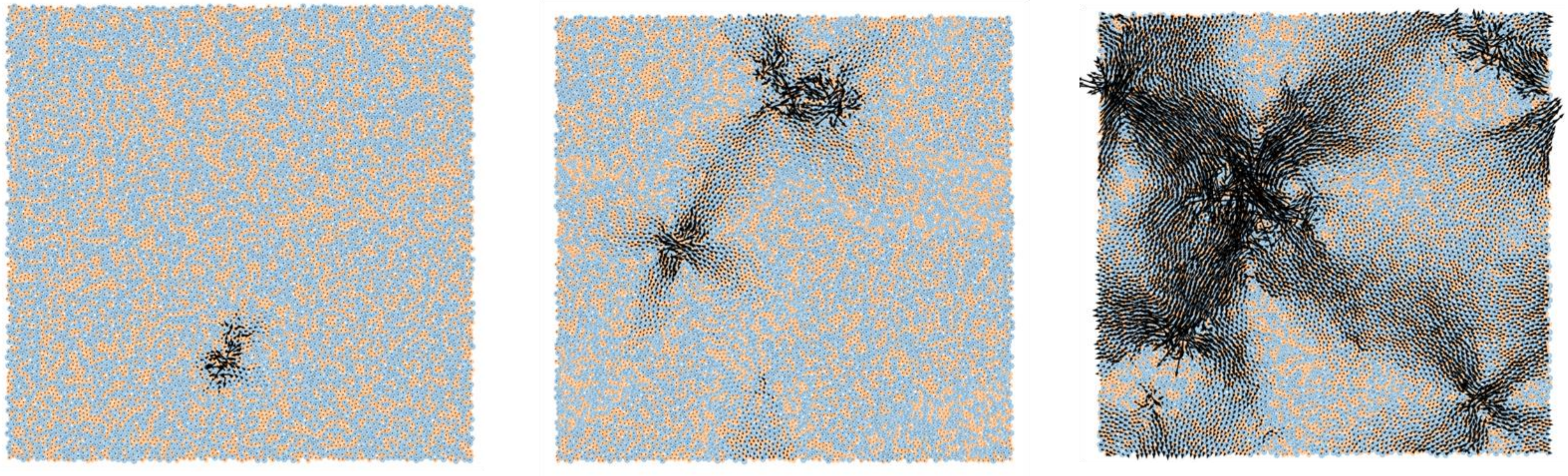
Avalanche criticality of rearrangements in aging glasses



Yuki Takaha, Hideyuki Mizuno, Atsushi Ikeda
The University of Tokyo

Outline

- **Introduction**
  - Intermittent dynamics in amorphous solids under shear
  - Avalanche critical phenomena
- **Model and Methods**
  - MD simulation
  - Analysis from the viewpoint of PEL
- **Results**
  - Displacement field of rearrangement events
  - Probability distribution of rearrangement events
- **Discussion**
  - Thermal EPM
  - Marginal stability and critical behavior

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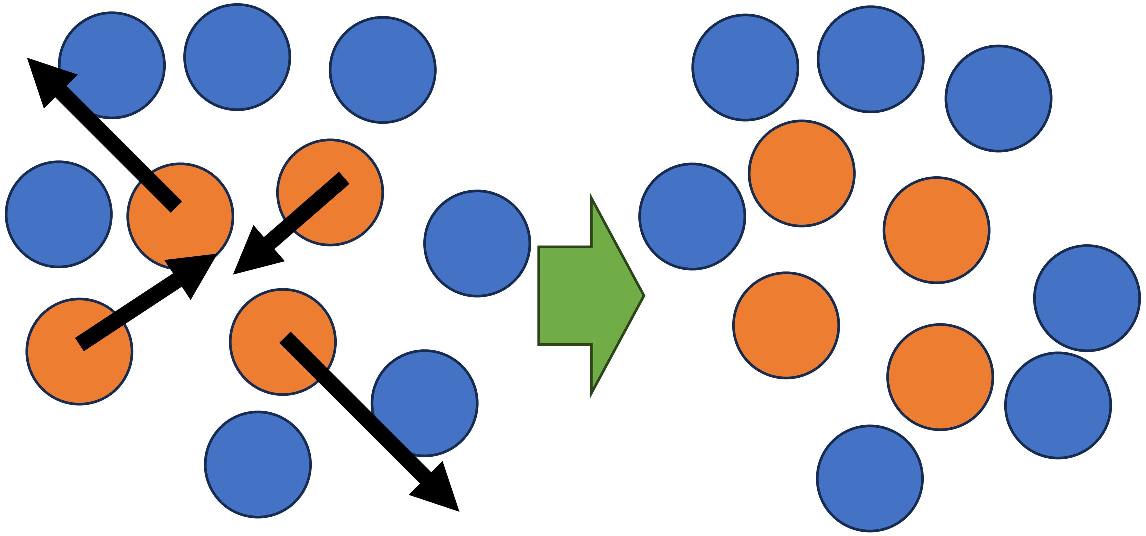
Intermittent particle rearrangements

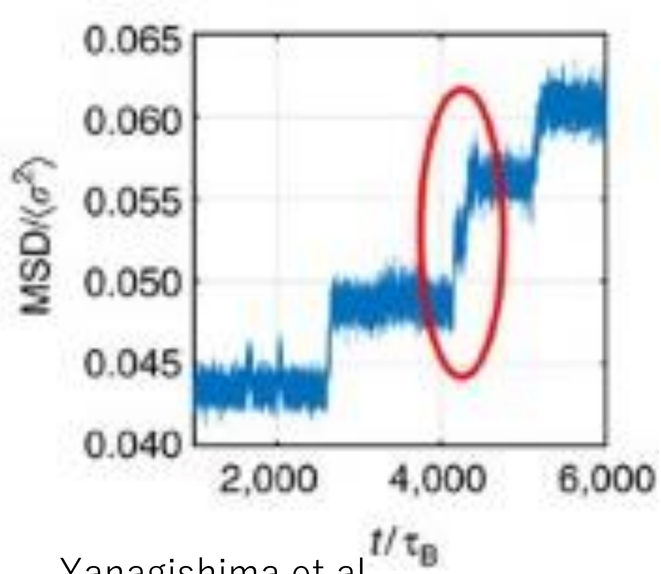
Particle rearrangement

- Elemental relaxation process
- Different from vibrational motion



Aging glass

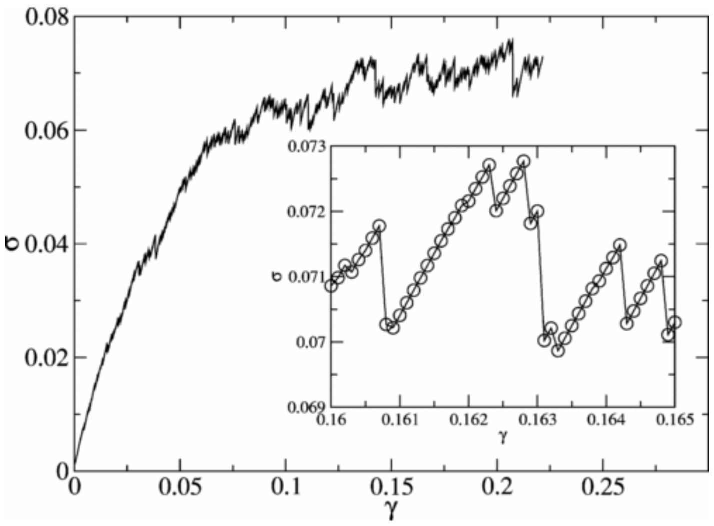
Thermal and quiescent



Yanagishima et al.
Nat. Commun. **8**, 15954(2017)

Stress drop under shear

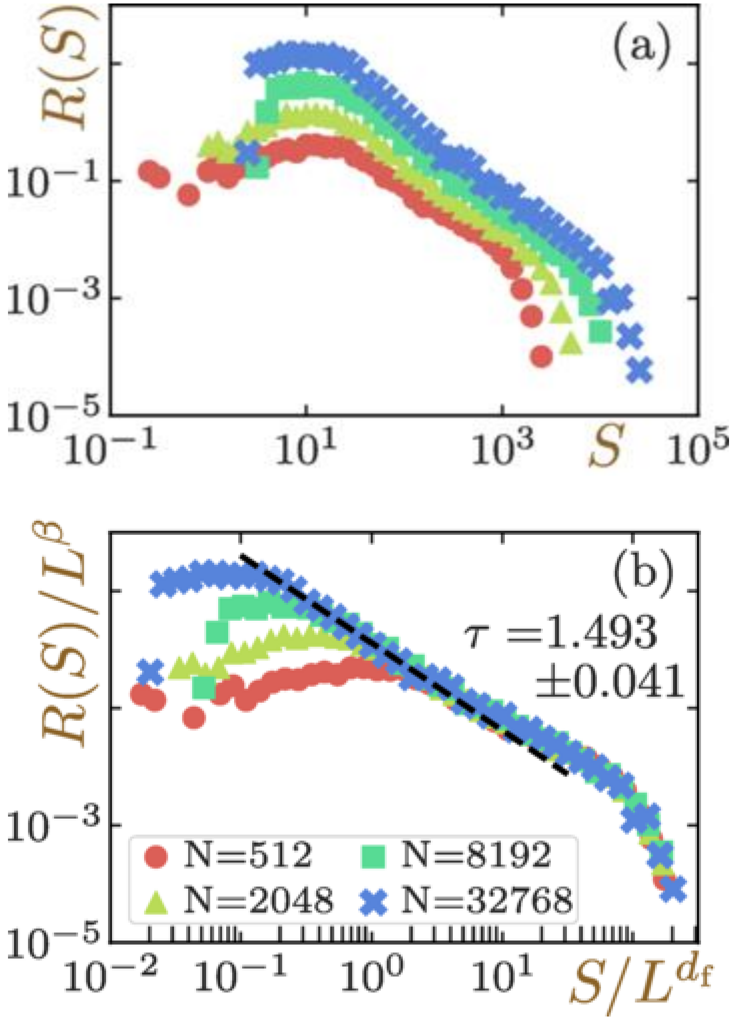
Sheard athermal system



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

Intermittent dynamics is ubiquitous in amorphous solids.

Avalanche critical phenomena under shear



Oyama et al,
Phys. Rev. E ***104***, 015002(2021)

Distribution of size of stress drop

- The power-law region
- Scaling relation of the distribution $R(S,L)$

$$R(S,L) \sim L^{\beta} f(S/L^{d_f})$$

- Finite size scaling

Avalanche critical phenomena

- Self-organized critical phenomena
- Earthquake

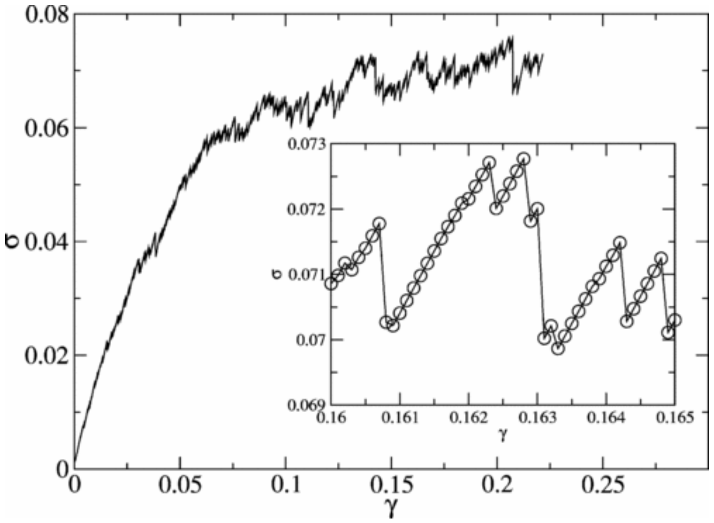
  (Fisher et al., *Phys. Rev. Lett.* **78**, 4885(1997))
- Crackling noise in crumpled sheet

  (Kramer and Lobkovsky, Phys. Rev. E 53, 1465(1996))

  and ⋯.

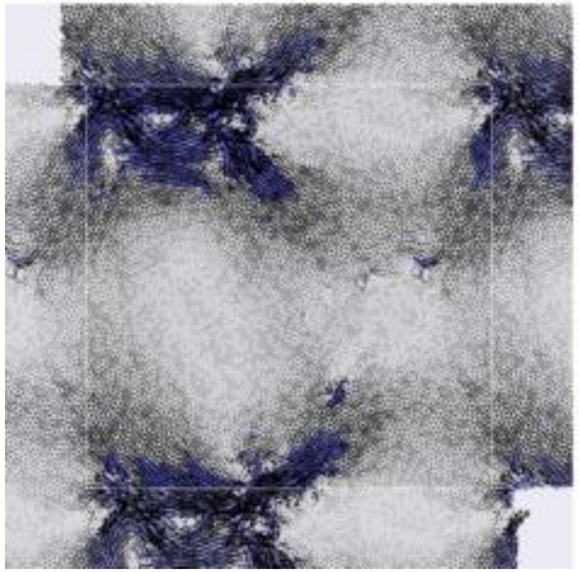
Elasticity & plasticity in sheared amorphous solids

Stress drop



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

Local plastic event and elastic field

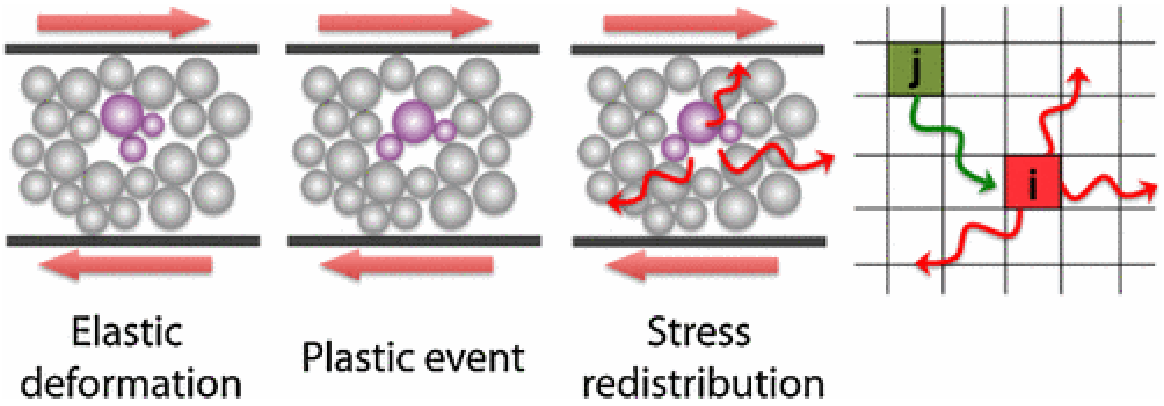


Oyama et al,
Phys. Rev. E ***10*4**, 015002(2021)

・Local regions in large motion
・Eshelby-like field

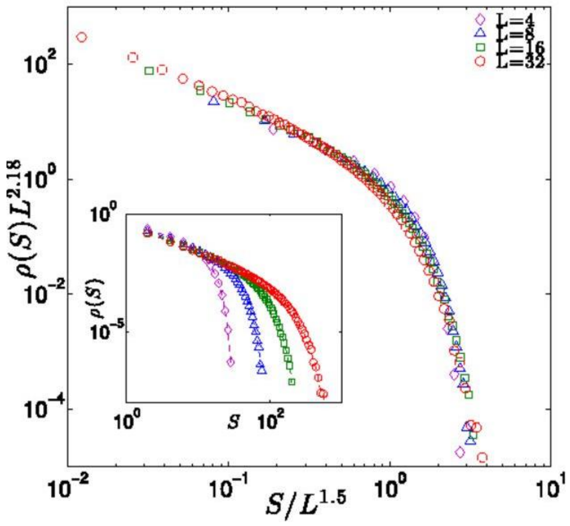
Intermittent events correspond to
local plastic events interacting via elastic fields.

Elastoplastic model(EPM)



Bocquet et al,
Phys. Rev. Lett. ***103***, 036001(2009)

Power-law distribution of stress drop



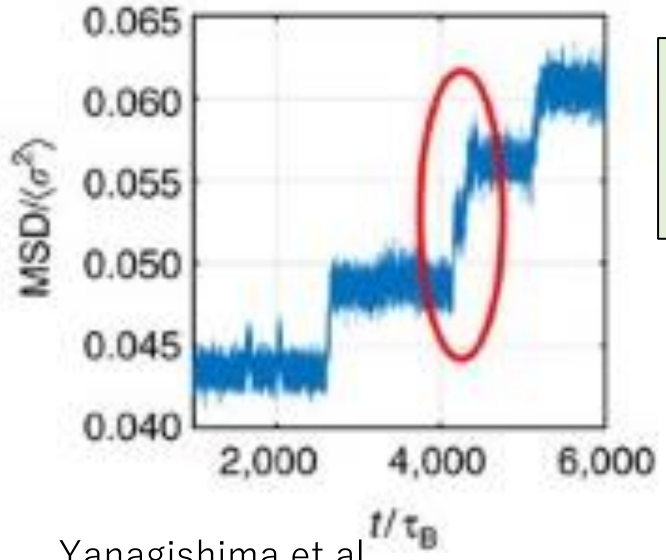
Lin et al.
Proc. Natl. Acad. Sci. USA **111(40)**, 14382-14387(2014)

- Local plastic event causes stress redistribution around the site.
- The stress change sometimes triggers other local events.
  ⇒ rare system-spanning event.
- Avalanche critical phenomena

Elasticity and plasticity play an important role to form avalanche.

How about aging glass?

Aging glass



Yanagishima et al.
Nat. Commun. **8**, 15954(2017)

Are elasticity and plasticity important?
Are there avalanche critical phenomena?

- Without shear, driven only by thermal noise

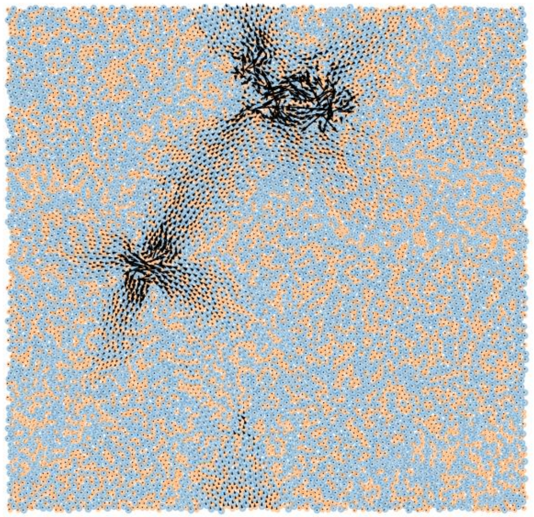
Particle rearrangements just after fast quench

Method

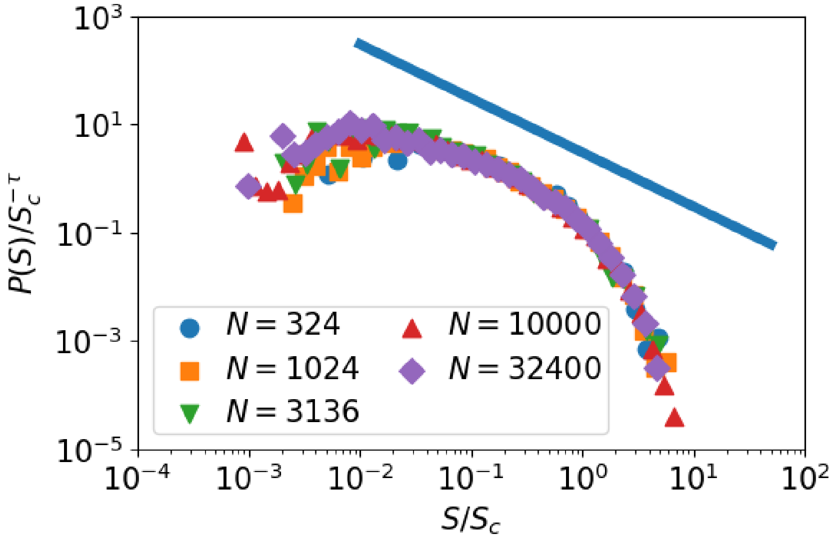
- Molecular dynamics(MD) simulation just after fast quench
- Analysis from the viewpoint of PEL

Results

Displacement field



Power-law distribution



We observe a critical phenomenon in a quiescent glass.

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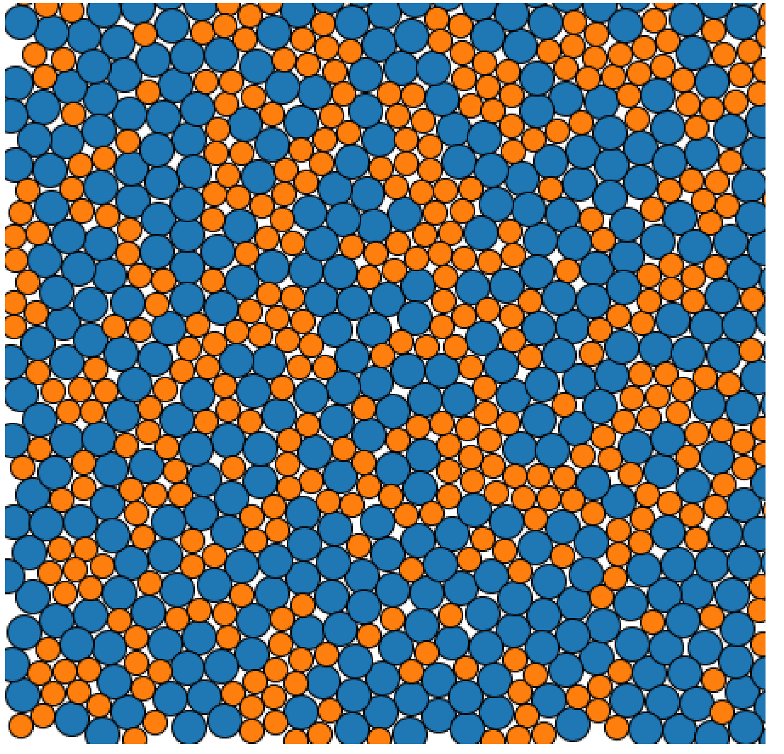
Methods: Binary mixture

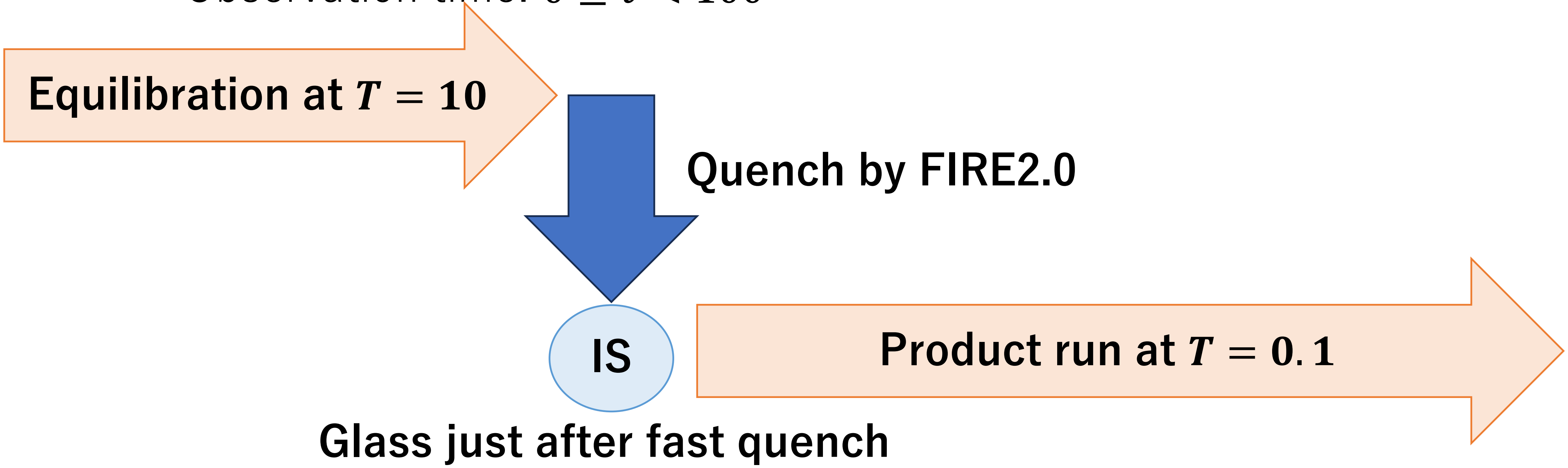
Model

- Binary in 2D
    - Effective diameter $\sigma_A : \sigma_B = 1 : 1.4$. Equimolar system.
    - $v_{12}(r) = \epsilon \left(\frac{\bar{\sigma}}{r}\right)^{12}, \bar{\sigma} = (\sigma_1 + \sigma_2)/2$
- Unit: length σ_A, mass m, time $\sigma_A\sqrt{m/\epsilon}$, temperature ϵ/k_B



Methods: MD simulation

- Initial state: Inherent structure(nearest minima of PEL, IS) of liquids($T = 10$)
- Dynamics: Underdamped Langevin equation with Stoke drag $\boldsymbol{f}_i^{\mathrm{drag}} = -\dot{\boldsymbol{r}}_i$.
    - Temperature: $T = 0.1$
    - Packing fraction: $\phi = 0.93$
    - Observation time: $0 \leq t < 100$



Equilibration at $\boldsymbol{T = 10}$

Quench by FIRE2.0

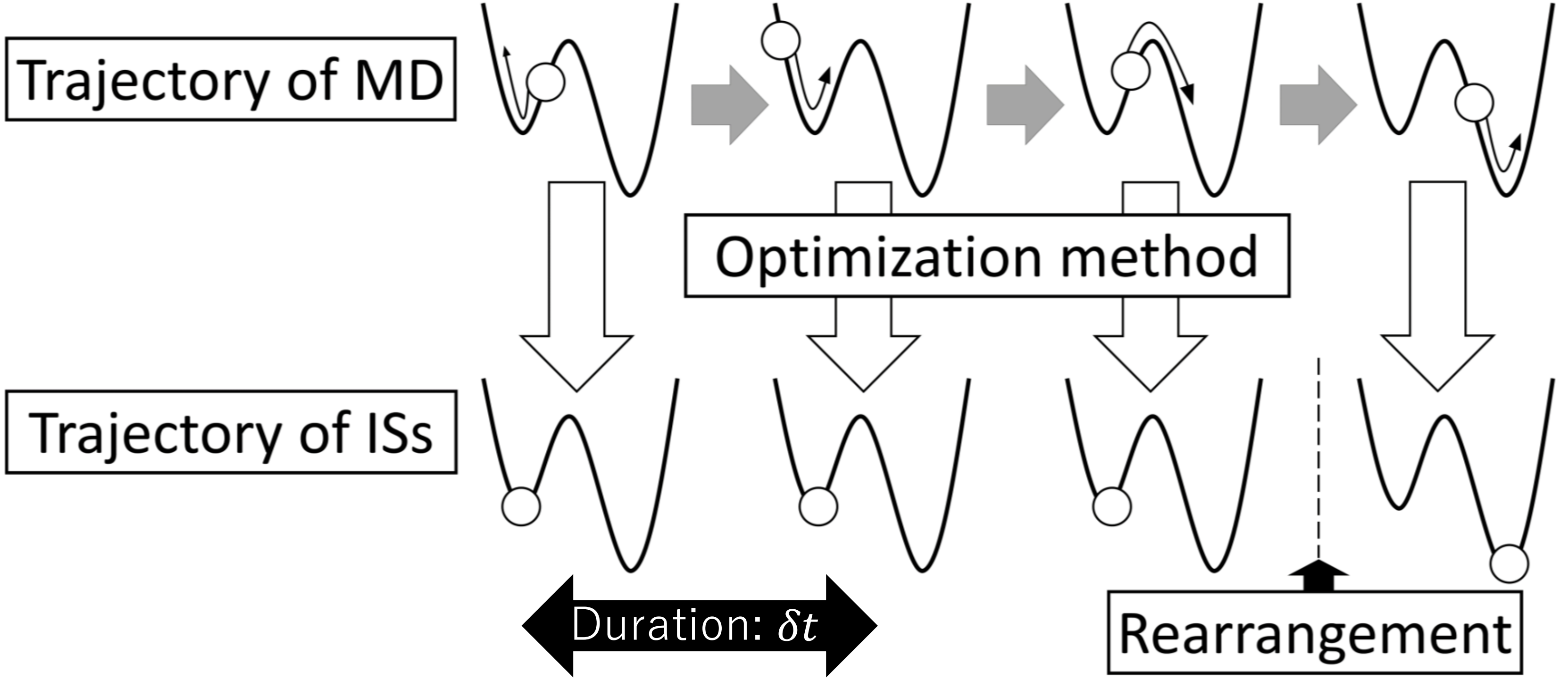
IS

Product run at $\boldsymbol{T = 0.1}$

Glass just after fast quench

Definition of particle rearrangements

Analysis from the viewpoint of PEL



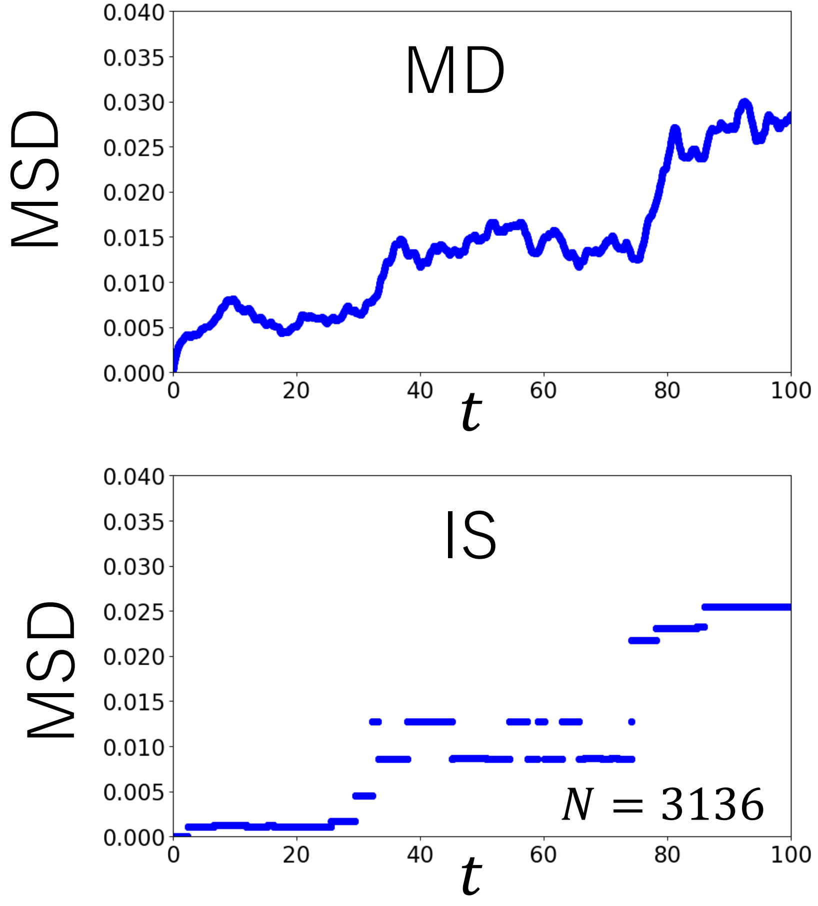
・$\delta t = 0.02$ to separate into individual events

・Intermittent event
=Transition between ISs

・Ignore vibration

We track the IS-trajectory and detect the rearrangements.

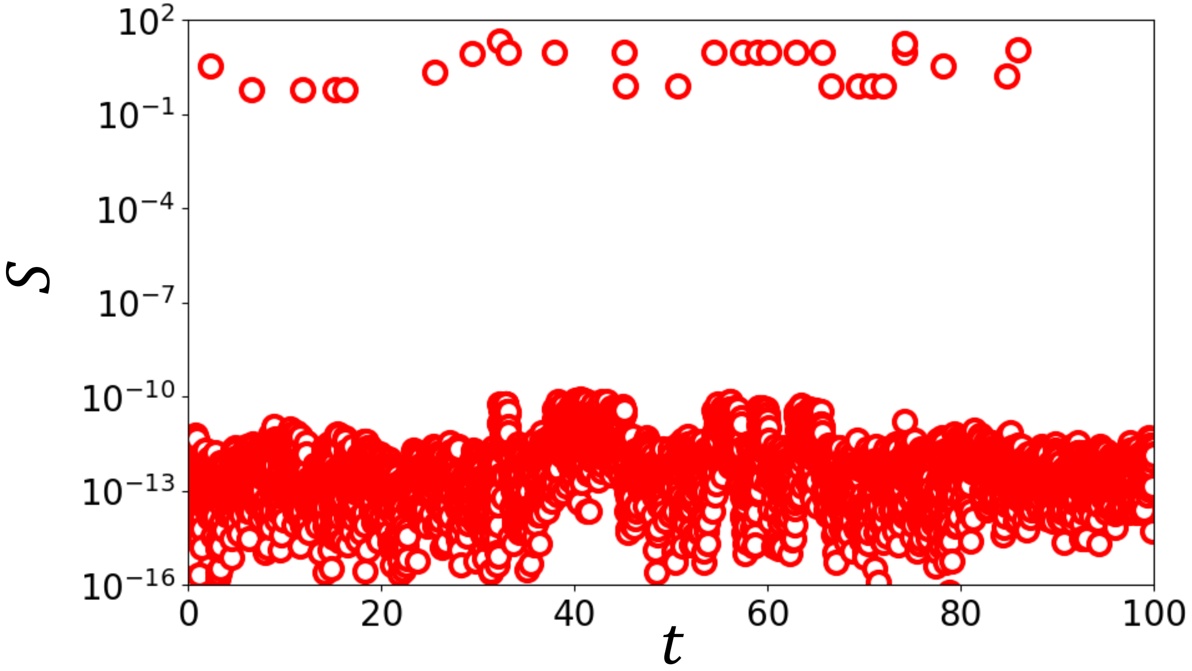
Definition of particle rearrangements



Clear intermittent events

$$S = \sum \left(\boldsymbol{r}_i^{IS}(t) - \boldsymbol{r}_i^{IS}(t + \delta t) \right)^2$$

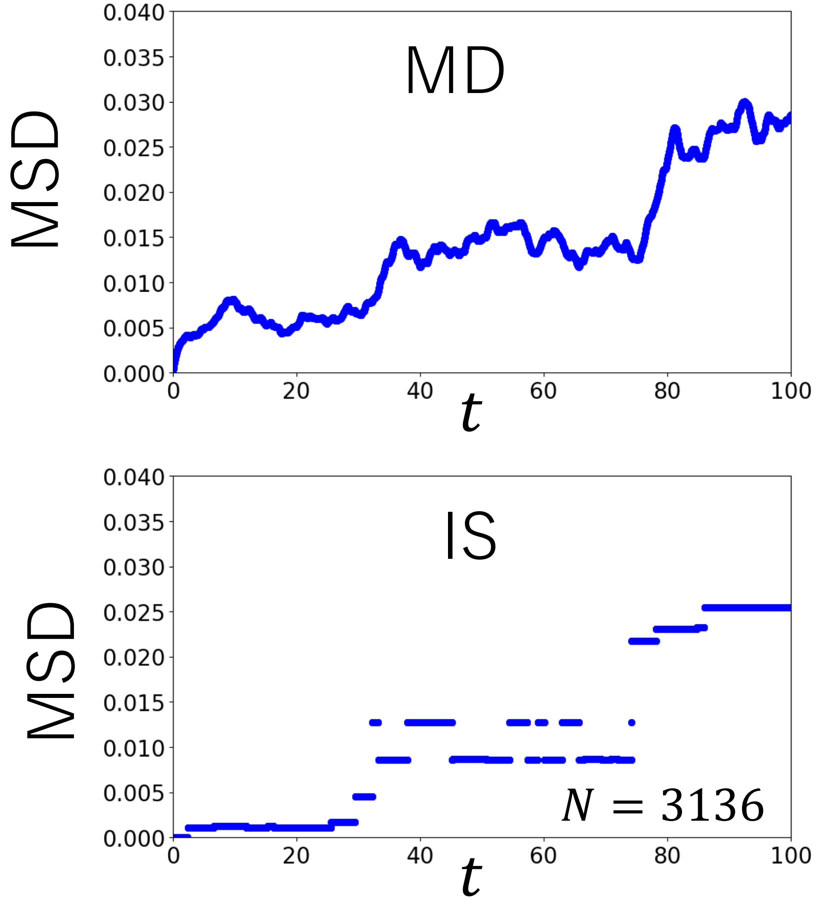
- $\delta t = 0.02$ to separate into individual events



We detect the rearrangements.

- Rearrangement events: $S > 10^{-6}$
- S: Size of rearrangement event

Definition of particle rearrangements



Clear intermittent events

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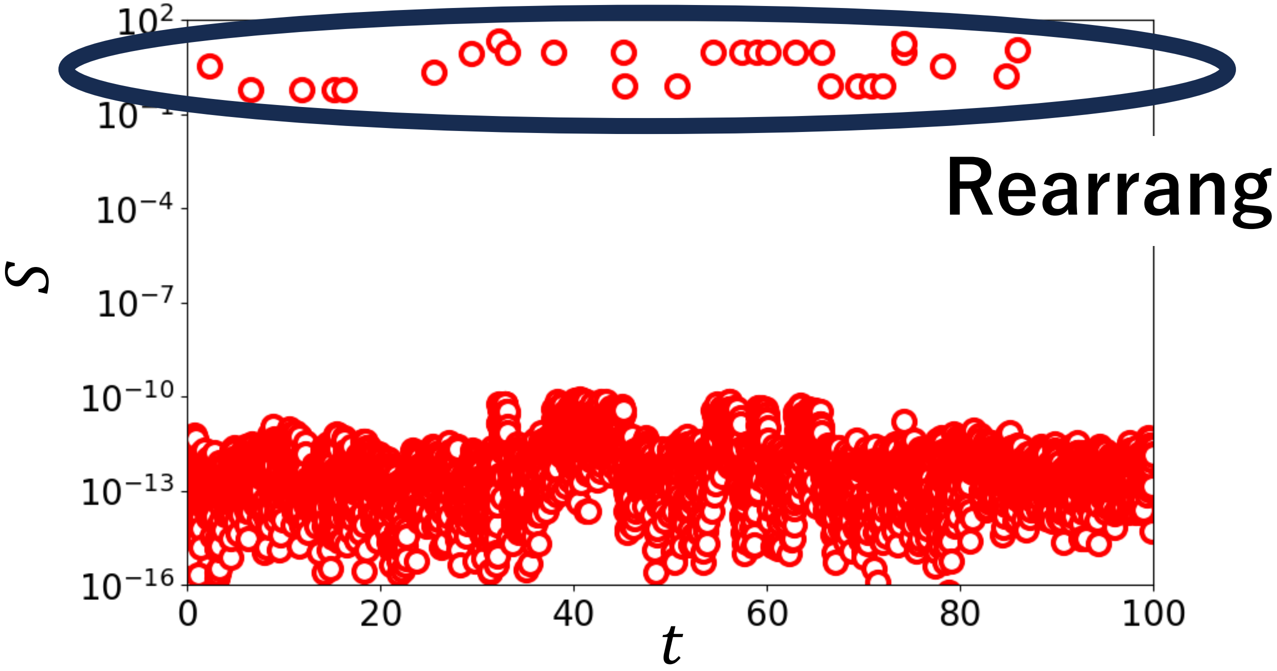

Rearrangements

We detect the rearrangements.

- Rearrangement events: $S > 10^{-6}$
- S: Size of rearrangement event

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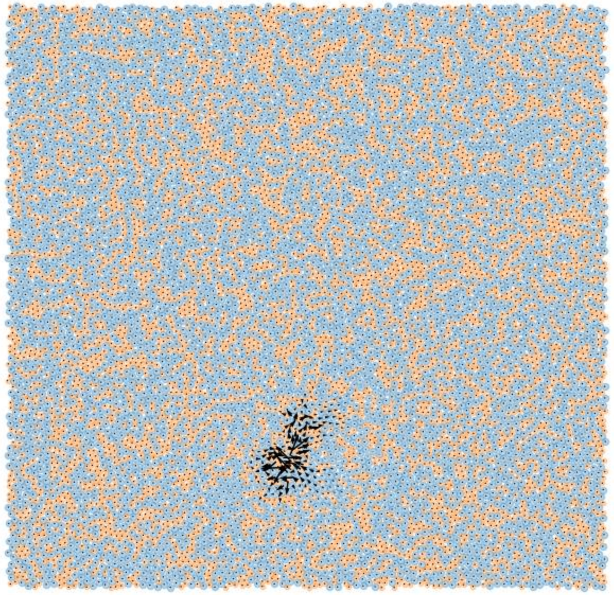
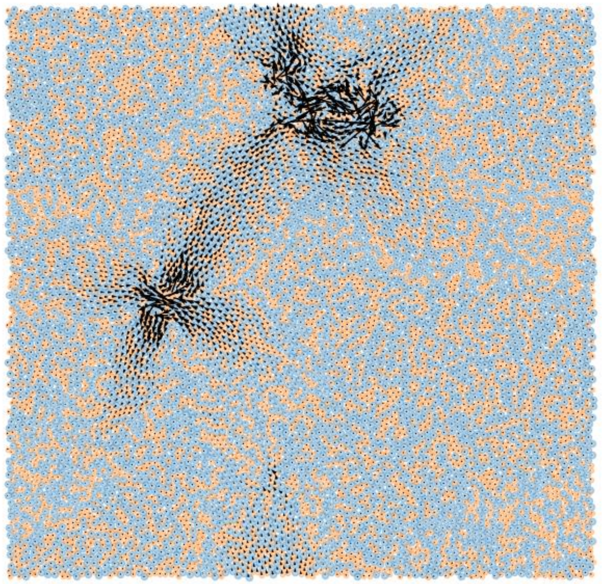
Displacement fields of particle rearrangements

Displacement fields between the ISs

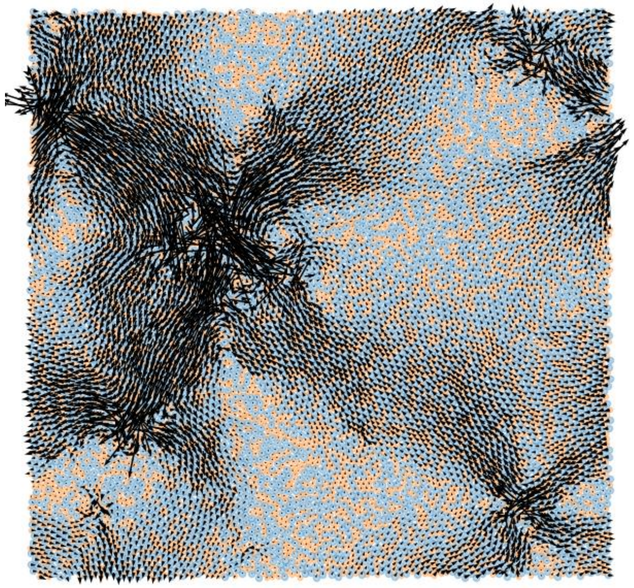
$S = 1$



$S = 10$

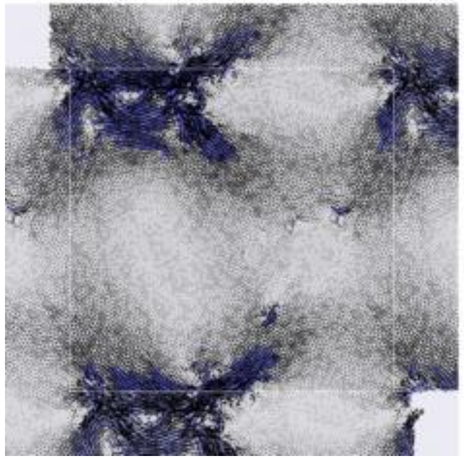


$S = 100$



N=10000

Under shear

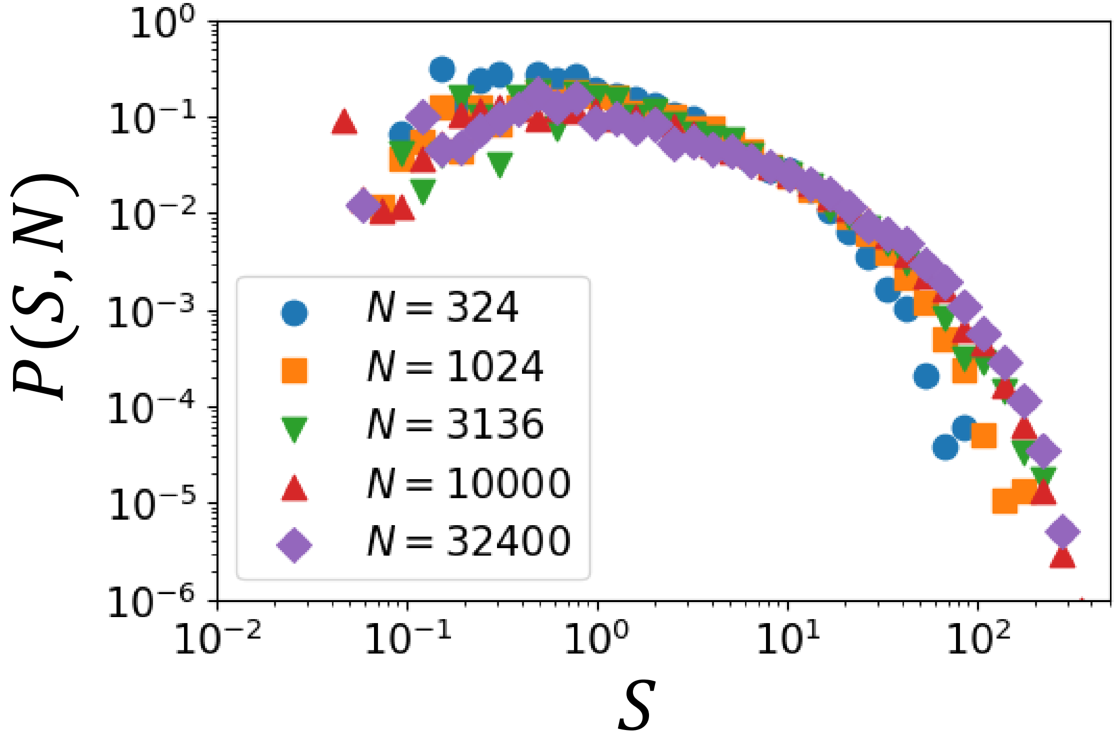


Oyama et al,
Phys. Rev. E ***104***, 015002(2021)

Local events coupled via Eshelby-like fileds

Rearrangement = Local plastic events interacting via elastic field

Statistical property of particle rearrangements

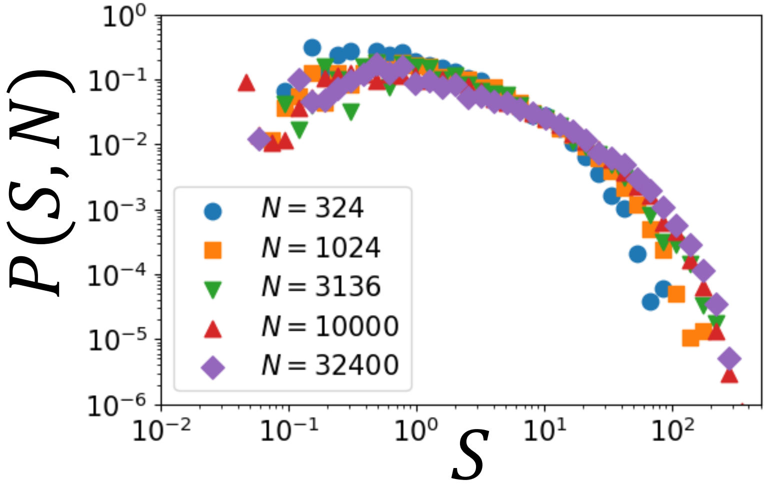


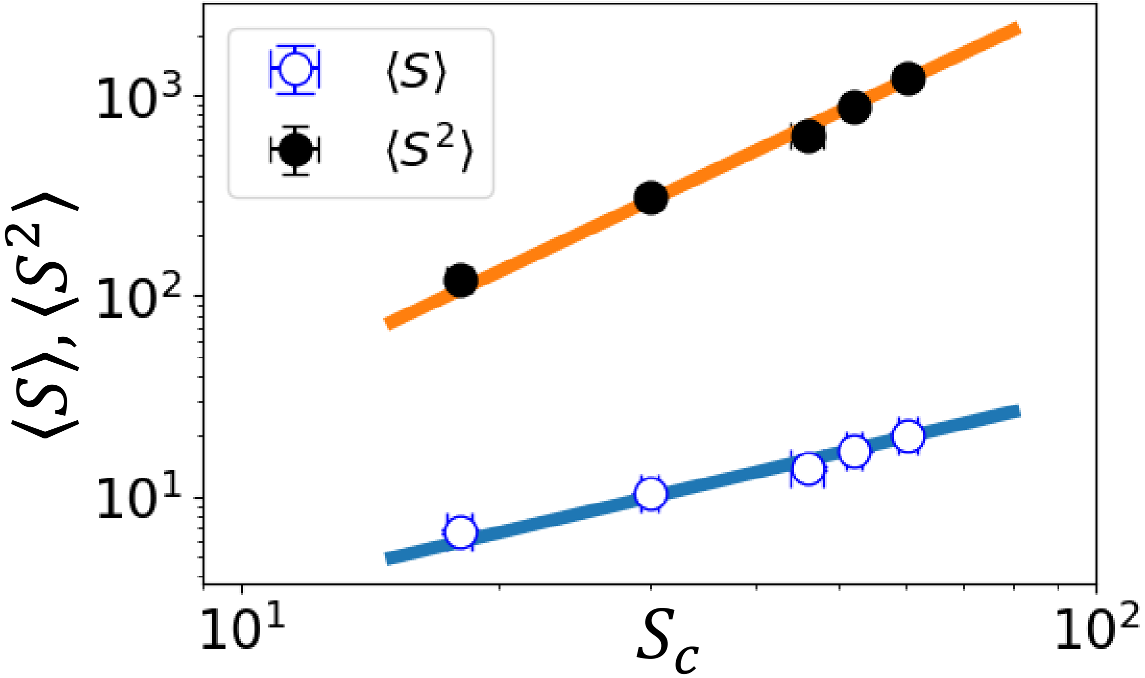
N	324	1024	3136	10000	32400
# of samples	1000	1000	100	100	10

$P(S,N)$: Probability distribution of the size S with the number N of particle

Power-law region
System-size dependence

Scaling analysis





Scaling assumption

$$P(S,N) \sim S^{-\tau} f(S/S_c) = S_c^{-\tau} g(S/S_c)$$

- τ: Predicted exponent
- S_c: Cutoff size

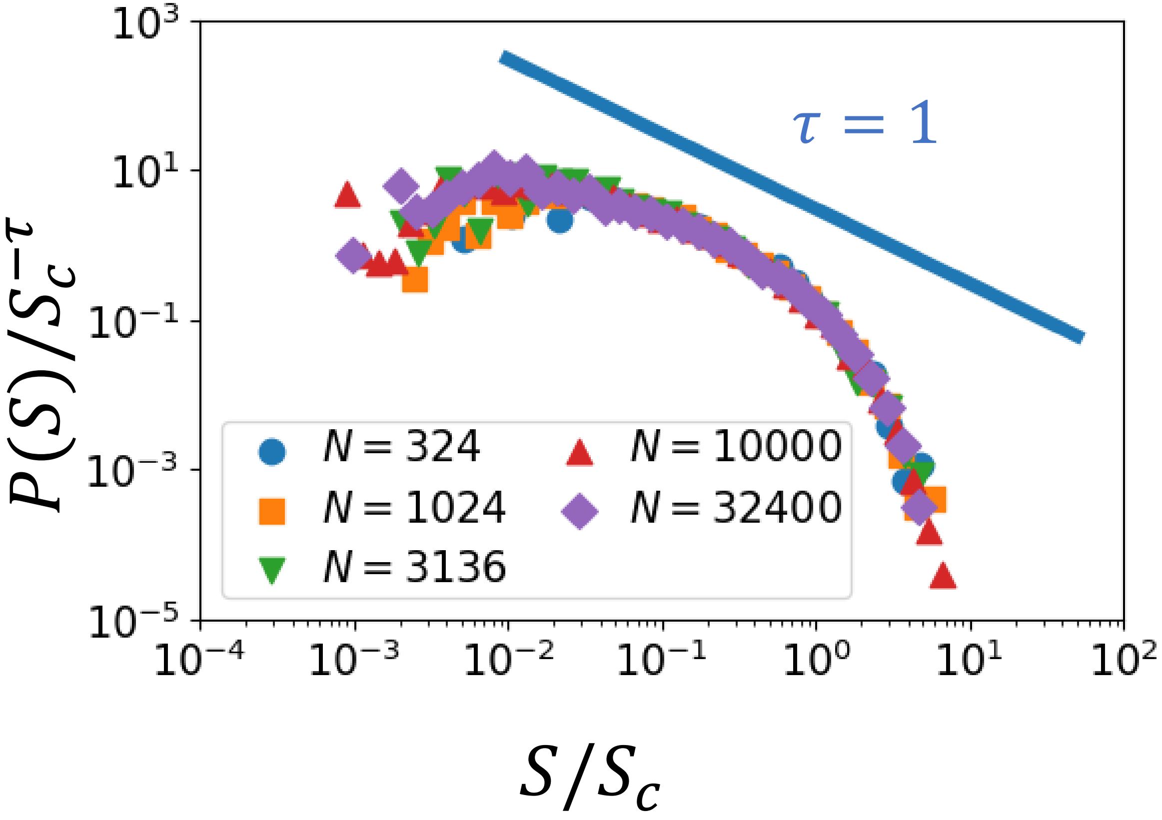
$$\Rightarrow \langle S\rangle \sim S_c^{2-\tau}, \langle S^2\rangle \sim S_c^{3-\tau}$$

We evaluate the cutoff $S_c = \langle S^2\rangle / \langle S\rangle$.

There is a power-law relation between moments and cutoff.

- $\tau \cong 1$

Collapse of the probability distribution



We check $P(S,N) \sim S_c^{-\tau} g(S/S_c)$.

We plot $P(S)/S_c^{-\tau}$ against S/S_c with $\tau = 1$.

The distribution collapse on the same curve.
The power-law region has the almost same exponent.
⇒**Particle rearrangements are critical phenomena.**

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Discussion: Why critical?

Why is our observation critical?

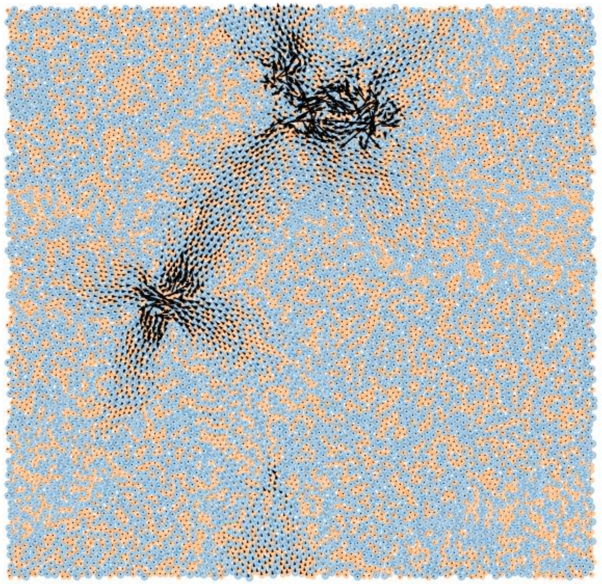
Examples of non-critical rearrangements in glasses.

- Aging after a finite waiting time (Masri et al, *Phys. Rev. E* ***82***, 031503(2010))
  - No system-spanning event
- Stationary dynamics in glasses(Mizuno et al, *J. Chem. Phys*. **153**, 154501(2020))
  - Intermittent dynamics does not have system-size dependence.

What does cause the difference?
⇒**We discuss from the viewpoint of elastoplasticity.**

Discussion: Elastoplasticity

Local plastic event & elastic interaction



Quiescent glass as an elastoplastic material

・Local plastic event causes stress redistribution around the site.

・The stress change sometimes triggers other local events.

・**Without shear, driven only by thermal noise**

EPM will help us understand the criticality.

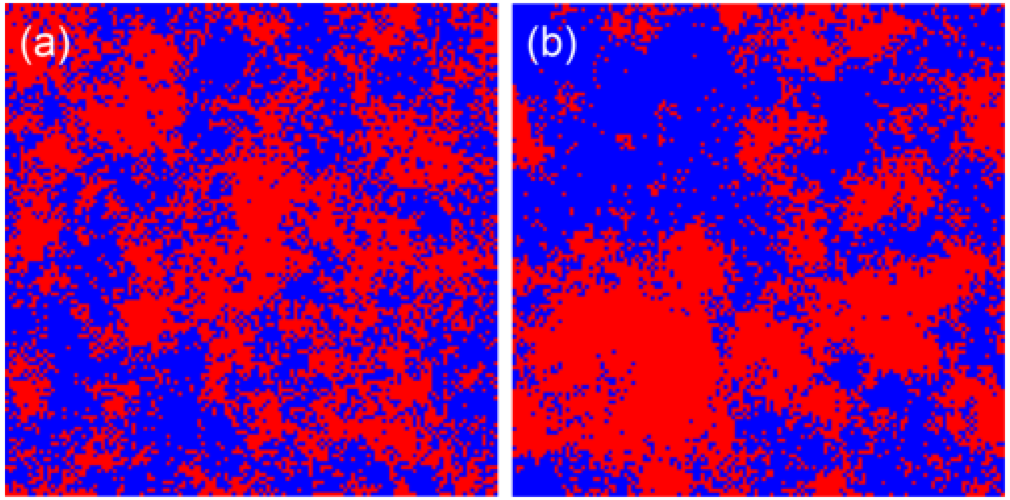
Discussion: Thermal EPM for supercooled liquids

Thermal EPM

(Ozawa and Biroli, *Phys. Rev. Lett.* **130**, 138201(2023))

- Driven by **only thermal noise**
- Elasticity facilitates dynamics.

Dynamical heterogeneity



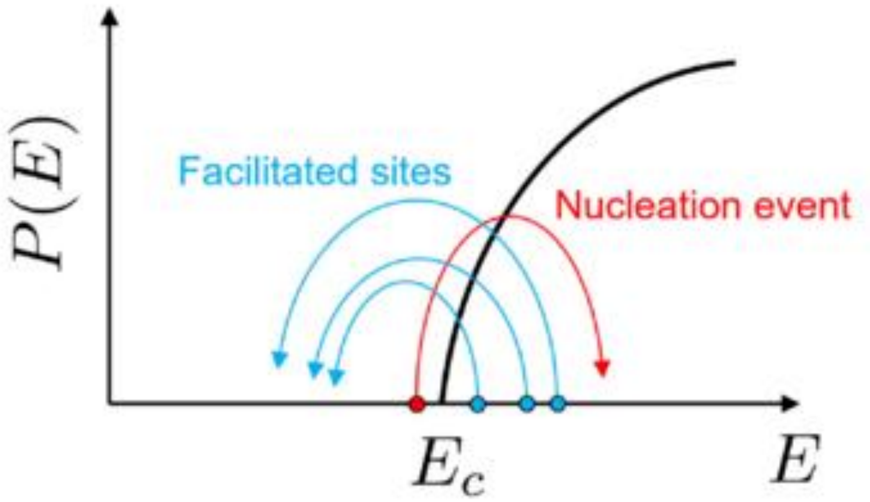
High temperature Low temperature

Elasticity and plasticity can explain dynamical heterogeneity.

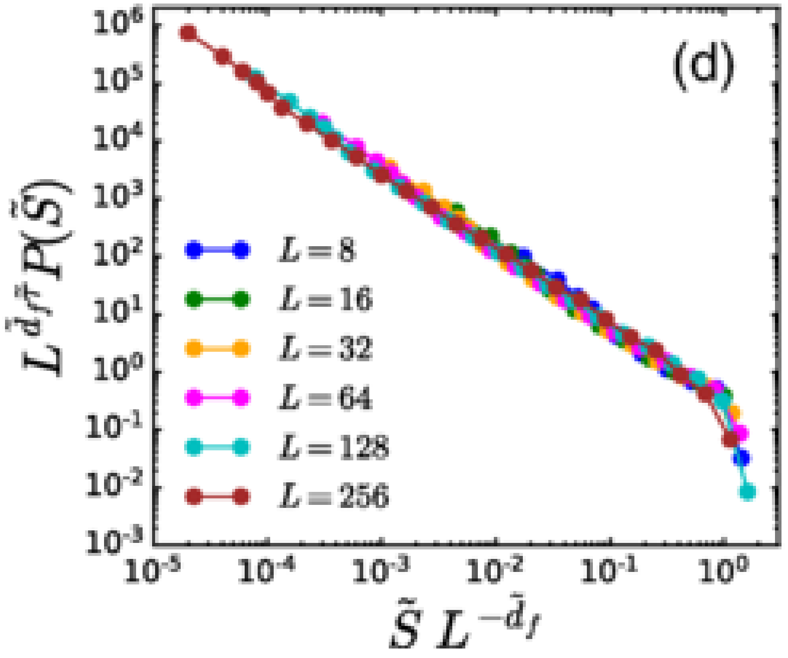
Discussion: Criticality in the thermal EPM

Stationary state with $T = 0^+$ in the thermal EPM

(Tahaei et al., *Phys. Rev. X* **13**, 031034(2023))



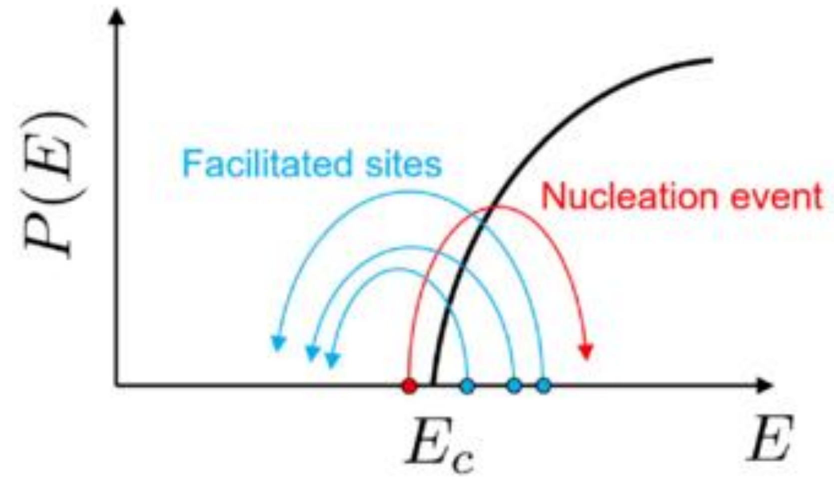
E_c defines $\tilde{S}$



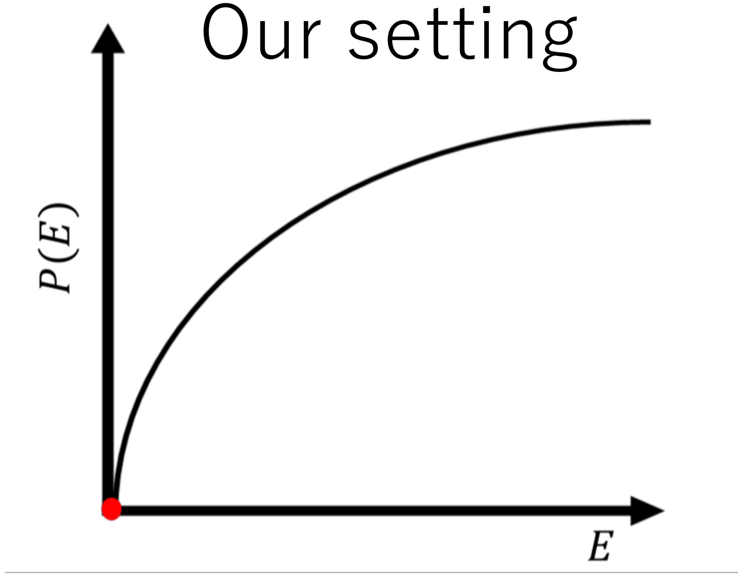
- Edge E_c of the distribution of activation energy E corresponds to the critical point.
- The size of relaxed events on a timescale $\tau \sim e^{E_c/k_B T}$ is critical.

Discussion: Criticality in our setting

Stationary state



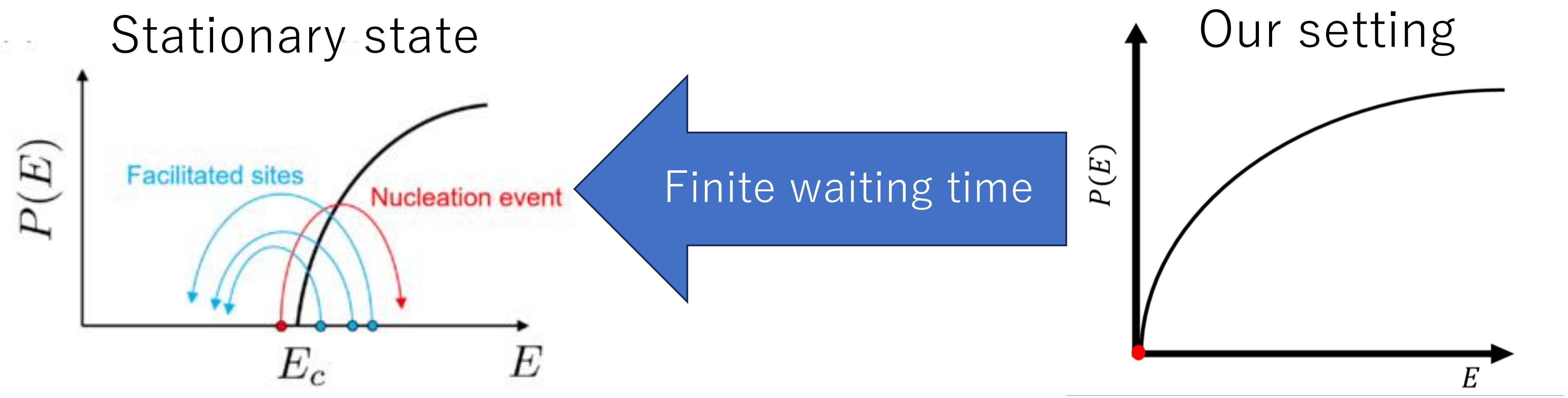
Our setting



Our setting: Glass just after a fast quench

- Marginally stable (Karmaker et al., *Phys. Rev. E* **82**, 055103(2010),
  Lin and Wyart, *Phys. Rev. X* **6**, 011005(2016))
  ⇒ $E_c = 0$ and corresponding timescale $\tau \sim e^{E_c/k_BT}$ is very small.
- **The size of particle rearrangements is critical.**

Discussion: Criticality in previous studies



Our setting: Glass just after a fast quench

- Marginally stable (Karmaker et al., *Phys. Rev. E* **82**, 055103(2010),
  Lin and Wyart, *Phys. Rev. X* **6**, 011005(2016))
  $\Rightarrow E_c = 0$ and corresponding timescale $\tau \sim e^{E_c/k_B T}$ is very small.
- **The size of particle rearrangements is critical.**

Previous studies: With finite waiting time

- $E_c > 0$. **The size of particle rearrangements is not critical.**

Summary

We study the particle rearrangements in glasses just after quench.

The particle rearrangements are critical.

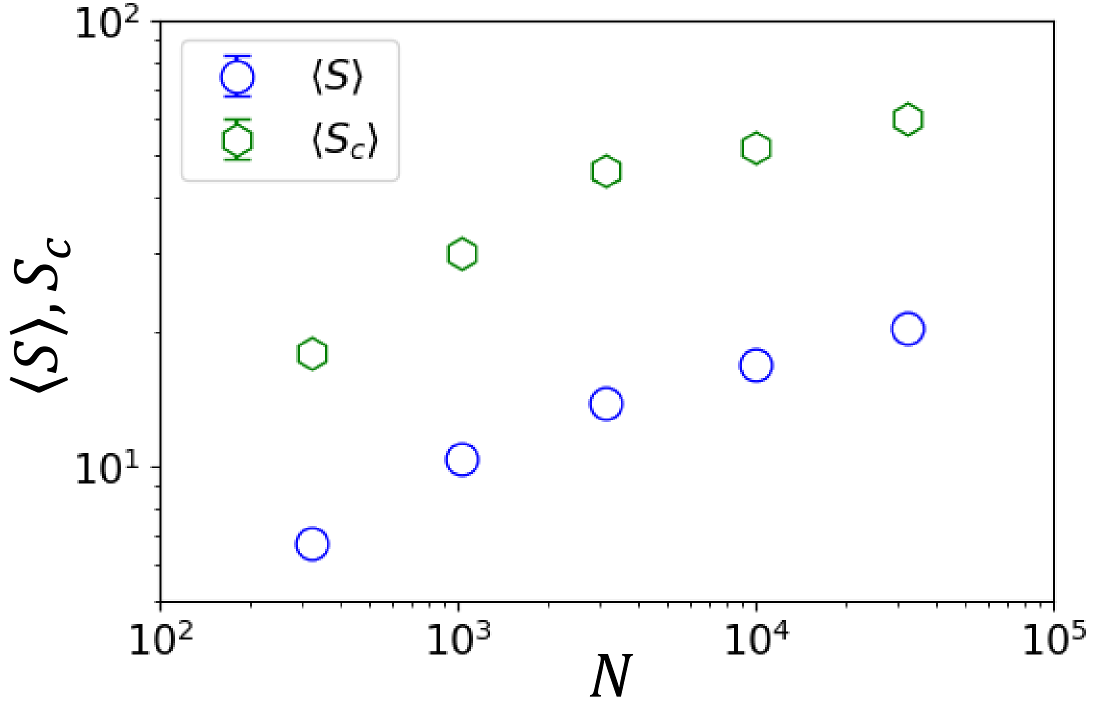
We can interpret the critical phenomena from the viewpoint of elastoplasticity.

Unclear point

・The system size dependence of S is not power-law.
・The value of the exponent τ is smaller than that observed in previous research.

Acknowledgement
・JSPS KAKENHI Grant Number 20H01868, 24H00192, 24KJ0589

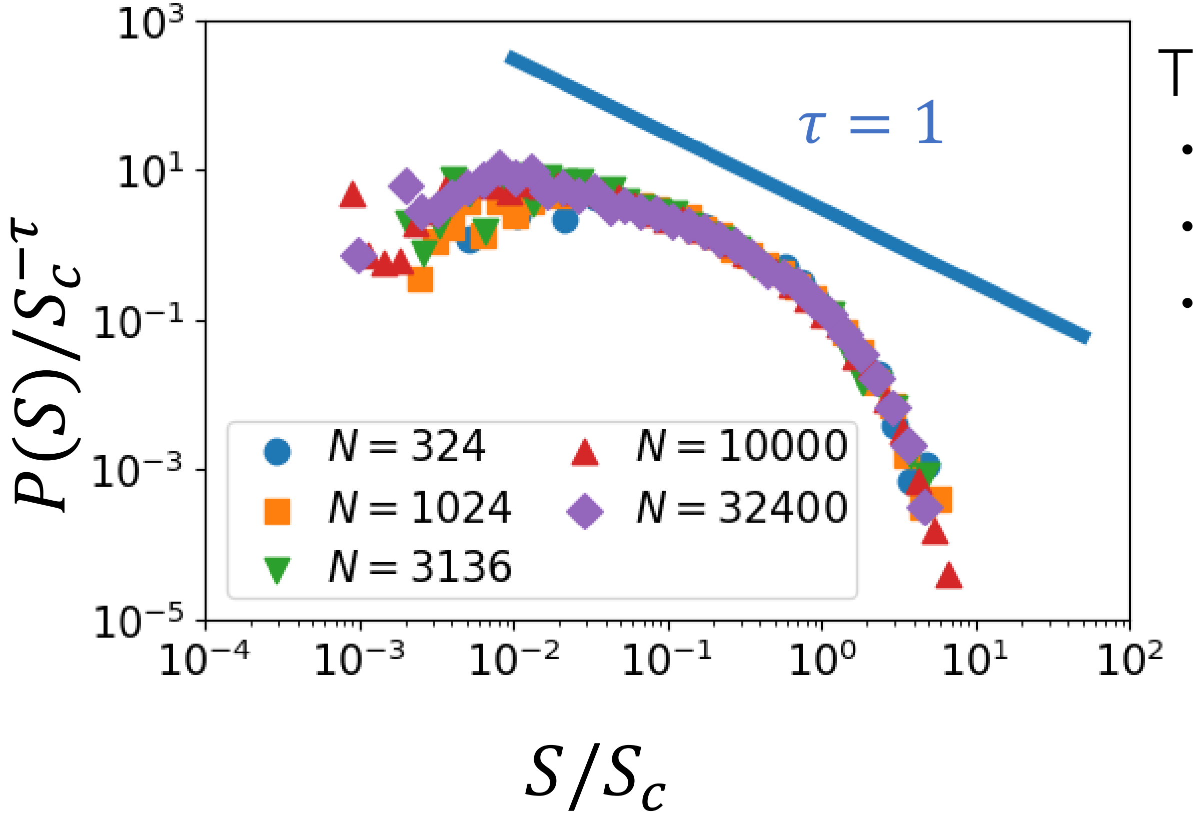
Unclear point: N-dependence of $\langle S\rangle$



$\langle S\rangle$ is not power-law dependent on N for large N.

We need more computational cost to refer the fully N-dependence.

Unclear point: exponent τ



The exponent $\tau = 1.2 \sim 1.5$ is usually observed.

- EPM under shear
- thermal EPM
- AQS MD under shear

$\tau = 1$ cases

- Elastic regime

(Shang et al., Proc. Natl. Acad. Sci. in USA **117(1)**, 86-92(2019))

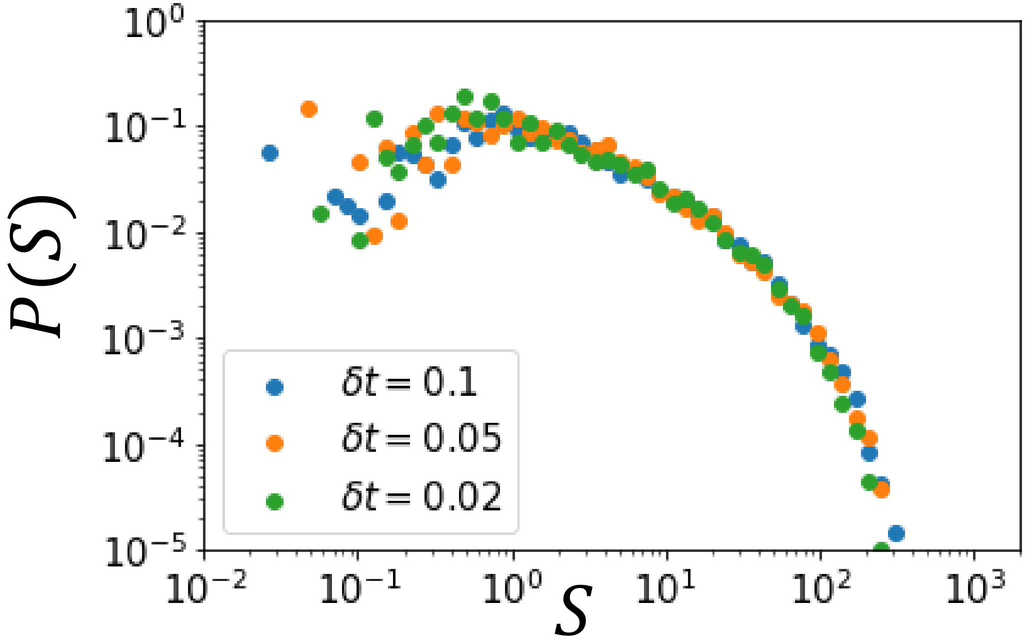
- EPM with a particular protocol

(Jagla, *Phys. Rev. E* **92**, 042135(2015))

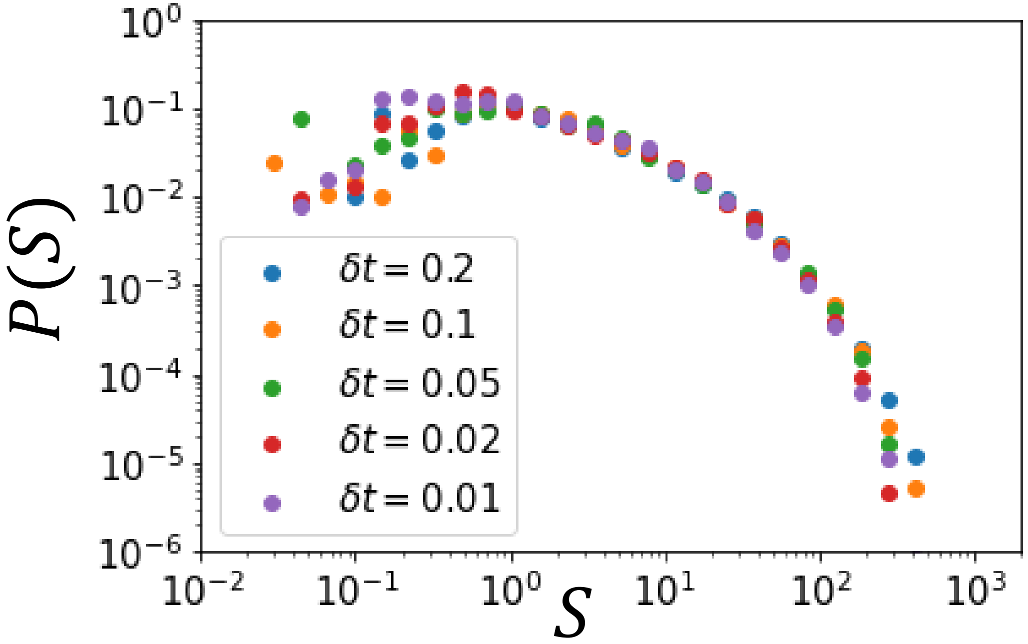
- Random energy model

(Franz and Spigler, *Phys. Rev. E* **95**, 022139(2017))

The dependence of time duration $\boldsymbol{\delta t}$



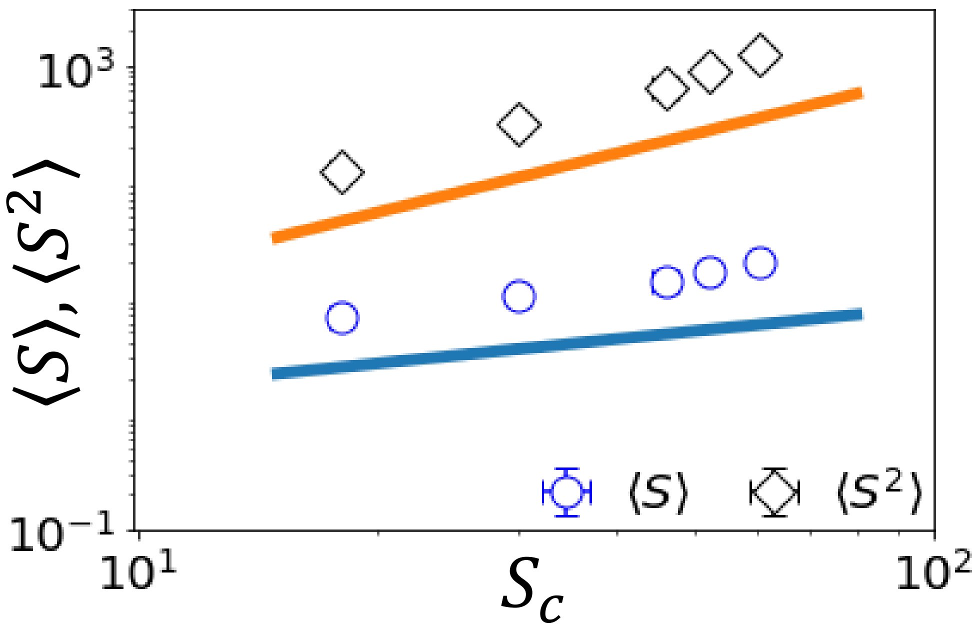
$N = 324$

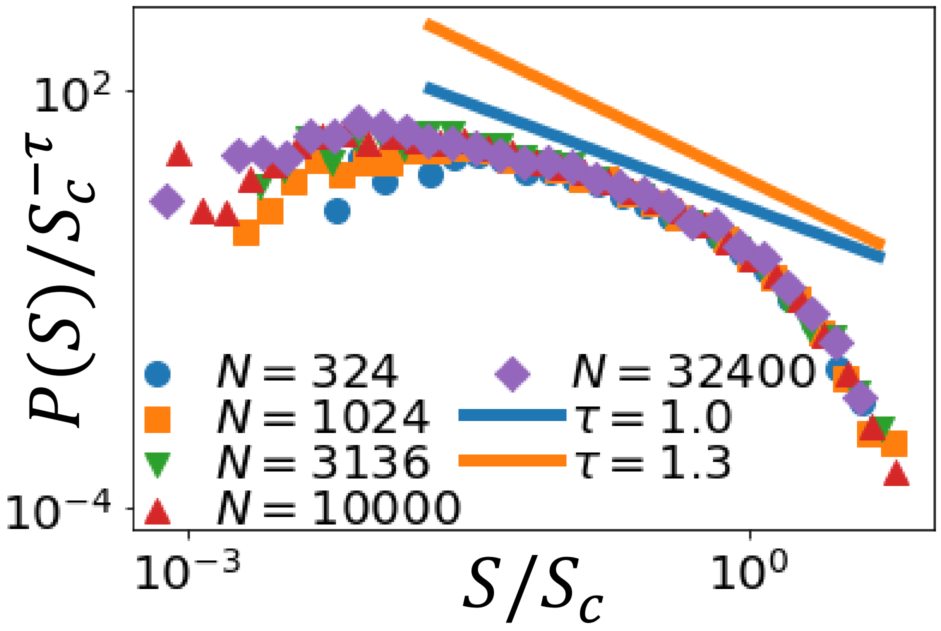


$N = 32400$

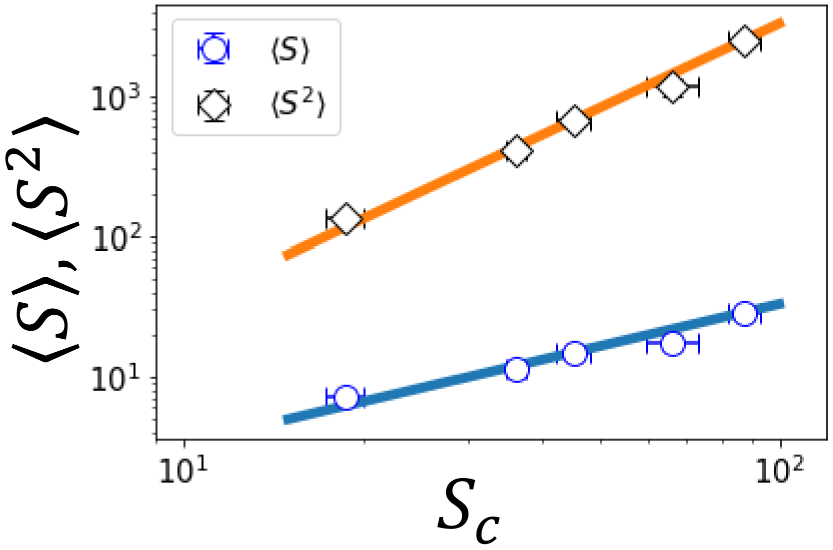
Evaluation of $\boldsymbol{\tau}$

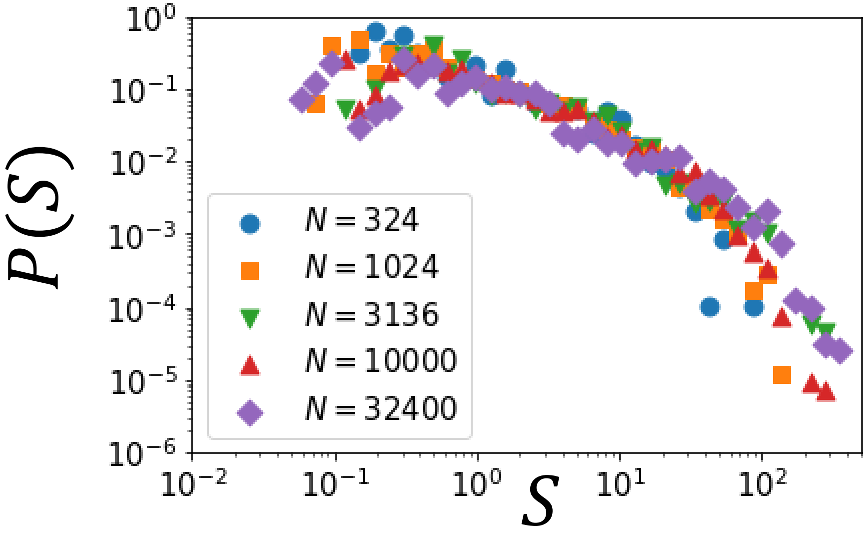
Scaling with $\tau = 1.3$



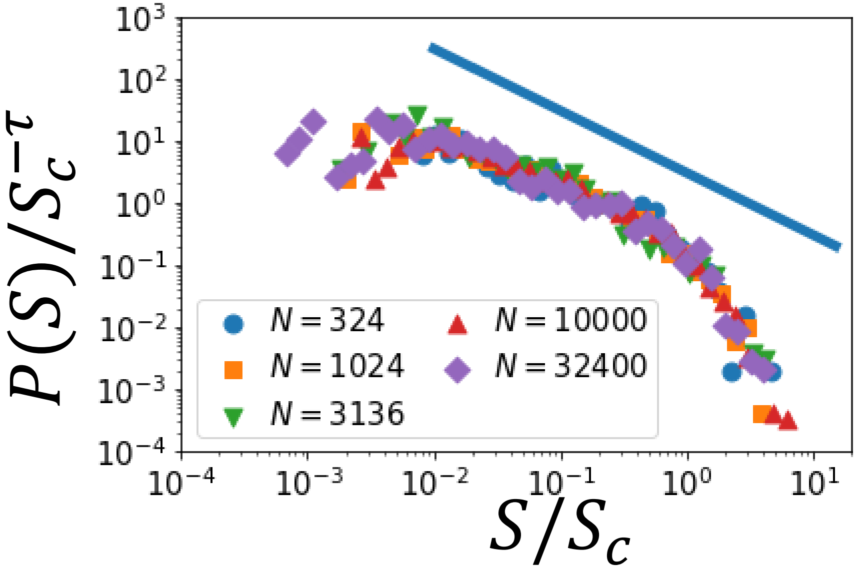


At low temperature($\boldsymbol{T = 0.02}$)

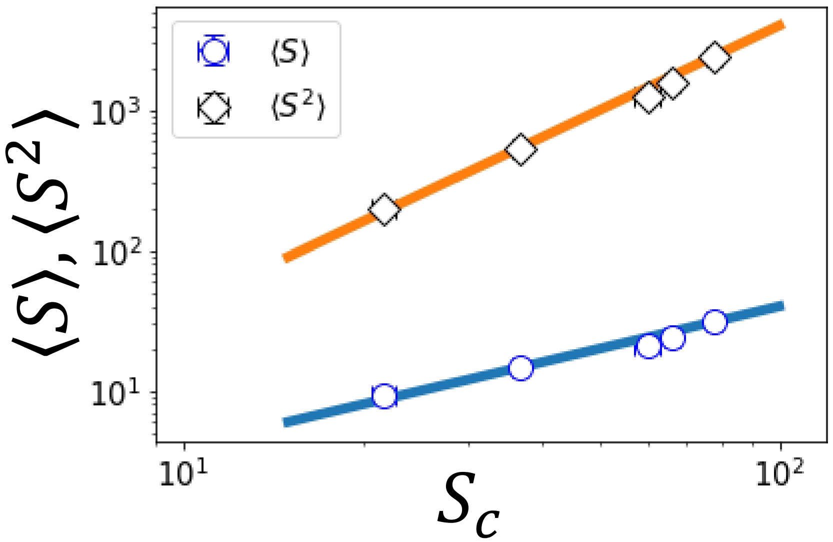


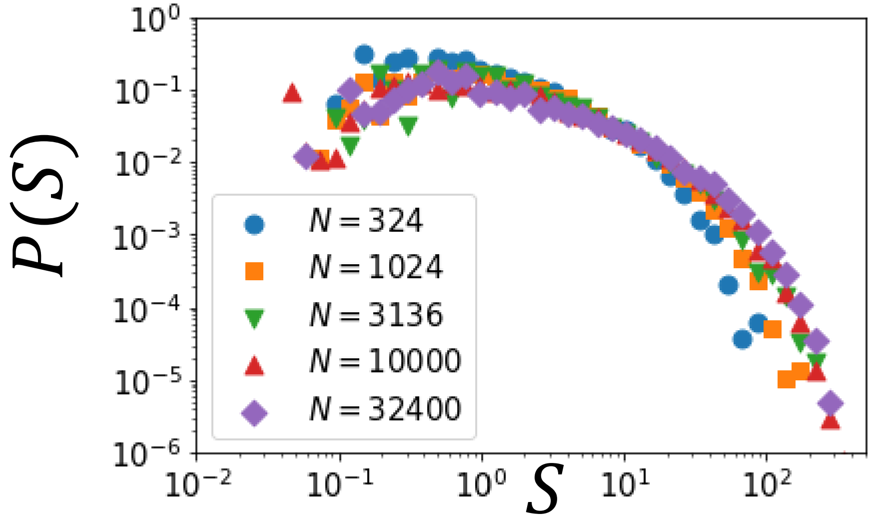


$\tau = 1$

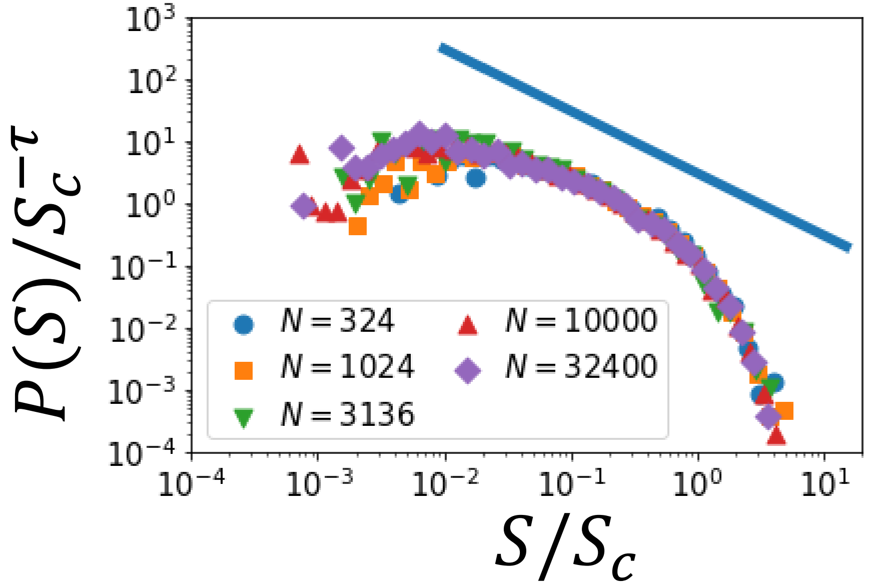


With shot time$(\mathbf{0} \leq \boldsymbol{t} < \mathbf{20})$

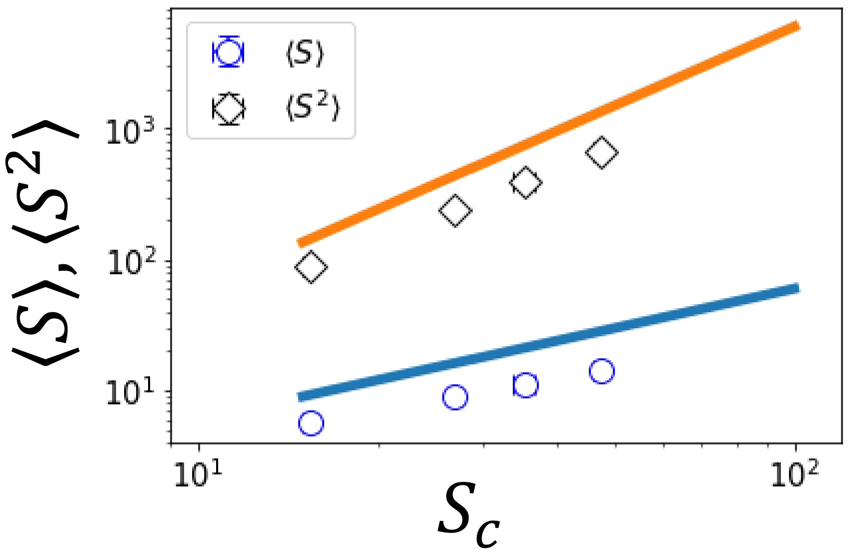


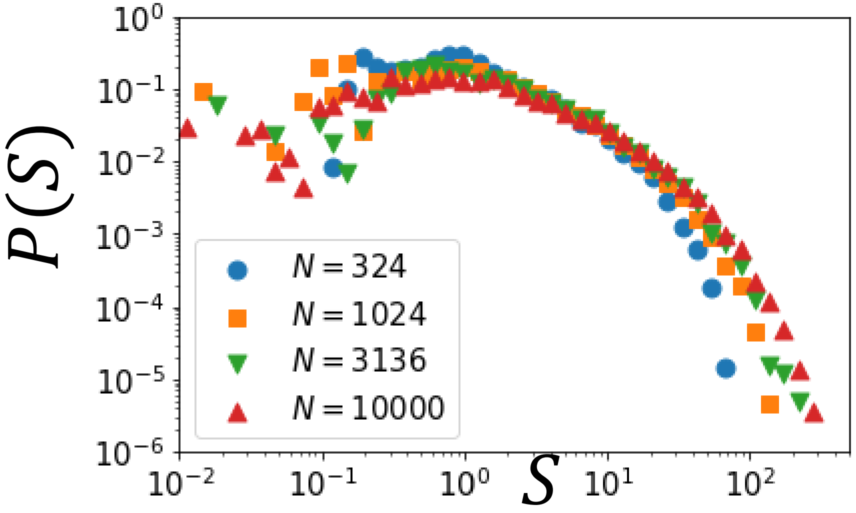


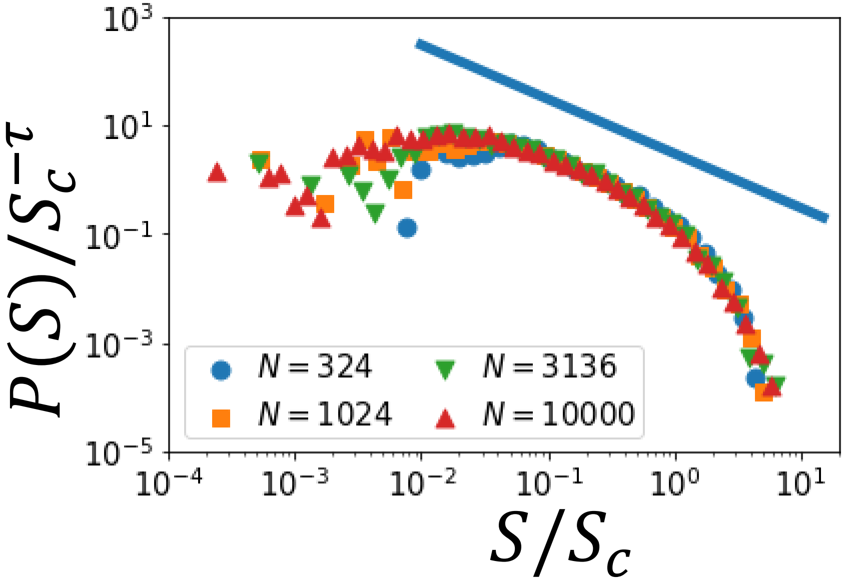
$\tau = 1$



With different thermostat(Nosé-Hoover)







$\tau = 1$