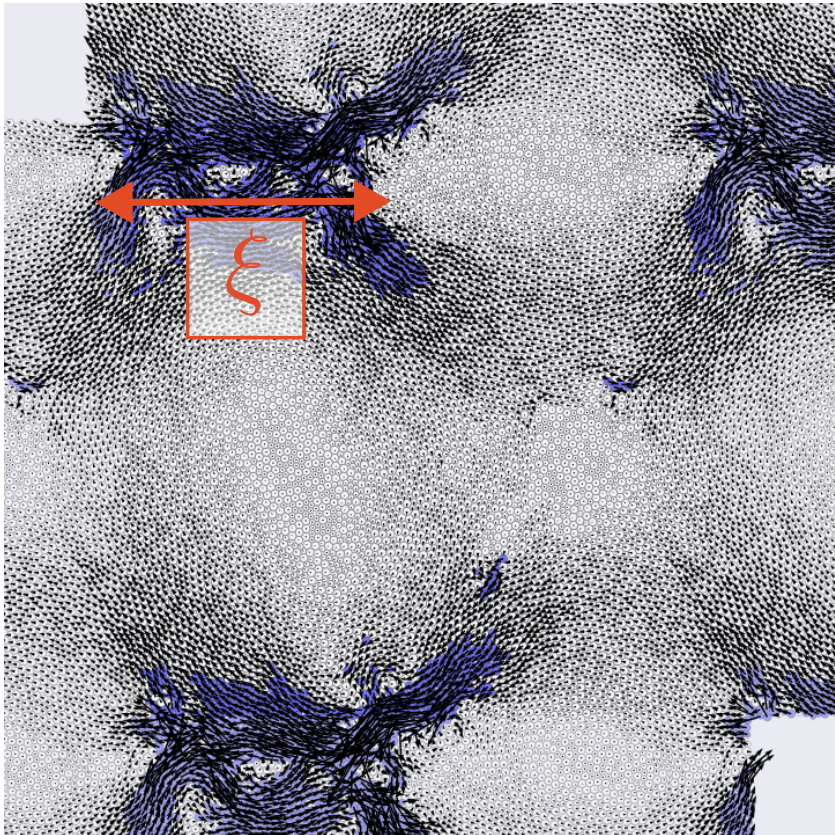
Cutoff avalanche size



- ▶  $\langle \Delta\gamma \rangle \sim N^{-\chi} \rightarrow 0 (N \rightarrow \infty)$ : consistent with MS
- ▶  $S_c \sim L^{d_f}$  will become important later

# Yielding: A Non-eq. Criticality?

## Scaling ansatzes



- Correlation length:  $\xi \sim |\sigma - \sigma_Y|^{-\nu}$ 
  - Maximum spanning of avalanches
- Macroscopic strain rate:  $\dot{\gamma} \sim |\sigma - \sigma_Y|^\beta$ 
  - Regarded as the order parameter
- Avalanche lifetime:  $T \sim \xi^z$ 
  - Inaccessible information
- Cutoff avalanche size:  $S_c \sim \xi^{d_f}$ 
  - Characterized by fractal dimension  $d_f$

# Effect of Structural Failure: Mechanical Aspect

- Structural origin of a universal rheological law -

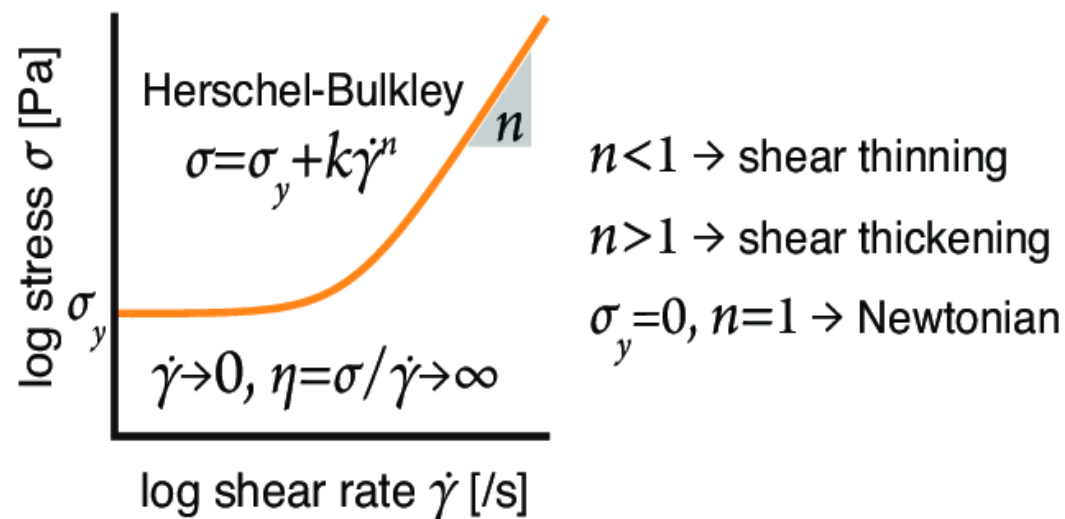
Oyama, Mizuno, and Ikeda, Phys. Rev. Lett. **127**, 108003 (2021)



# Herschel-Bulkley Law

- Universal constitutive relation -  
Herschel and Bulkley, Kolloid Zeitschrift **39**, 291 (1926)

## Schematic Flow Curve



de Kort, PhD Thesis (2016)

## Vegetables and Fruits



<http://www.kuroda-dryer.co.jp>,  
Diamante and Umemoto, Int. J. Food. Prop. **18**, 1191 (2015)

- ▶ Glasses, foams, emulsions, suspensions, blood, etc.
- ▶ Yield stress and power-law offset from it
- ▶ **Structural origin** is not yet clarified

# MD Simulation under Finite-Rate Shear

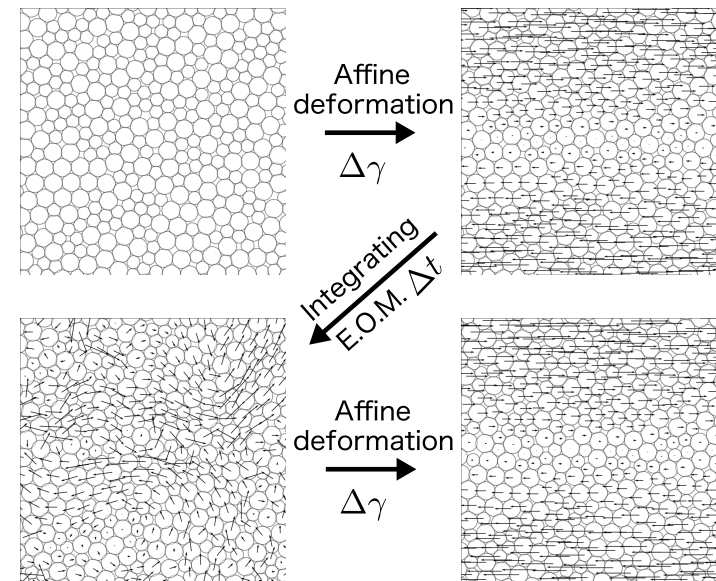
- Athermal system with mechanical noises -

Equation of motion

$$\frac{d\delta\mathbf{v}_i}{dt} = - \sum_{j \in \partial i} \frac{\partial V(r_{ij})}{\partial \mathbf{r}_i} - \eta \delta\mathbf{v}_i$$

$$\frac{d\mathbf{r}_i}{dt} = \delta\mathbf{v}_i + \dot{\gamma} y_i \mathbf{e}_x$$

Sketch of algorithm

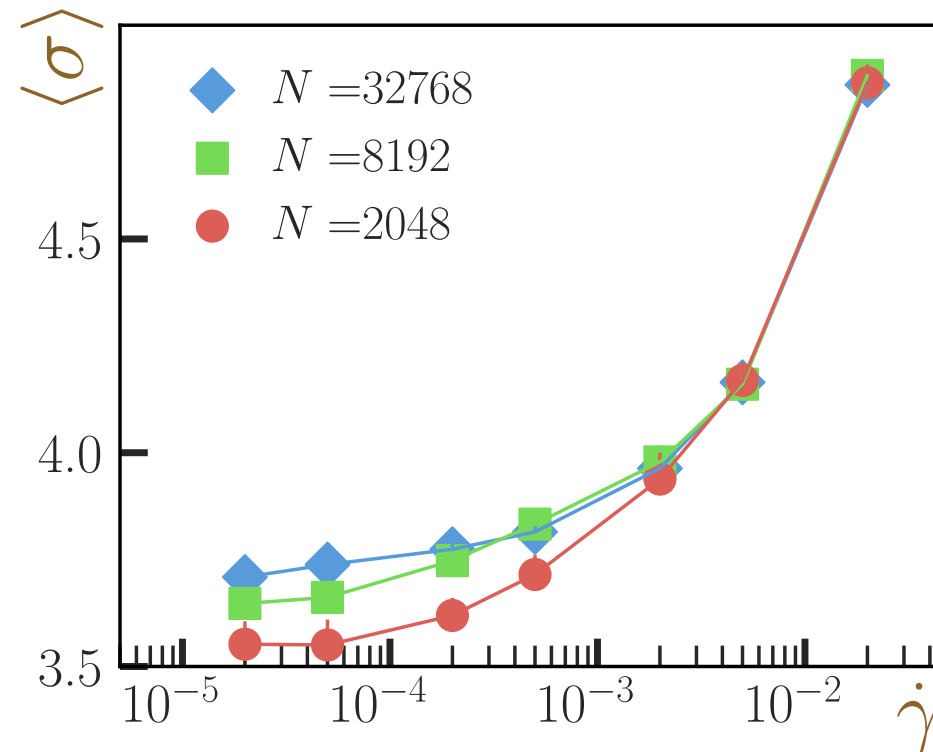


- ▶  $2 \times 10^{-5} < \dot{\gamma} \equiv \Delta\gamma/\Delta t < 2 \times 10^{-2}$
- ▶ Focus on purely structurally-induced rheology: zero temperature (still treated as a classical system)
- ▶ Dissipation: Stokes drag



# Flow Curves

- Shear-rate dependent mechanical response -

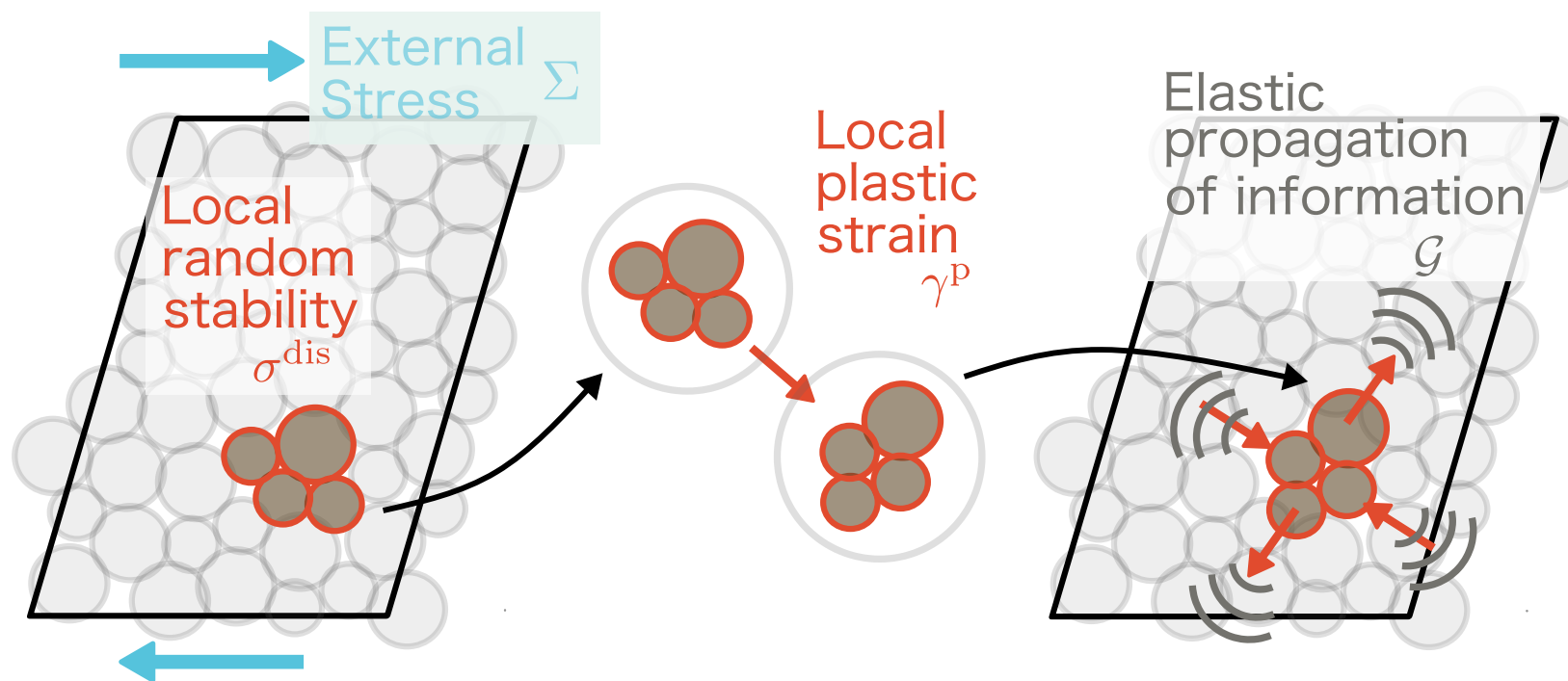


- ▶ Herschel-Bulkley law:  $\langle \sigma \rangle = \sigma_Y + k\dot{\gamma}^n$
- ▶ Strong finite size effect (FSE)
- ▶ HB parameters cannot be obtained by simple fitting

# Plasticity in Sheared Glasses

- Phenomenological description -

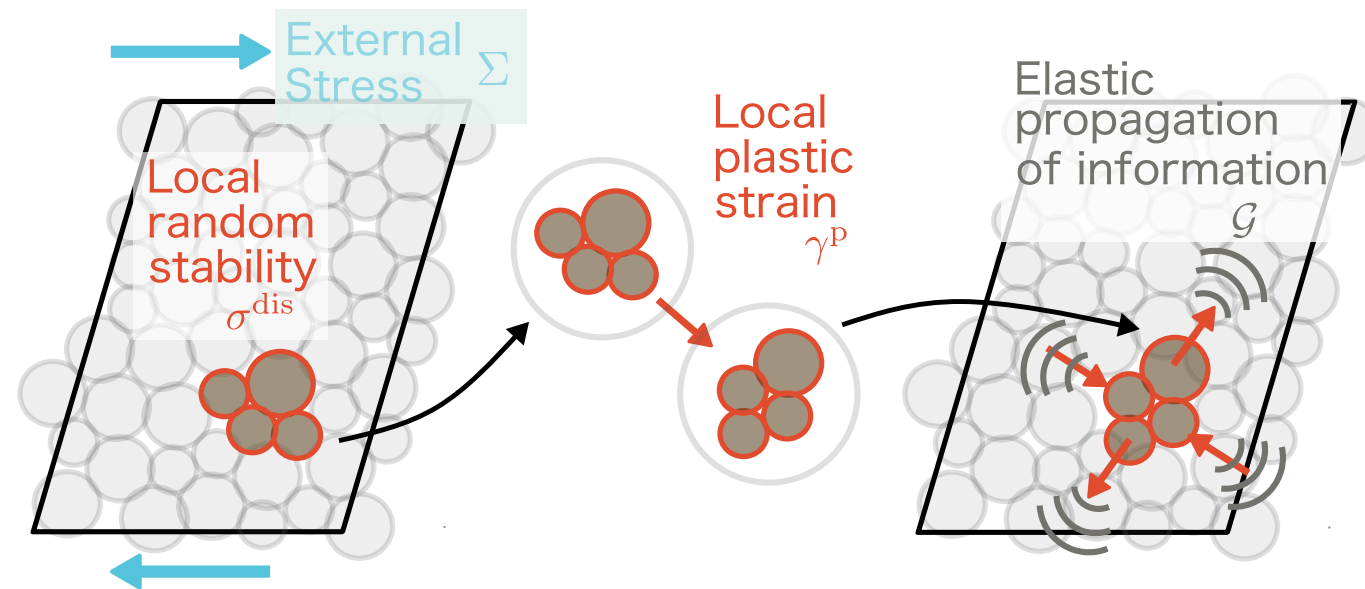
Schematic picture of cause and effect of plastic events



- ▶ Driven by **external shear stress**
- ▶ **Local stability** is randomly distributed
- ▶ Local instability triggers **plastic events**
- ▶ **Local plastic strain** propagate through elastic kernel

# Theoretical Formulation

- Continuum description -



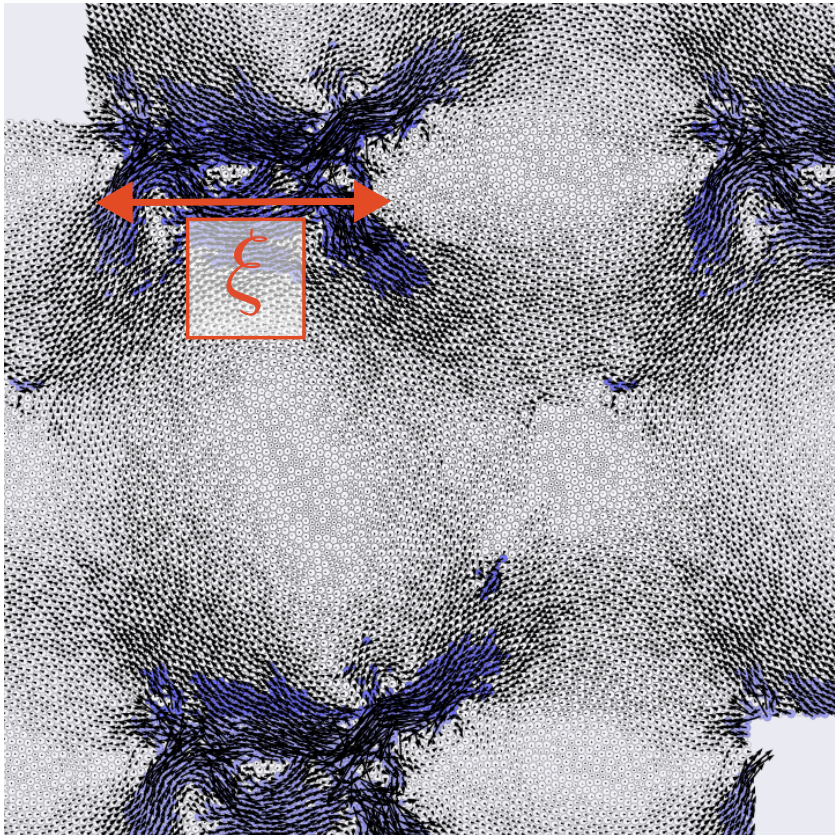
$$\eta \partial_t \gamma(\mathbf{r}, t) = \Sigma + \int_{\mathbf{r}'} \mathcal{G}(\mathbf{r} - \mathbf{r}') \gamma(\mathbf{r}', t) - \sigma^{\text{dis}}[\gamma(\mathbf{r}, t), \mathbf{r}]$$

Lin et al., PNAS 111, 14382 (2014)

- ▶ External stress  $\Sigma$ : Spatially uniform and time independent
- ▶ Local yield stress  $\sigma^{\text{dis}}[\gamma, \mathbf{x}]$ : Not explicitly depend on time (controlled solely by the applied total shear  $\gamma \rightarrow$  so is  $\gamma^p$ )
- ▶ Interaction kernel  $\mathcal{G}$ : Eshelby-type quadrupolar propagator (Nonmonotonicity is crucial to reproduce MS:  $\langle \Delta \gamma \rangle \sim N^{-x}$ )

# Yielding: A Non-eq. Criticality?

## Scaling ansatzes



- Interaction kernel:  $\mathcal{G} \sim \xi^0$  (non-monotonic)
  - Eshelby-like quadrupolar pattern  
( $\mathcal{G}(\mathbf{k}) = 4k_x^2 k_y^2 / k^4$  in  $\mathbf{k}$ -space)
- Correlation length:  $\xi \sim |\sigma - \sigma_Y|^{-\nu}$ 
  - Maximum spanning of avalanches
- Macroscopic strain rate:  $\dot{\gamma} \sim |\sigma - \sigma_Y|^\beta$ 
  - Regarded as the order parameter
- Avalanche lifetime:  $T \sim \xi^z$
- Cutoff avalanche size:  $S_c \sim \xi^{d_f}$ 
  - Characterized by fractal dimension  $d_f$

► Useful hyperscaling relations among them?

# Statistical Tilt Symmetry (STS)

- Special symmetry of the system -

## Introduction of "tilt"

$$\begin{aligned}\eta\partial_t\gamma(\mathbf{r}, t) &= \Sigma + \sigma^{\text{tilt}} + \int_{\mathbf{r}'} \mathcal{G}(\mathbf{r} - \mathbf{r}')\gamma(\mathbf{r}', t) - \sigma^{\text{dis}}[\gamma(\mathbf{r}, t), \mathbf{r}] \\ \Leftrightarrow \eta\partial_t\tilde{\gamma}(\mathbf{r}, t) &= \Sigma + \int_{\mathbf{r}'} \mathcal{G}(\mathbf{r} - \mathbf{r}')\tilde{\gamma}(\mathbf{r}', t) - \sigma^{\text{dis}}[\tilde{\gamma} - \int \mathcal{G}^{-1}\sigma^{\text{tilt}}, \mathbf{r}]\end{aligned}$$

Narayan and Fisher, Phys. Rev. B **48**, 7030 (1993); [Lin et al., PNAS \*\*111\*\*, 14382 \(2014\)](#).

- ▶ Tilt  $\sigma^{\text{tilt}}$ : random stress field with vanishing spatial average  
(tilted strain field:  $\tilde{\gamma}(\mathbf{r}) = \gamma(\mathbf{r}) + \int_{\mathbf{r}'} \mathcal{G}^{-1}(\mathbf{r} - \mathbf{r}')\sigma^{\text{tilt}}(\mathbf{r}')$ )
- ▶ Absorbed by the random local yield stress distribution  $\sigma^{\text{dis}}$
- ▶ On average (over randomness), tilt does not matter:  $\overline{\delta\tilde{\gamma}/\delta\sigma^{\text{tilt}}} = 0$

# Consequences of STS

- Scaling relations from susceptibility -

## *Susceptibility estimated by tilt*

$$\chi_1 \equiv \frac{\overline{\partial\gamma}}{\partial\sigma^{\text{tilt}}} = \frac{\overline{\partial(\tilde{\gamma} + \int \mathcal{G}^{-1} \sigma^{\text{tilt}})}}{\partial\sigma^{\text{tilt}}} \sim \mathcal{G}^{-1} \sim \xi^0$$

- Tilt does not play any role:  $\overline{\partial\tilde{\gamma}}/\partial\sigma^{\text{tilt}} = 0$
- Interactino kernel is nonmonotonic:  $\mathcal{G} \sim \xi^0$

## *Susceptibility estimated by global stress increment*

$$\chi_2 \equiv \frac{\Delta\gamma}{\Delta|\sigma - \sigma^Y|} \sim \frac{\xi^{d_f}/\xi^d}{\xi^{-1/\nu}} \sim \xi^{1/\nu+d_f-d}$$

- Perturbing  $\sigma$  induces avalanche with size  $\xi \sim |\sigma - \sigma_Y|^{-\nu}$
- Strain: (avalanche volume  $\xi^{d_f}$ ) / (total volume  $\xi^d$ )

Narayan and Fisher, Phys. Rev. B **48**, 7030 (1993); Lin et al., PNAS **111**, 14382 (2014).

► Hyperscaling relation:  $\chi_1 \sim \chi_2 \Rightarrow \nu = 1/(d - d_f)$



# Simple Scaling Argument

- Other useful relations -

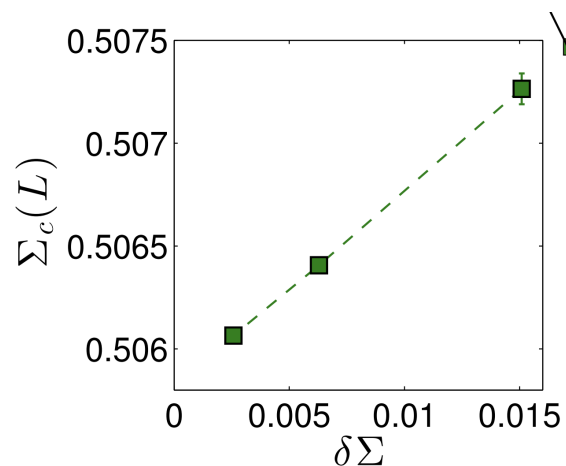
## Scaling relation for strain rate

$$\dot{\gamma} = \frac{\gamma}{T} \sim \frac{\xi^{d_f} / \xi^d}{\xi^z} \sim \xi^{d_f - d - z}$$

$$\dot{\gamma} \sim |\sigma - \sigma_Y|^\beta \sim \xi^{-\beta/\nu}$$

$$\therefore \beta = \nu(z + d - d_f)$$

## Determination of the intrinsic yield stress



$$\xi \sim |\sigma - \sigma_Y|^{-\nu} \Leftrightarrow \langle \sigma \rangle(\xi) = \sigma_Y + k_1 \xi^{-1/\nu}$$

$$\Delta_\sigma(\xi) \sim \langle \sigma \rangle(\xi) - \sigma_{rmY} \sim k_2 \xi^{-1/\nu}$$

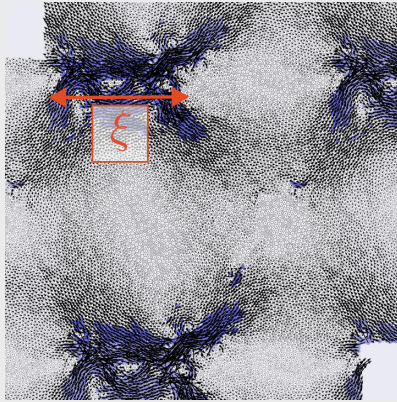
$$\therefore \langle F \rangle(\xi) = F_c^* + k_3 \sigma_F(\xi)$$

( $\Delta_\sigma(\xi)$ : Standard deviation of  $\sigma(\xi)$ )

Vandembroucq et al., Phys. Rev. E 70, 051101 (2004)

# Yielding: A Non-eq. Criticality?

## Scaling ansatzes



- Interaction kernel:  $\mathcal{G} \sim \xi^0$  (non-monotonic)  
( $\mathcal{G}(\mathbf{k}) = 4k_x^2 k_y^2 / k^4$  in  $k$ -space)
- Correlation length:  $\xi \sim |\sigma - \sigma_Y|^{-\nu}$
- Macroscopic strain rate:  $\dot{\gamma} \sim |\sigma - \sigma_Y|^\beta \sim \xi^{-\beta/\nu}$
- Avalanche lifetime:  $T \sim \xi^z$
- Cutoff avalanche size:  $S_c \sim \xi^{d_f}$

## Hyperscaling relation

- Correlation length:  $\nu = 1/(d - d_f)$
- Strain rate:  $\beta = \nu(z + d - d_f)$
- Critical stress estimation:  $\langle \sigma \rangle(\xi) = \sigma_Y + k\Delta_\sigma(\xi)$

► These relations were verified using continuum model

Lin et al., PNAS 111, 14382 (2014)

► No verification for particle-based data -> WHY?



# Yielding: A Non-eq. Criticality?

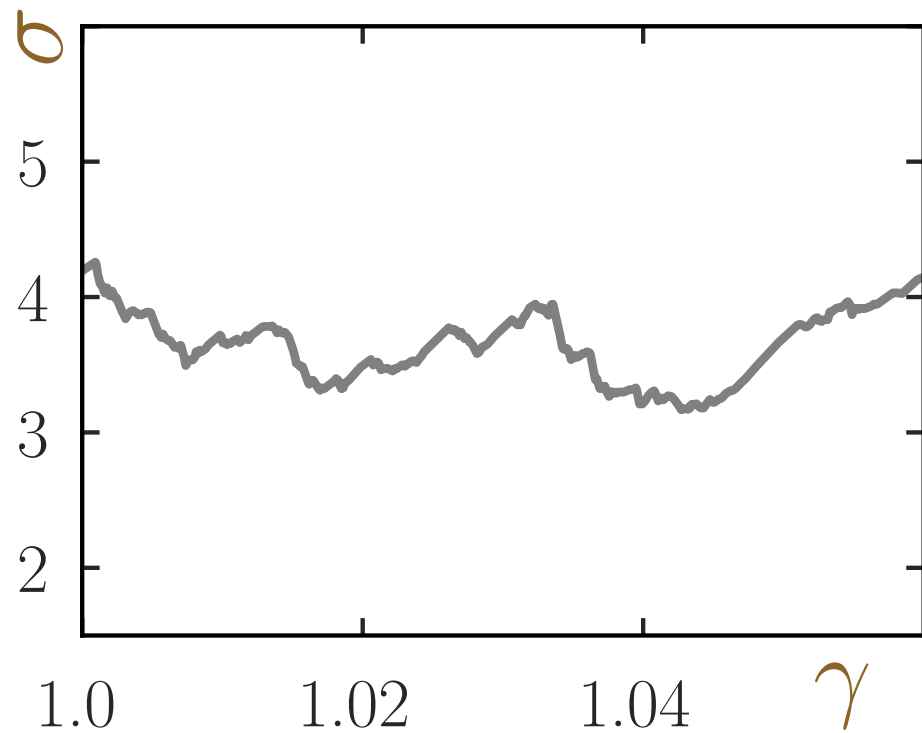
## Hyperscaling relation

- Correlation length:  $\nu = 1/(d - d_f)$
  - Strain rate:  $\beta = \nu(z + d - d_f)$
  - Critical stress estimation:  $\langle \sigma \rangle(\xi) = \sigma_Y + k \Delta_\sigma(\xi)$
- ▶ **Red values** can be measured by quasistatic simulation  
Oyama, Mizuno, and Ikeda, PRE **104**, 015002 (2021)
- ▶ **Critical stress  $\sigma_Y$**  is determined!  
(HB law:  $\dot{\gamma} \sim |\sigma - \sigma_Y|^\beta$ )
- ▶ **HB exponent  $\beta$**  can be obtained if  $z$  is measured, but...

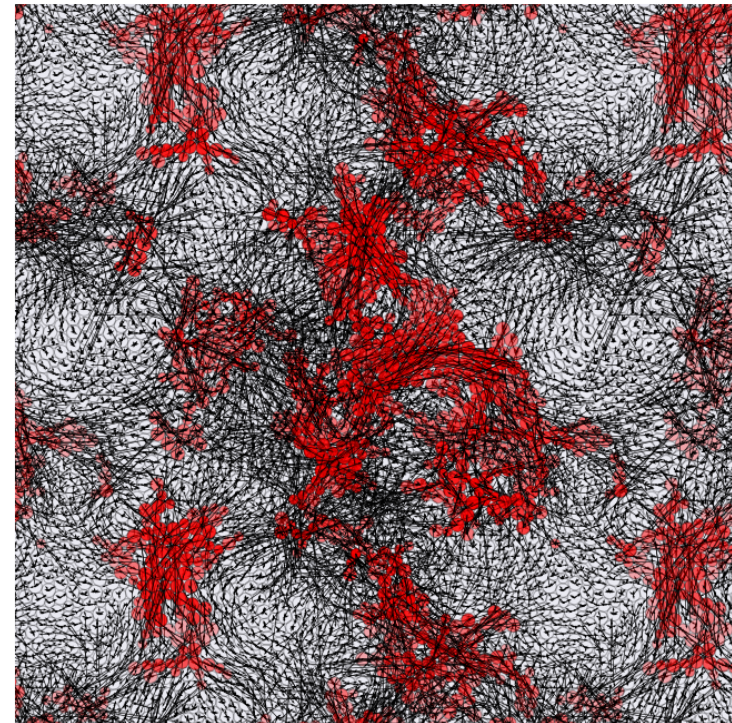
# Dynamical information?

- Inaccessible information -

Stress-strain curve



"Displacement" field



- ▶ Avalanche lifetime:  $T \sim \xi^z$
- ▶ Both  $T$  and  $\xi$  cannot be extracted unambiguously
- ▶ Cannot utilize this relation for particle data...

# Our Strategy and Aim

- To by-pass the problem above... -

Utilize the microscopic structures  
that are available only in MD simulations

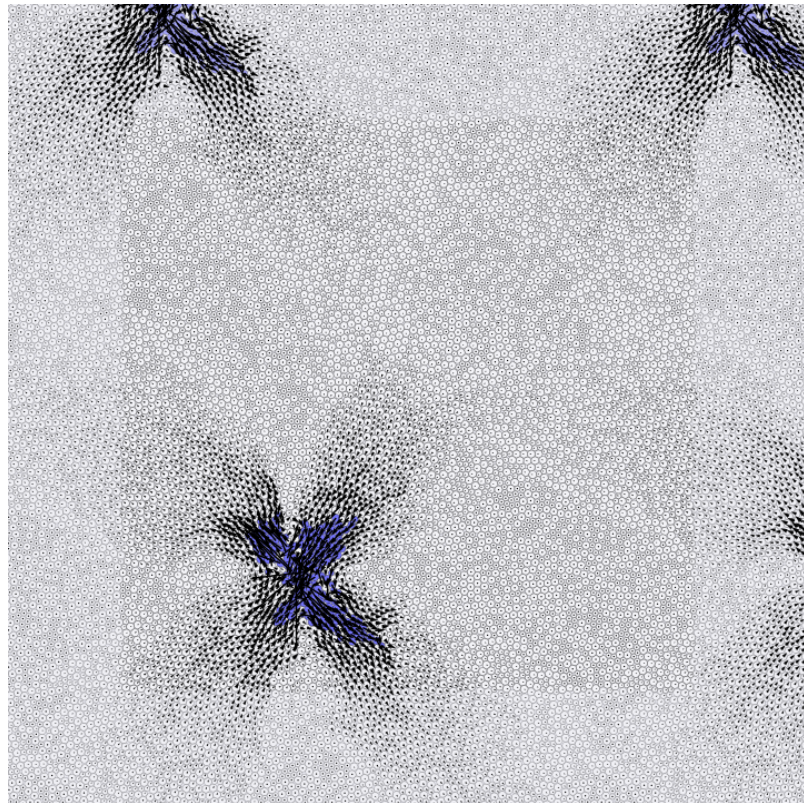
▶ **(Instantaneous) Normal Modes**



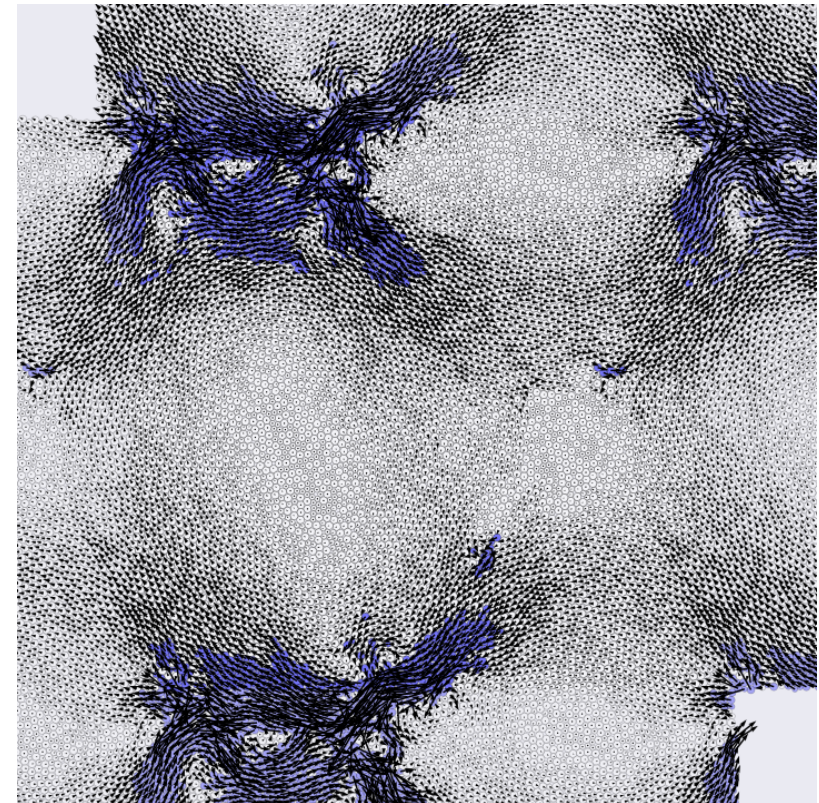
# Shear Transformations (STs)

- Elementary processes of plasticity -

Single ST



Avalanche of STs



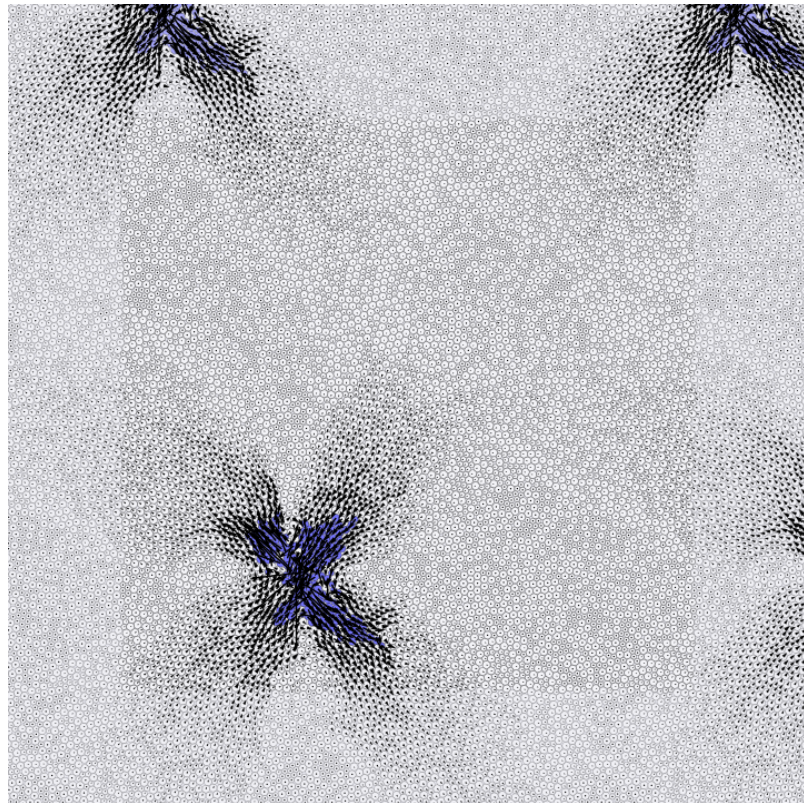
- ▶ Considered to be the elementary process
- ▶ Sometimes form "avalanches"



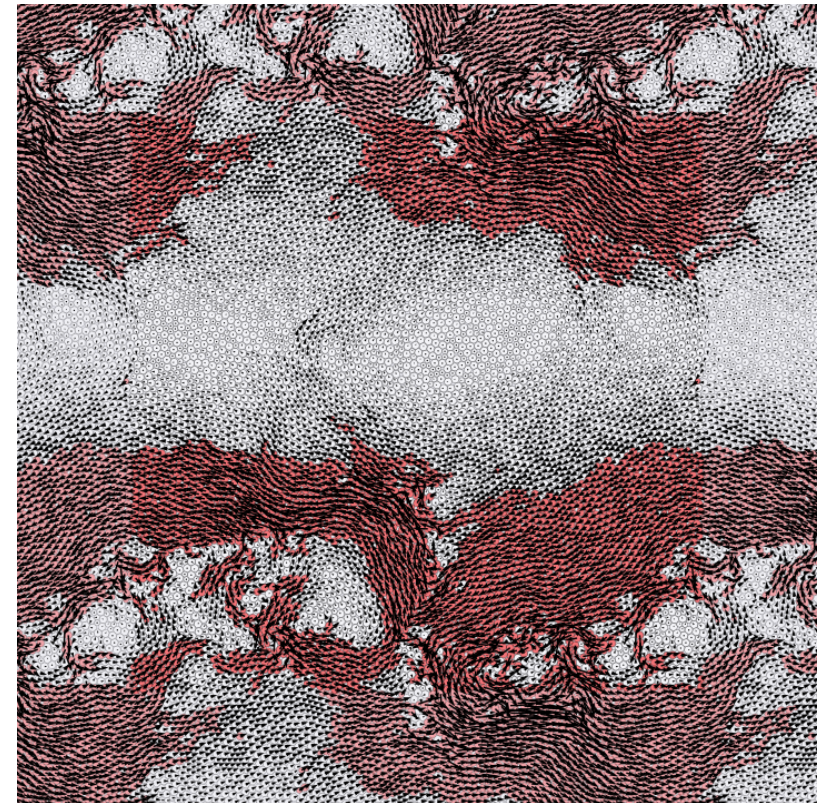
# Shear Transformations (STs)

- Elementary processes of plasticity -

Single ST



System-spanning Avalanche



- ▶ Considered to be the elementary process
- ▶ Sometimes form "avalanches"

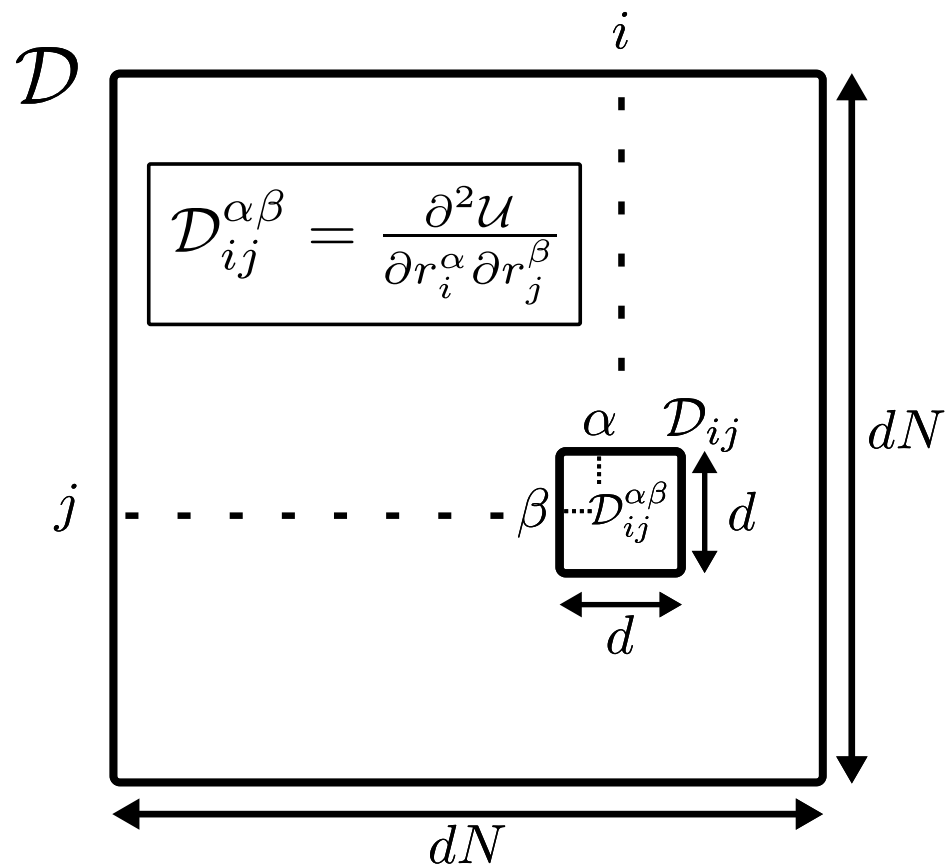


# Knowledge Under Quasistatic Shear

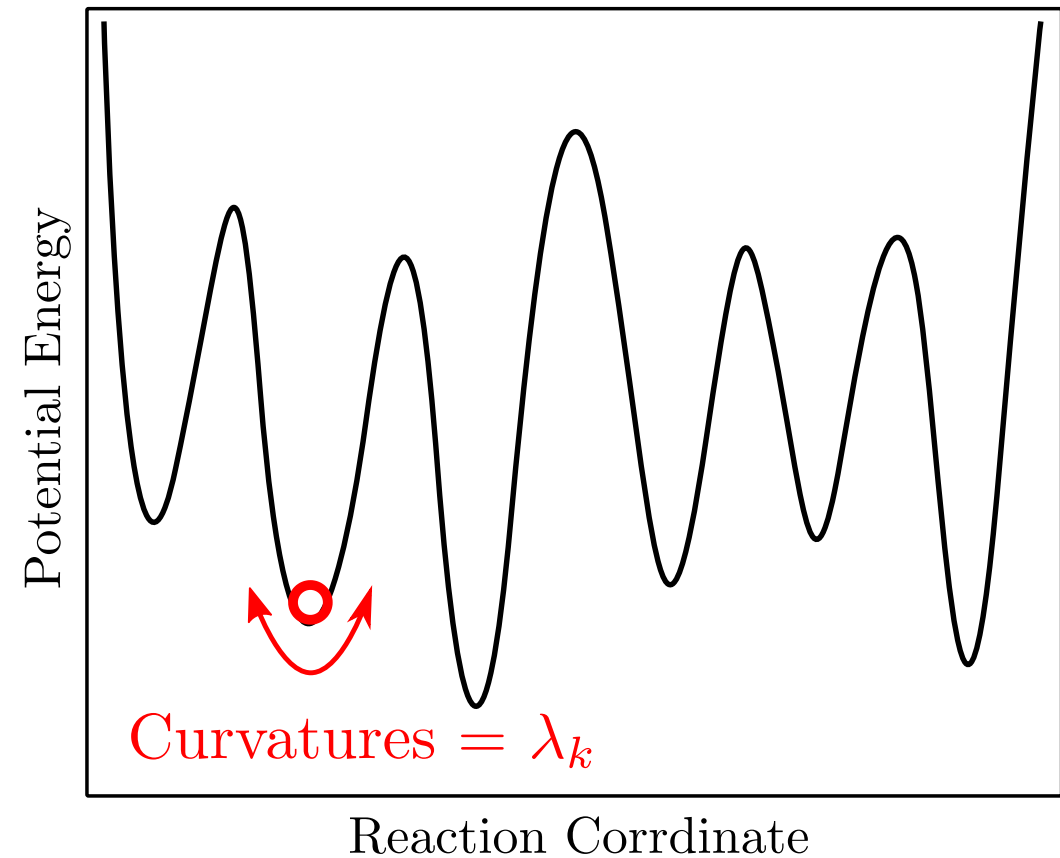
- How are plastic events evoked? -

# Normal Mode Analysis

## Dynamical Matrix



## Potential energy landscape (PEL)

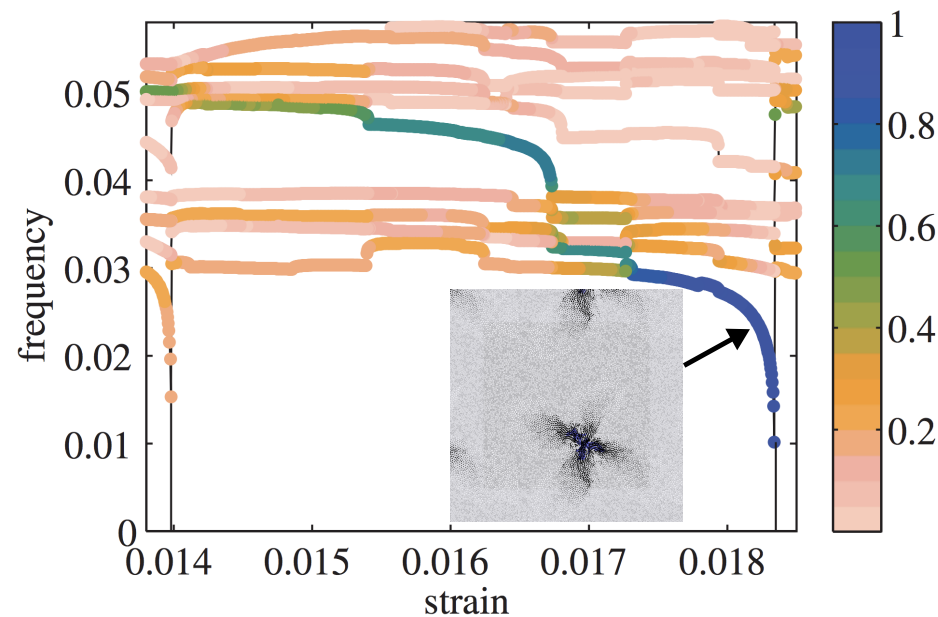


- ▶ Measured with no noise sources (basin bottom of PEL)
- ▶ All eigenvalues  $\lambda_k$  are positive in this case
- ▶ Eigenvalues  $\lambda_k$  give the curvatures of the PEL
- ▶  $\omega_k \equiv \sqrt{\lambda_k}$ : eigen-frequencies along the curvature

# "Cause" of Plastic Events

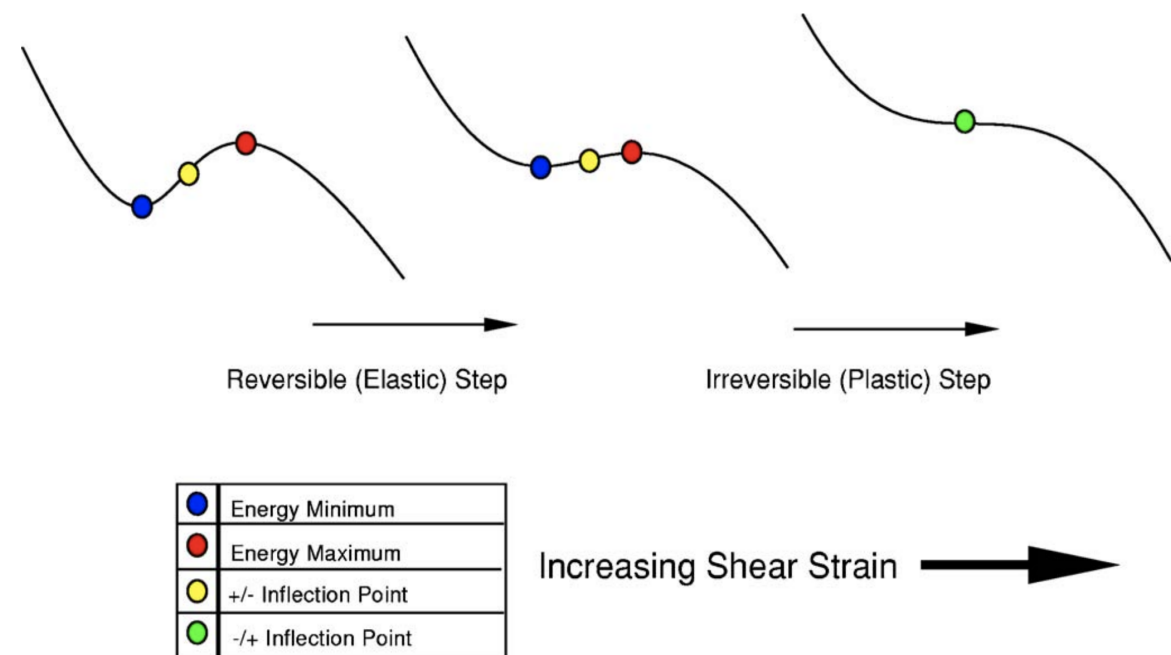
- Under athermal quasistatic shear -

## Evolution of normal modes



Manning and Liu, Phys. Rev. Lett. **107**,108302 (2011)

## Evolution of potential energy landscape



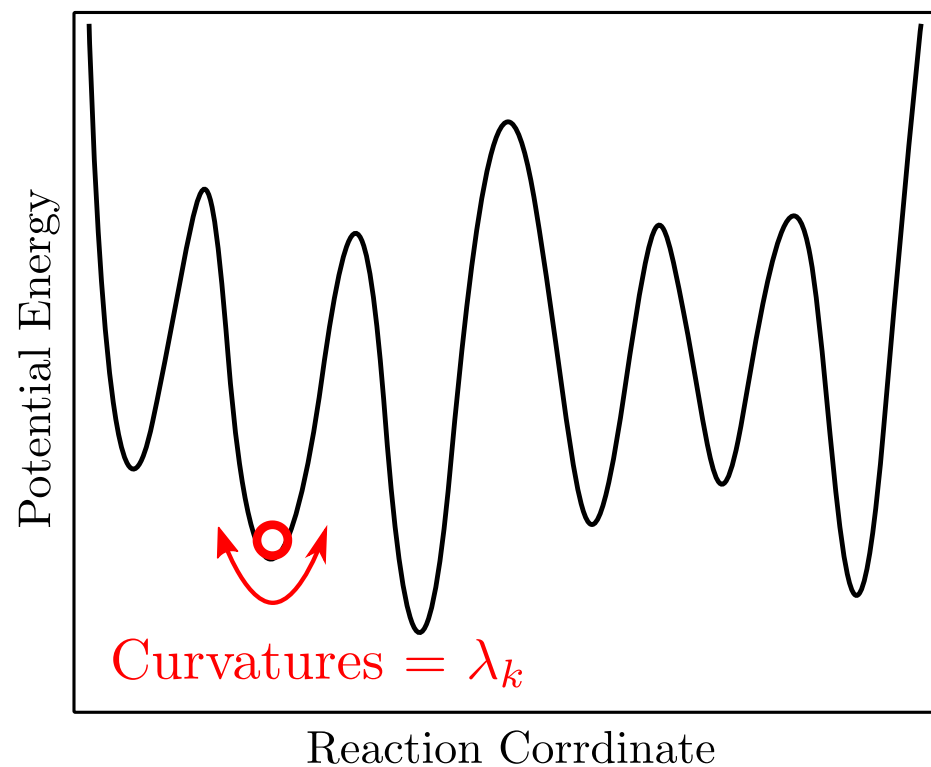
Maloney and Lemaître, Phys. Rev. E **74**,016118 (2006)

- ▶ Lowest eigenvalue goes to zero just before plastic event
- ▶ The decaying mode has a quadrupolar pattern
- ▶ Disappearance of energy basin: saddle-node bifurcation
- ▶ What if under **finite-rate** shear?

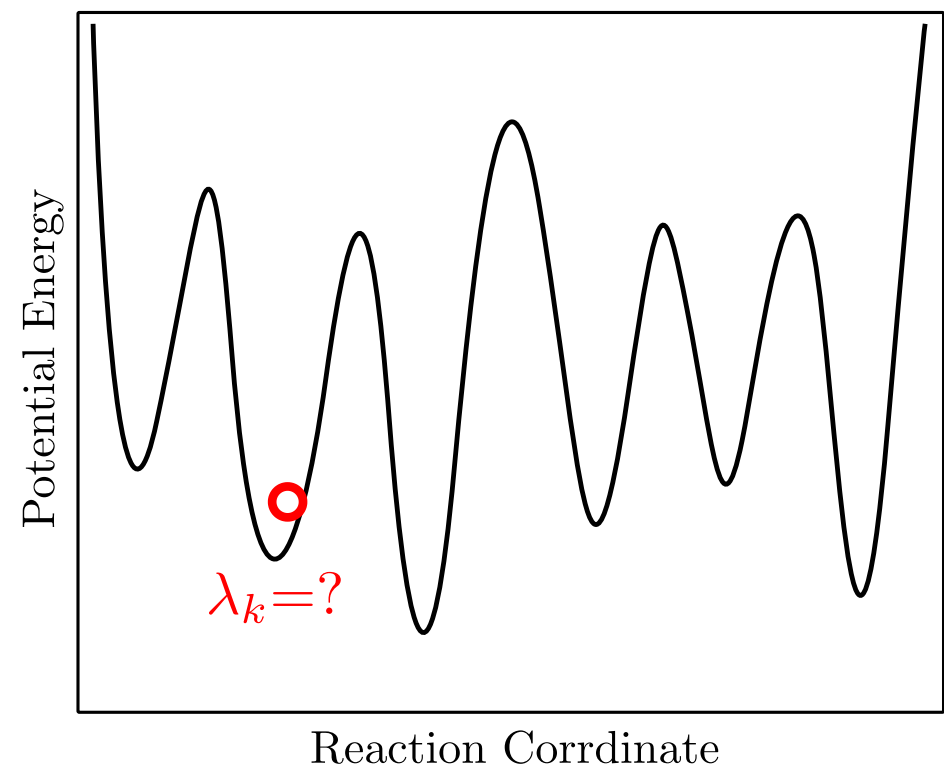
# Normal Modes Under Finite-rate Shear

- Generalization of normal mode analysis -

Standard NM analysis



NM analysis under finite-rate shear

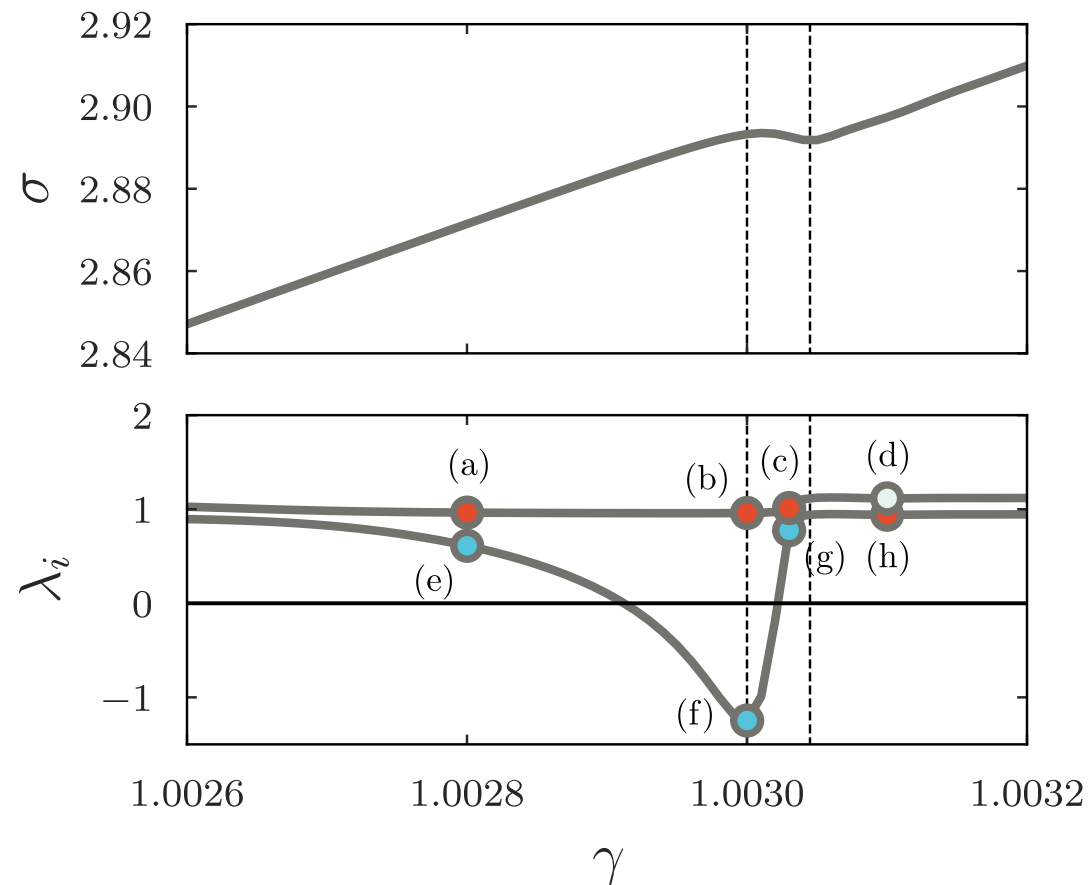


► What do eigenmodes stand for in such a situation?

# Emergence of Negative Mode?

- Cause of plasticity under finite-rate shear -

At very slow rate:  $\dot{\gamma} = 2 \times 10^{-5}$



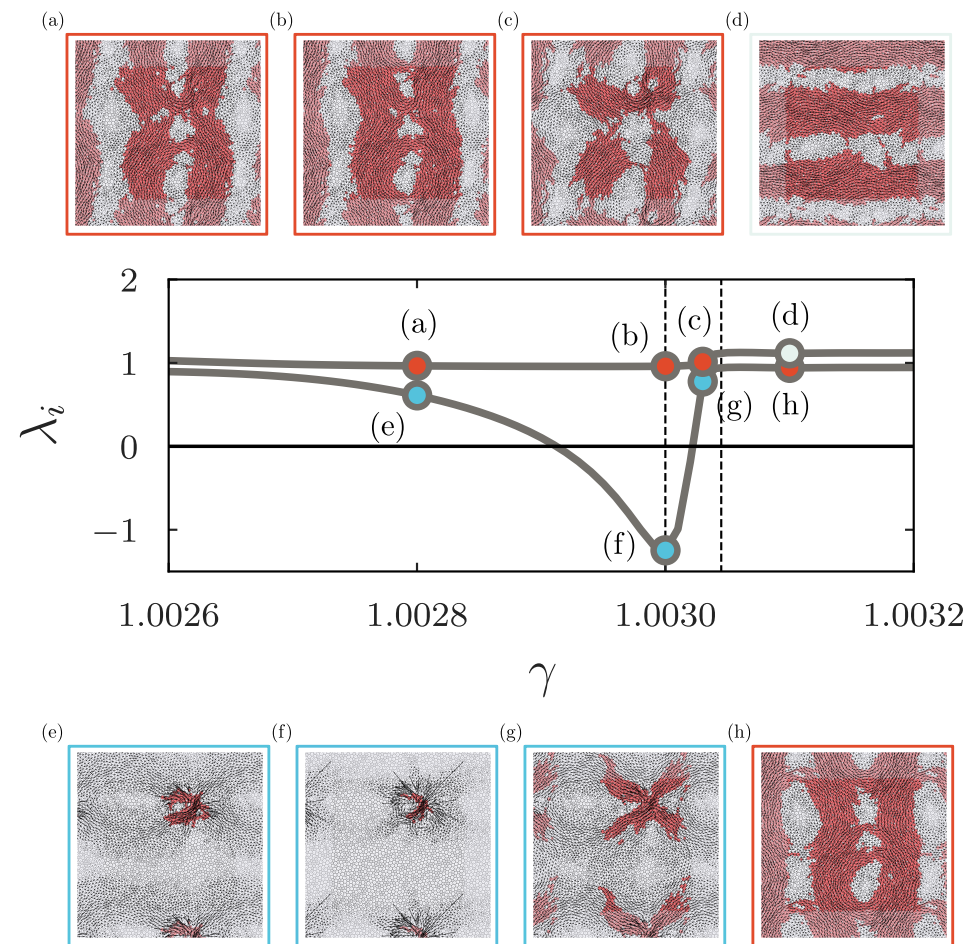
- ▶ Lowest eigenvalue goes down similarly to quasistatic case
- ▶ No stress drop (plasticity) at the onset of  $\lambda_1 = 0$



# Emergence of Negative Mode?

- Cause of plasticity under finite-rate shear -

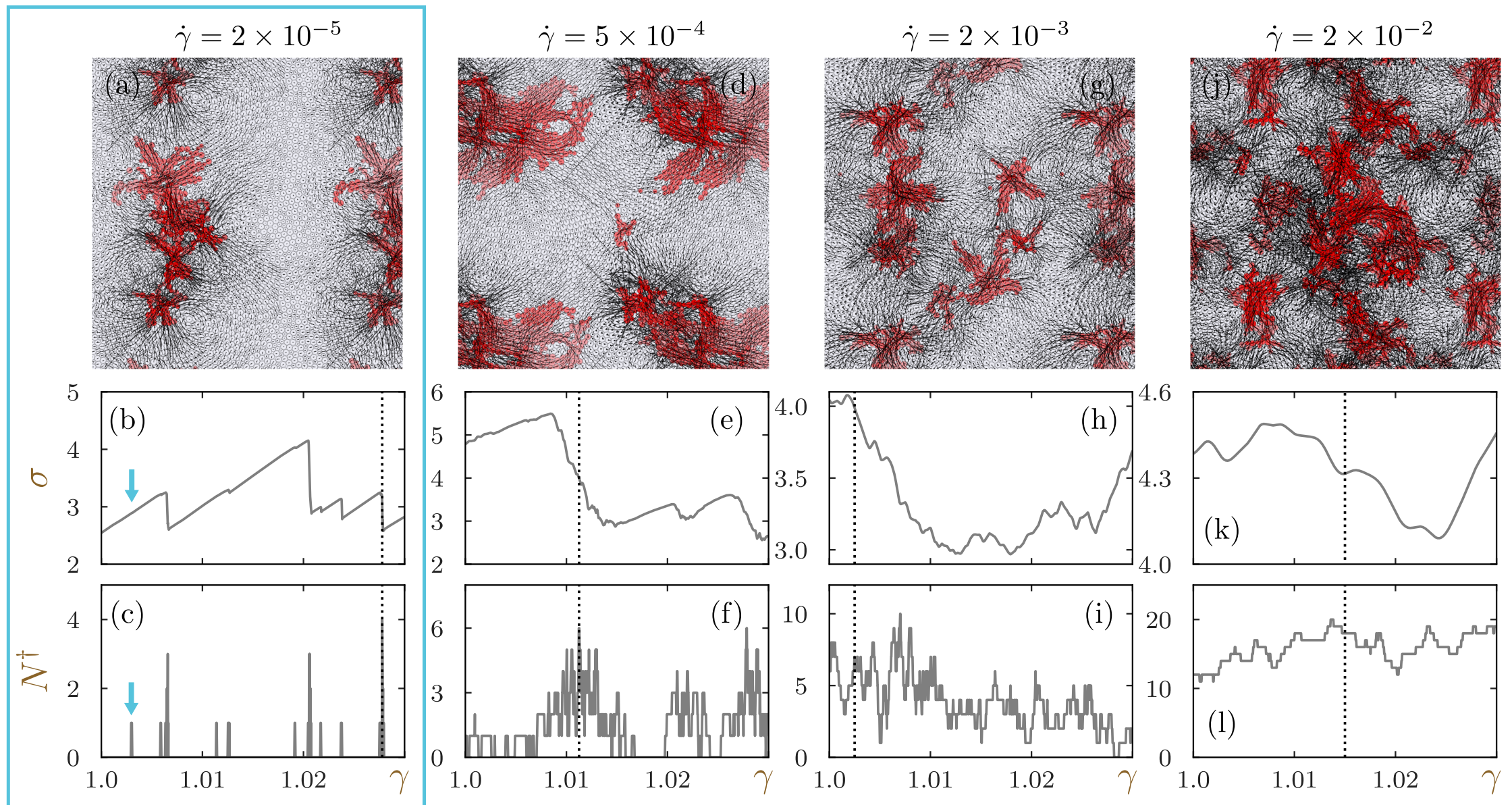
At very slow rate:  $\dot{\gamma} = 2 \times 10^{-5}$



- ▶ Mode crossing zero: ST-inducing eigenvector -> phonon
- ▶ **Negative** normal mode corresponds to "active" ST

# Number of Negative Modes $N^\dagger$

- Shear rate dependent change in morphology of avalanches -

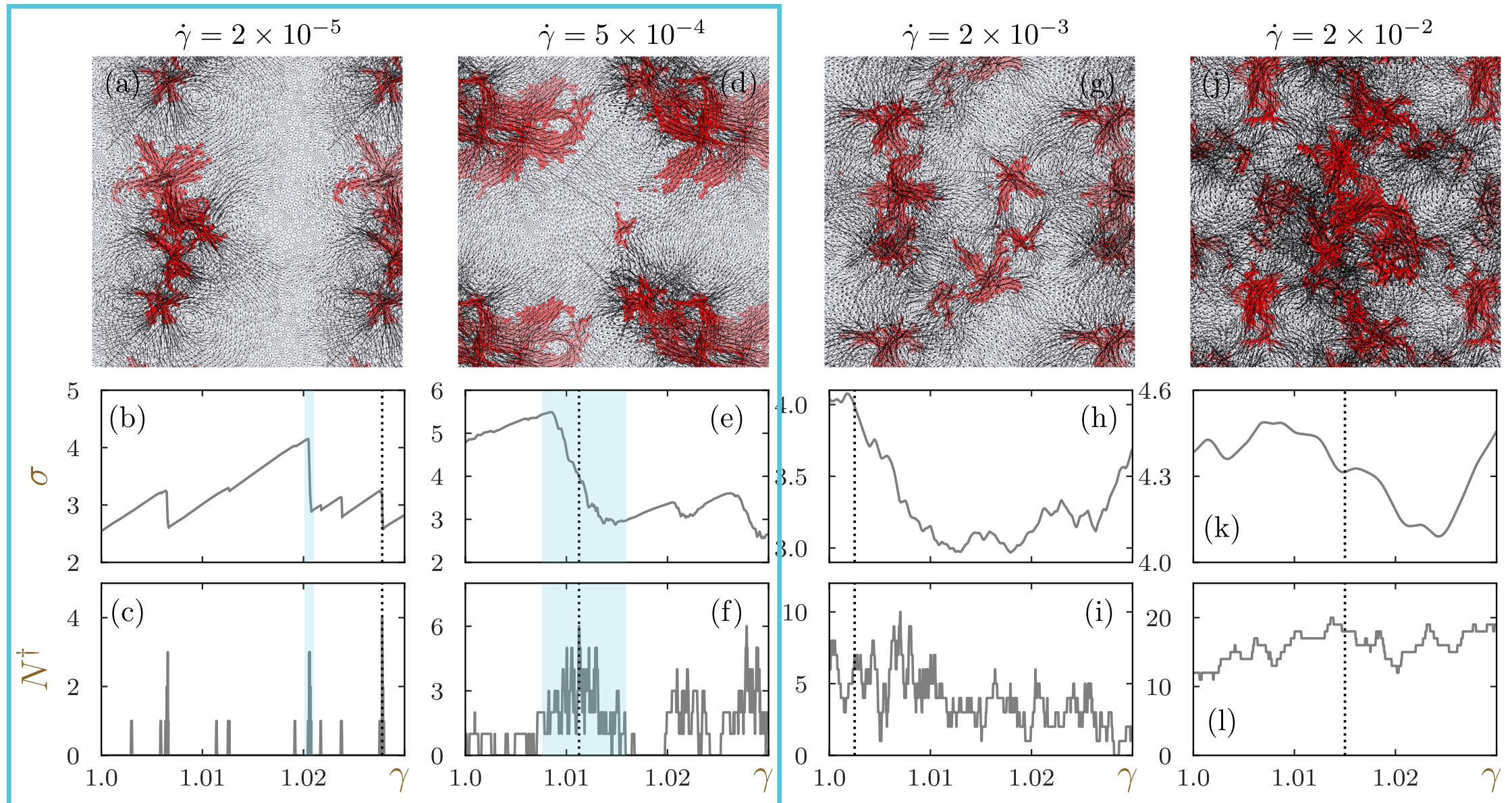


► Sometimes form avalanches: large stress drop and  $N^\dagger > 1$



# Number of Negative Modes $N^+$

- Shear rate dependent change in morphology of avalanches-

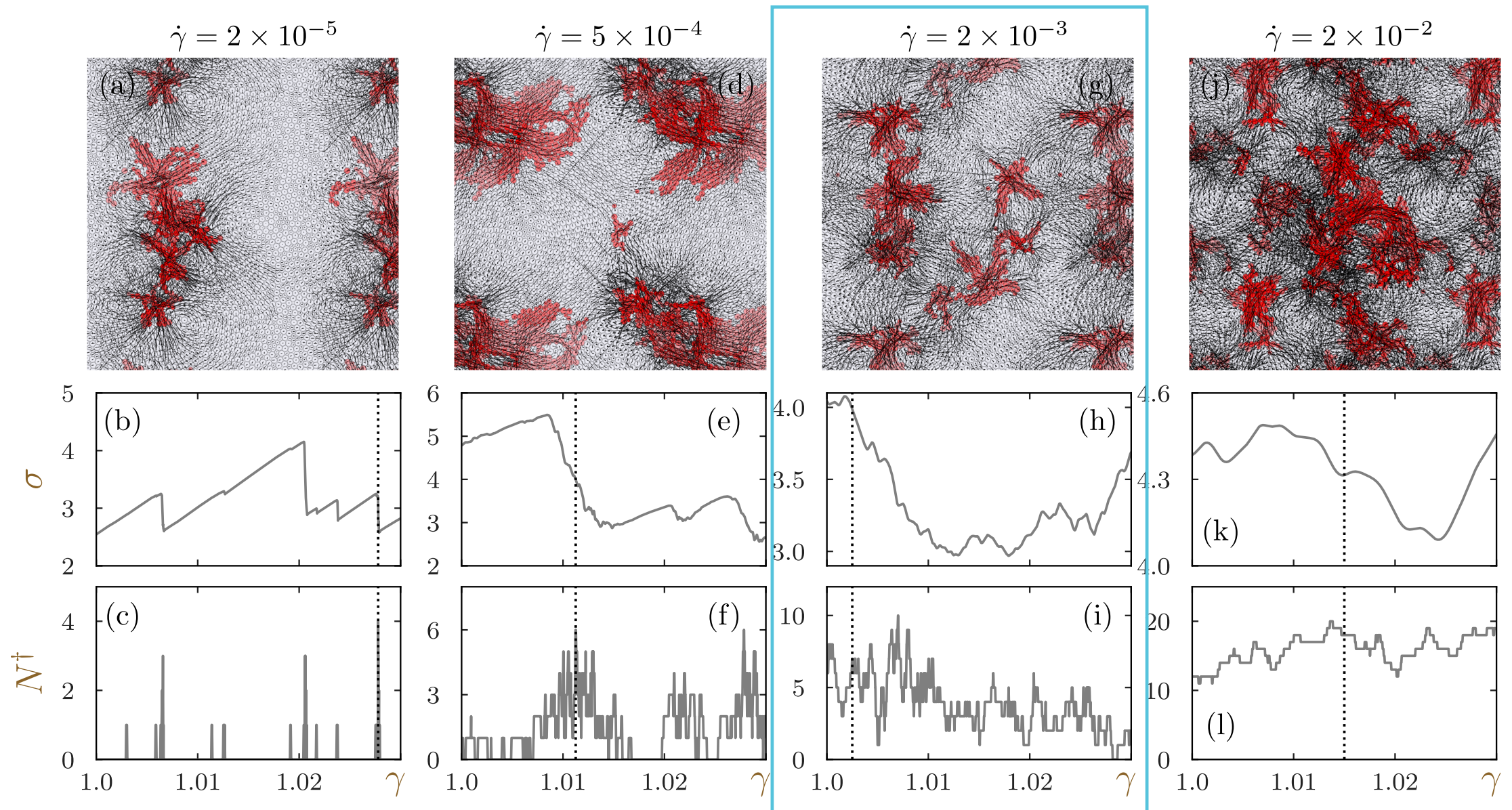


► Stress drop events span broad (abscissa :  $\gamma$ , not  $t$ )



# Number of Negative Modes $N^+$

- Shear rate dependent change in morphology of avalanches -

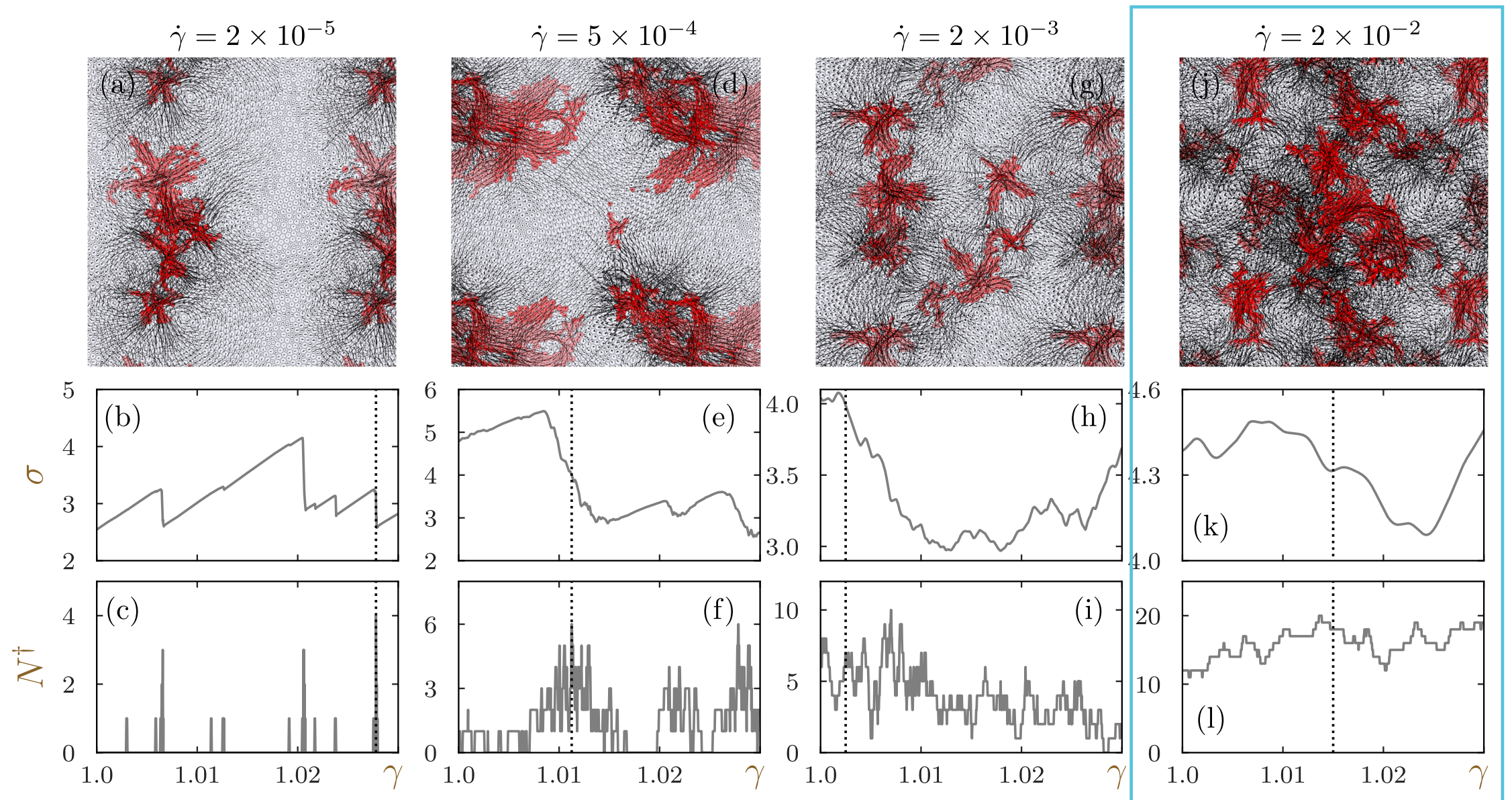


► Multiple avalanches (cause of decrease in  $\xi$ )



# Number of Negative Modes $N^+$

- Shear rate dependent change in morphology of avalanches-

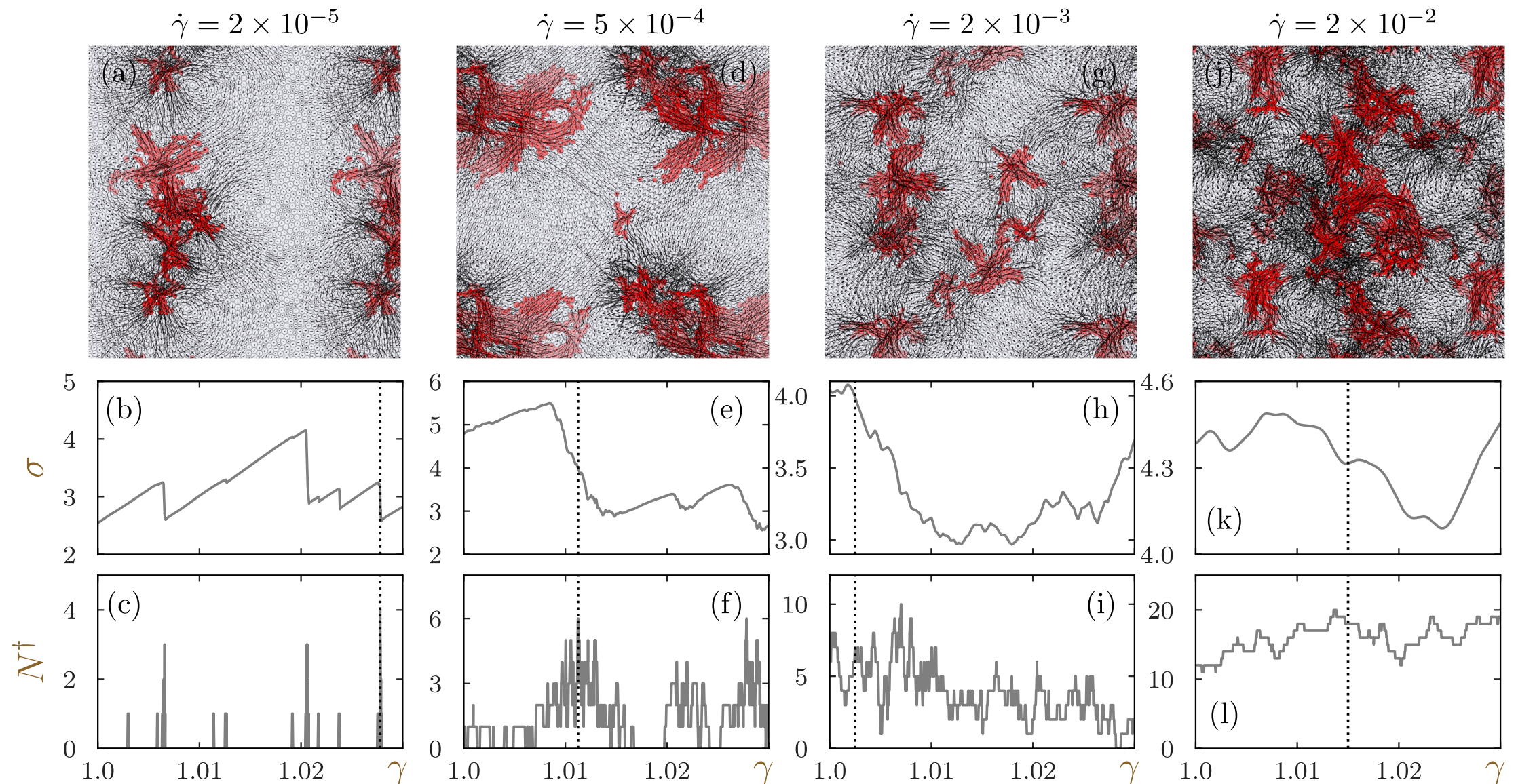


► Complicated spatial pattern (avalanches cannot be identified)



# Number of Negative Modes $N^\dagger$

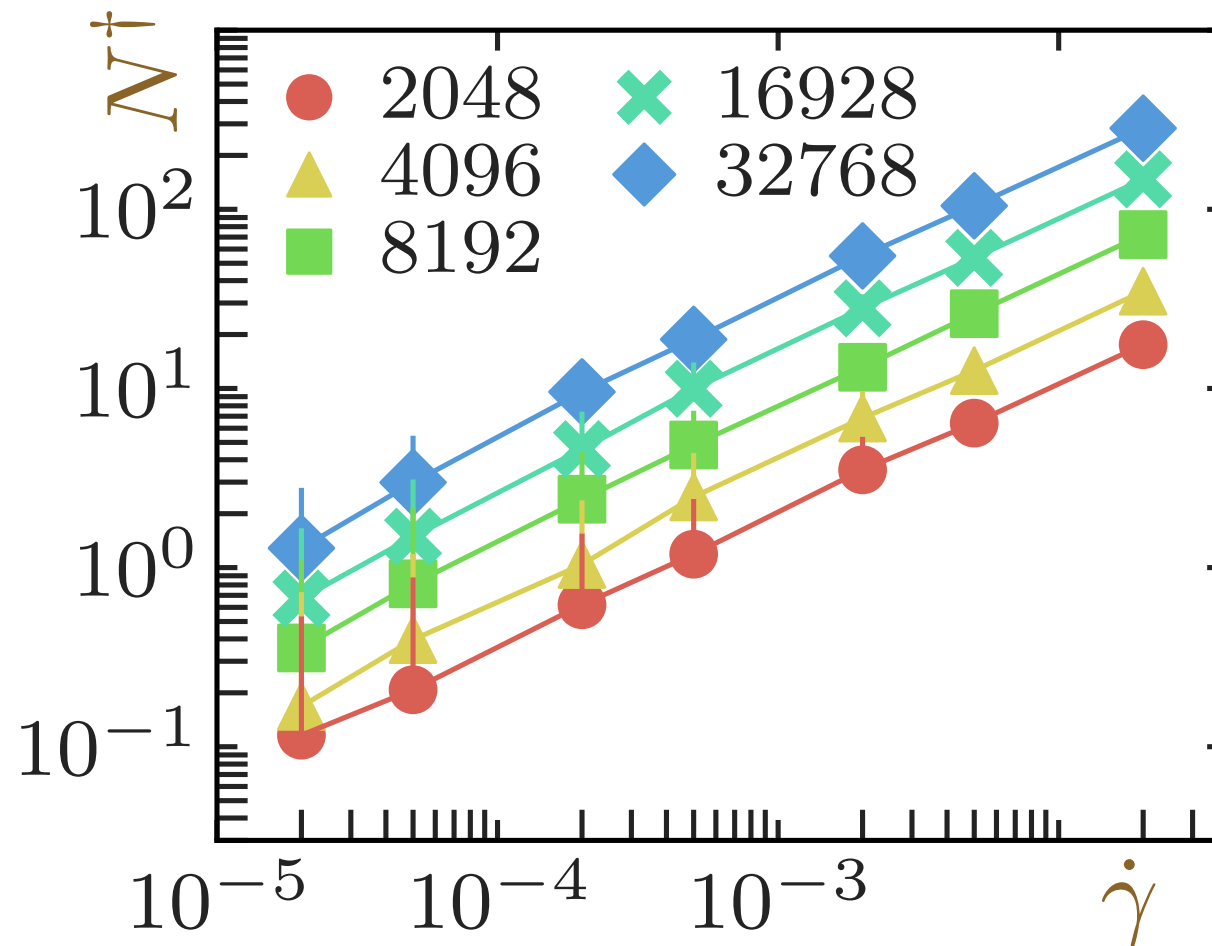
- Shear rate dependent change in morphology of avalanches -



► Information of shape and number of avalanches is encoded in  $N^\dagger$ ?

# Statistics of Number of Negative Modes $N^+$

- Structural information about plasticity -

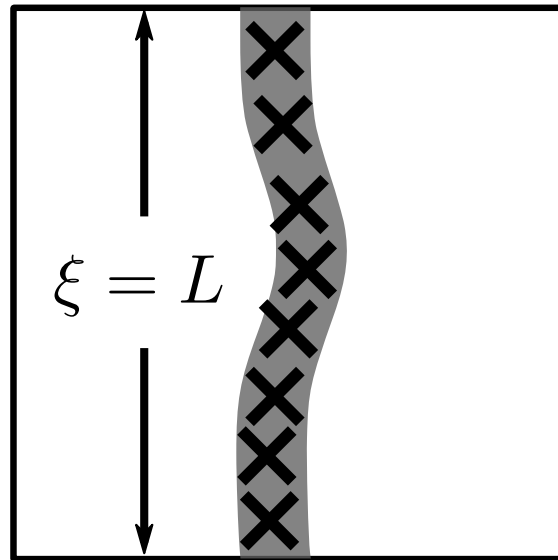


► Power-law function of  $\dot{\gamma}$ ?

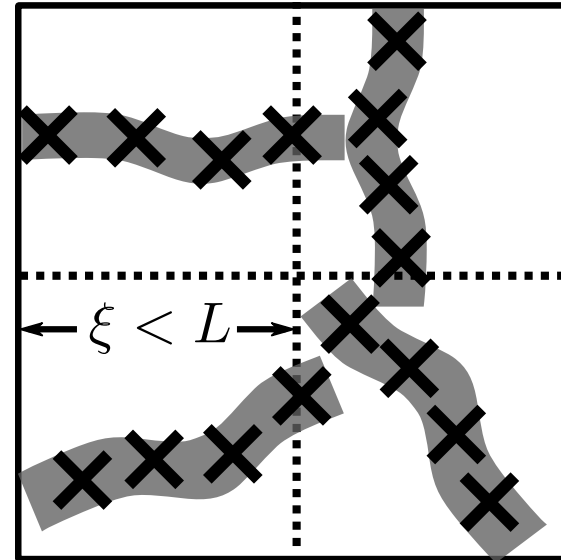
# Scaling Estimation of $N^\dagger$

- Plastic "structures" indicate mechanics -

$$\xi = L$$



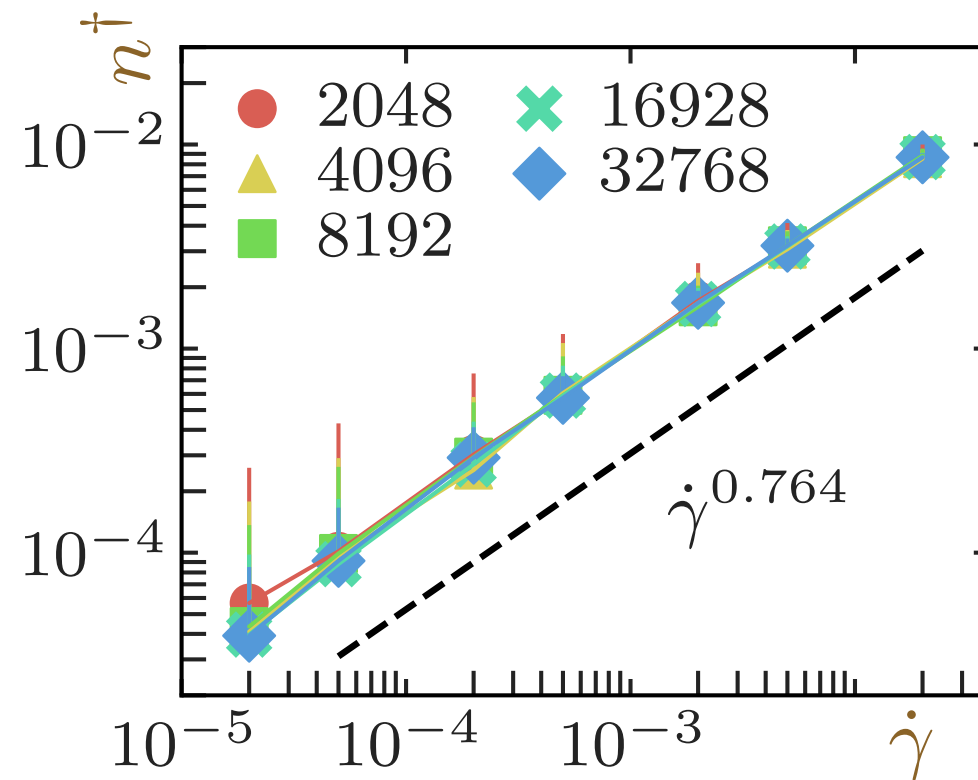
$$\xi < L$$



- ▶ # of avalanches:  $N_{\text{ava}} \sim L^d / \xi^d$   
White and Dahmen, PRL **91**, 085702 (2003), Lin et al., PNAS **111**, 14382 (2014)
- ▶ # of STs per avalanche:  $N_{\text{ST}/\text{ava}} \sim \xi^{d_f}$
- ▶  $N^\dagger = N_{\text{ava}} \times N_{\text{ST}/\text{ava}} \sim L^d \xi^{d_f - d} \sim N \dot{\gamma}^{1/\beta}$
- ▶ Number density:  $n^\dagger \equiv N^\dagger / N \sim N^0 \dot{\gamma}^{1/\beta}$

# Number Density of Negative Modes $n^\dagger$

- Validation of scaling law 1 -



$$n^\dagger \sim N^0 \dot{\gamma}^{1/\beta}$$

- ▶  $n^\dagger$  for different  $N$  are collapsed as predicted!
- ▶  $\beta$  is determined to be  $\beta \approx 1/0.764 \approx 1.31$

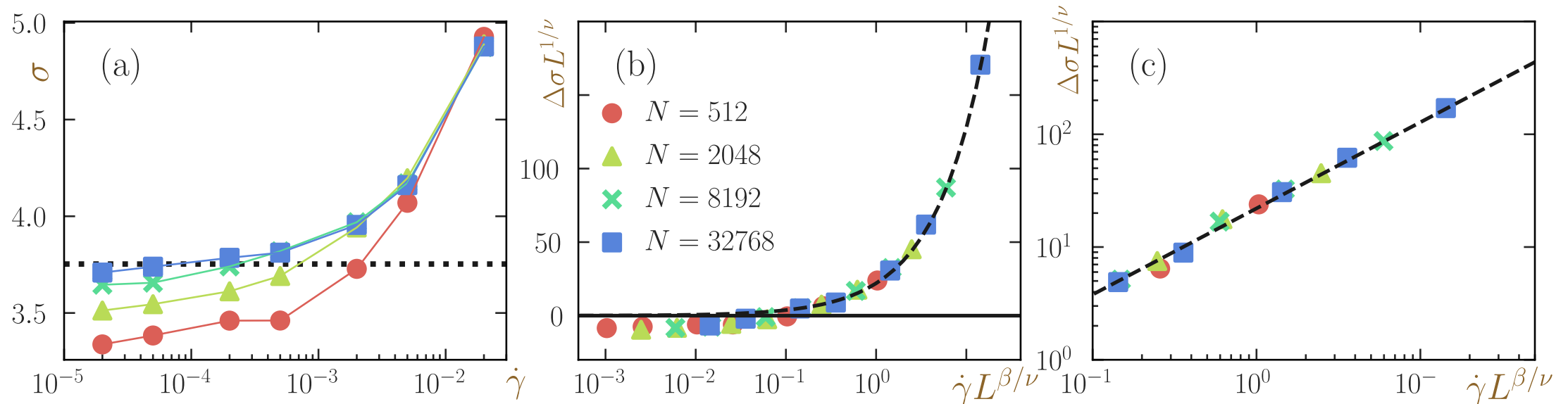
# Scaling Collapse of Flow Curves

- Validation of scaling law 2 -

Unscaled plot

Scaled semi-log plot

Scaled log-log plot



$$\begin{aligned} \dot{\gamma} &\sim \Delta\sigma^\beta f(\Delta\sigma/\Delta\sigma_0(L)) \\ &\sim L^{-\beta/\nu} (\Delta\sigma \cdot L^{1/\nu})^\beta f(\Delta\sigma L^{1/\nu}) \\ \Leftrightarrow \dot{\gamma} L^{\beta/\nu} &\sim (\Delta\sigma \cdot L^{1/\nu})^\beta f(\Delta\sigma L^{1/\nu}) \end{aligned}$$

- ▶ Beautiful collapse with  $\beta$  obtained by negative NM analysis
- ▶ Negative modes serve as **the structural signature** of HB law



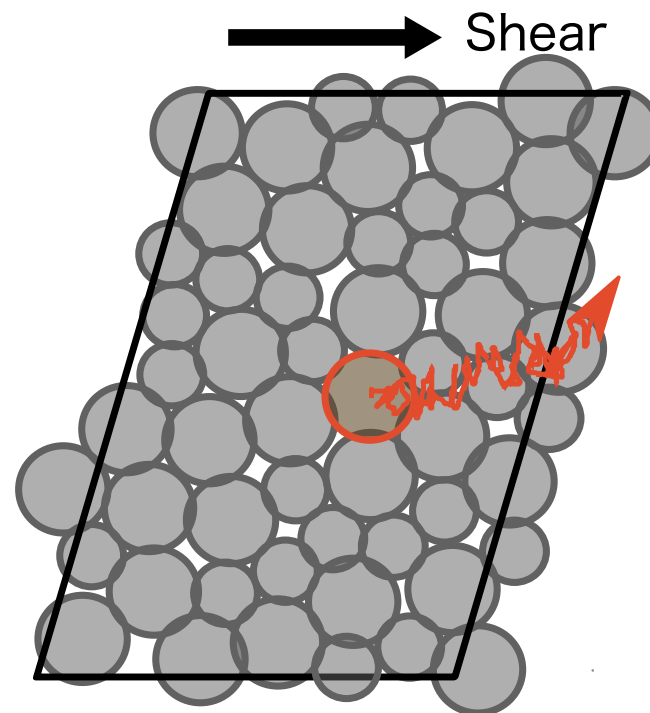
# Effect of Structural Failure: Dynamical Aspect

- A distinct correlation length emerges? -

Oyama, Kawasaki, Kim, and Mizuno, in preparation

# Effective Diffusion under Shear

- Purely mechanically induced diffusivity -



- ▶ Diffusive motion in perpendicular direction to shear
- ▶ Quantified by mean squared displacements (MSD)  $\Delta^\perp$ :

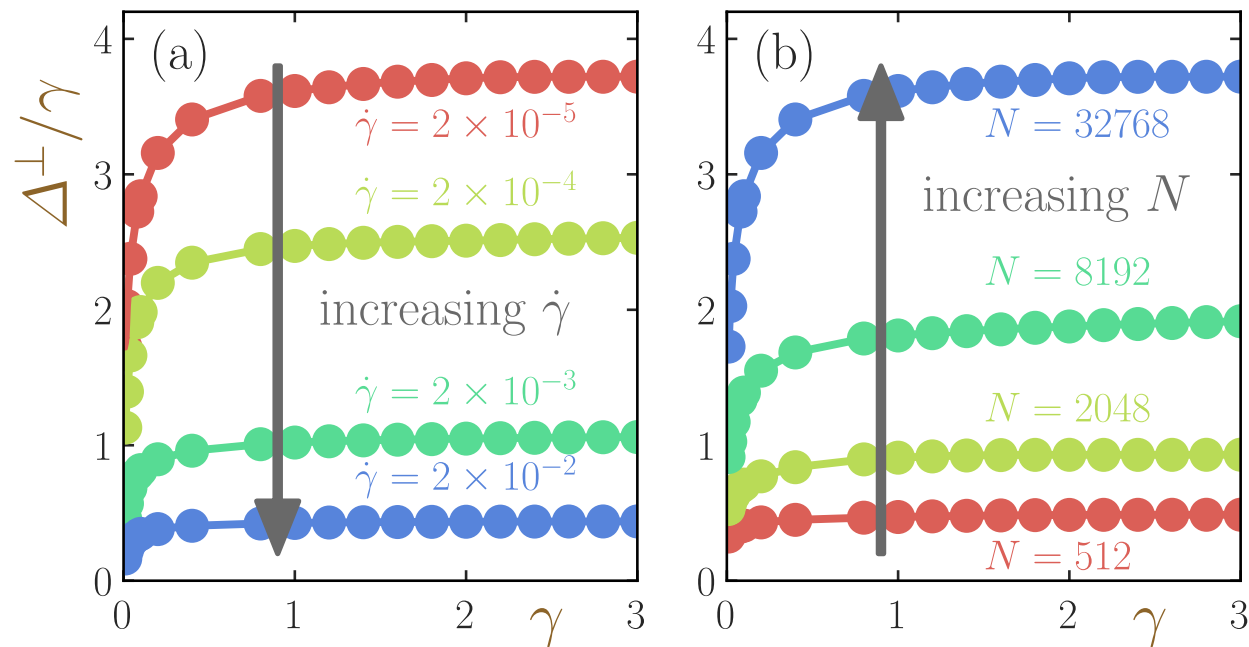
$$\Delta^\perp(t) \equiv \frac{1}{N} \sum_i \langle y_i(t_0 + t) y_i(t_0) \rangle_{t_0}$$

# Mean Squared Displacements

- Shear-rate dependent dynamical response -

Constant  $N$   
( $N = 32768$ )

Constant  $\dot{\gamma}$   
( $\dot{\gamma} = 2 \times 10^{-5}$ )

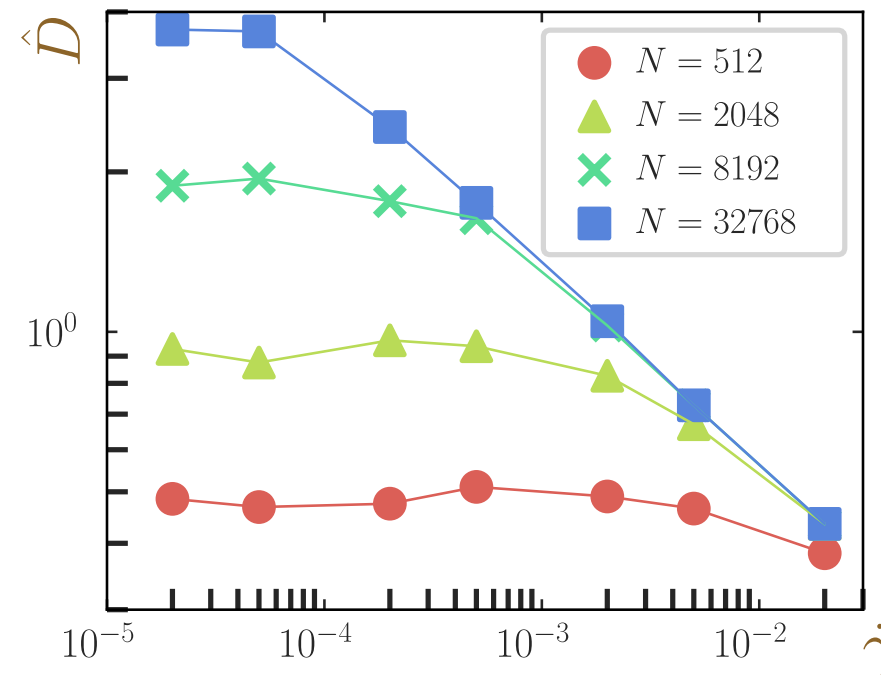


- ▶  $\Delta^\perp$  decreases with shear rate  $\dot{\gamma}$
- ▶  $\Delta^\perp$  increases with system size  $N$
- ▶ Quantified by per-strain diffusion constant

$$\hat{D} \equiv D^\perp / \dot{\gamma} = \lim_{\gamma \rightarrow \infty} \Delta^\perp / \gamma$$

# Per-strain Diffusion Constant

- Total parameter dependence -



- ▶  $\hat{D}$  decreases with shear rate as:  $\hat{D}(\dot{\gamma} \gg 0) \sim \dot{\gamma}^{-\nu}$ ?
- ▶  $\hat{D}$  increases with system size as:  $\hat{D}_0 \equiv \hat{D}(\dot{\gamma} \rightarrow 0) \sim L$
- ▶ Consistent with a previous work

Lemaître and Caroli, Phys. Rev. Lett. **103**, 065501 (2009)

# Summary

- Take-home messages -

- ☑ Structural failures of glasses: yielding criticality
  - ▶ Closely related to marginal stability
- ☑ Universal rheological law: Herschel-Bulkley law
  - ▶ Governed by the correlation length  $\xi$
- ☑ Shear-induced self-diffusion dynamics active STs
  - ▶ Can be governed by another length  
(depending on dissipation mechanism)

# Overview

- What should be done next? -

- Checking the "universality" of the finding
  - ▶ Potentials, dissipation sources, ...
- Taking into account thermal fluctuations
  - ▶ Phase diagram gets complicated
- Thermal relaxation without shear?
  - ▶ Is there any connection?