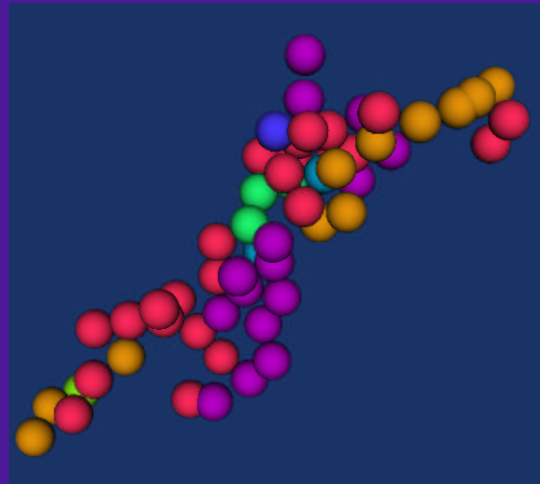


Self-Organized Criticality Below The Glass Transition

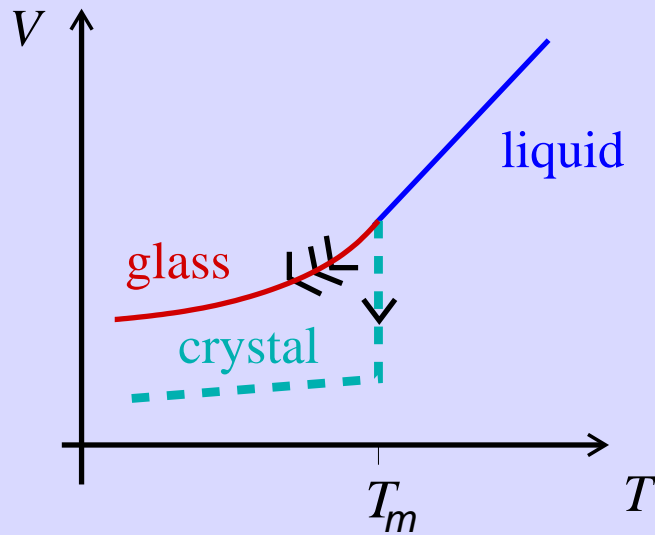
Katharina Vollmayr-Lee, Bucknell University

May 15, 2008



Thanks: E. A. Baker, A. Zippelius, K. Binder, and J. Horbach

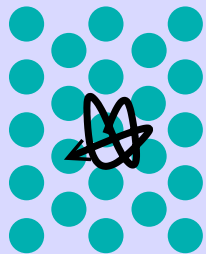
Introduction



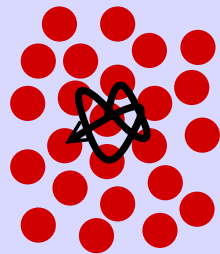
Glass:

→ system falls
out of equilibrium

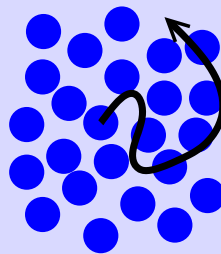
Crystal



Glass



Liquid



Structure: disordered

Dynamics: frozen in

Complex Dynamics

Model

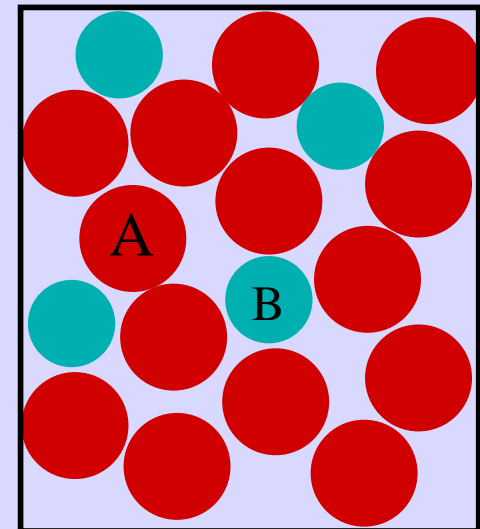
Binary Lennard-Jones System

$$V_{\alpha\beta}(r) = 4 \epsilon_{\alpha\beta} \left(\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right)$$

$$\sigma_{AA} = 1.0 \quad \sigma_{AB} = 0.8 \quad \sigma_{BB} = 0.88$$

$$\epsilon_{AA} = 1.0 \quad \epsilon_{AB} = 1.5 \quad \epsilon_{BB} = 0.5$$

[W. Kob and H.C. Andersen, PRL 73, 1376 (1994)]



800 A and 200 B

Simulations

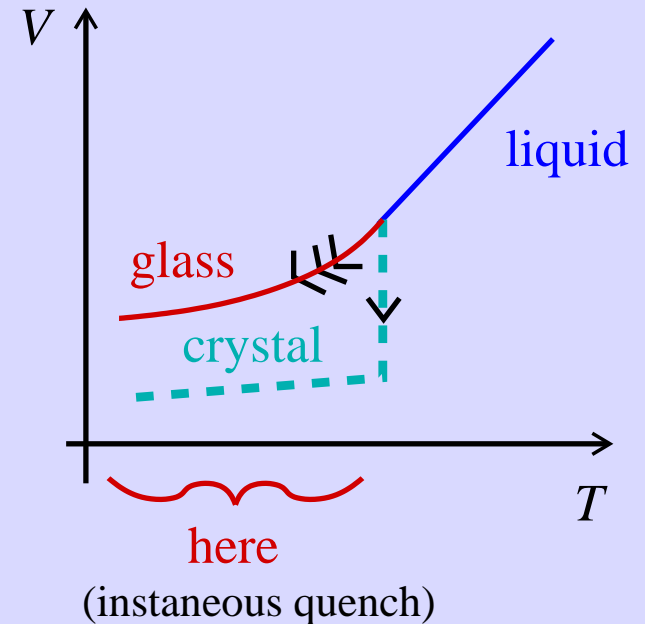
Molecular Dynamics Simulations

Velocity Verlet

below glass transition:

$$T = 0.15 - 0.43$$

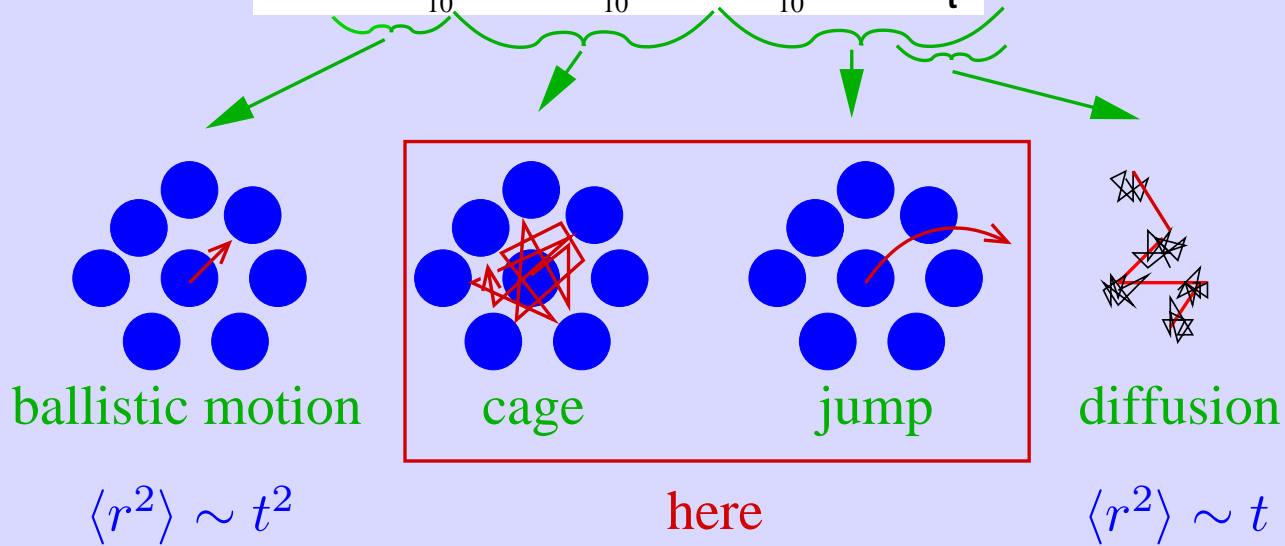
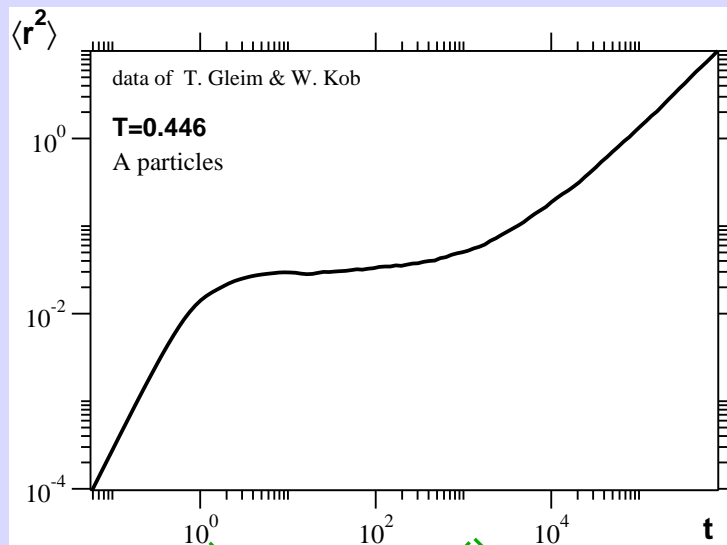
$$\text{MCT: } T_c = 0.435 \quad [\text{W. Kob et al., PRL 73 (1994)}]$$



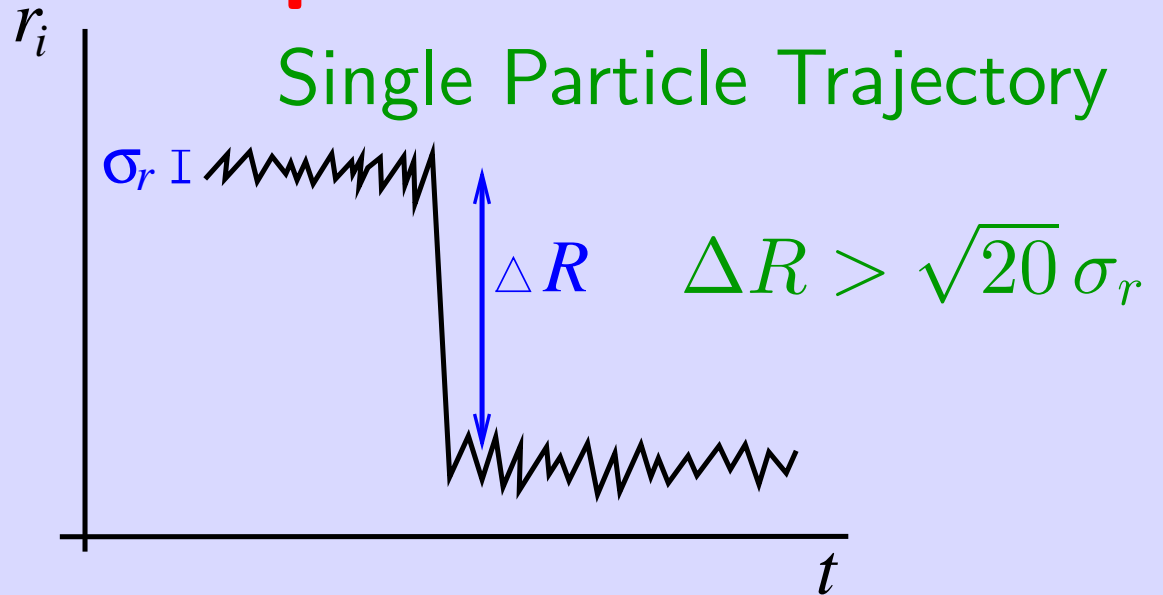
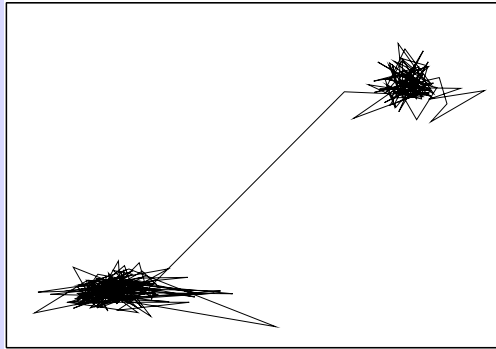
History Production Runs

Cage-Picture

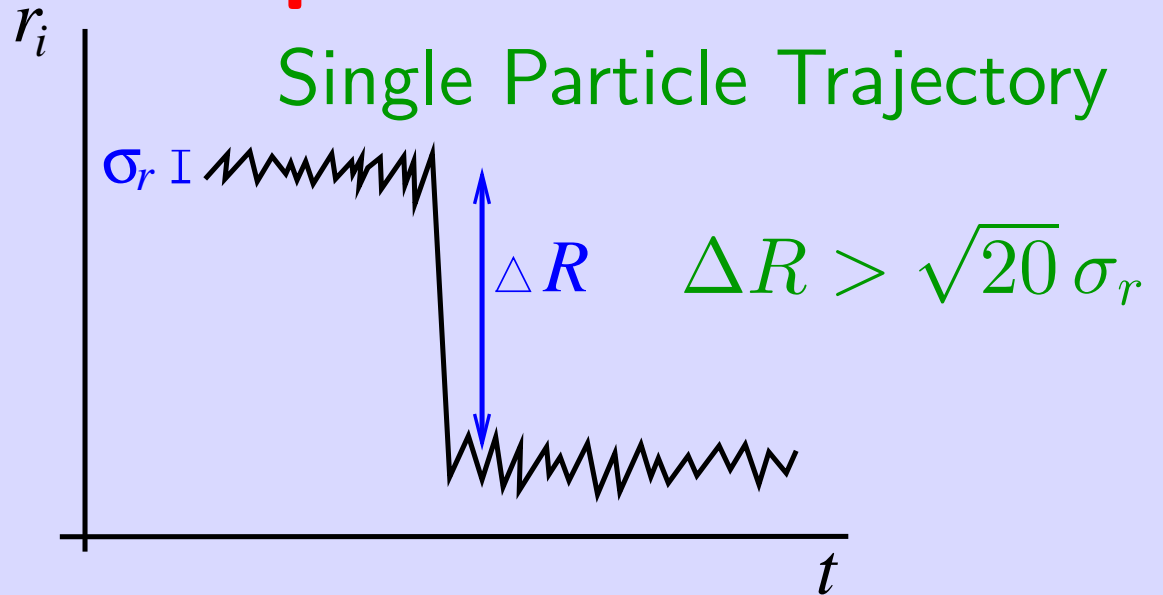
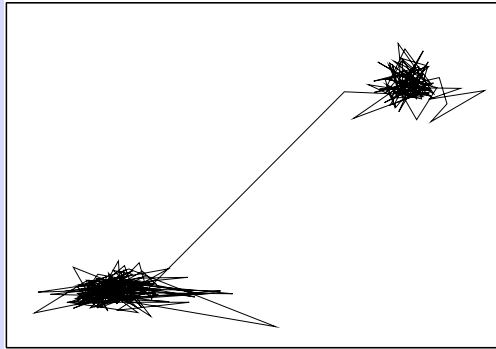
Mean-Squared Displacement: $\langle r^2 \rangle(t) = \left\langle \frac{1}{N} \sum_{i=1}^N (\underline{r}_i(t) - \underline{r}_i(0))^2 \right\rangle$



Definition: Jump Occurrence

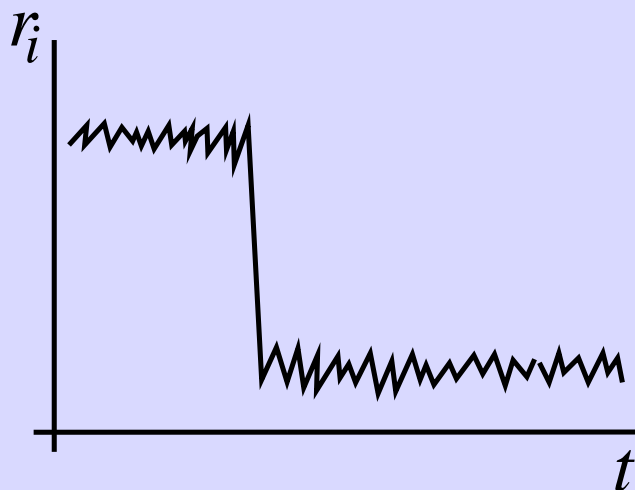


Definition: Jump Occurrence

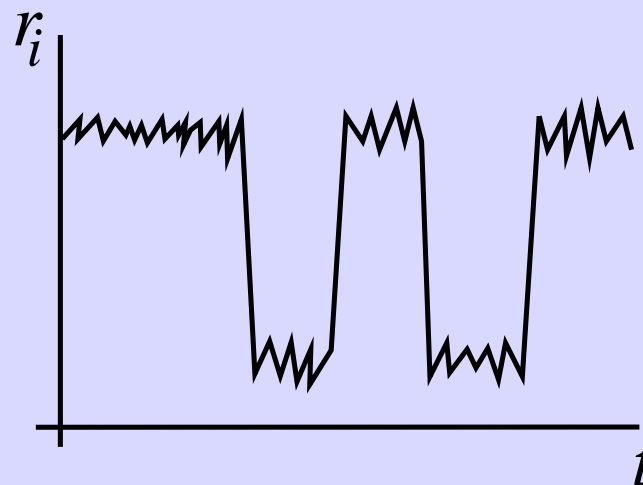


Definition: Jump Type

Irreversible Jump



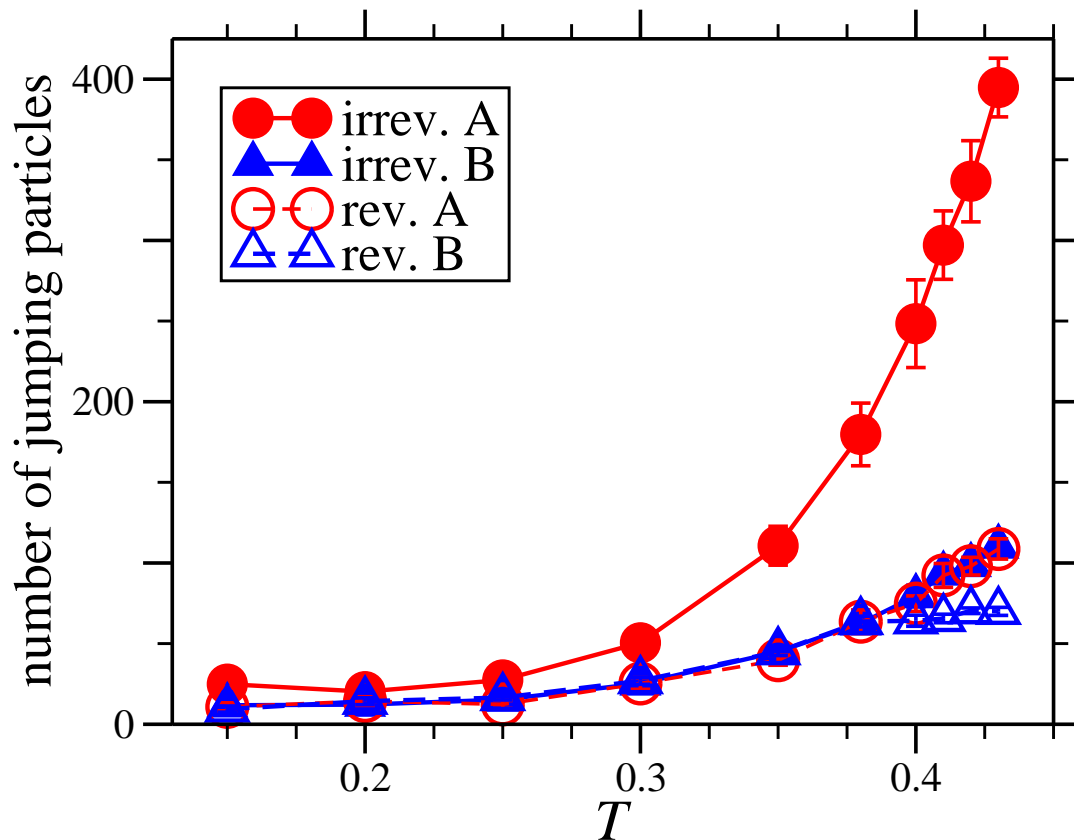
Reversible Jump



Outline

- Jump Statistics
- Correlated Single Particle Jumps
- History Dependence
- Summary & Outlook

Number of Jumping Particles



⇒ increasing with increasing T

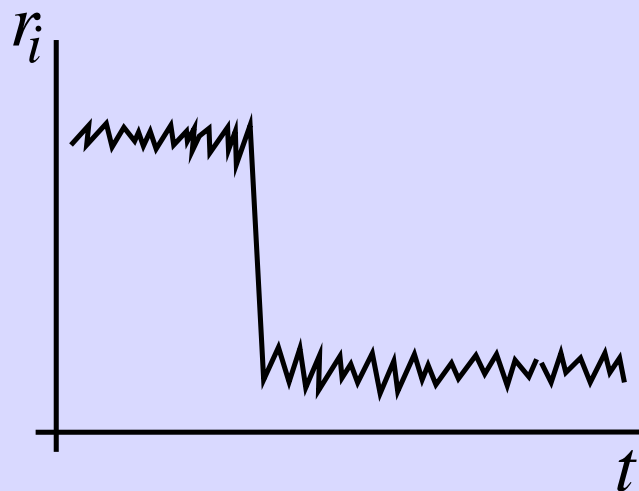
⇒ both A & B particles jump

⇒ irrev. & reversible jumps at all temperatures T

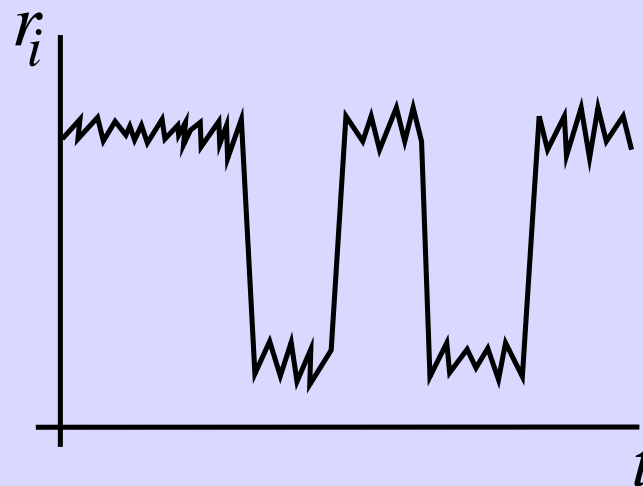
Fraction of Irreversibly Jumping Particles

$$\text{fraction of irrev. jumpers} = \frac{\text{number of irrev. jump. part.}}{\text{number of jump. part.}}$$

Irreversible Jump

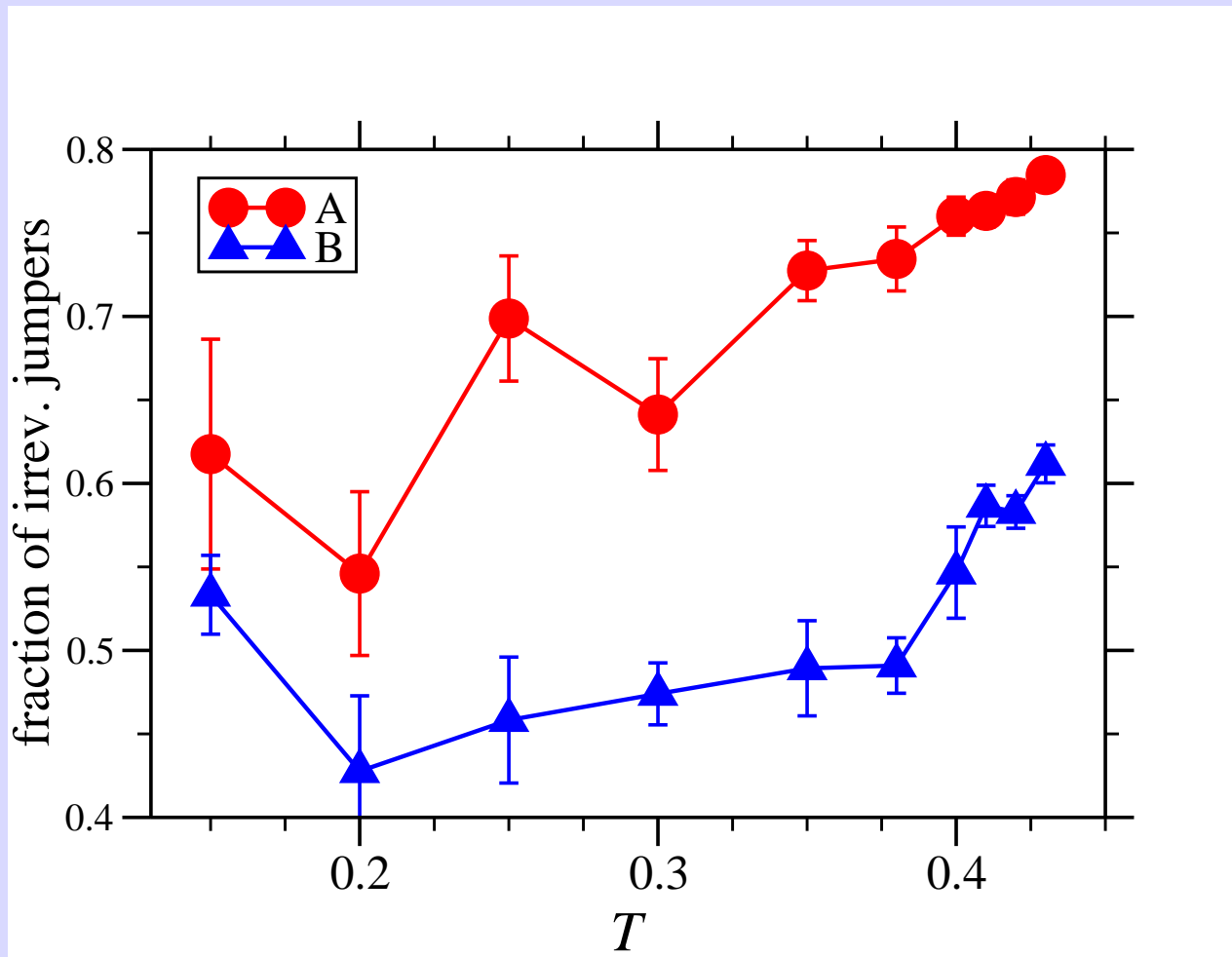


Reversible Jump



Fraction of Irreversibly Jumping Particles

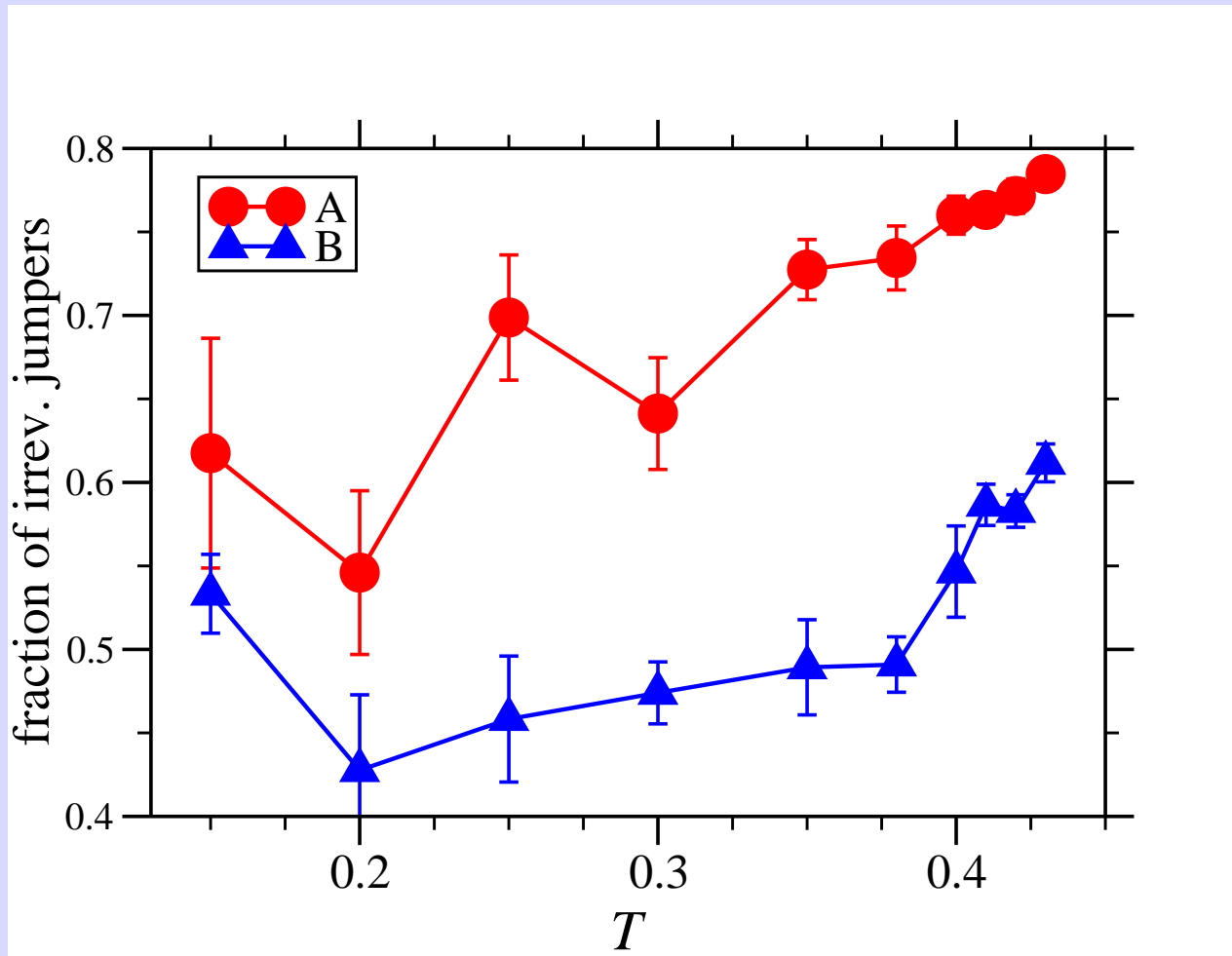
$$\text{fraction of irrev. jumpers} = \frac{\text{number of irrev. jump. part.}}{\text{number of jump. part.}}$$



⇒ fraction of irrev. jumpers increases with increasing T

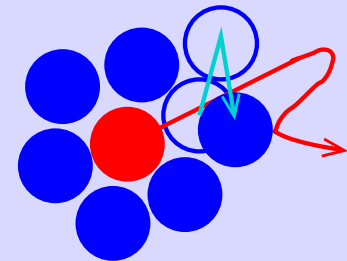
Fraction of Irreversibly Jumping Particles

$$\text{fraction of irrev. jumpers} = \frac{\text{number of irrev. jump. part.}}{\text{number of jump. part.}}$$

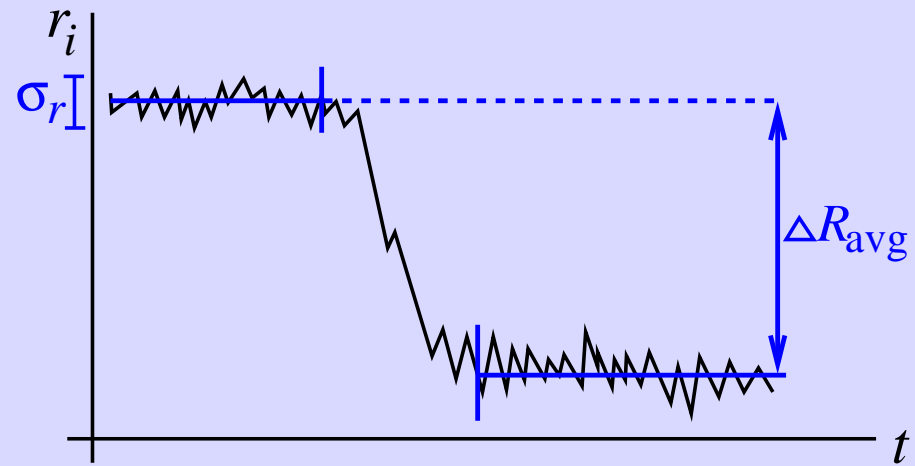


⇒ fraction of irrev. jumpers increases with increasing T

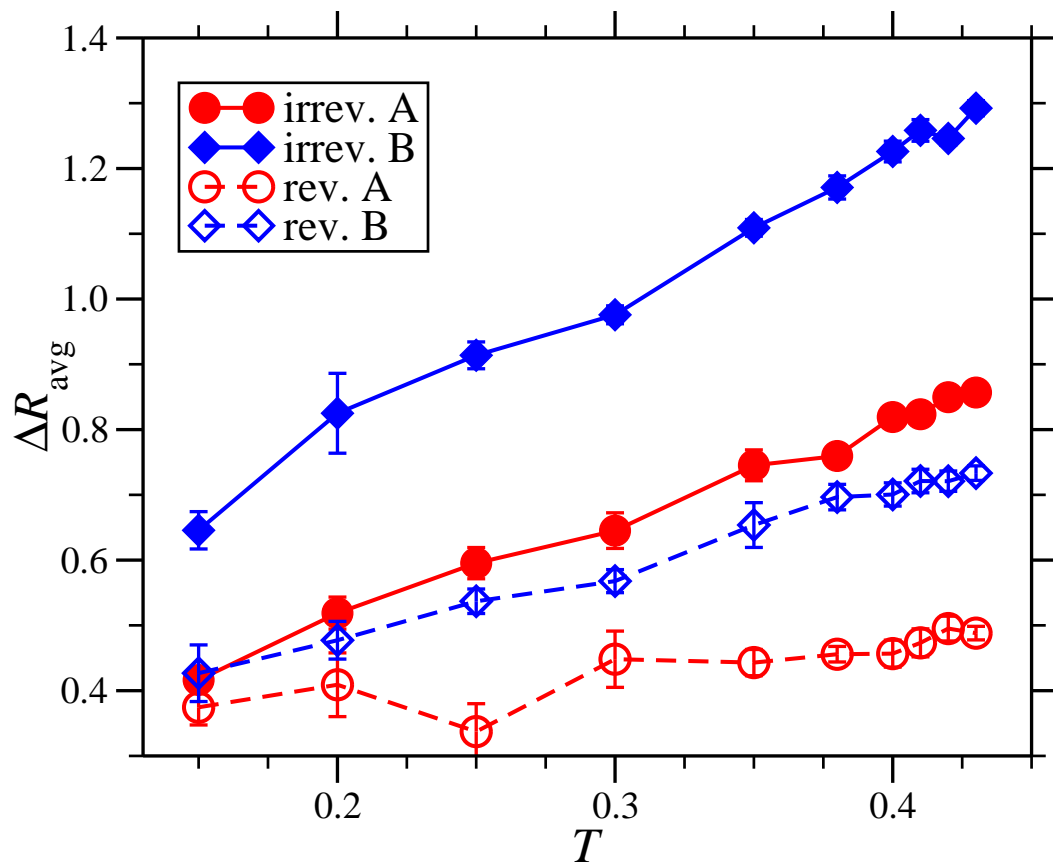
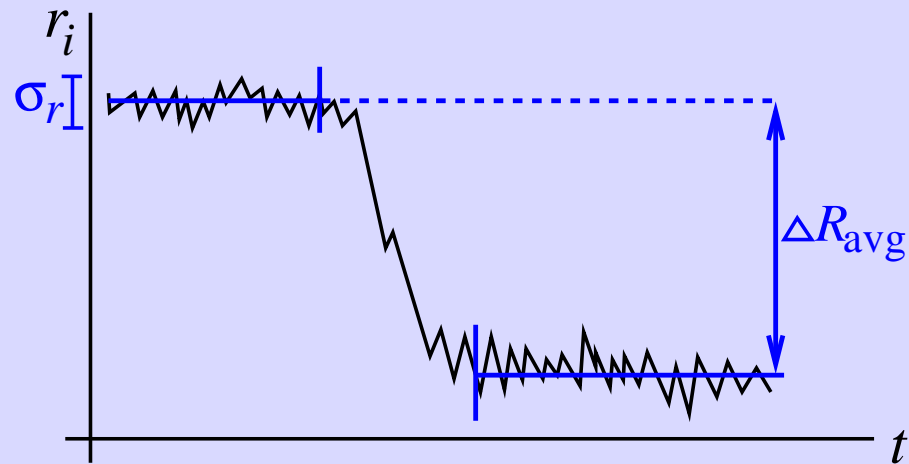
interpretation: door closing



Jump Size



Jump Size

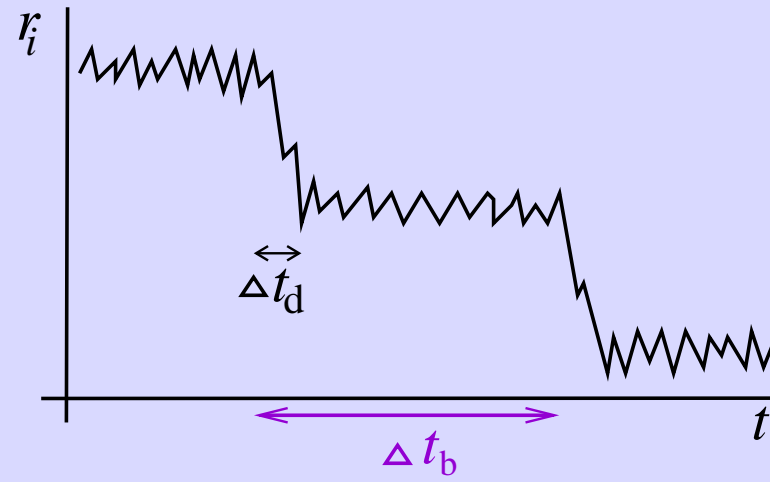


⇒ increasing with increasing T

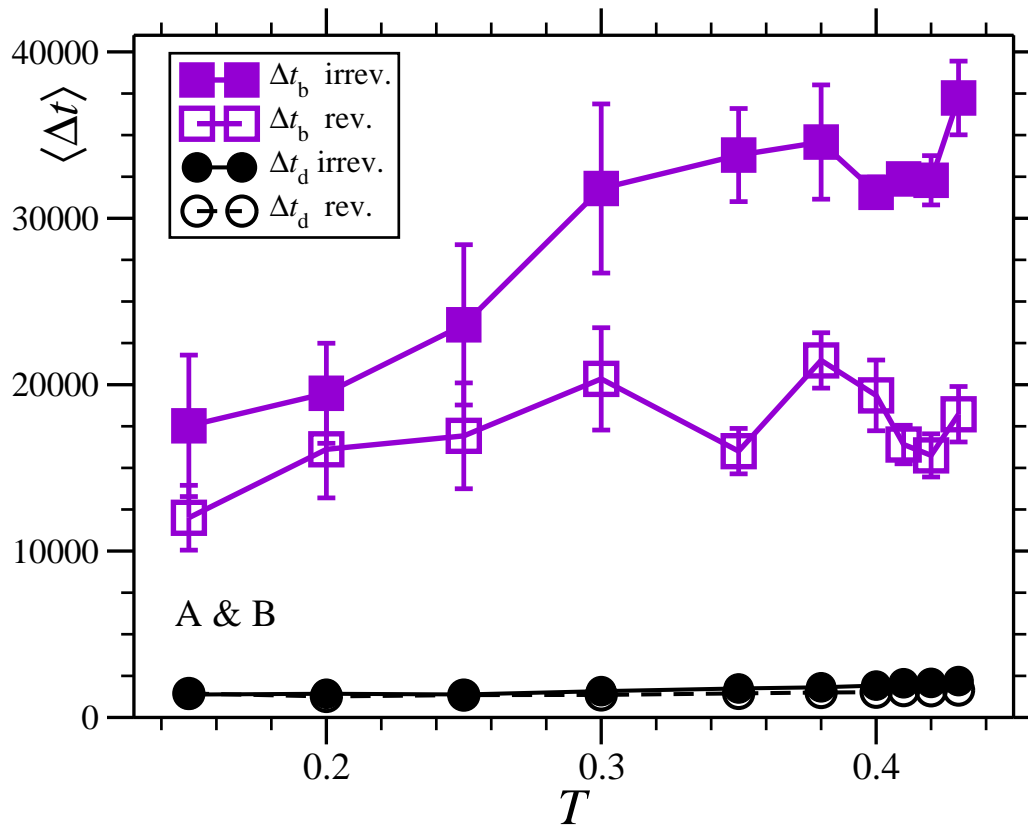
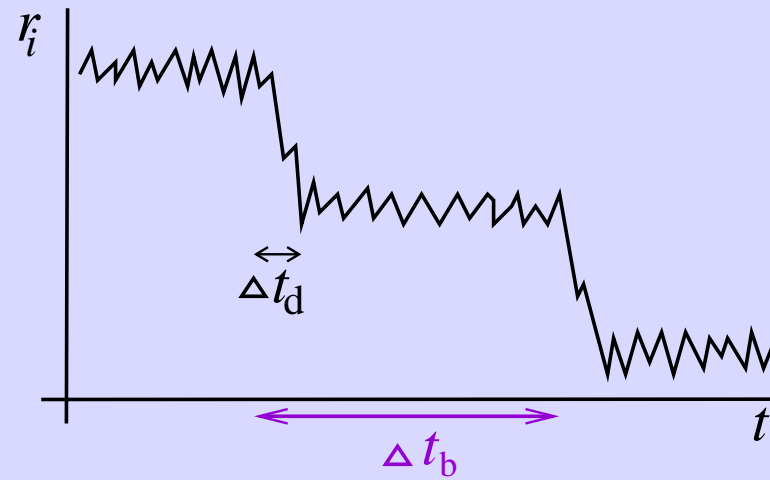
⇒ (smaller) B-particles jump farther

⇒ irreversible jumps farther

Time Scale



Time Scale



$$\implies \Delta t_b \gg \Delta t_d$$

$\implies \Delta t_b$ independent
of temperature

(whole simulation 10^5)

Summary: Jump Statistics

At larger temperature relaxation:

- not via Δt_b (indep. of T)
- via larger jumpsizes
- via more jumping particles

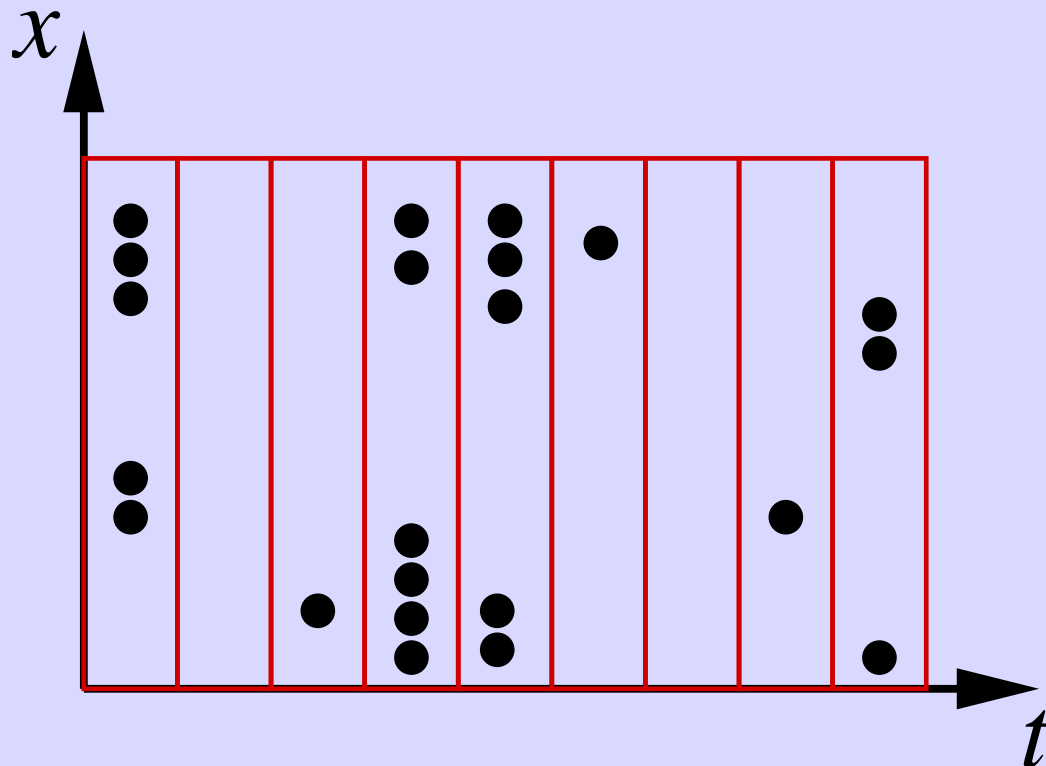
[J. Chem. Phys. **121**, 4781 (2004)]

Outline

- Jump Statistics
- Correlated Single Particle Jumps
 - ◇ Simultaneously Jumping Particles
 - ◇ Temporally Extended Cluster
- History Dependence
- Summary & Outlook

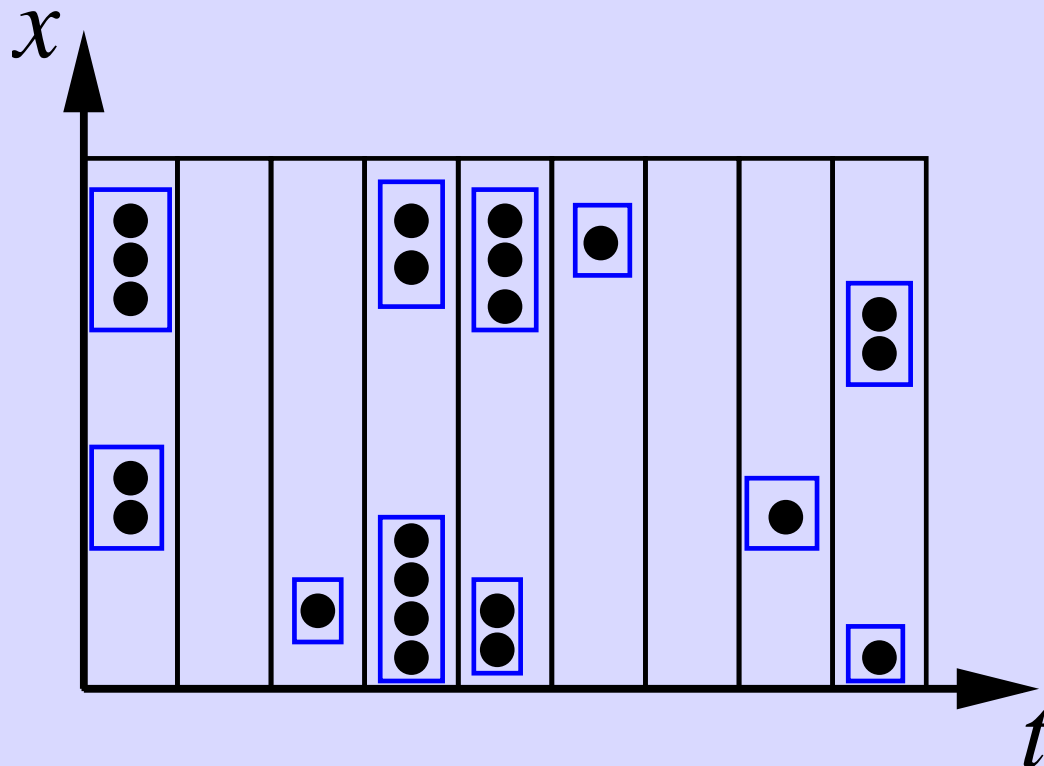
Simultaneously Jumping Particles

Definition: Correlated in Time & Space



Simultaneously Jumping Particles

Definition: Correlated in Time & Space

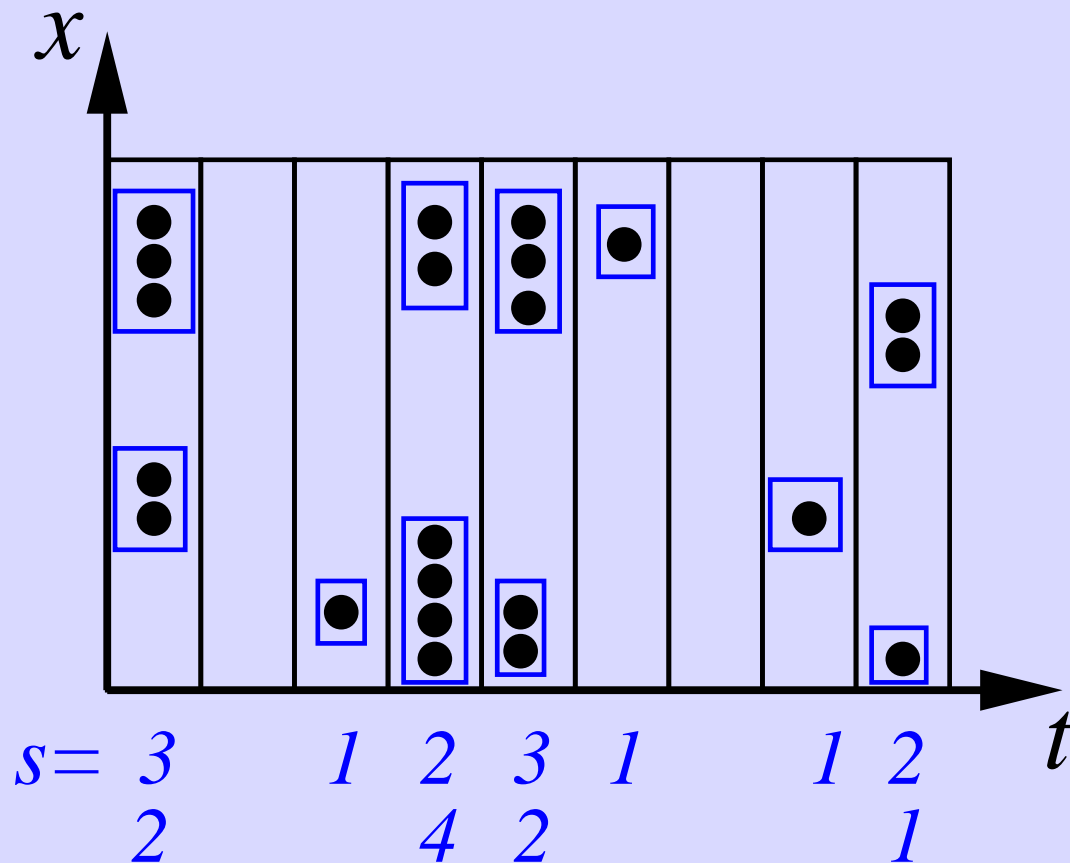


Cluster:

nearest neighbor
connections
(via $g(r)$)

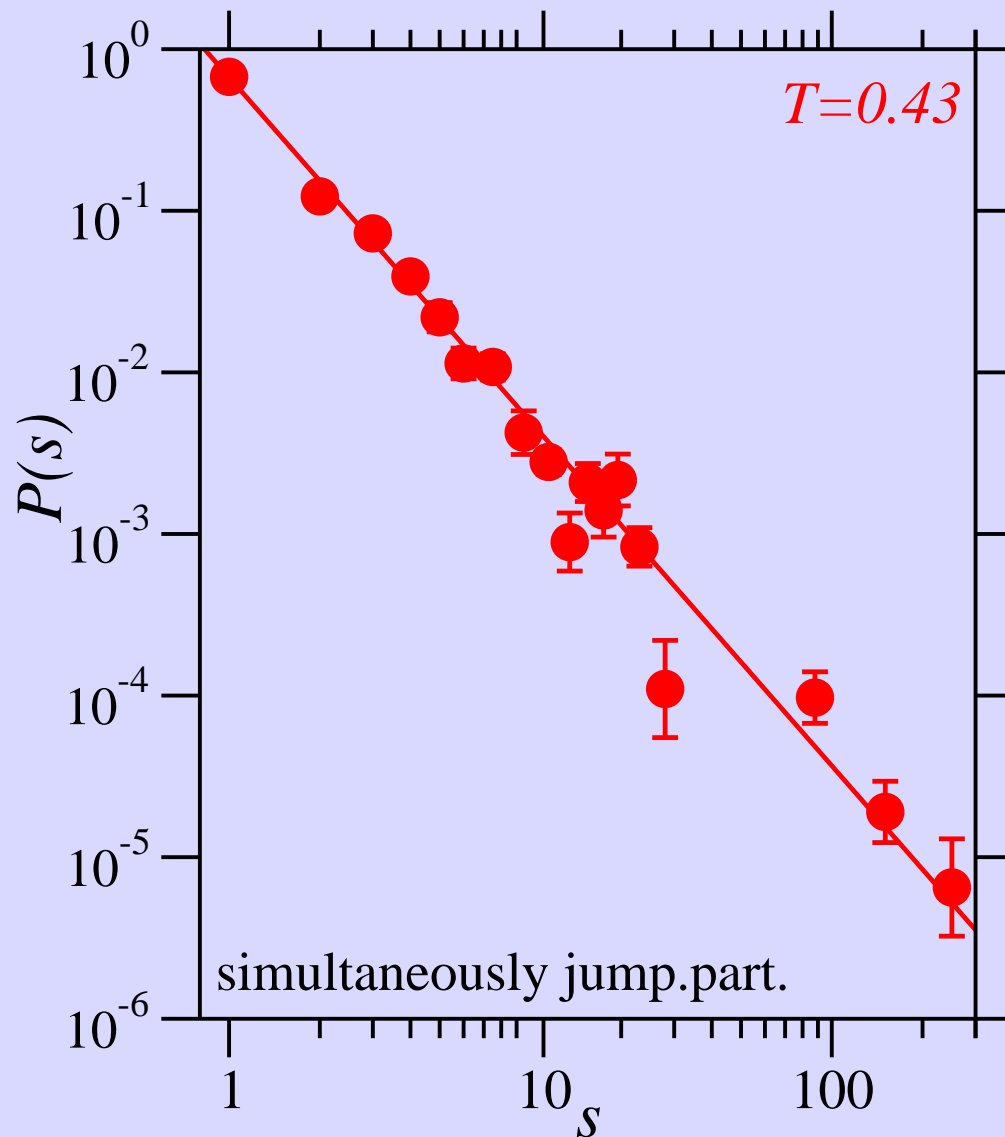
Simultaneously Jumping Particles

Cluster Size = number of particles in cluster



Cluster:
nearest neighbor
connections

Cluster Size Distribution of Simultaneously Jumping Particles



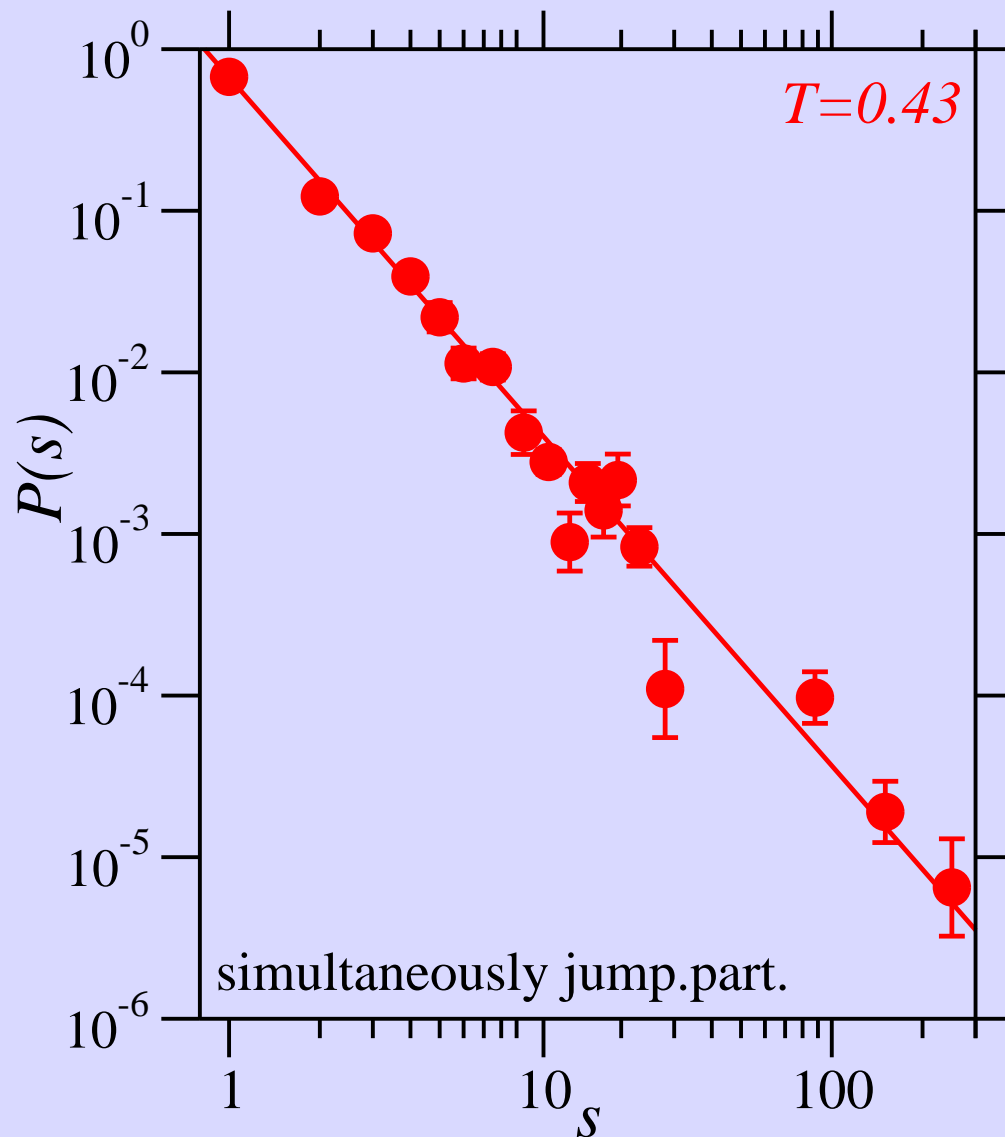
$$\Rightarrow \ln P = a - \tau \ln s$$

$$\Rightarrow P(s) \sim s^{-\tau}$$

$$\tau = 1.89 \pm 0.03$$

\Rightarrow critical behavior

Cluster Size Distribution of Simultaneously Jumping Particles



$$\Rightarrow \ln P = a - \tau \ln s$$

$$\Rightarrow P(s) \sim s^{-\tau}$$

$$\tau = 1.89 \pm 0.03$$

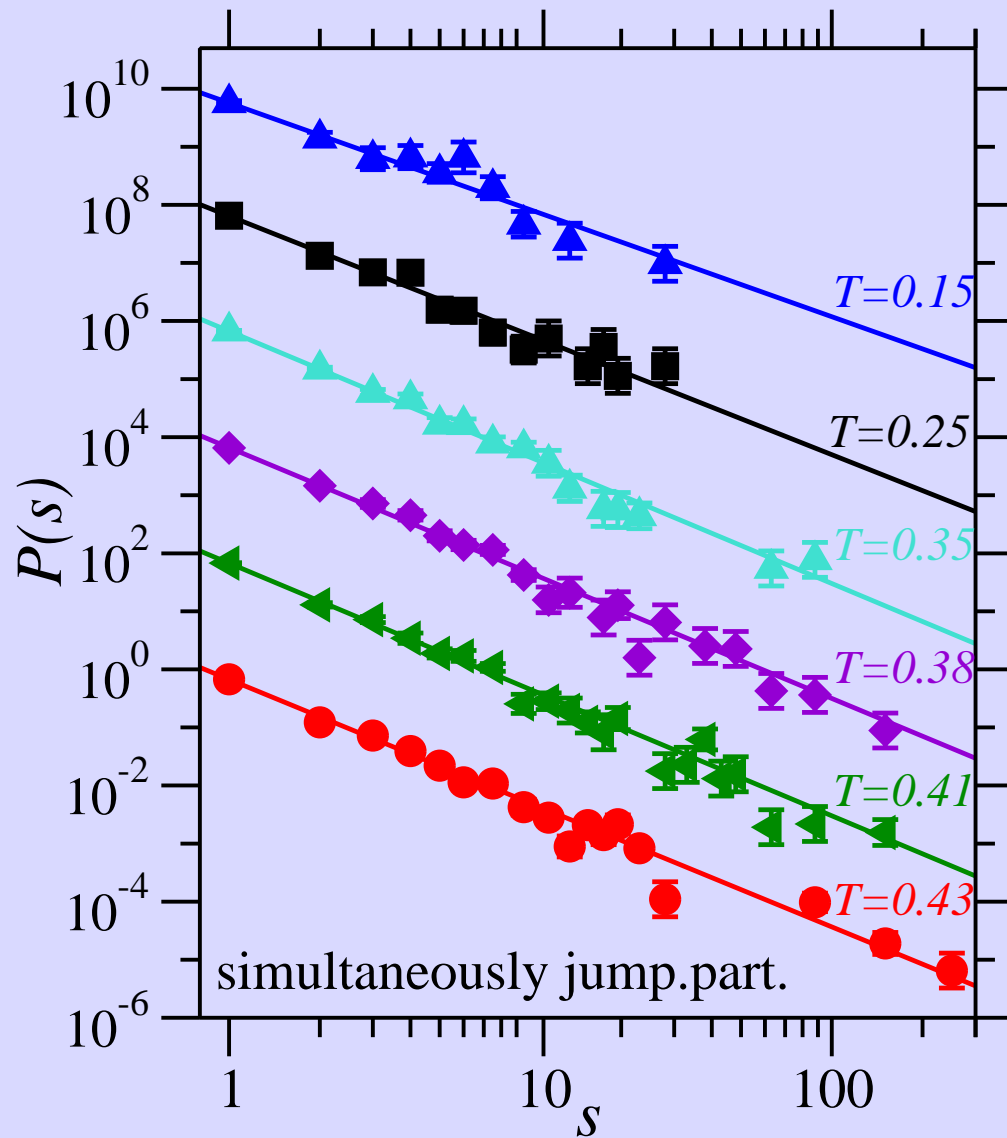
\Rightarrow critical behavior

\Rightarrow Percolation?

$$\tau_{\text{MF}} = 2.5$$

$$\tau_{3\text{d}} = 2.2$$

Cluster Size Distribution of Simultaneously Jumping Particles



$$\implies P(s) \sim s^{-\tau}$$

percolation?

NO because

\implies power law for
all temperatures

\implies self-organized
criticality

$\tau(T)$

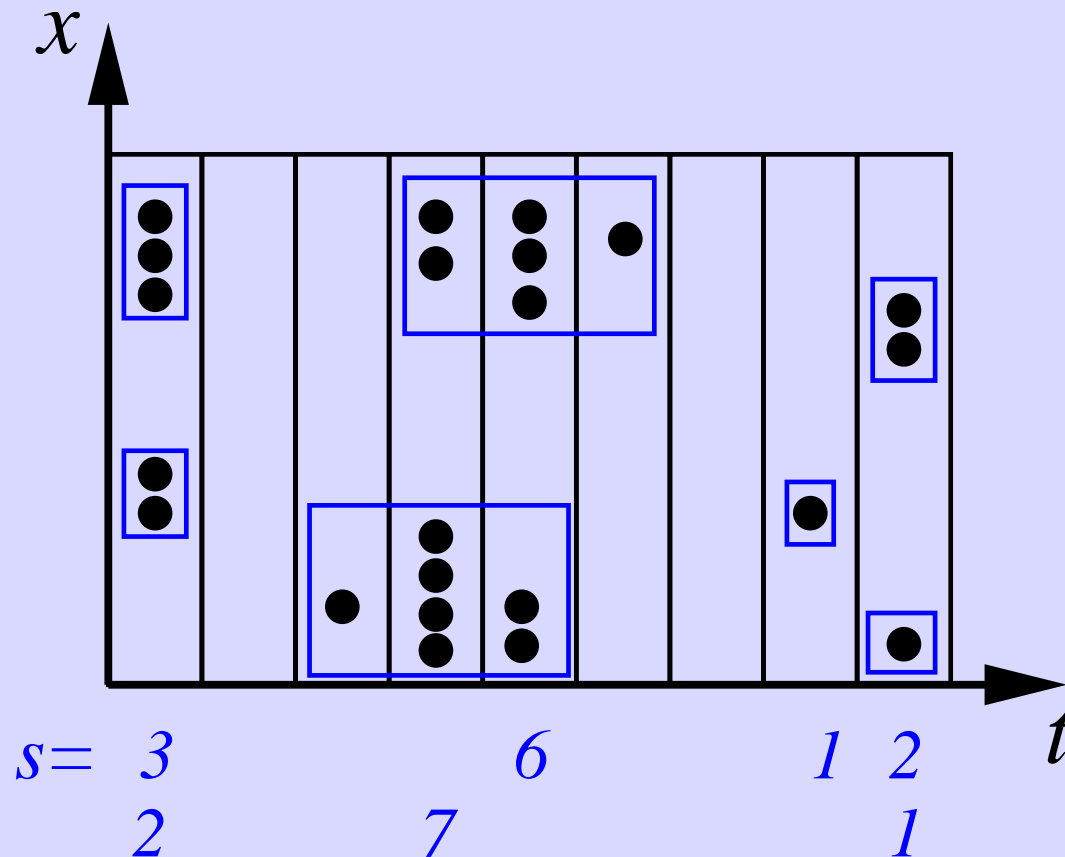
Self-Organized Criticality: Similarities

- power law (critical behavior)
not only at T_c but for **all** $T < T_c$
- out of equilibrium
- wide range of time scales
- avalanches

Outline

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Temporally Extended Cluster

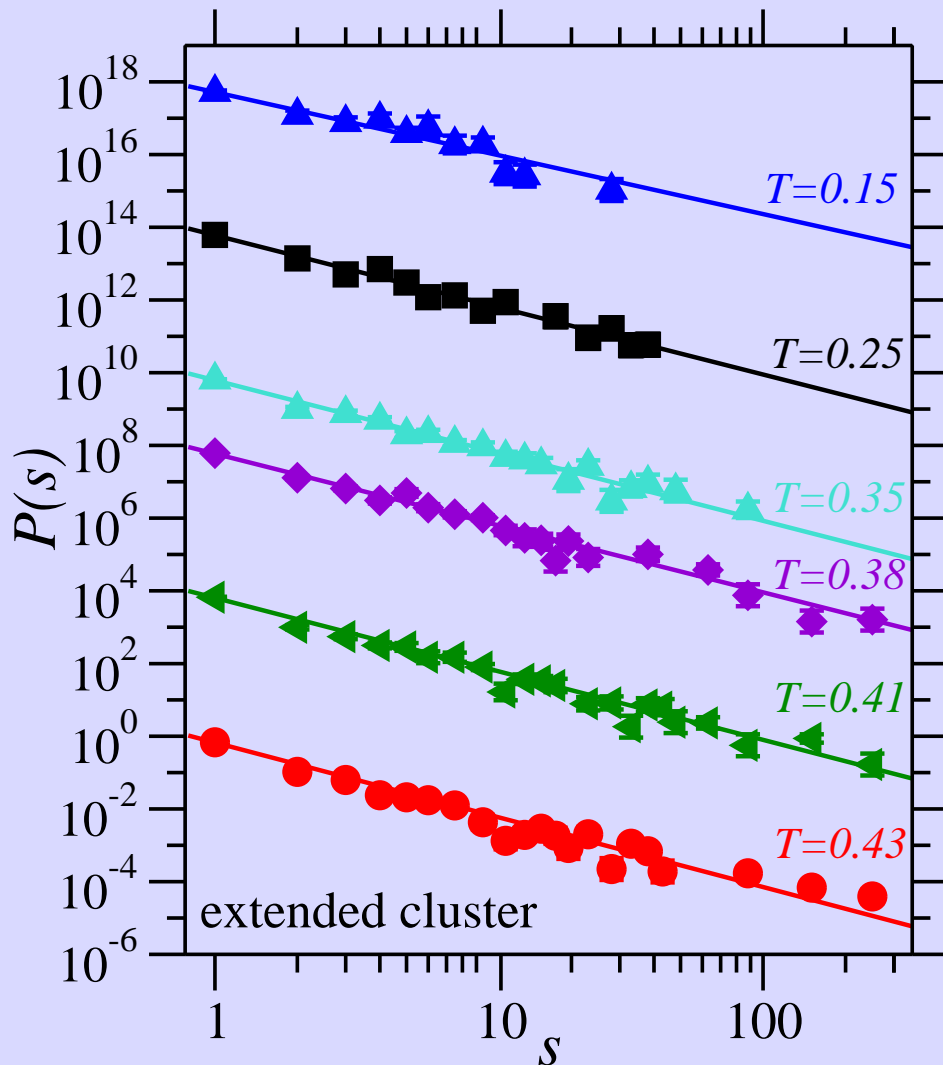


Definition:

cluster of events (\mathbf{r}_i, t_i)
connected if:

$$\Delta r < r_{\text{cutoff}} \quad \text{and}$$
$$\Delta t < t_{\text{cutoff}}$$

Cluster Size Distribution of Temporally Extended Clusters

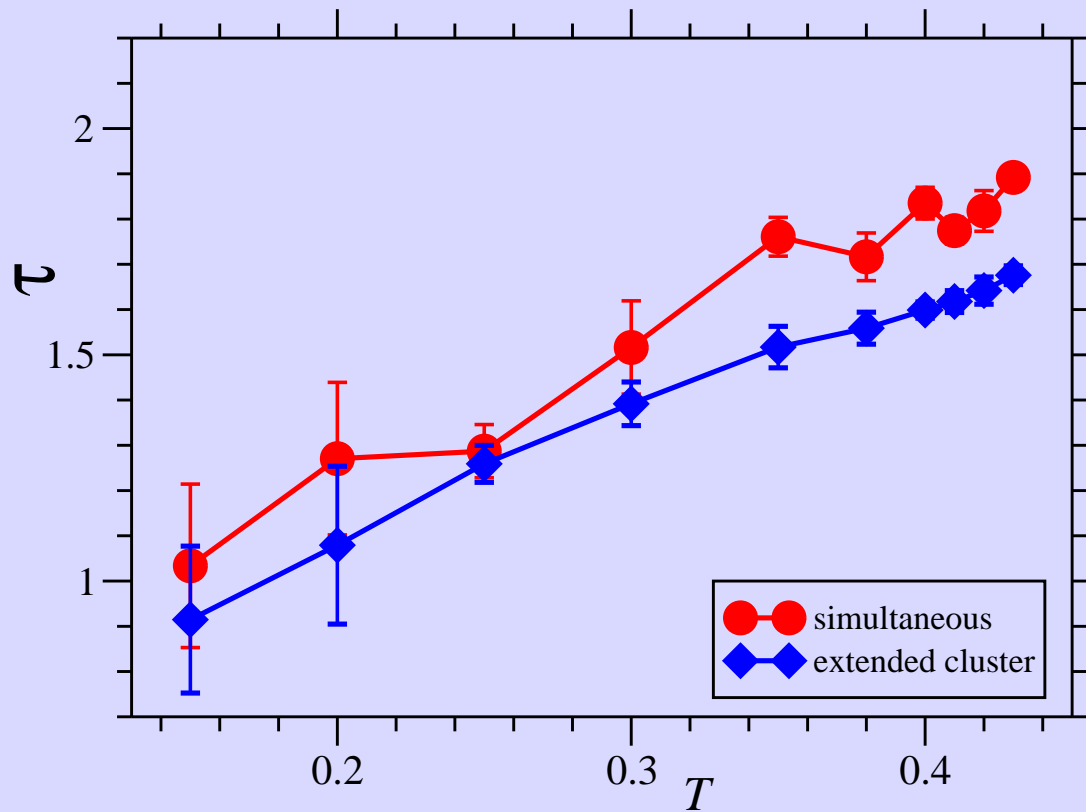


$$\implies P(s) \sim s^{-\tau}$$

\implies for all temperatures
(self-organized crit.)

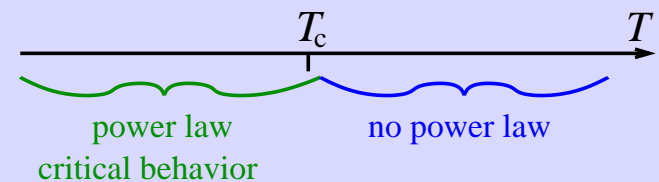
Exponent $\tau(T)$

$$P(s) \sim s^{-\tau}$$



slightly above T_c $\tau \approx 1.86$

[Donati et al. 1999]



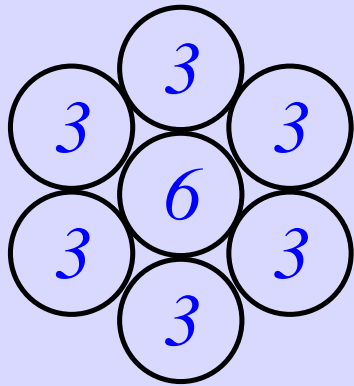
P simult.

Shape of Clusters

z = number of nearest neighbors within cluster

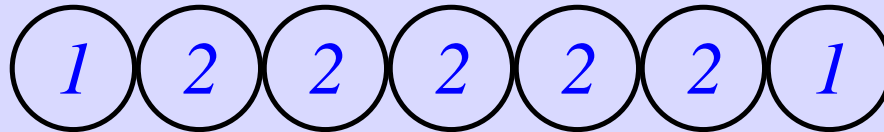
s = number of particles (cluster size)

$\langle z \rangle$ = average of z over particles $1, \dots, s$



$$s=7$$

$$\langle z \rangle = 3.4$$



$$s=7$$

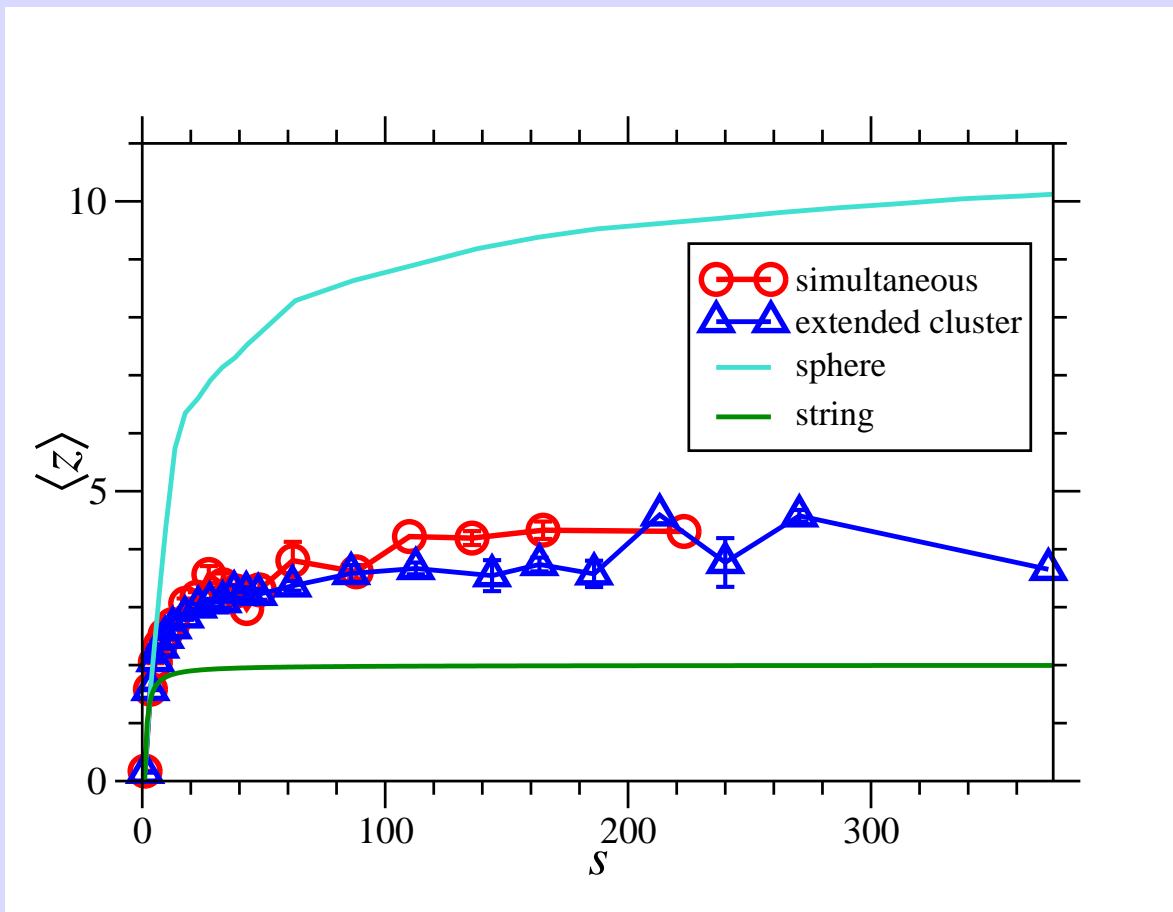
$$\langle z \rangle = 1.7$$

Shape of Clusters

z = number of nearest neighbors within cluster

s = number of particles (cluster size)

$\langle z \rangle$ = average of z over particles $1, \dots, s$



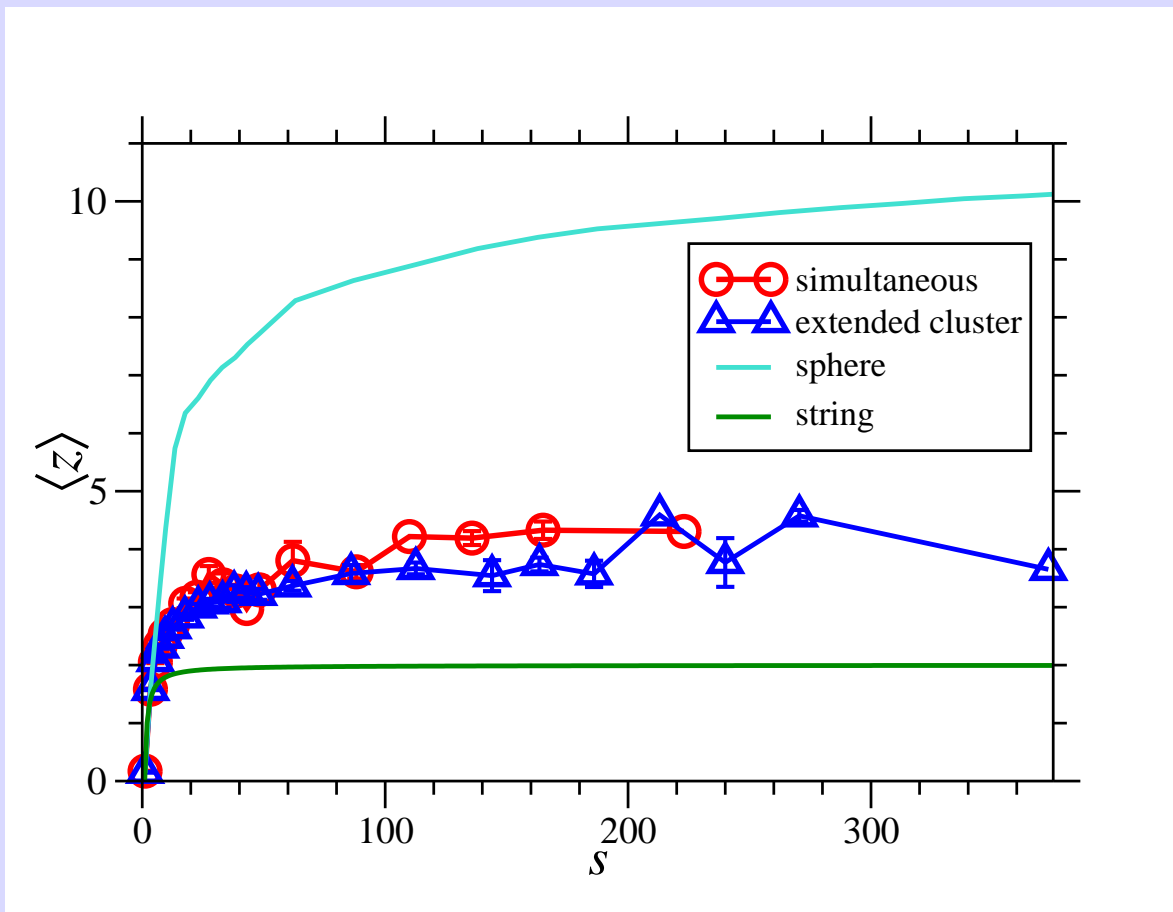
⇒ string-like clusters

Shape of Clusters

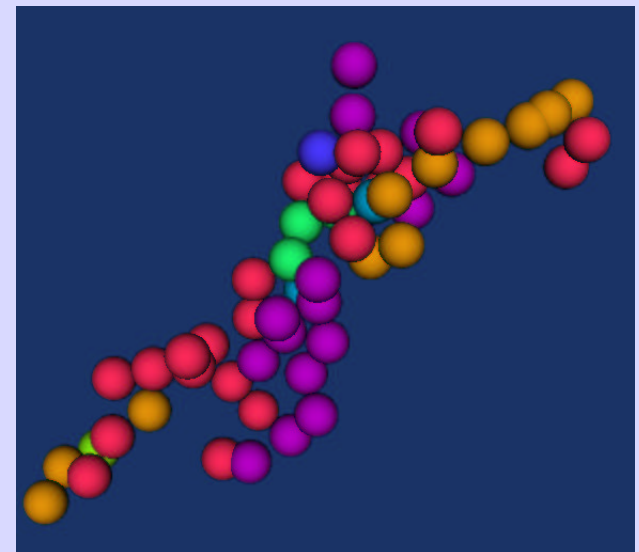
z = number of nearest neighbors within cluster

s = number of particles (cluster size)

$\langle z \rangle$ = average of z over particles $1, \dots, s$



⇒ string-like clusters

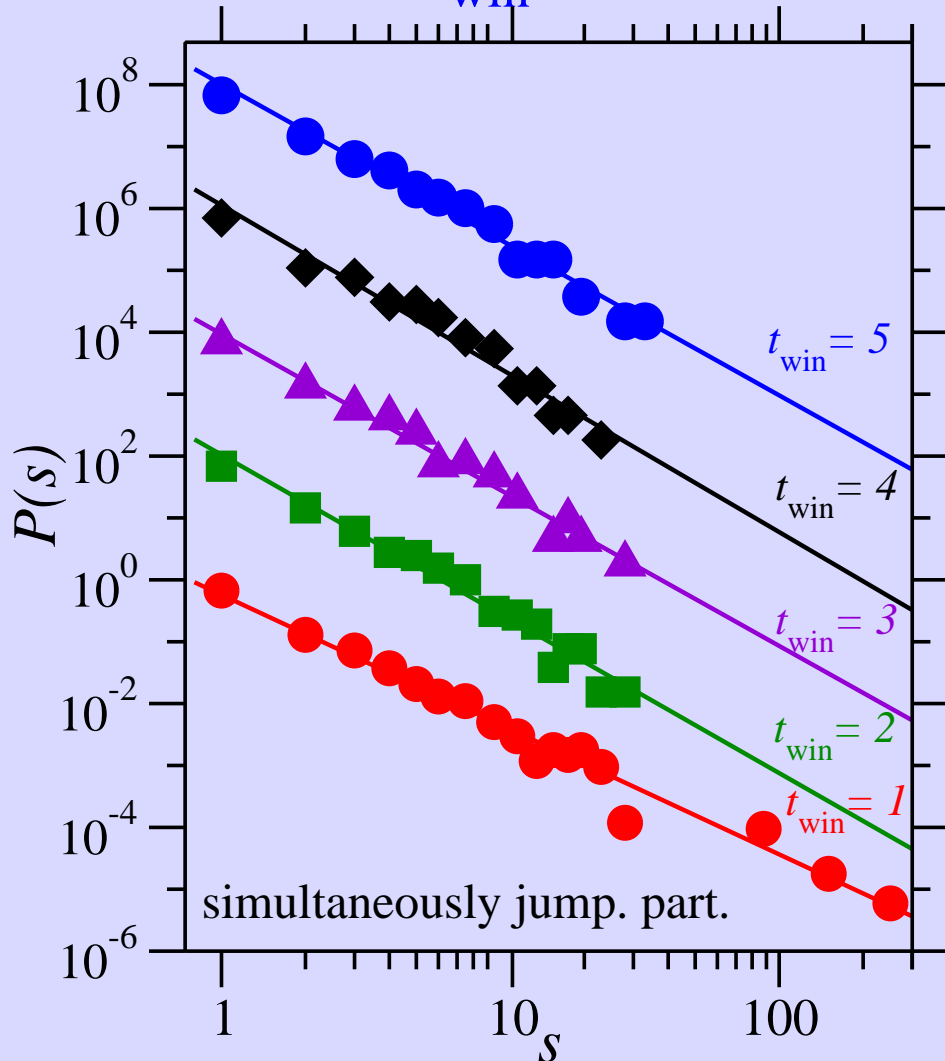
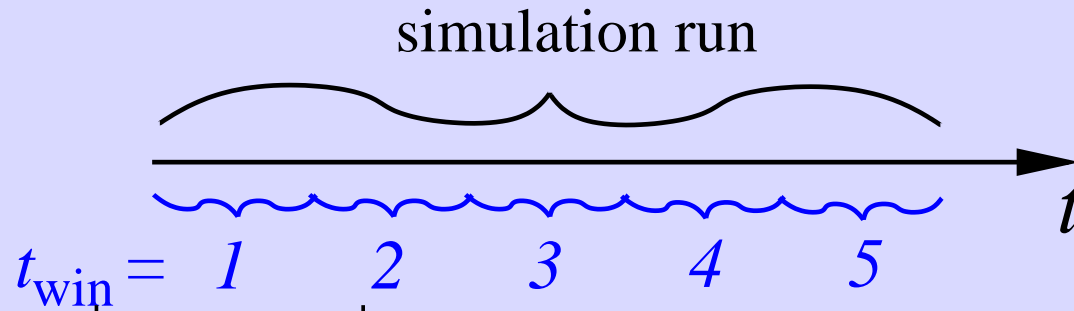


same color = same time

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History Dependence



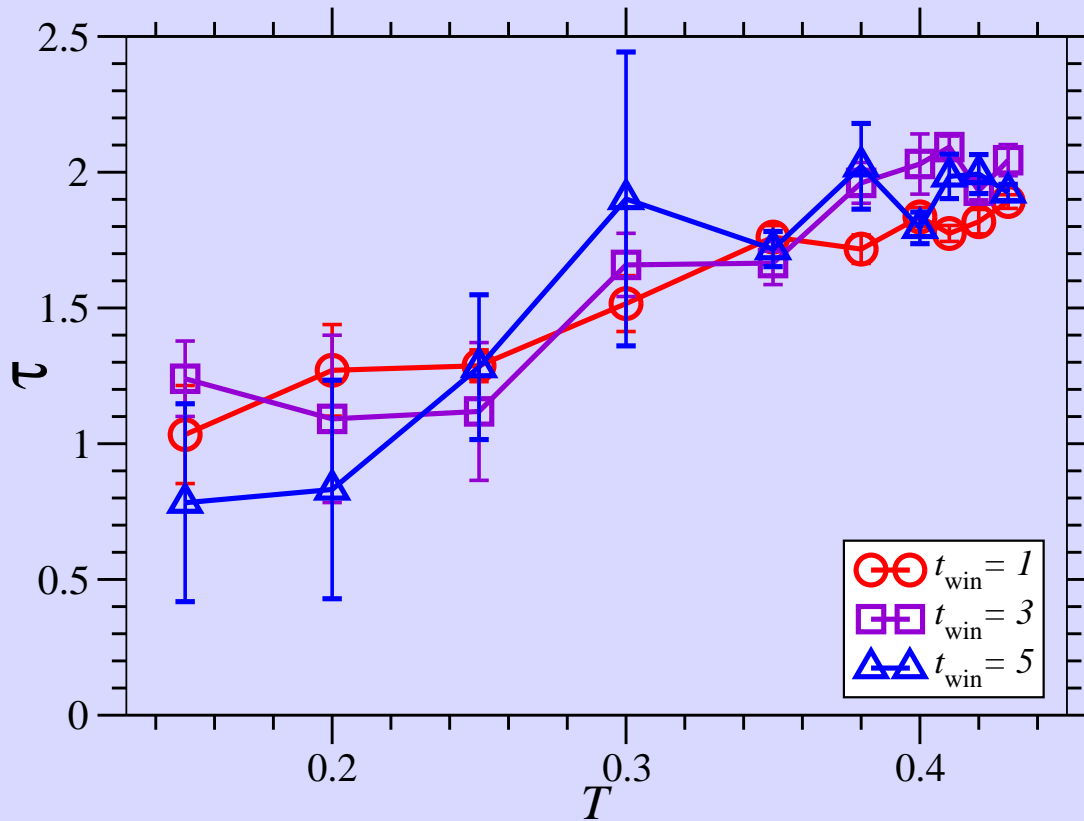
Power Law

(Simultan. Jump. Part.)

\implies aging independent

Exponent $\tau(T)$

$$P(s) \sim s^{-\tau}$$



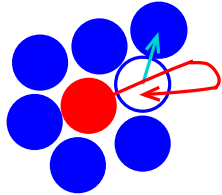
\Rightarrow aging independent

Outline

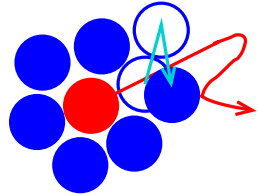
- Jump Statistics
- Correlated Single Particle Jumps
 - ◇ Simultaneously Jumping Particles
 - ◇ Temporally Extended Cluster
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- Summary & Outlook

Summary: Jump Statistics

reversible and irreversible jumps:



reversible jump

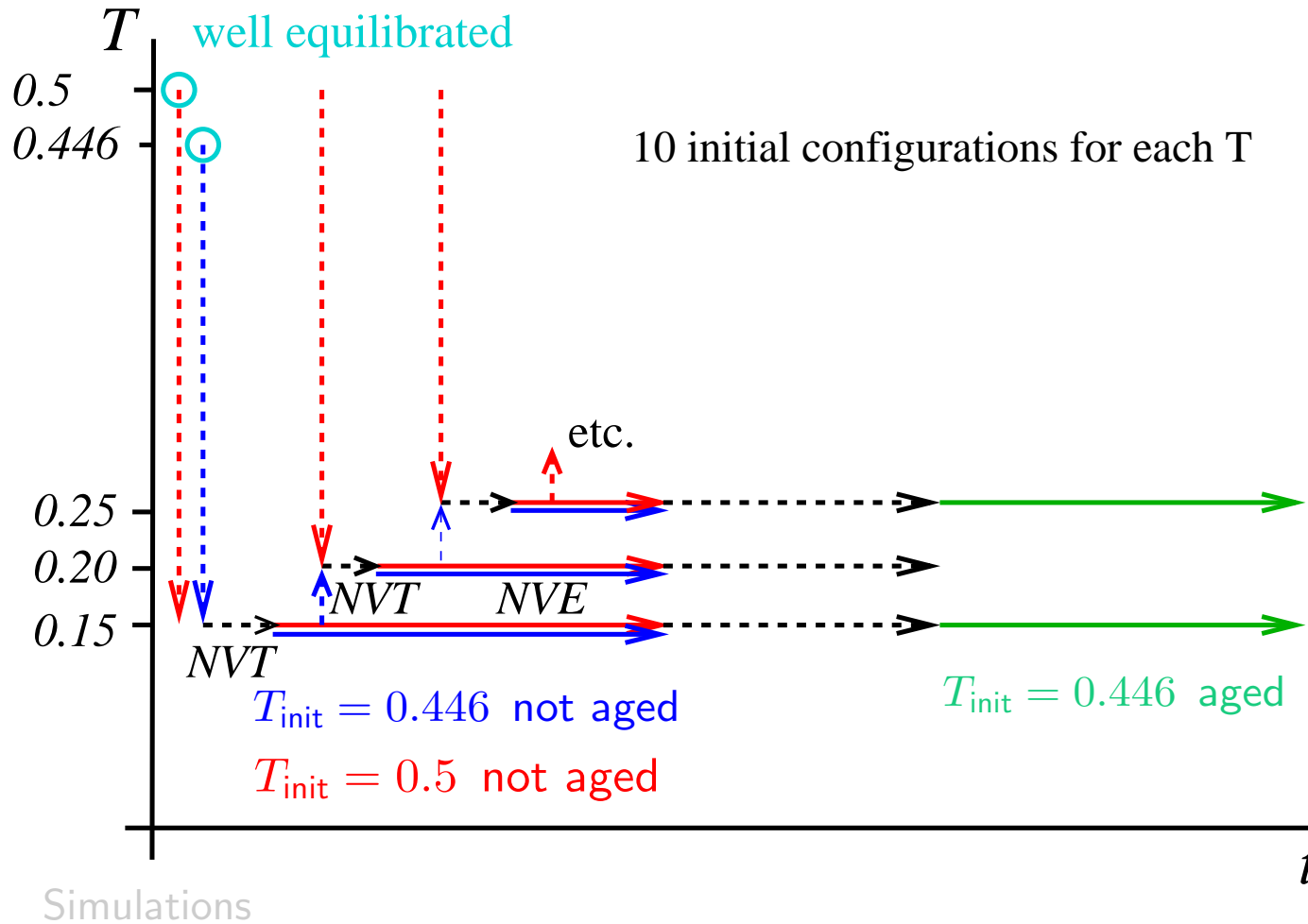


irreversible jump

At larger temperature relaxation:

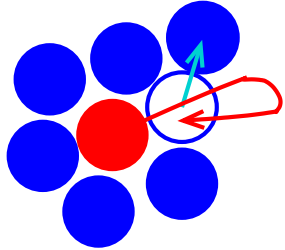
- via more jumping particles
- via larger jumpsizes
- not via Δt_b (indep. of T)

History of Production Runs

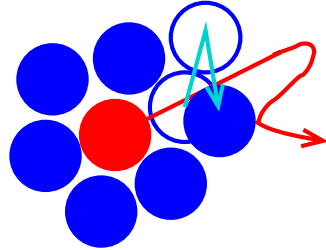


Summary: Jump Statistics

reversible and irreversible jumps:



reversible jump



irreversible jump

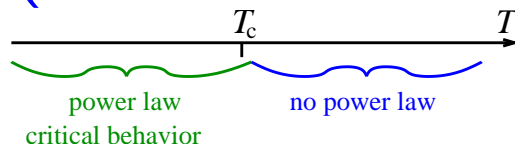
At larger temperature relaxation:

- via more jumping particles history dependent
- via larger jumpsizes history independent
- not via Δt_b (indep. of T) history independent

Summary: Correlated Single Particle Jumps

simultaneously jump. part. & extended clusters

- jumps are correlated spatially and temporally
- string-like clusters
- Distribution of Cluster Size: $P(s) \sim s^{-\tau}$
 - ◇ aging independent
 - ◇ for all temp. \longrightarrow **self-organized criticality**
(critical behavior gets frozen in)



[Europhys. Lett. **76**, 1130 (2006)]

Future/Present

- SiO_2
(R. A. Bjorkquist & J. A. Roman & J. Horbach)
- granular media
(T. Aspelmeier & A. Zippelius)

Acknowledgments

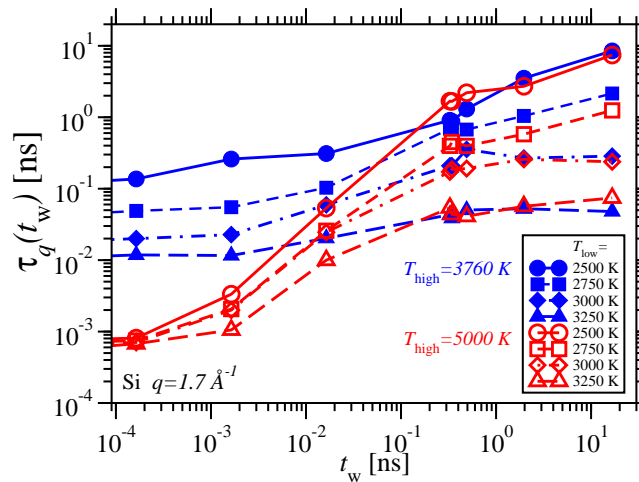
A. Zippelius, K. Binder, E. A. Baker, J. Horbach

Support from Institute of Theoretical Physics, University Göttingen,

SFB 262 and DFG Grant No. Zi 209/6-1

Out-of-Equilibrium to In-Equilibrium: SiO₂

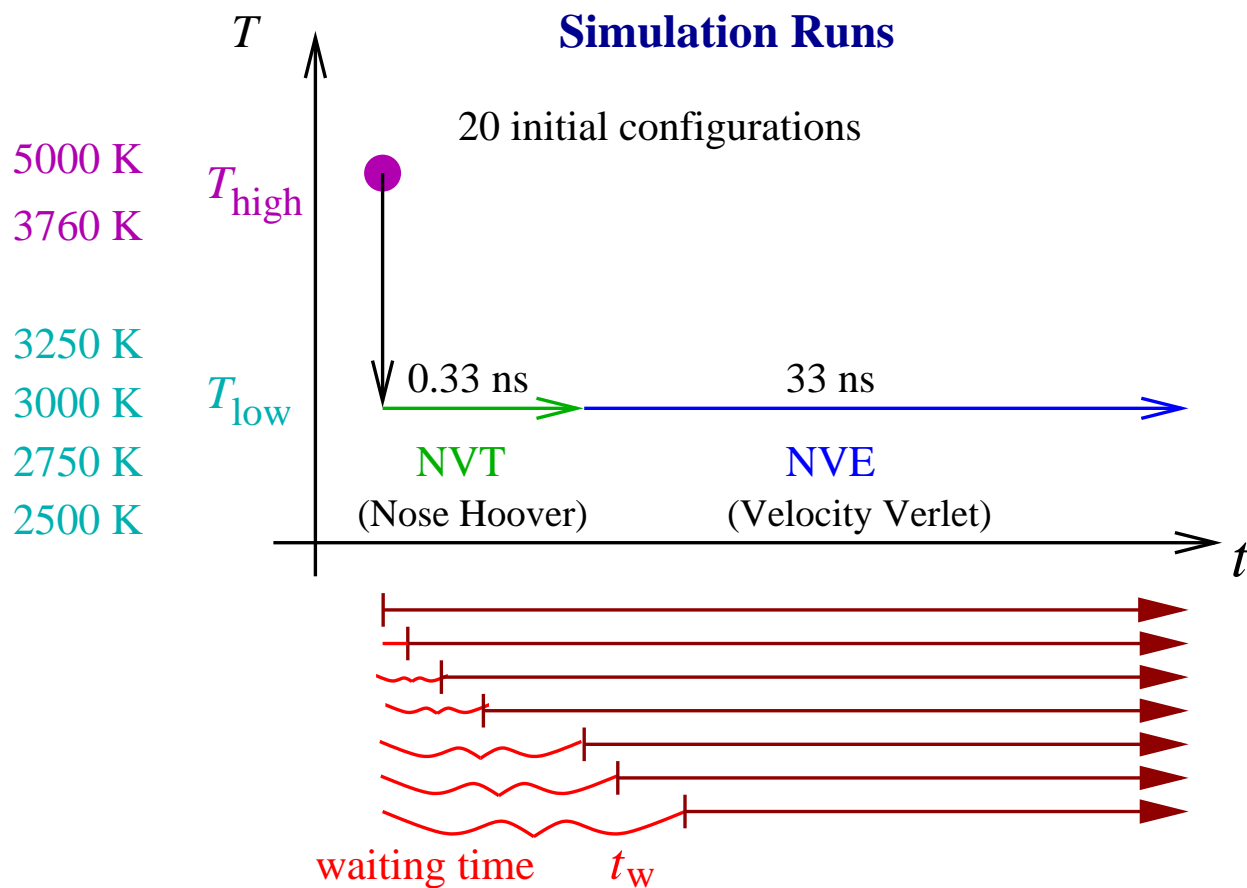
- jump statistics
- intermediate incoherent scattering function

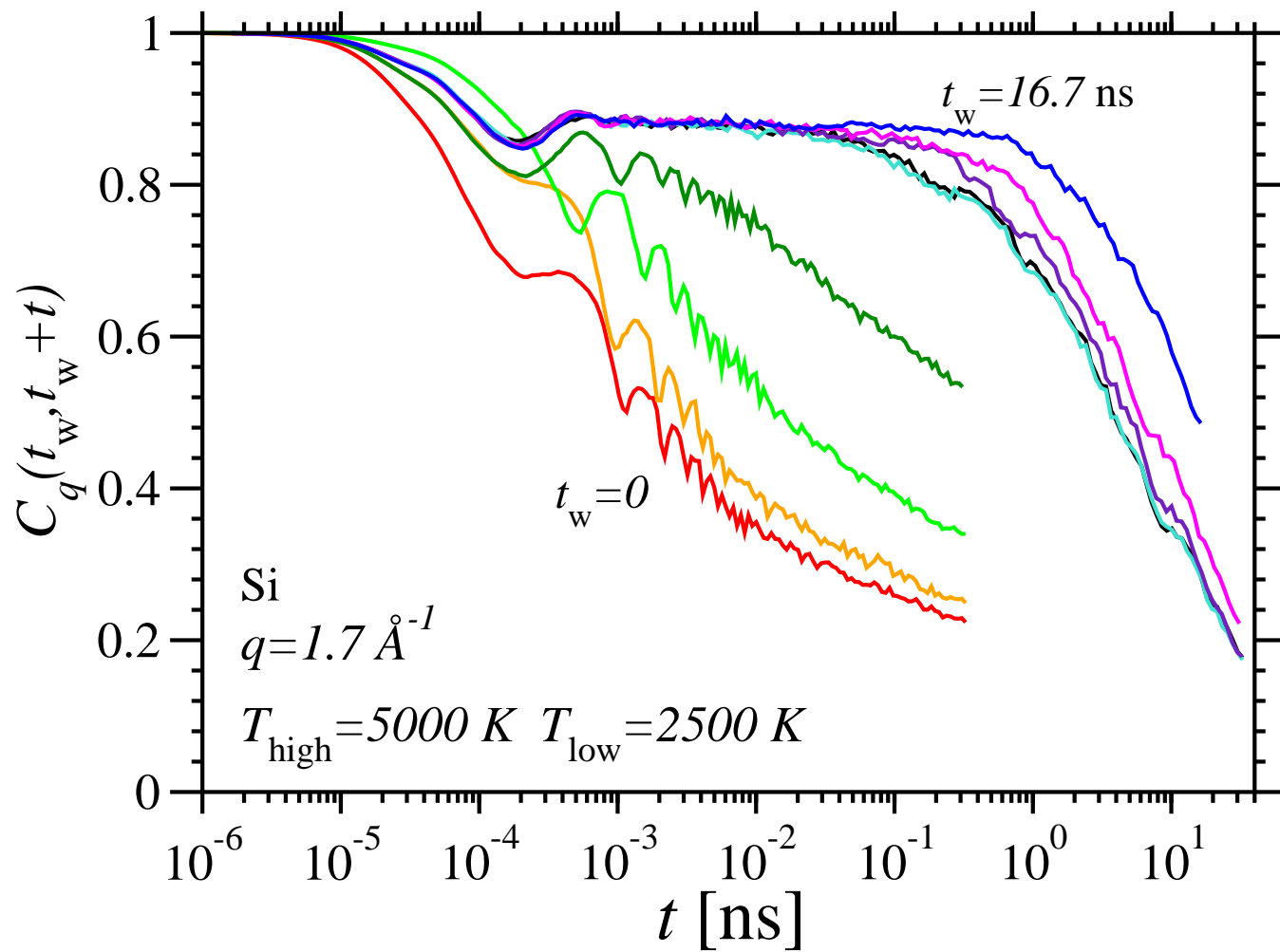


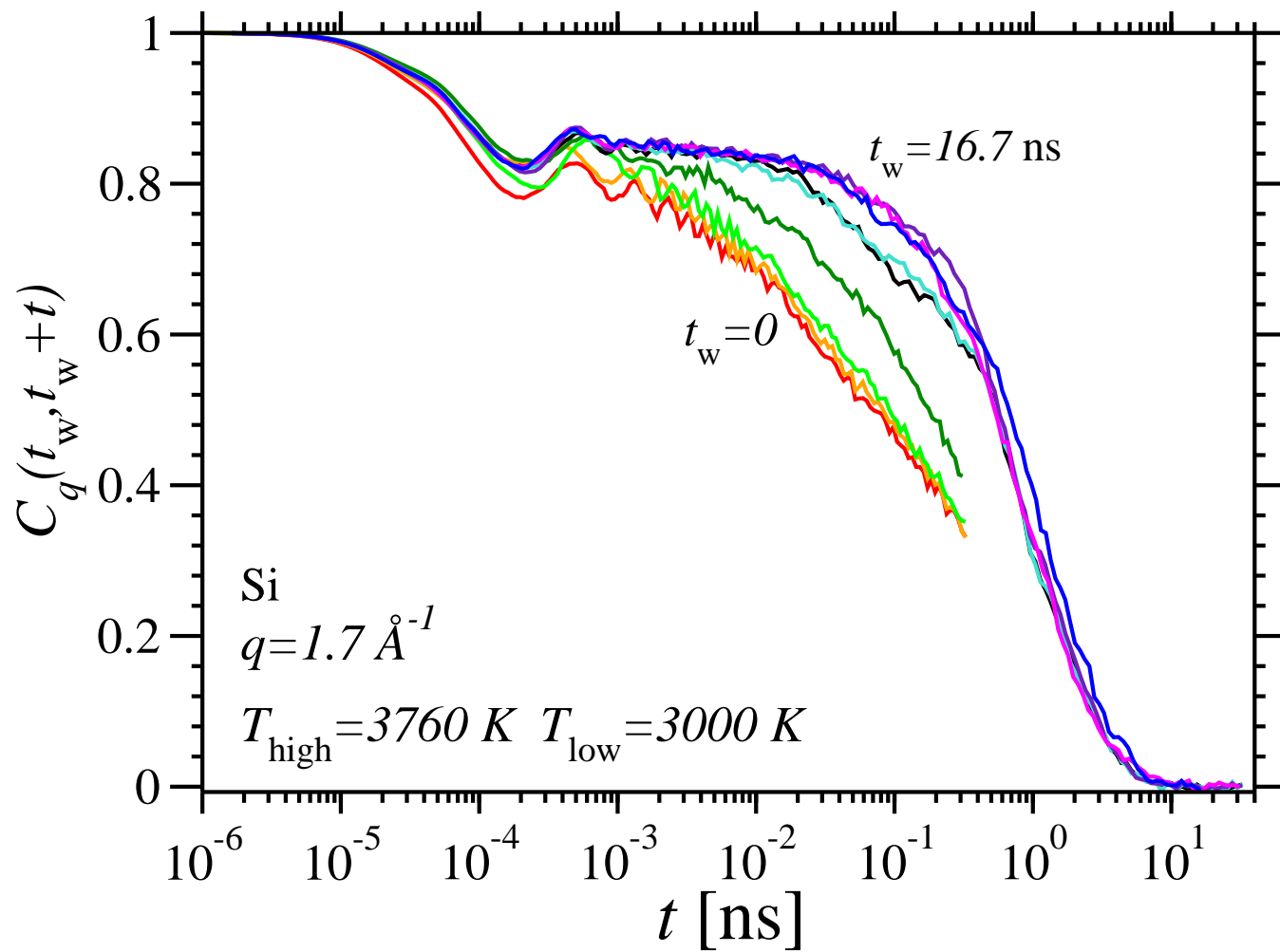
three t_w ranges:

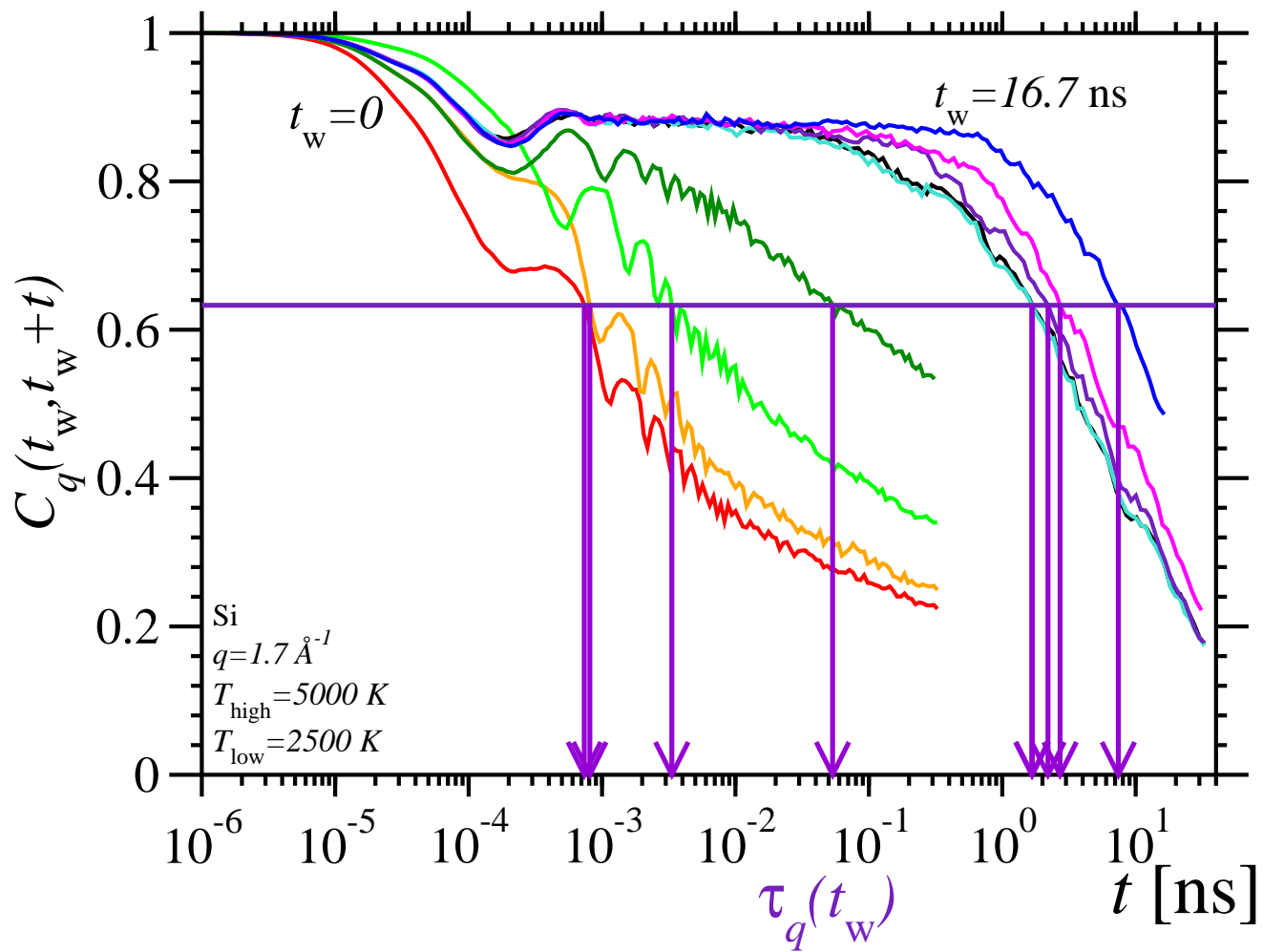
t_w too small: aging regime: equilibrium
 $C_q^{\text{AG}}(t/\tau)$
 $C_q^{\text{AG}}(h(t_w + t)/h(t_w))$

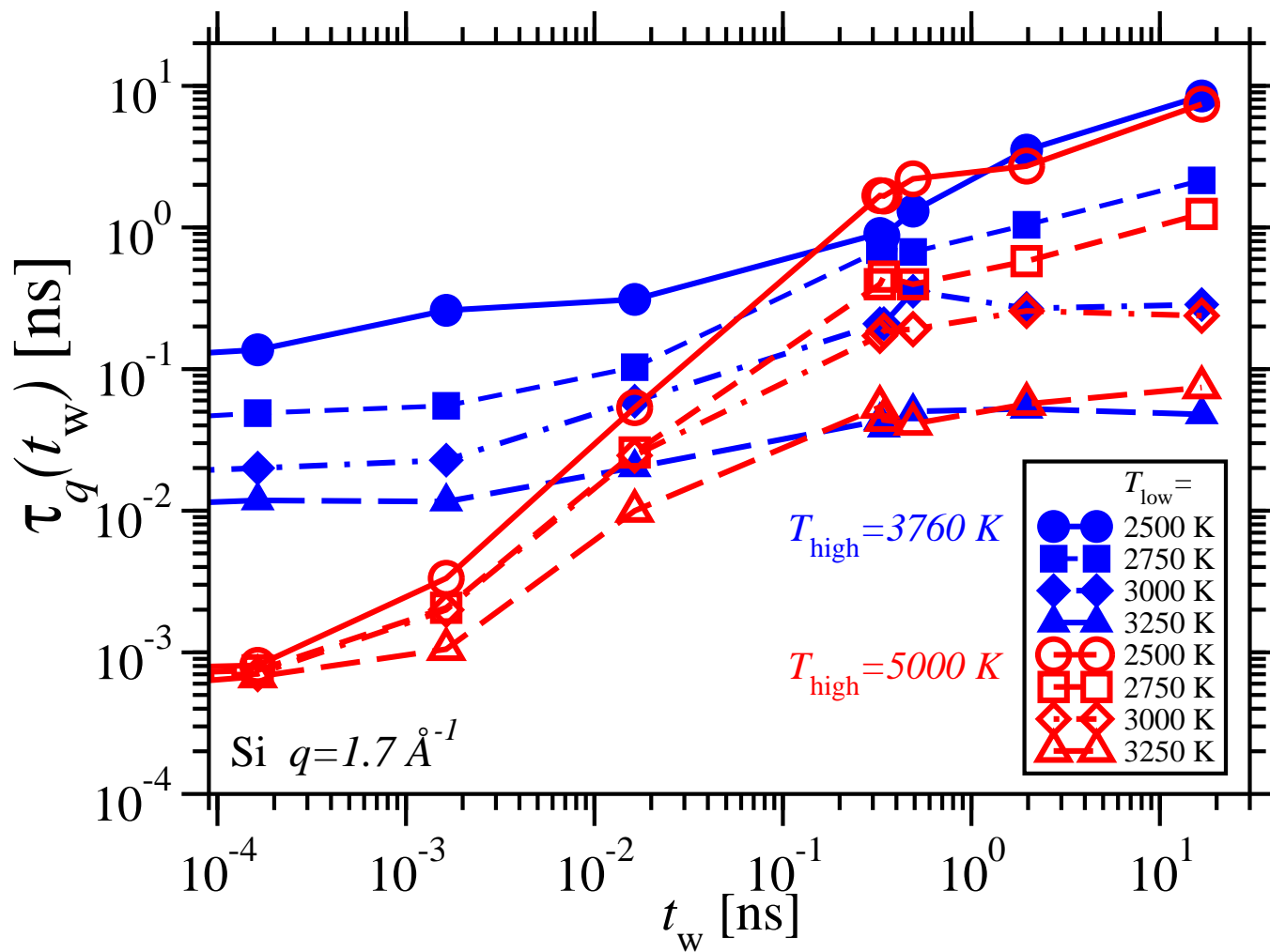
Simulation Runs

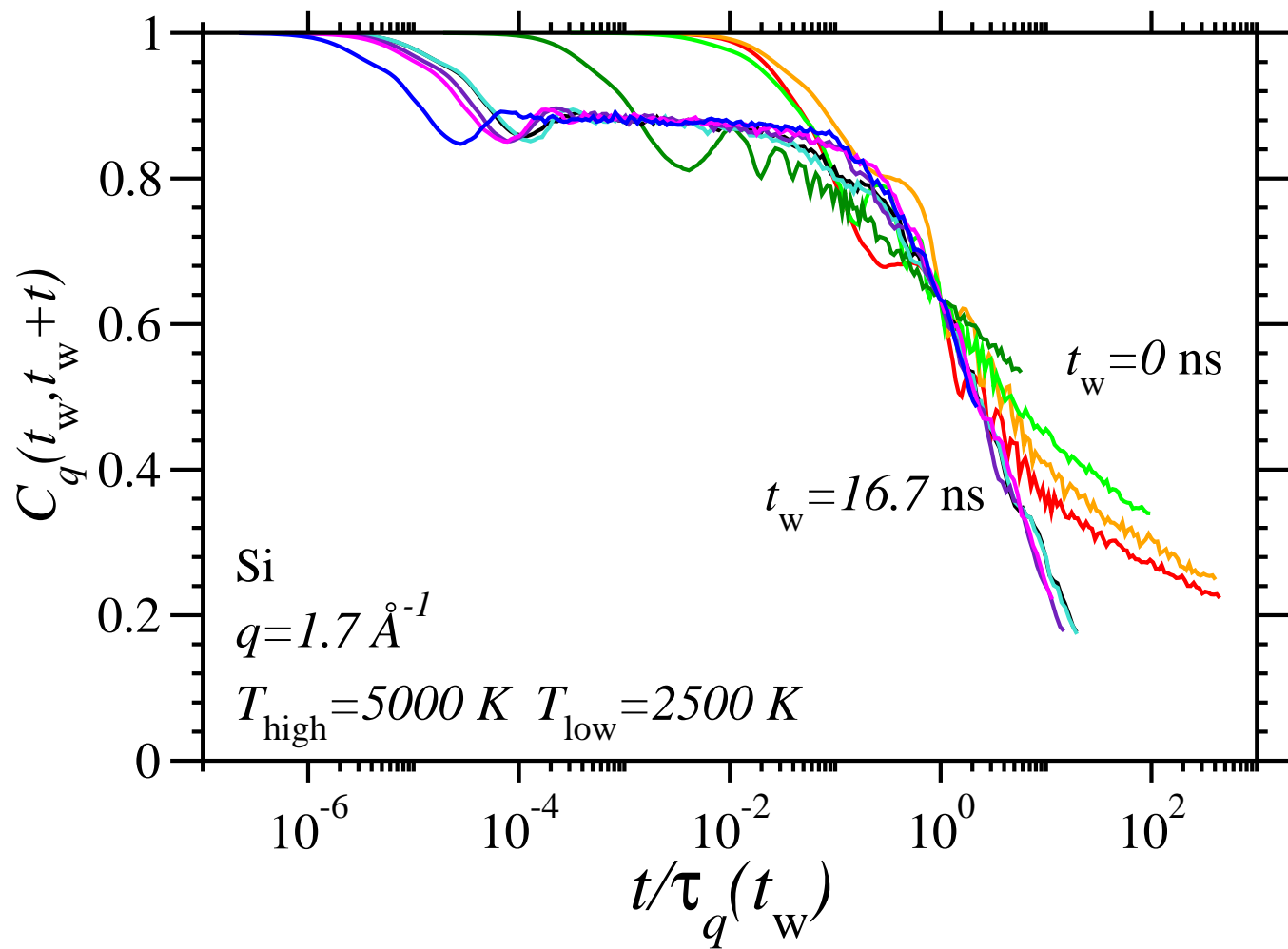


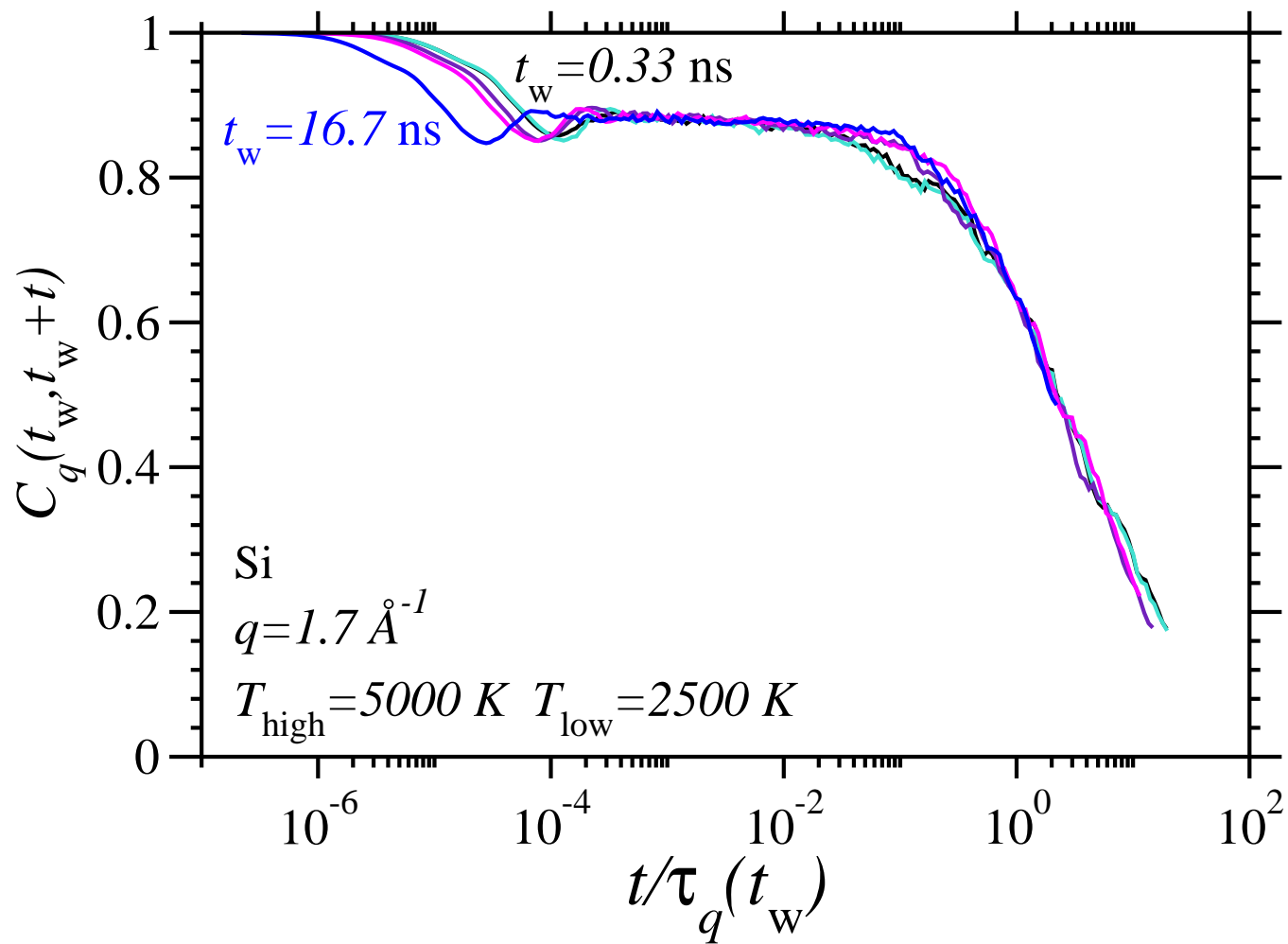


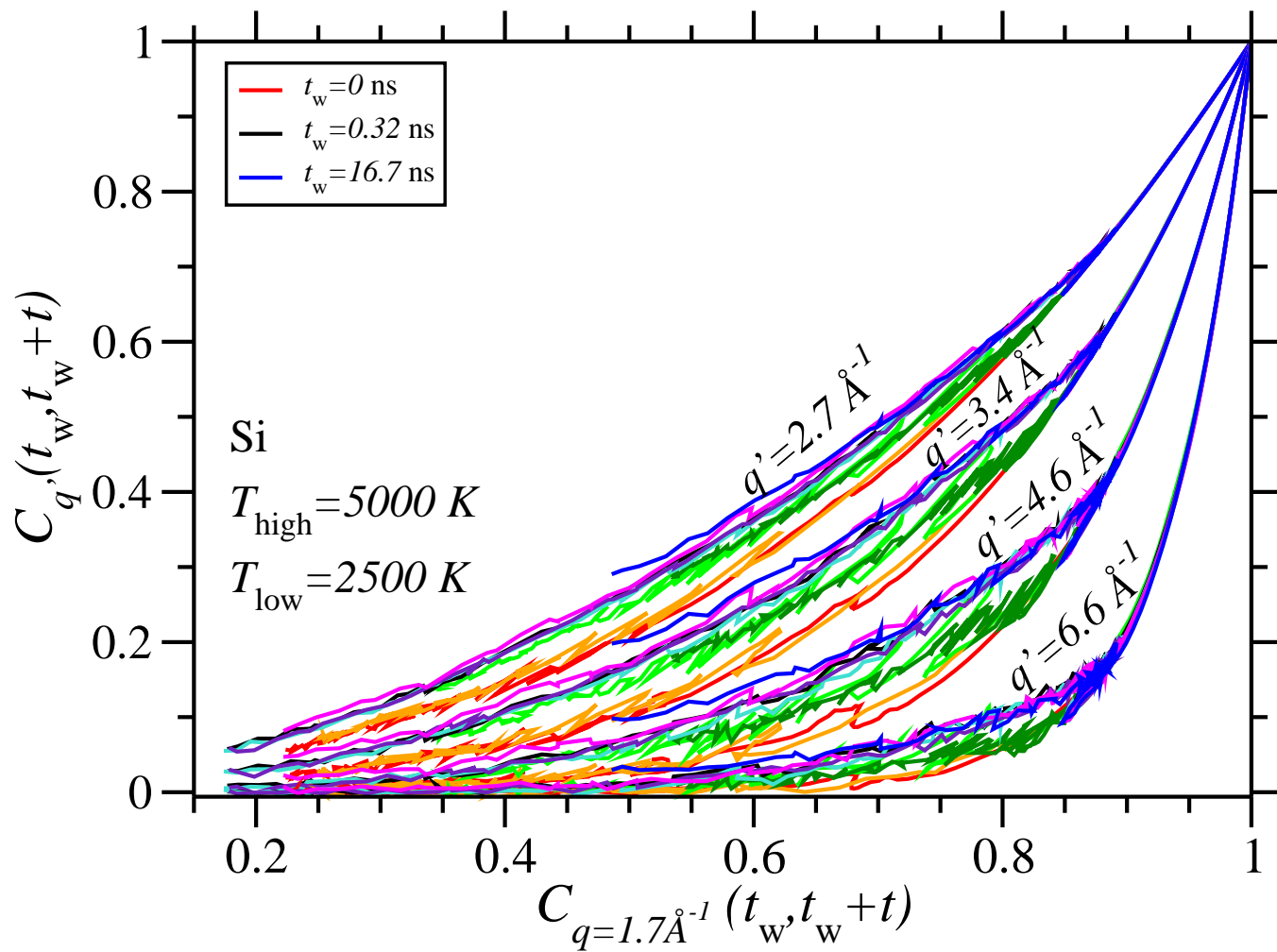


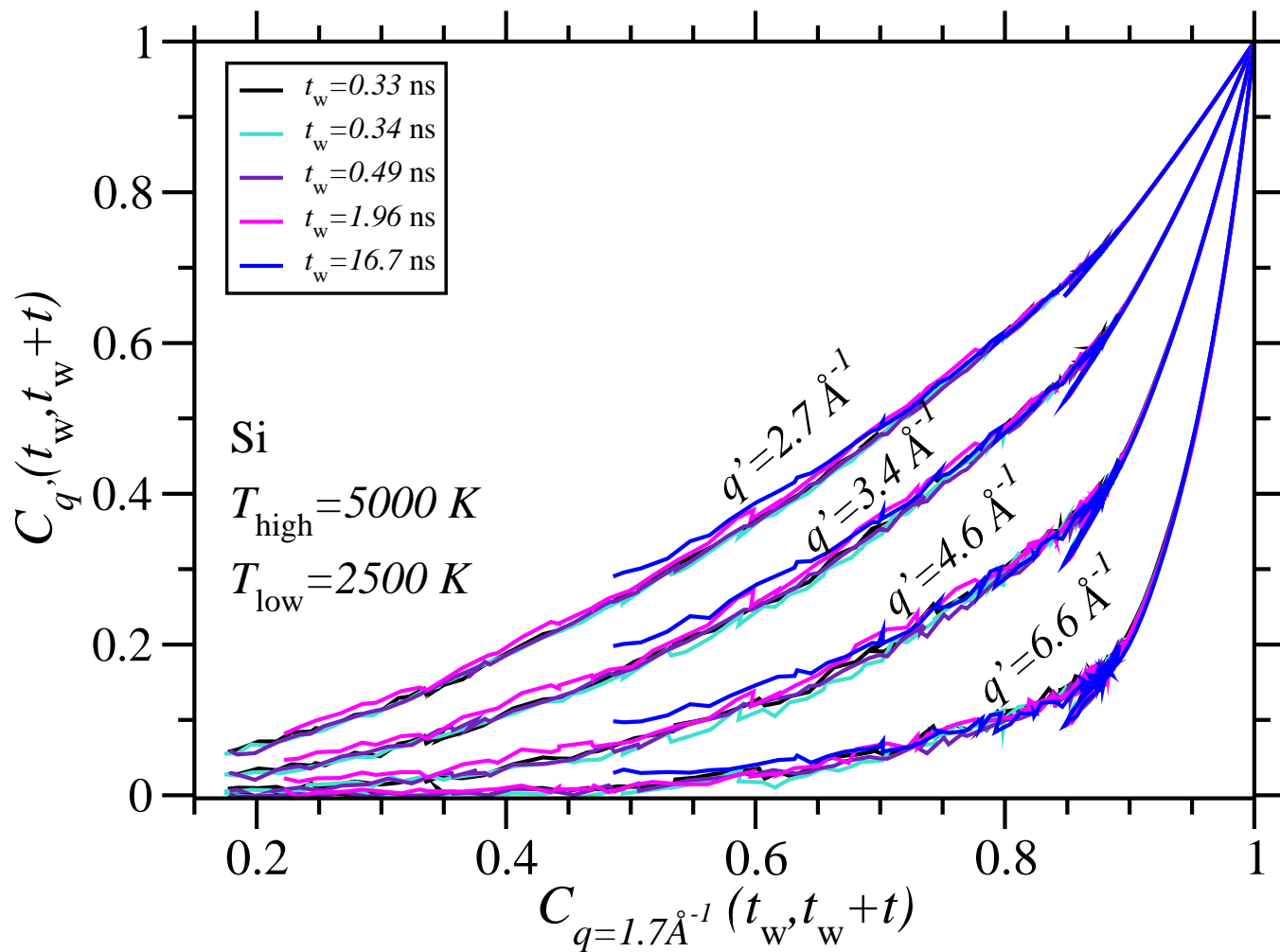








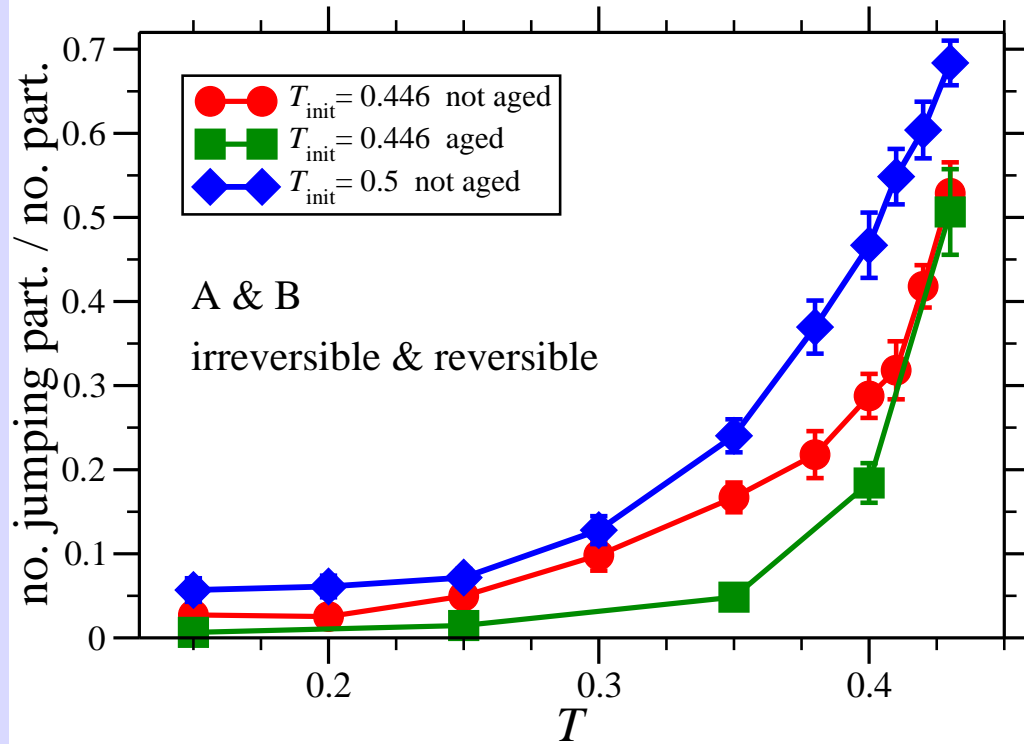
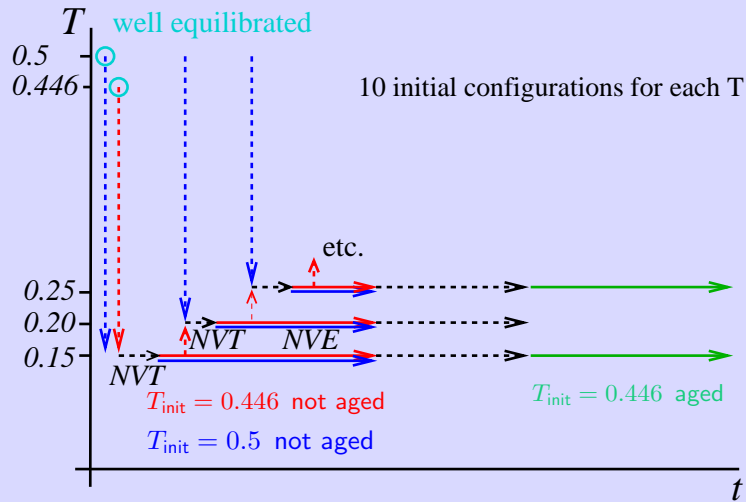




Time Scales

- one MD step: 0.02 time units, Ar: $3 \cdot 10^{-13} \text{s} \cdot 0.02 = 6 \text{fs}$
- one oscillation: 100 MD steps, 0.6 ps
- time a jump takes: 200 MD steps, 1.2 ps
- time resolution (time bin): 40000 MD steps, 240 ps
- time betw. successive jumps Δt_b : $1.5 \cdot 10^6$ MD steps, 9 ns
- whole simulation run: $5 \cdot 10^6$ MD steps, 30 ns

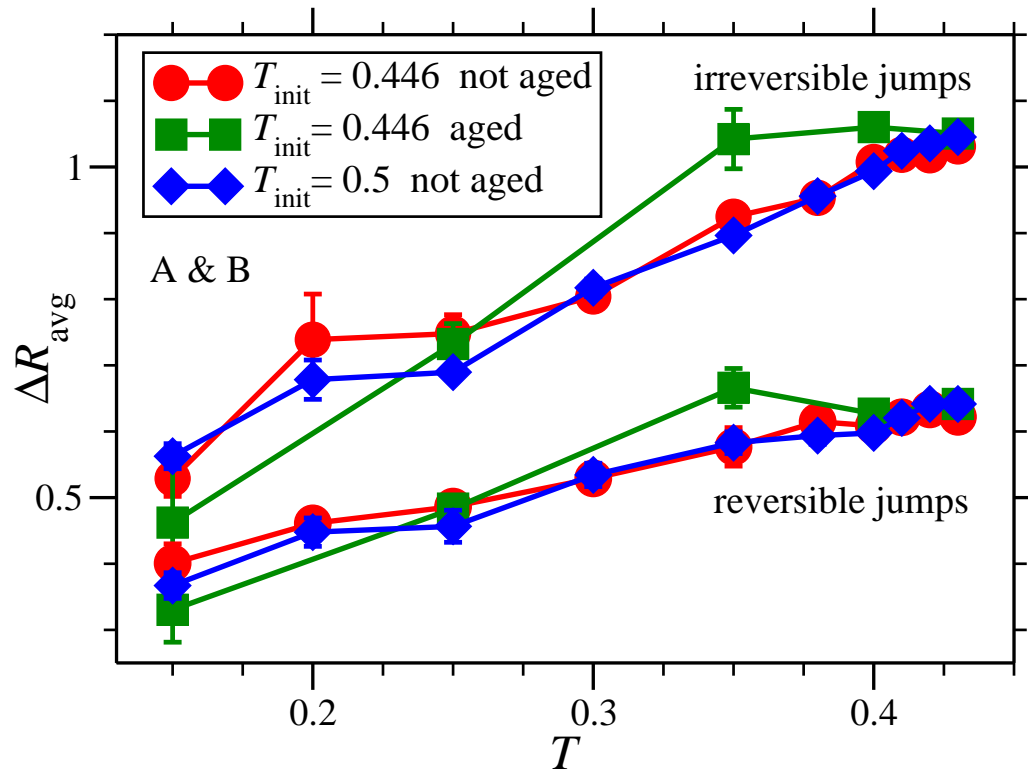
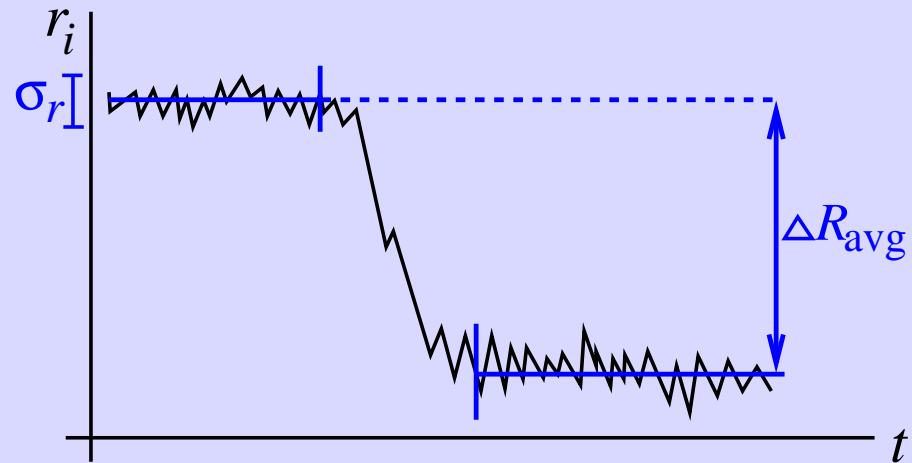
History Dependence



Number of Jump. Part.

⇒ history dependent

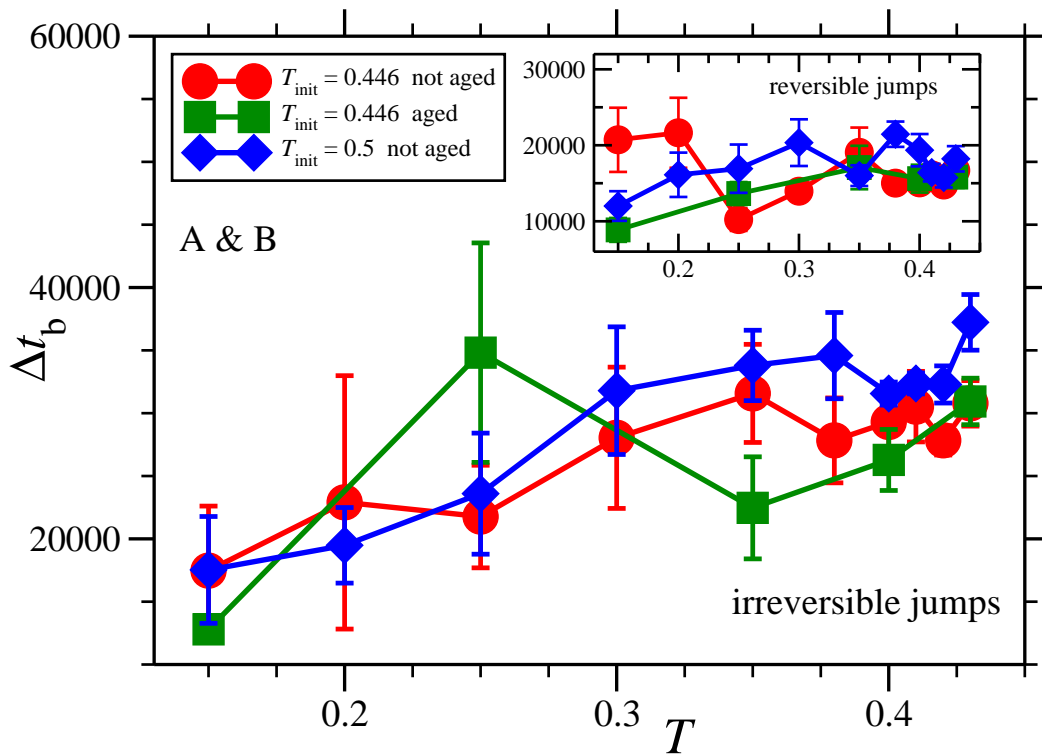
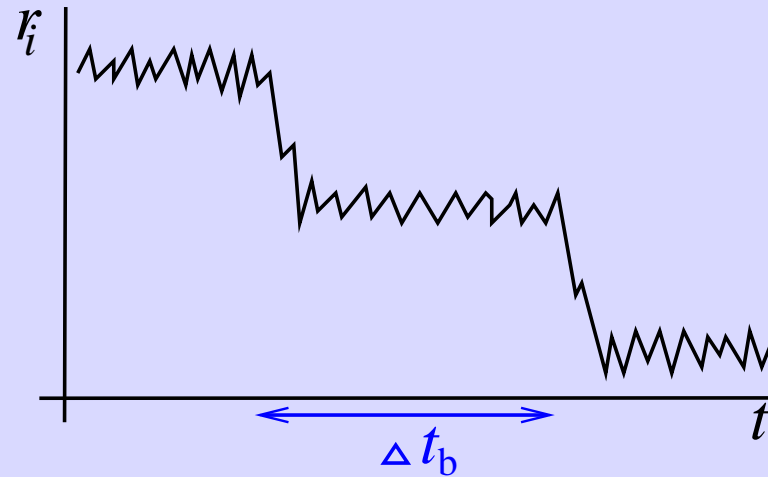
History Dependence



Jump Size

\implies history independent

History Dependence

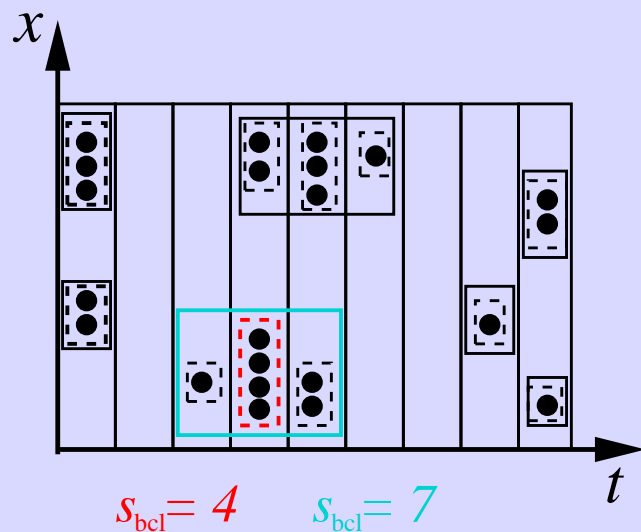


Time Between Jumps

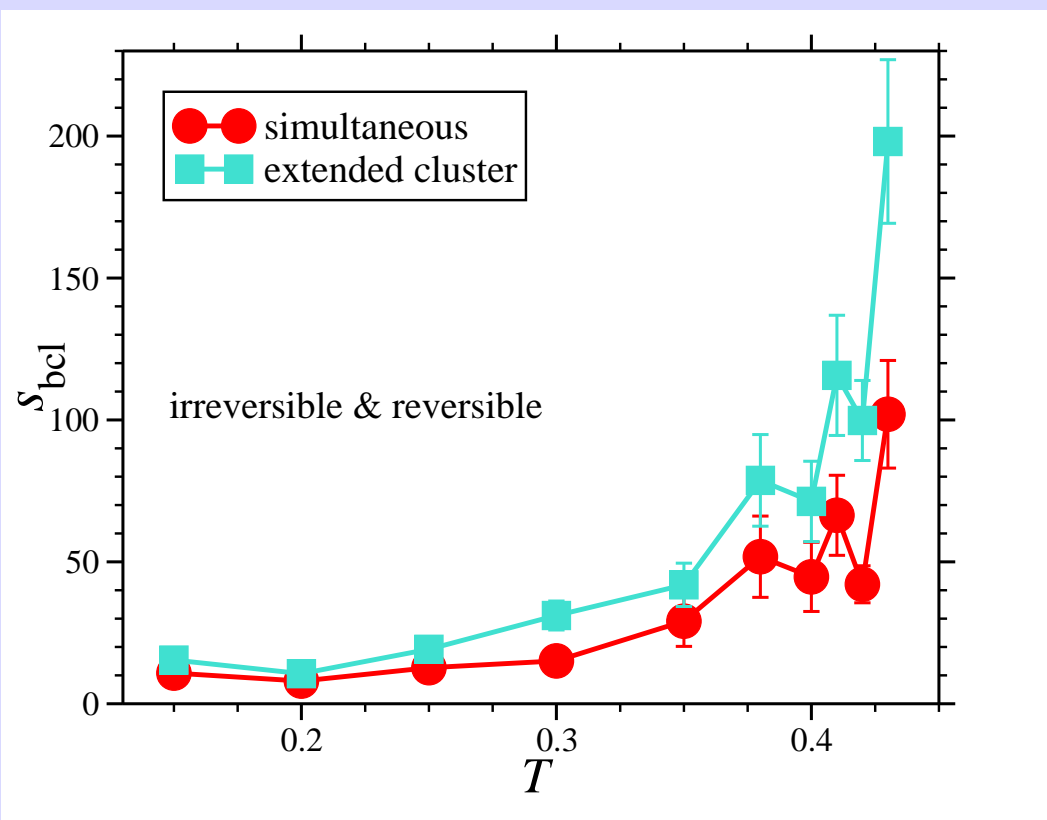
⇒ history independent

Summary: Jump Statistics

Most Cooperative Processes



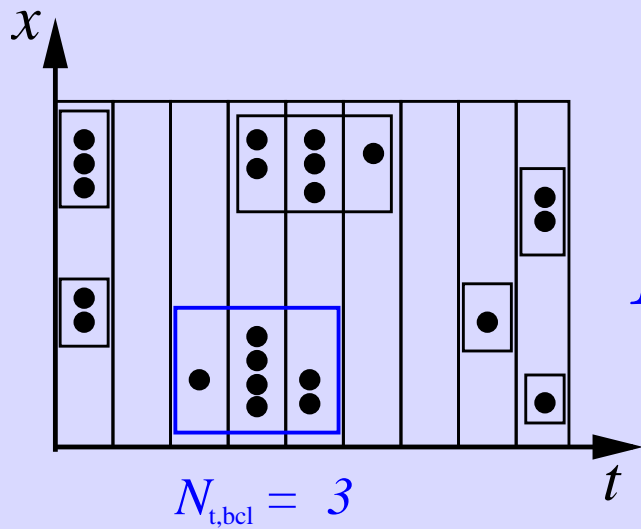
$s_{\text{bcl}} =$ largest cluster size



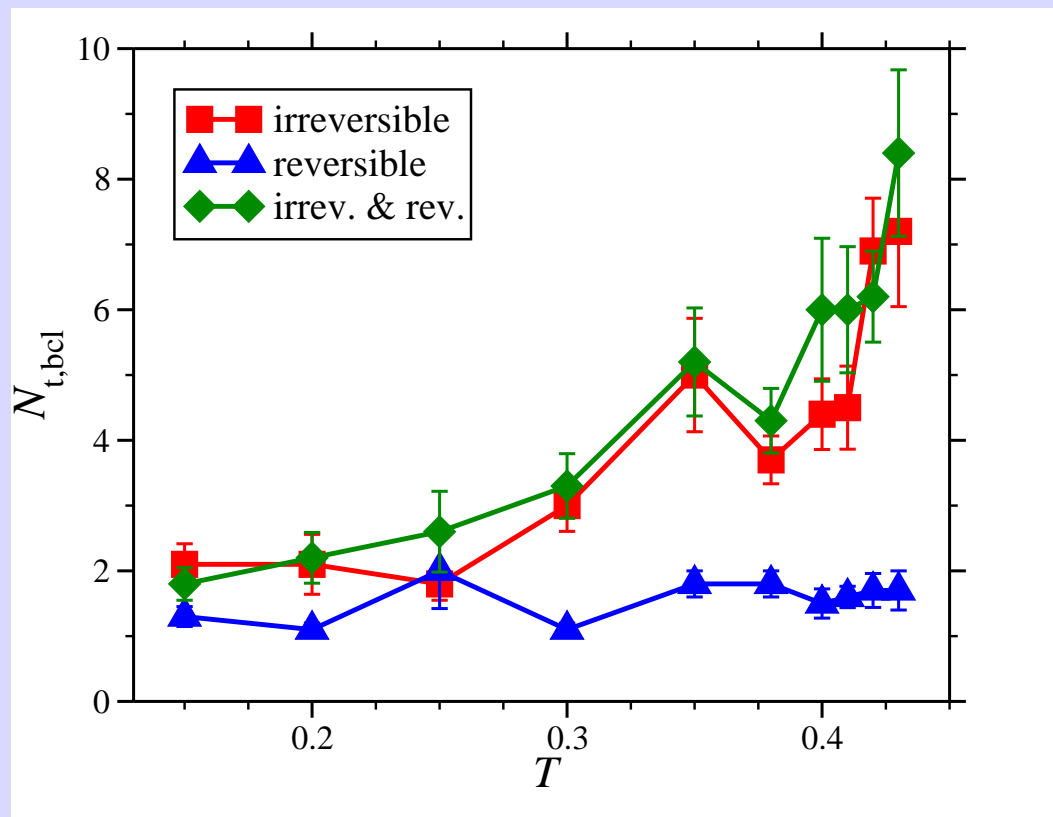
\Rightarrow highly correlated
single particle
jumps

● many particles

Most Cooperative Processes



$N_{t,bcl}$ = no. of time bins of largest cluster



⇒ highly correlated
single particle
jumps

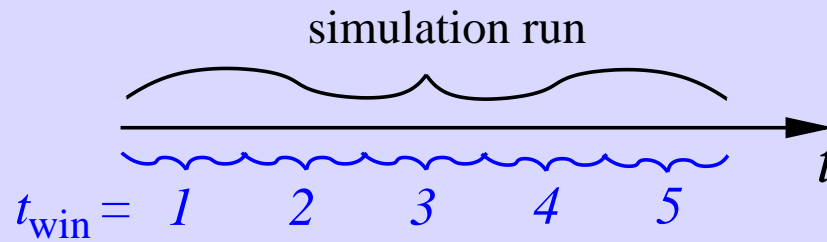
● many particles

● many time bins

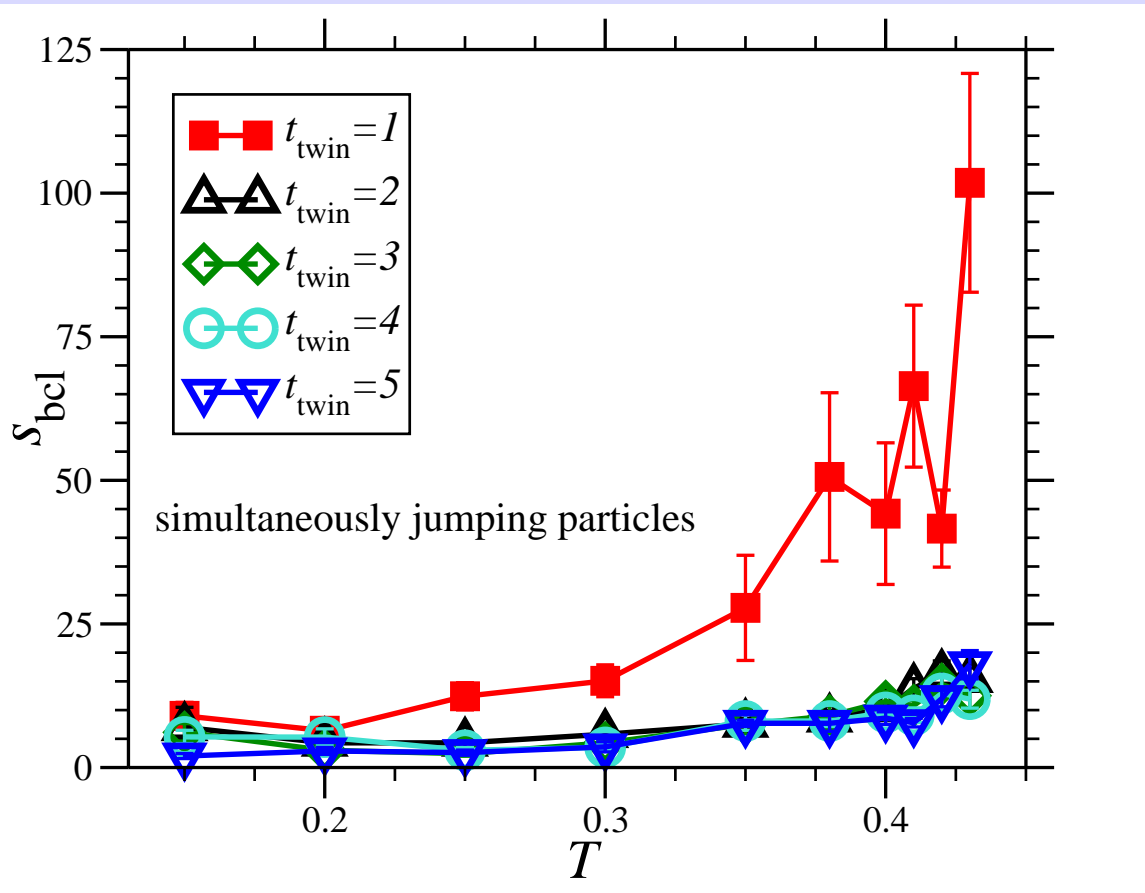
(maximum = 125)

Time Scales Extra

History Dependence



$s_{\text{bcl}} = \text{largest cluster size}$



\Rightarrow aging dependent

- 1st t-window:

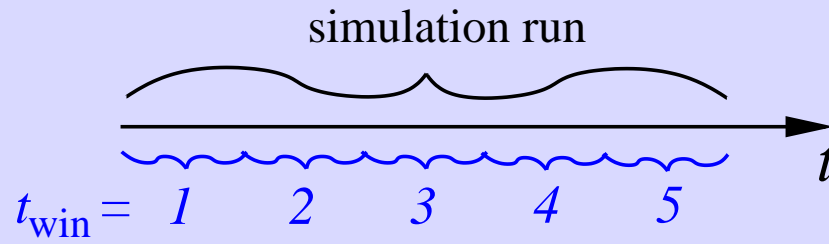
highly cooperative

- 2nd - 5th t-window:

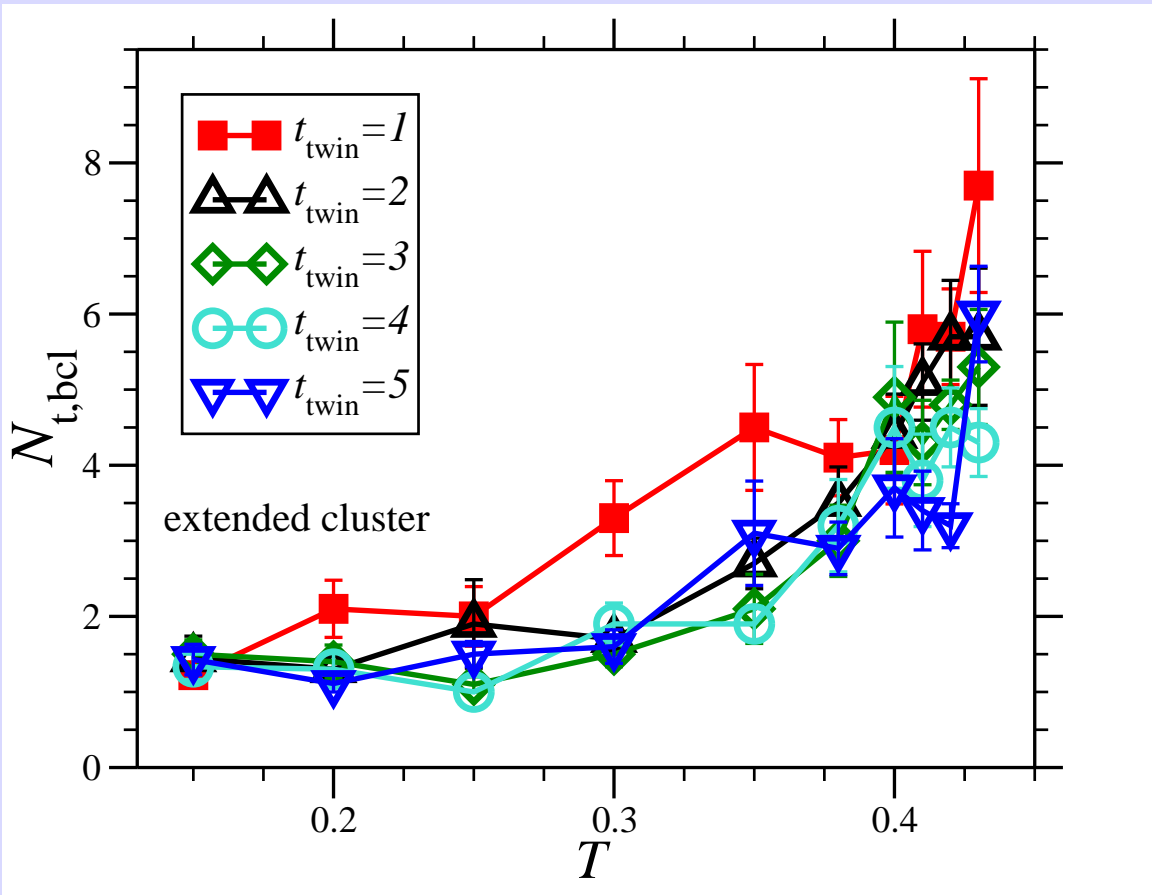
same, cooperative

s_{bcl} extended cluster

History Dependence



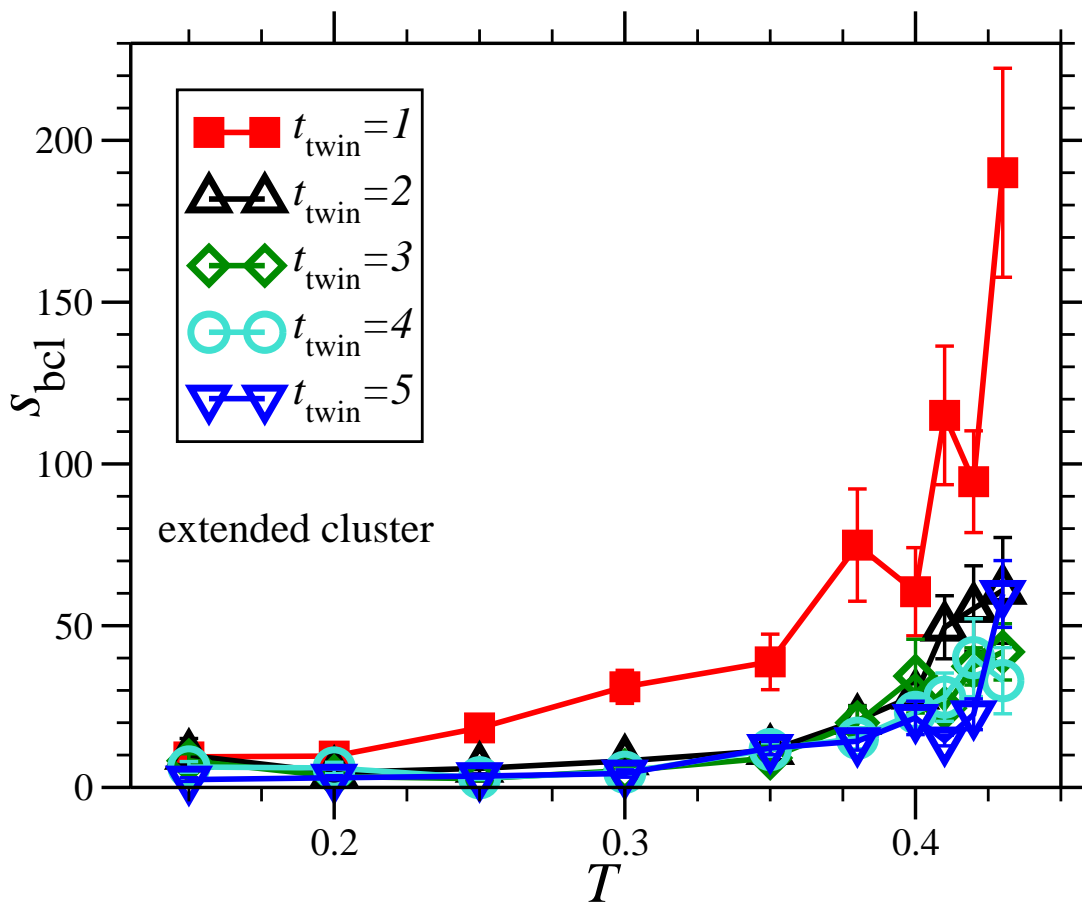
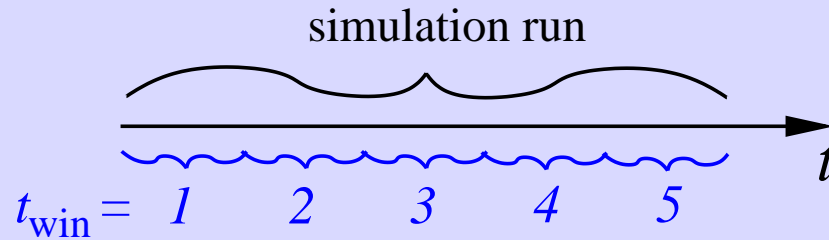
$N_{t,\text{bcl}}$ = no. of t-bins of largest cluster



⇒ less aging dependent

⇒ highly cooperative

History Dependence



\Rightarrow aging dependent

- 1st t-window:

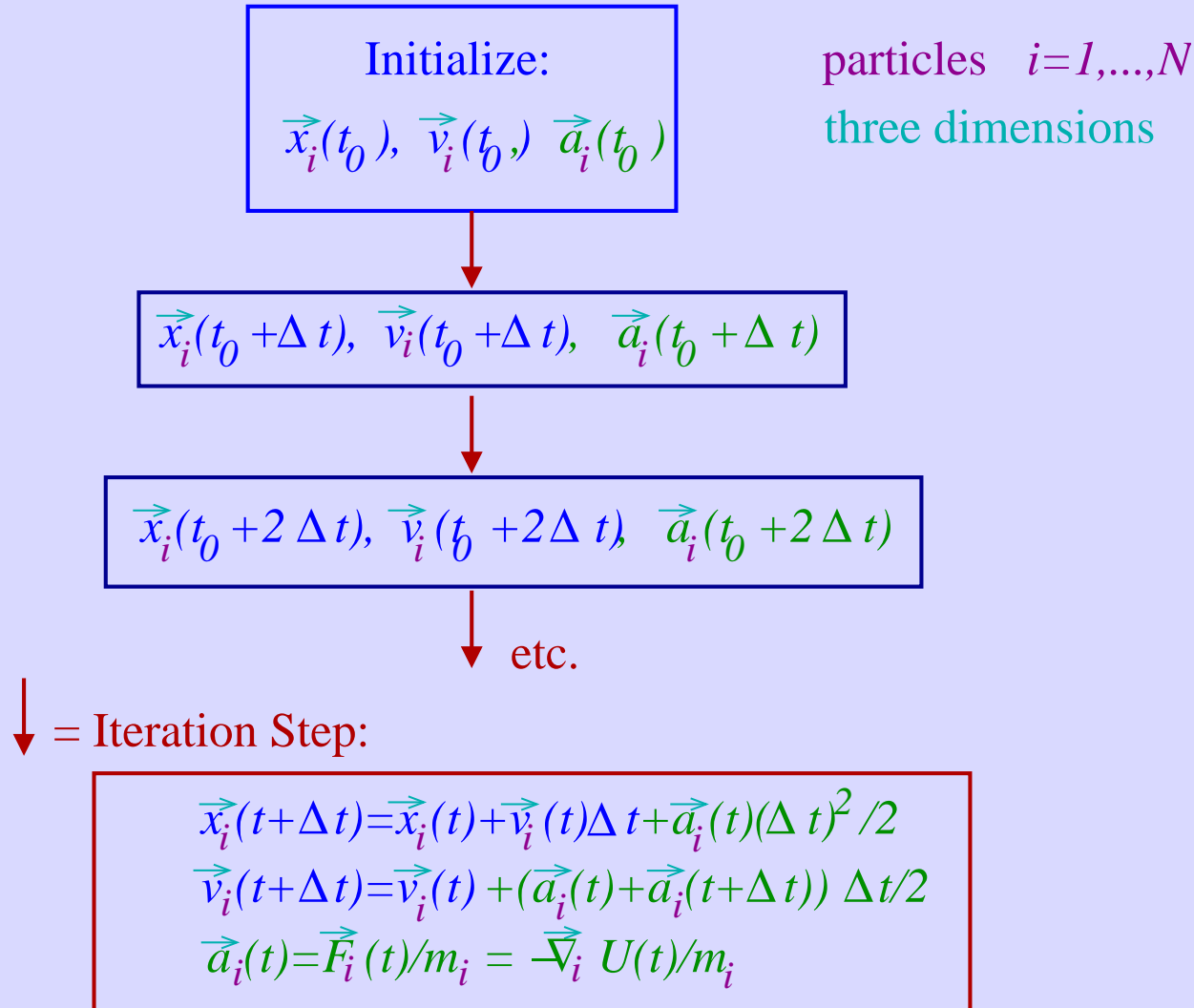
highly cooperative

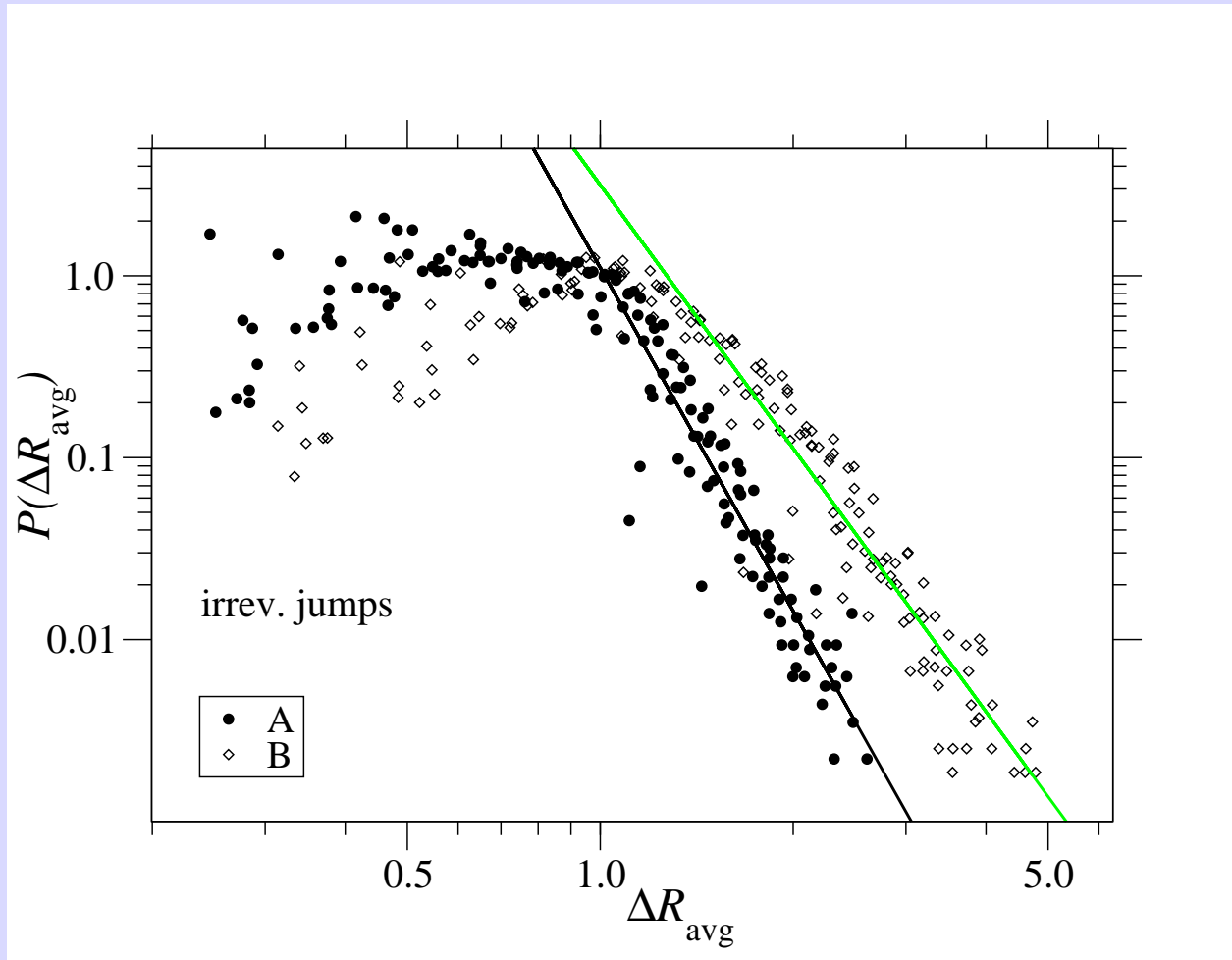
- 2nd - 5th t-window:

same, cooperative

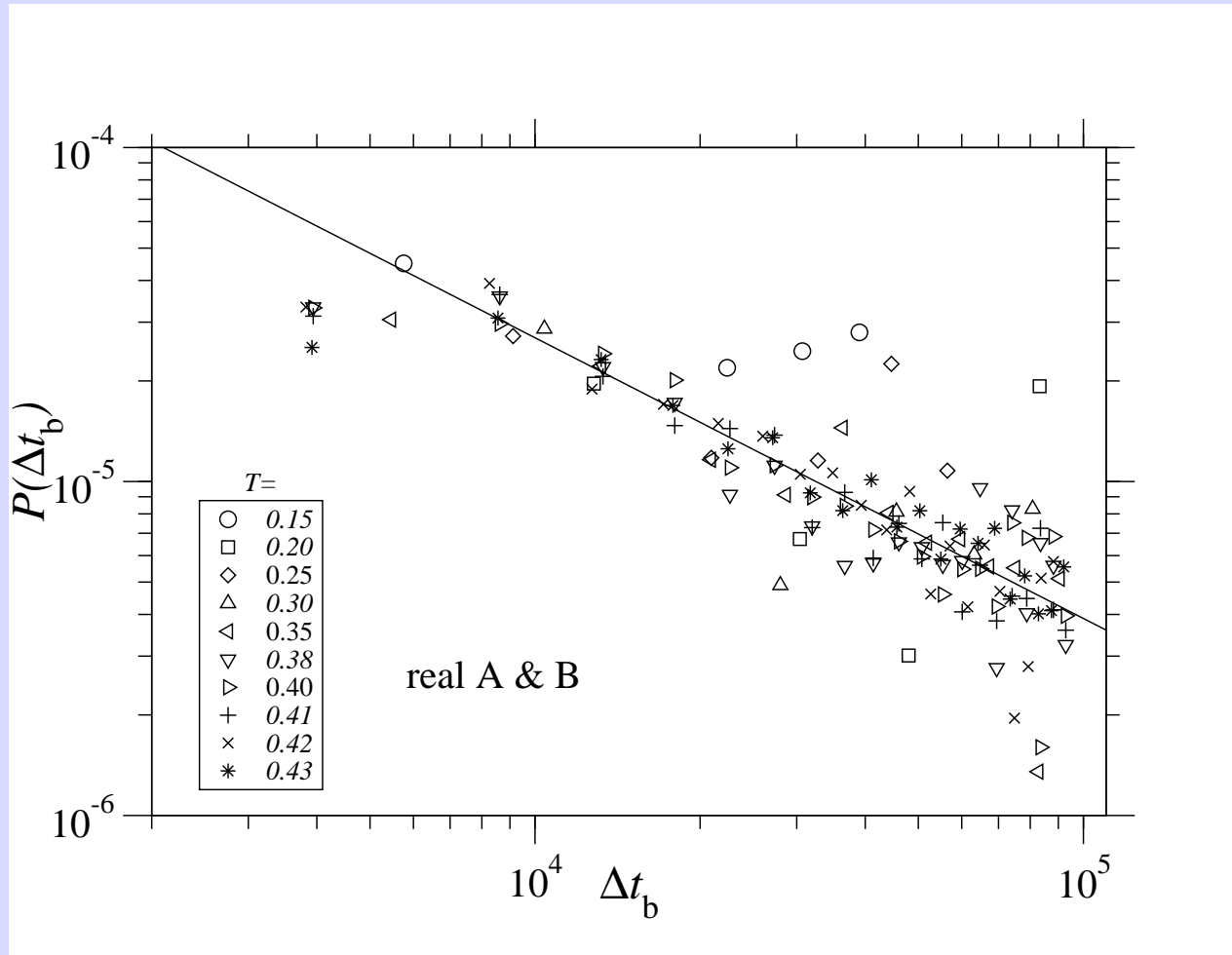
s_{bcl} simult. jump.

Molecular Dynamics Simulation





slopes -6.3 for A and -4.8 for B particles \longrightarrow subdiffusive



slopes -0.84 → subdiffusive

Critical Behavior: power law \longleftrightarrow scale invariance

Critical Point at Phase Transition:

power law at specific fine tuned external parameter

e.g. percolation: $P(s)=s^{-\tau}$ at $p=p_c$ at all other p no power law

e.g. jumping particle clusters: $P(s)=s^{-\tau}$ (would be) at $T=T_c$ only

Self-Organized Criticality:

power law for whole range of external parameter

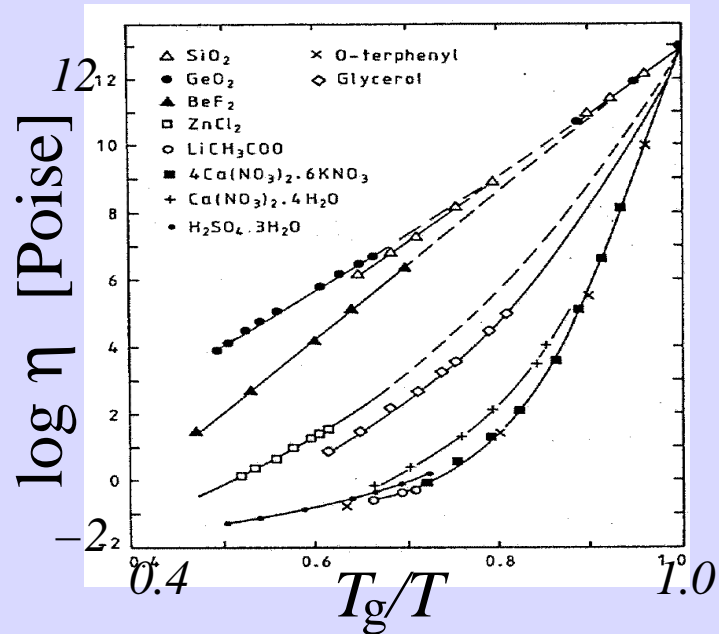
here jumping particle clusters: $P(s)=s^{-\tau}$ for all $T=0.15-0.43$

Other Examples:

- sandpile avalanches
- forest fire
- financial market
- earth quakes

[P. Bak, C. Tang, and K. Wiesenfeld, PRL 59, 381 (1987)]

Introduction



[C.A. Angell and W. Sichina, Ann. NY Acad.Sci. 279, 53 (1976)]

Dynamics:

→ slowing down
of many decades