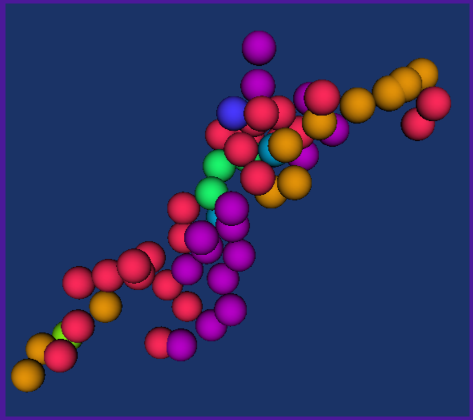
Computer Simulation of Glasses: Jumps and Self-Organized Criticality

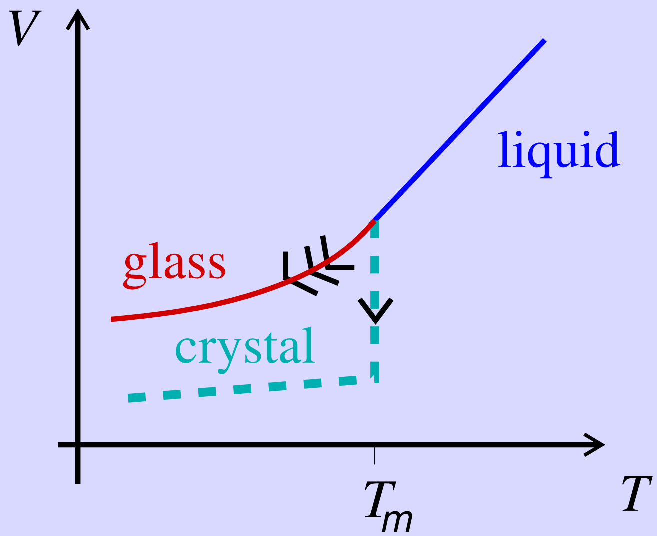
Katharina Vollmayr-Lee, Bucknell University

March 10, 2009



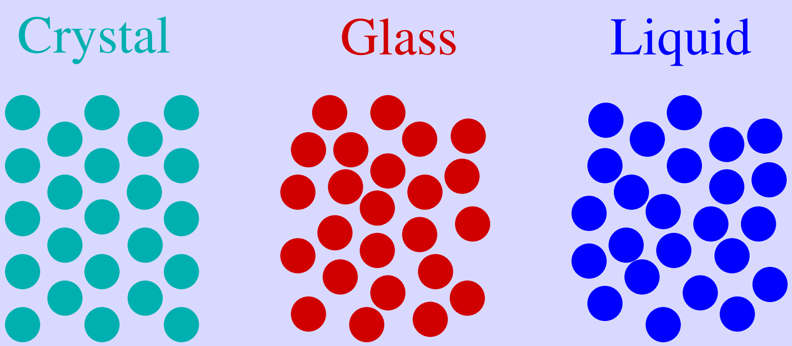
Thanks: E. A. Baker, A. Zippelius, K. Binder, and J. Horbach

Introduction



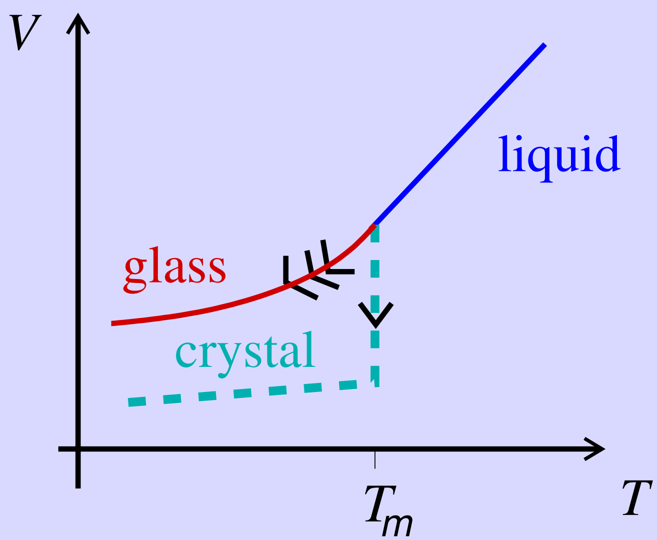
Glass:

→ system falls out of equilibrium



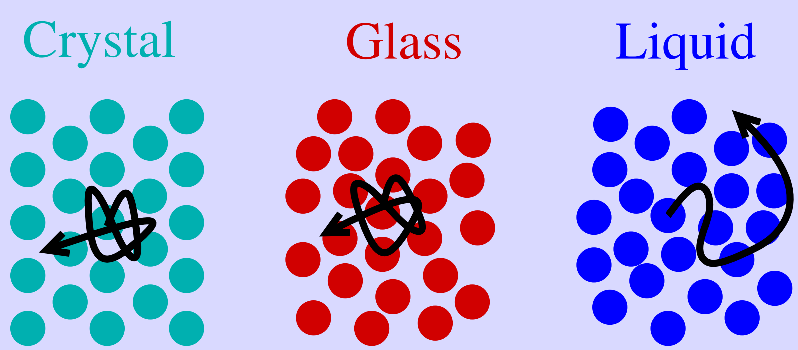
Structure: discordered

Introduction



Glass:

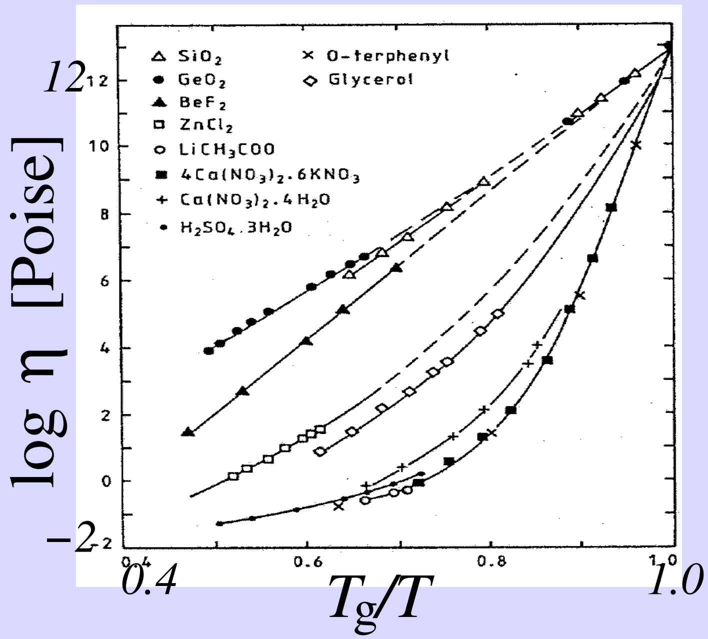
→ system falls out of equilibrium



Structure: discordered

Dynamics: frozen in

Introduction



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

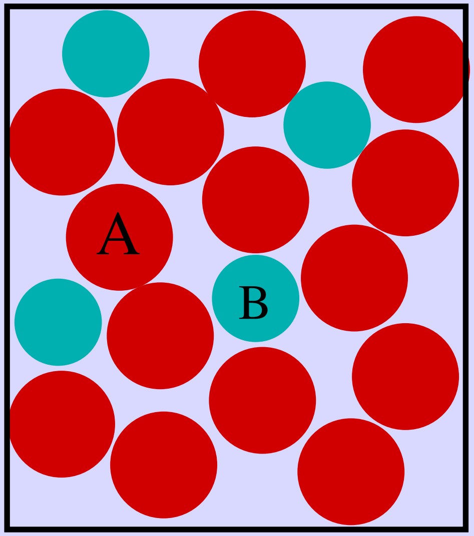
Dynamics:

⟶ slowing down of many decades

Model

Binary Lennard-Jones System

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



800 A and 200 B

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

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

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

Numerical Solution: Euler Step

Initialize:

$x(t_0),\ v(t_0),\ a(t_0)$

↓

$x(t_0+\Delta t),\ v(t_0+\Delta t),\ a(t_0+\Delta t)$

↓

$x(t_0+2\,\Delta t),\ v(t_0+2\,\Delta t),\ a(t_0+2\,\Delta t)$

↓ etc.

↓ = Iteration Step:

$$x(t+\Delta t)=x(t)+v(t)\Delta t$$

$$v(t+\Delta t)=v(t)+a(t)\Delta t$$

$$a(t)=F(t)/m=-(dU/dx)(t)$$

Molecular Dynamics Simulation

particles $i=1,...,N$
three dimensions

Initialize:
$\vec{x}_i(t_0),\ \vec{v}_i(t_0),\ \vec{a}_i(t_0)$

↓

$\vec{x}_i(t_0+\Delta t),\ \vec{v}_i(t_0+\Delta t),\ \vec{a}_i(t_0+\Delta t)$

↓

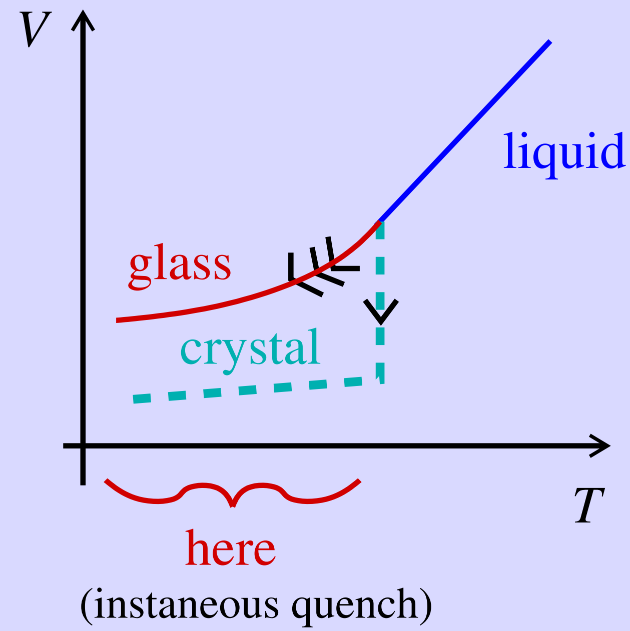
$\vec{x}_i(t_0+2\Delta t),\ \vec{v}_i(t_0+2\Delta t),\ \vec{a}_i(t_0+2\Delta t)$

↓ etc.

↓ = Iteration Step: (Velocity Verlet)

$$\vec{x}_i(t+\Delta t)=\vec{x}_i(t)+\vec{v}_i(t)\Delta t+\vec{a}_i(t)(\Delta t)^2/2$$
$$\vec{v}_i(t+\Delta t)=\vec{v}_i(t)+(\vec{a}_i(t)+\vec{a}_i(t+\Delta t))\,\Delta t/2$$
$$\vec{a}_i(t)=\vec{F}_i(t)/m_i=-\vec{\nabla}_i\,U(t)/m_i$$

Simulations



Molecular Dynamics Simulations

Velocity Verlet

below glass transition:

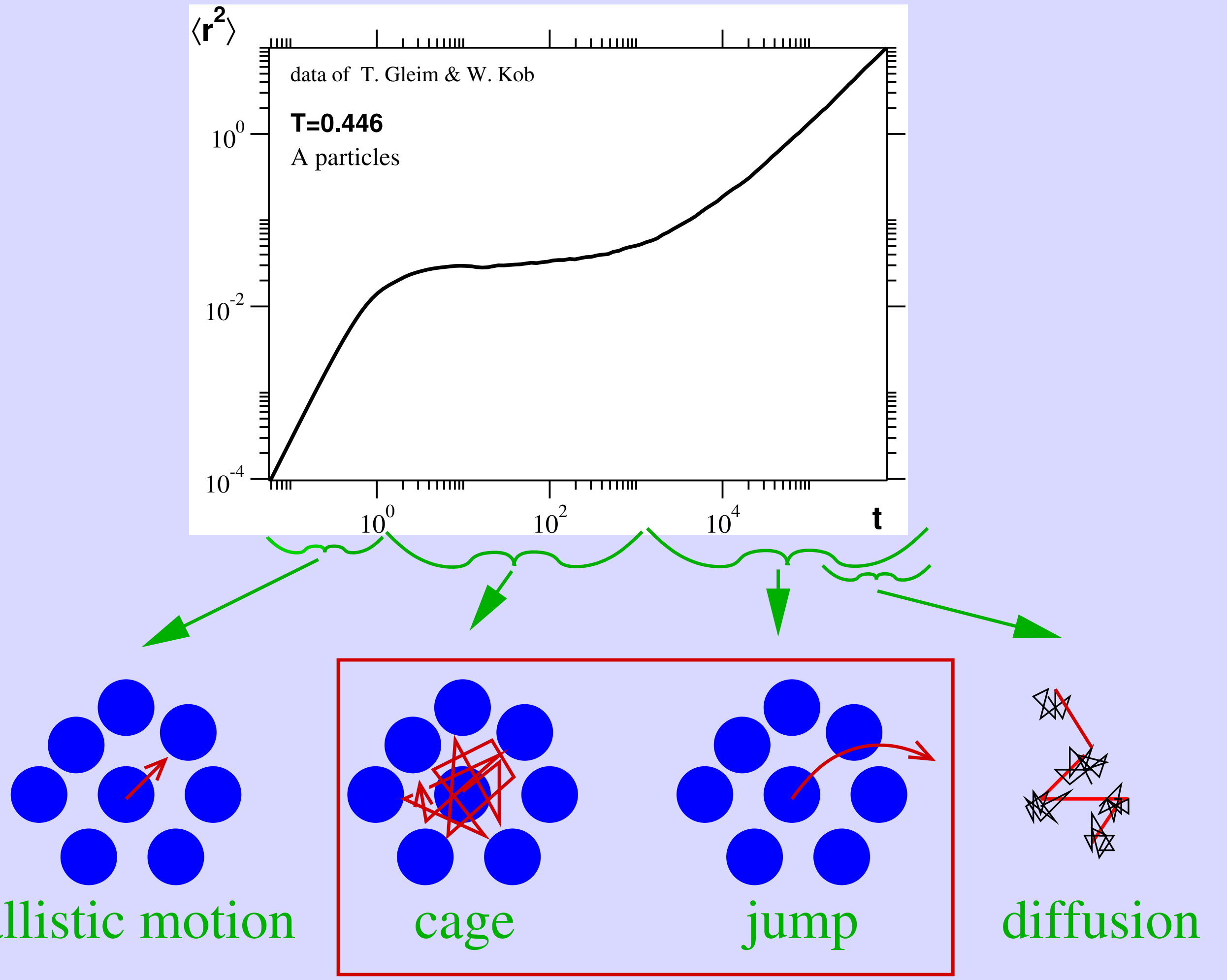
$T = 0.15 - 0.43$

MCT: $T_{\mathsf{c}} = 0.435$ [W. Kob et al., PRL 73 (1994)]

History Production Runs

Cage-Picture

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

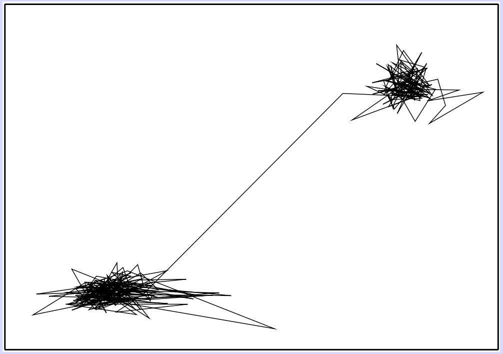


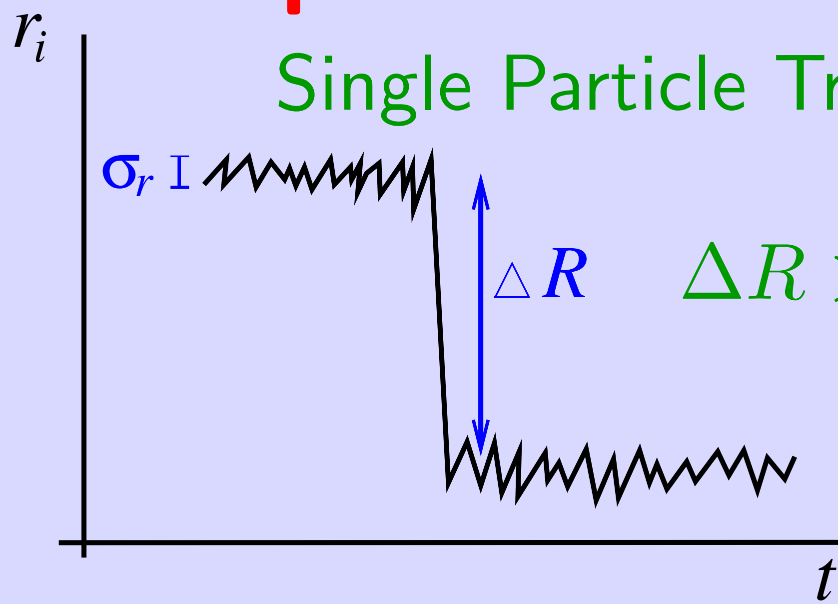
$\langle r^2 \rangle \sim t^2$

here

$\langle r^2 \rangle \sim t$

Definition: Jump Occurrence

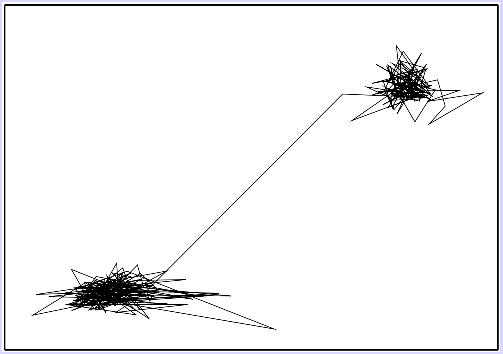


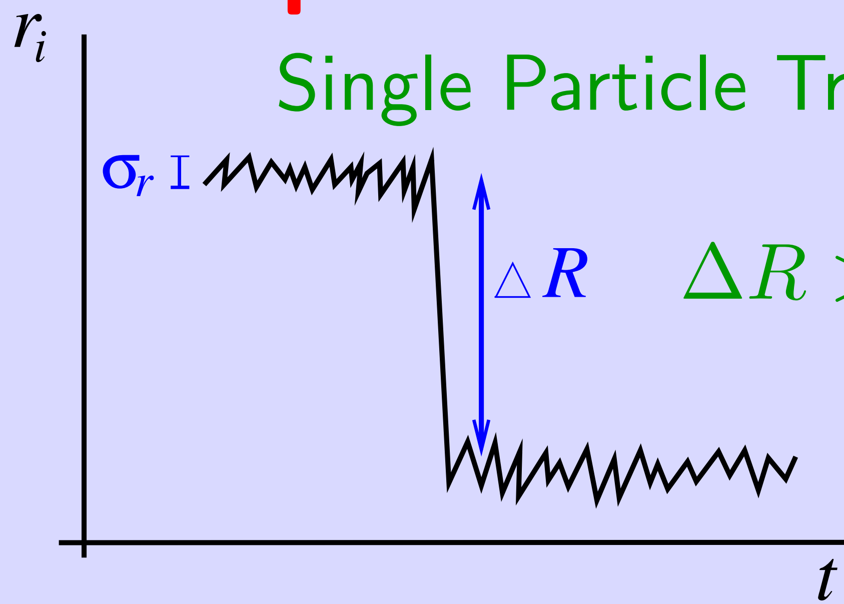


Single Particle Trajectory

$$\Delta R > \sqrt{20}\,\sigma_r$$

Definition: Jump Occurrence



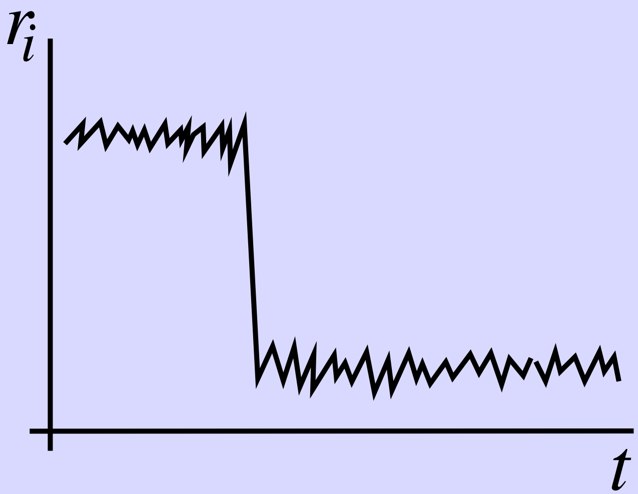


Single Particle Trajectory

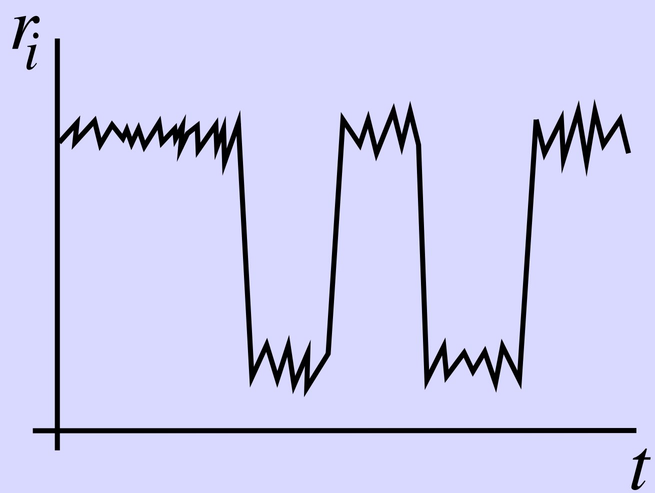
$$\Delta R > \sqrt{20}\,\sigma_r$$

Definition: Jump Type

Irreversible Jump



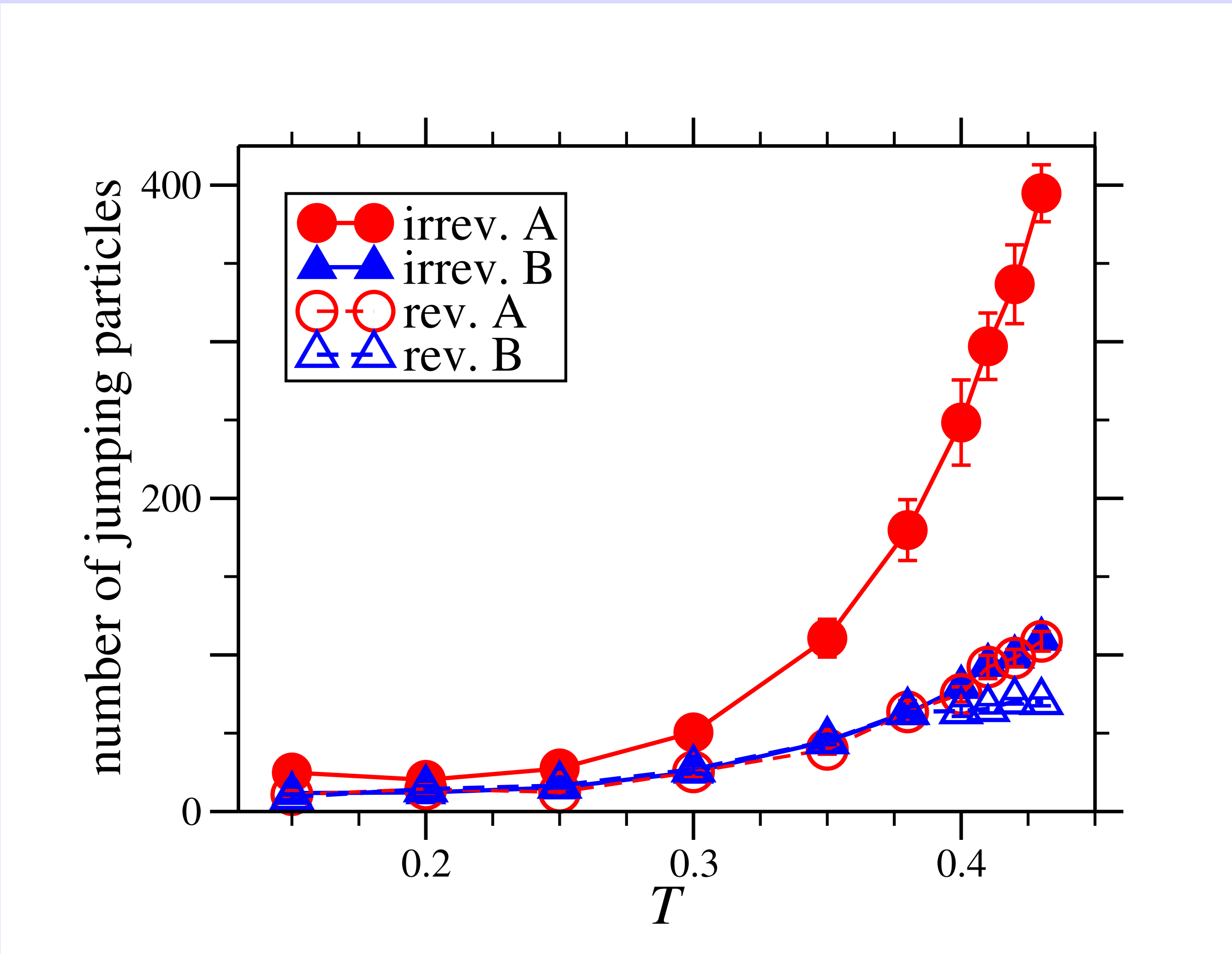
Reversible Jump



Outline

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

Number of Jumping Particles



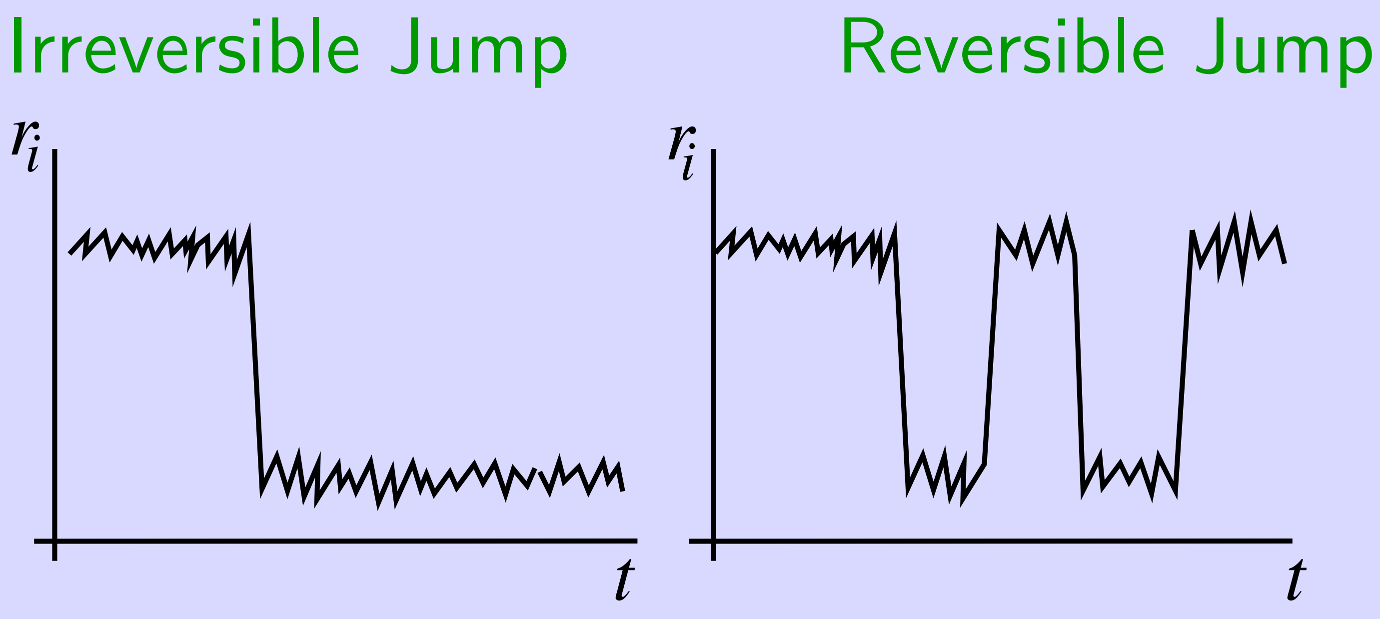
$\Longrightarrow$ increasing with increasing T

$\Longrightarrow$ both A & B particles jump

$\Longrightarrow$ irrev. & reversible jumps at all temperatures T

Fraction of Irreversibly Jumping Particles

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



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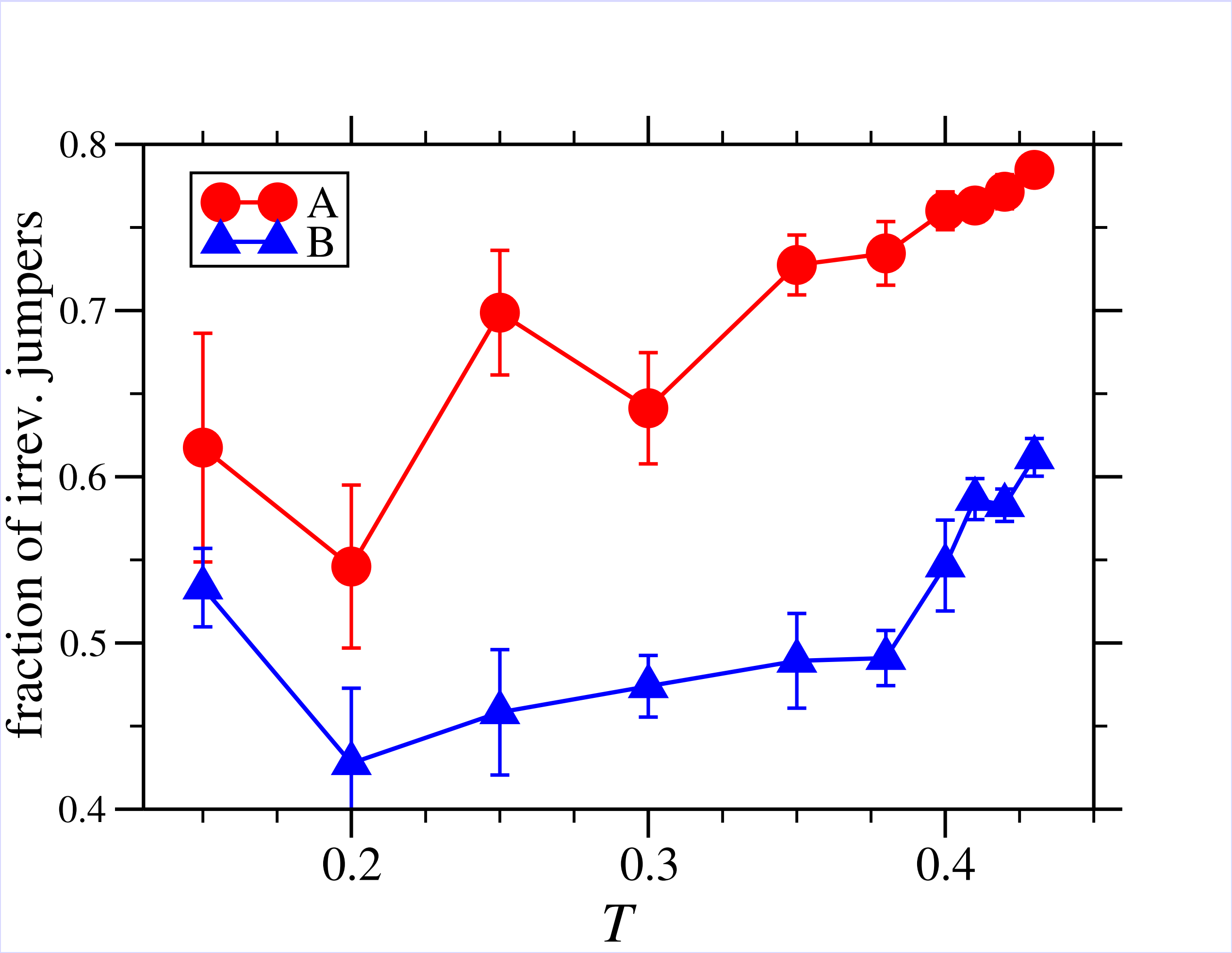
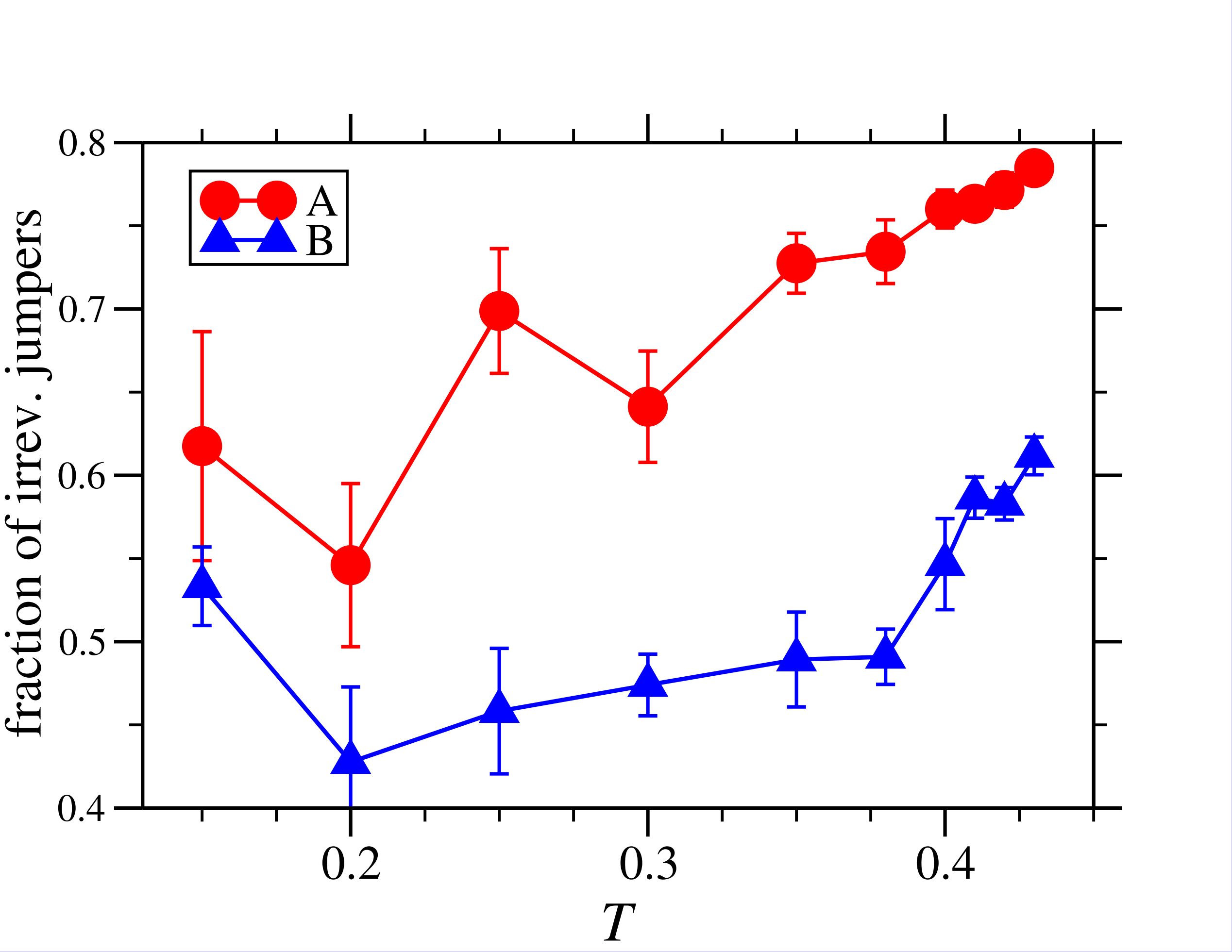


$\Longrightarrow$ fraction of irrev. jumpers increases with increasing T

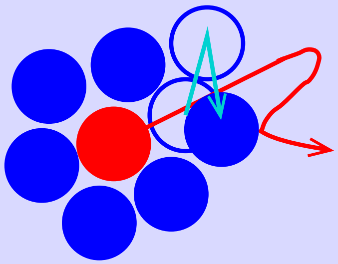
Fraction of Irreversibly Jumping Particles

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

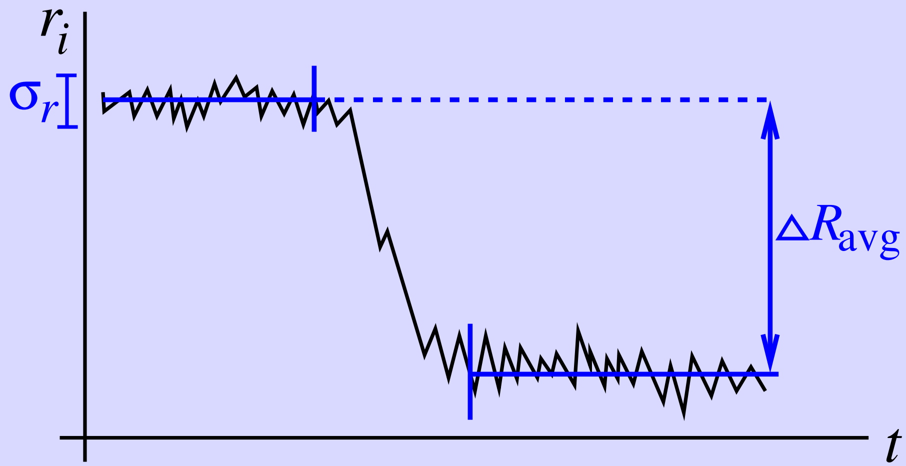


$\Longrightarrow$ fraction of irrev. jumpers increases with increasing T

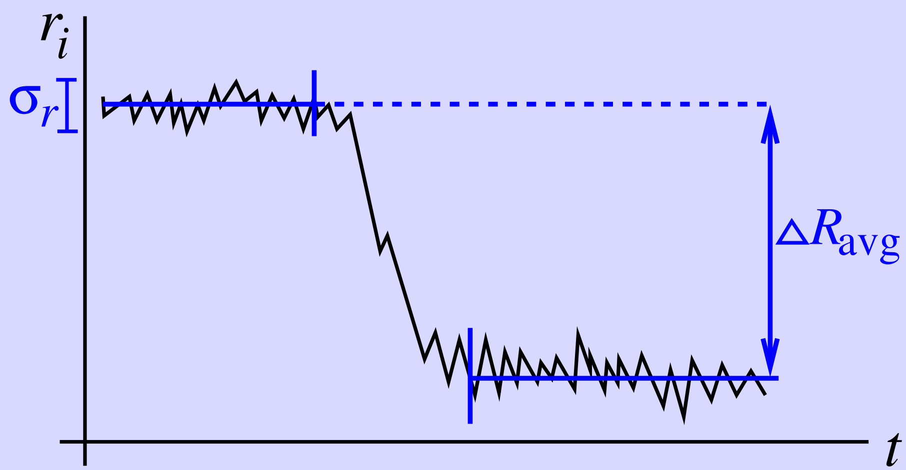
interpretation:
door closing

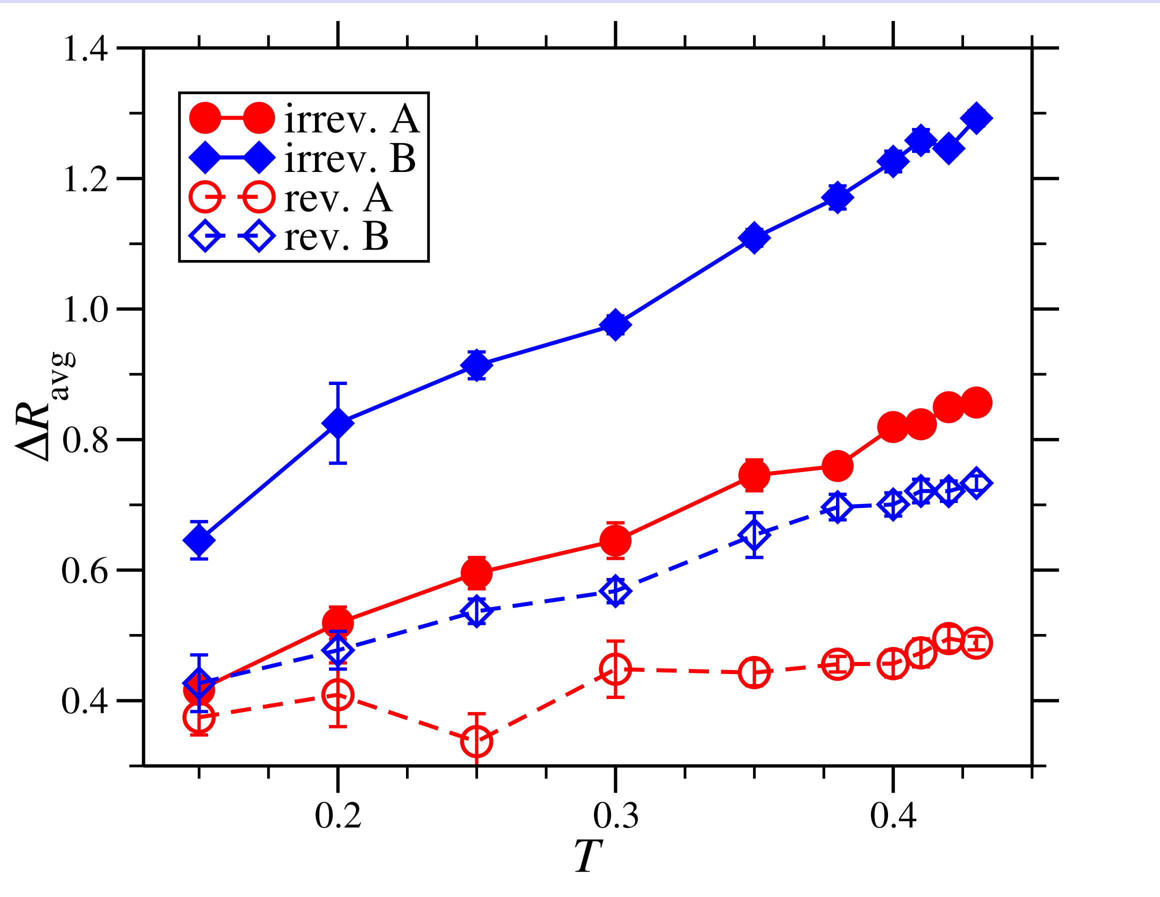


Jump Size



Jump Size



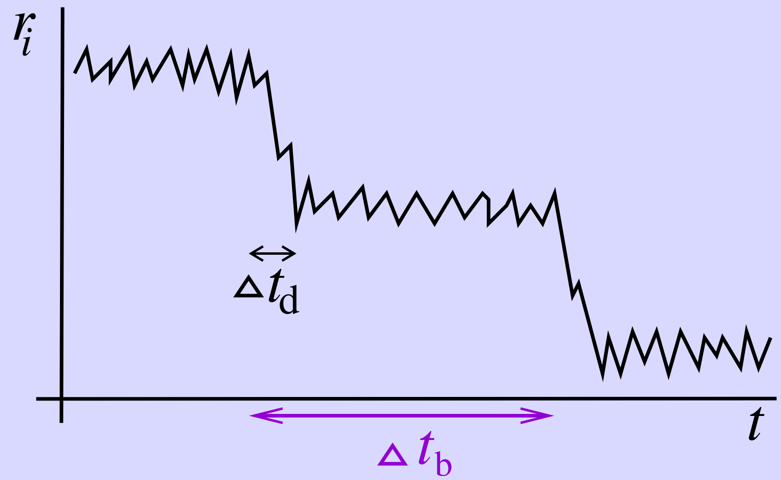


$\Longrightarrow$ increasing with increasing T

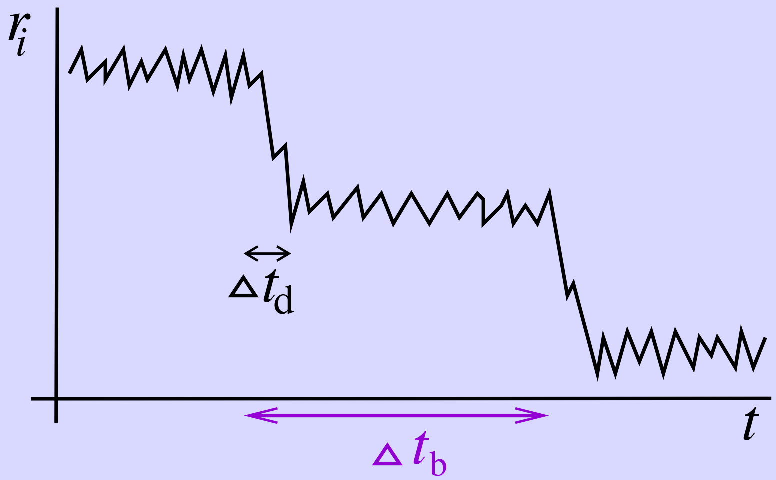
$\Longrightarrow$ (smaller) B-particles jump farther

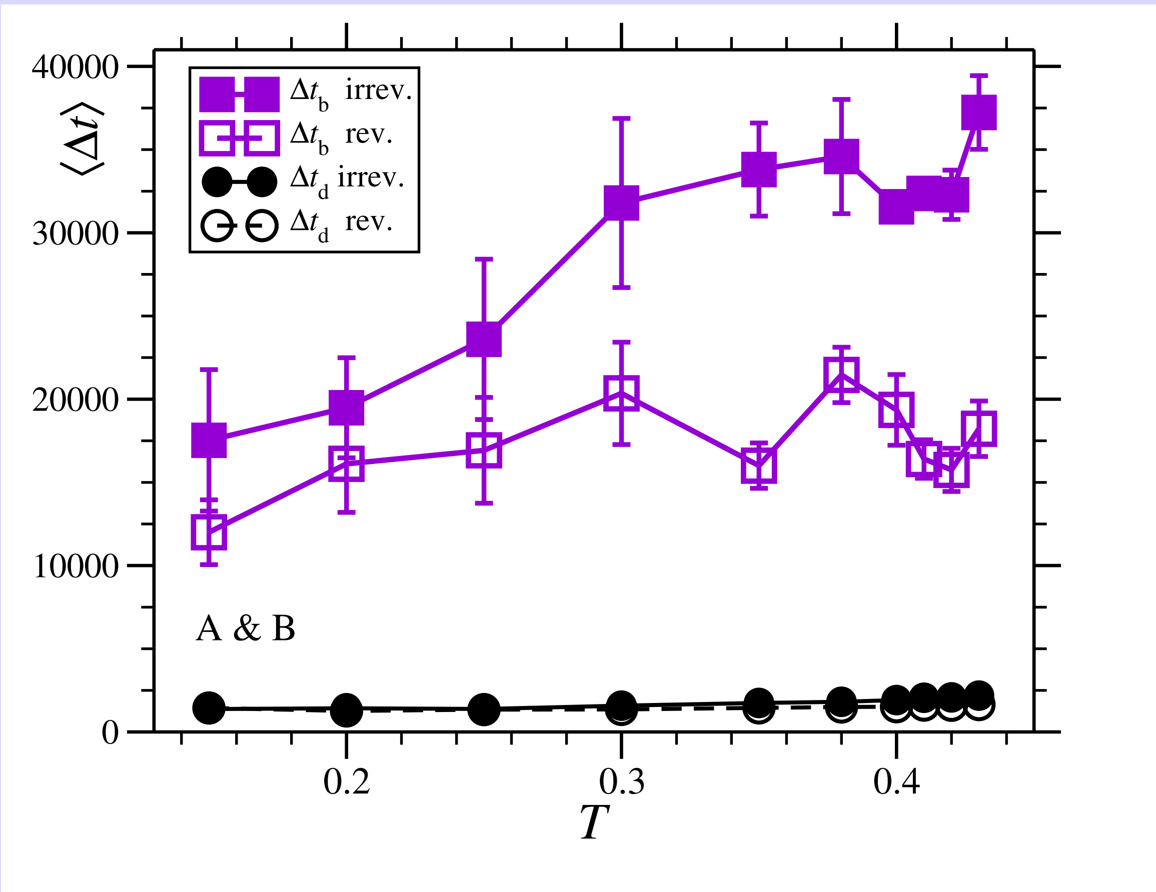
$\Longrightarrow$ irreversible jumps farther

Time Scale



Time Scale





$\Longrightarrow \Delta t_b \gg \Delta t_d$

$\Longrightarrow \Delta t_b$ 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

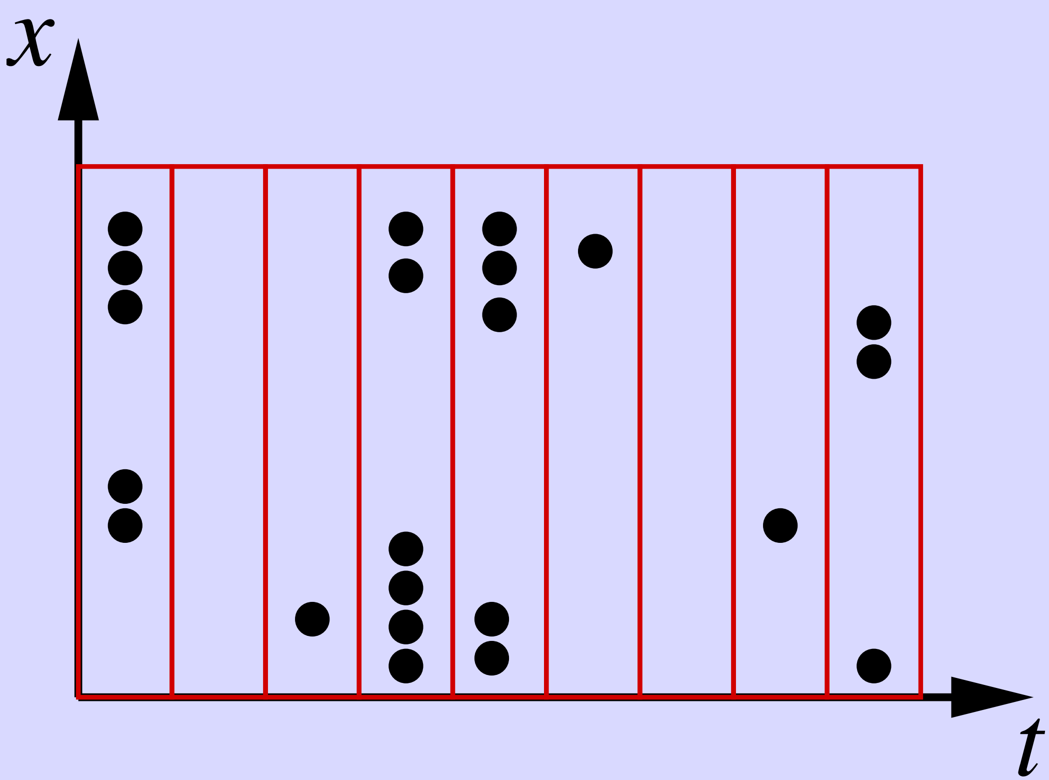
[J. Chem. Phys. **121**, 4781 (2004)]

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

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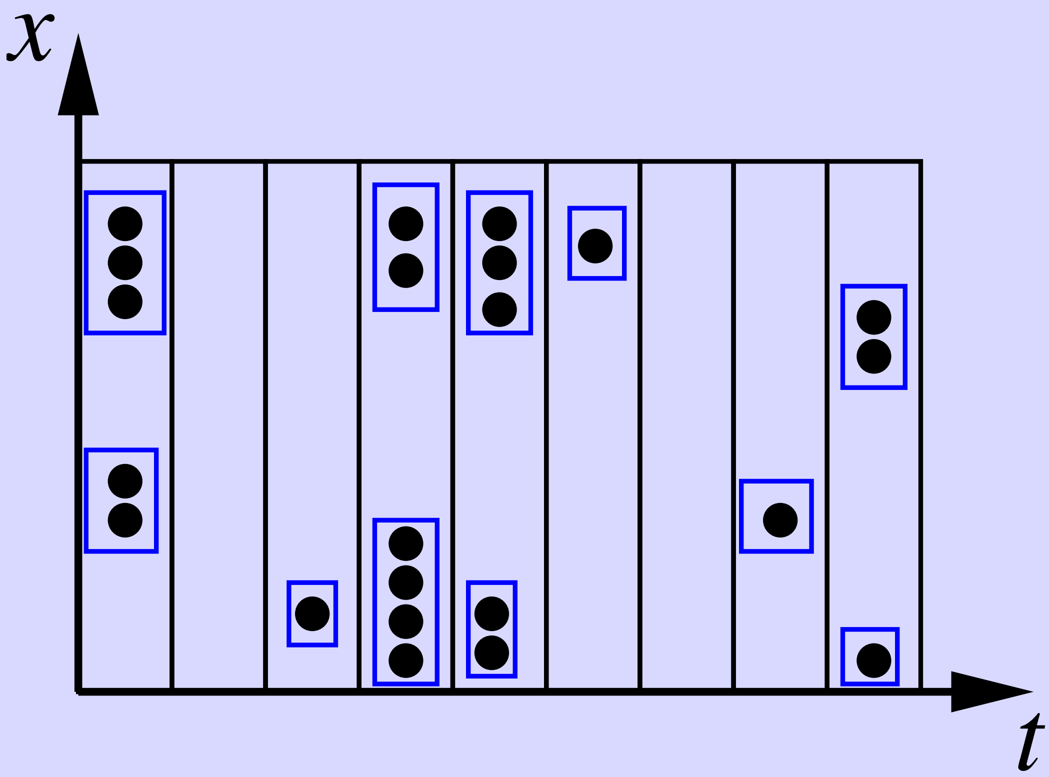
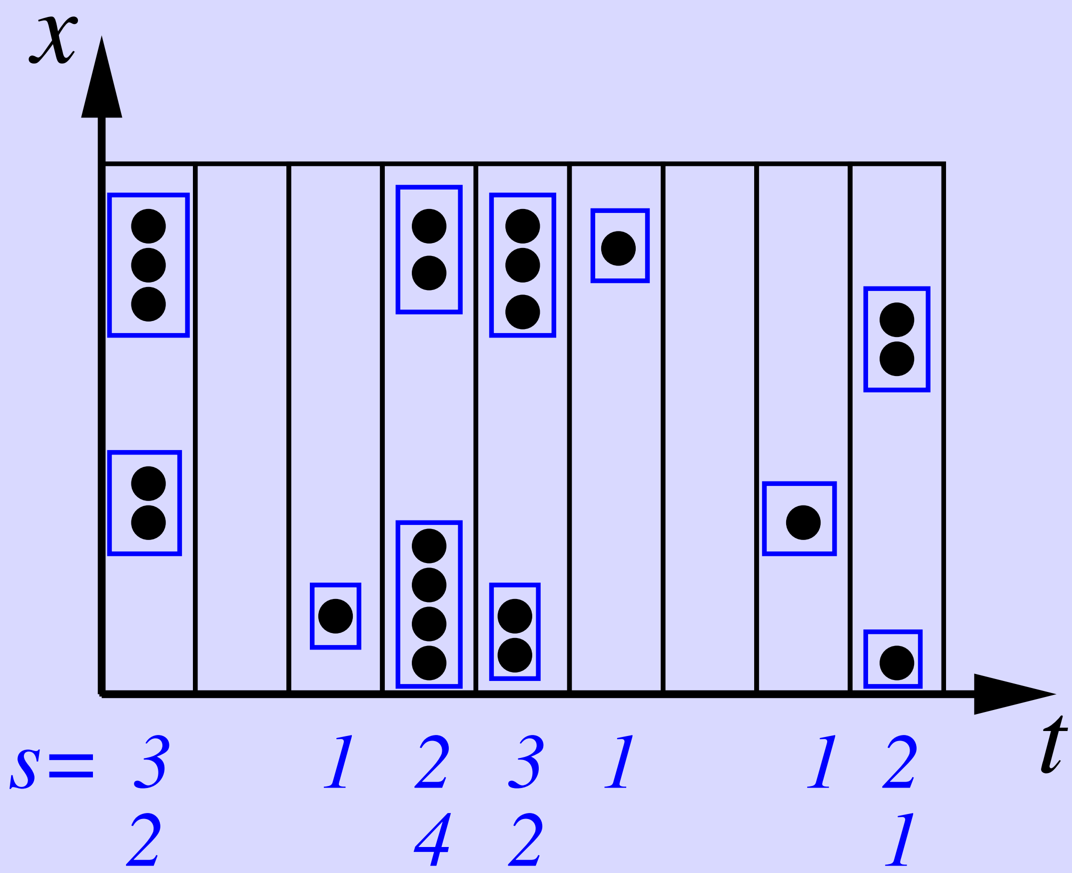


Cluster:

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

Simultaneously Jumping Particles

Cluster Size = number of particles in cluster

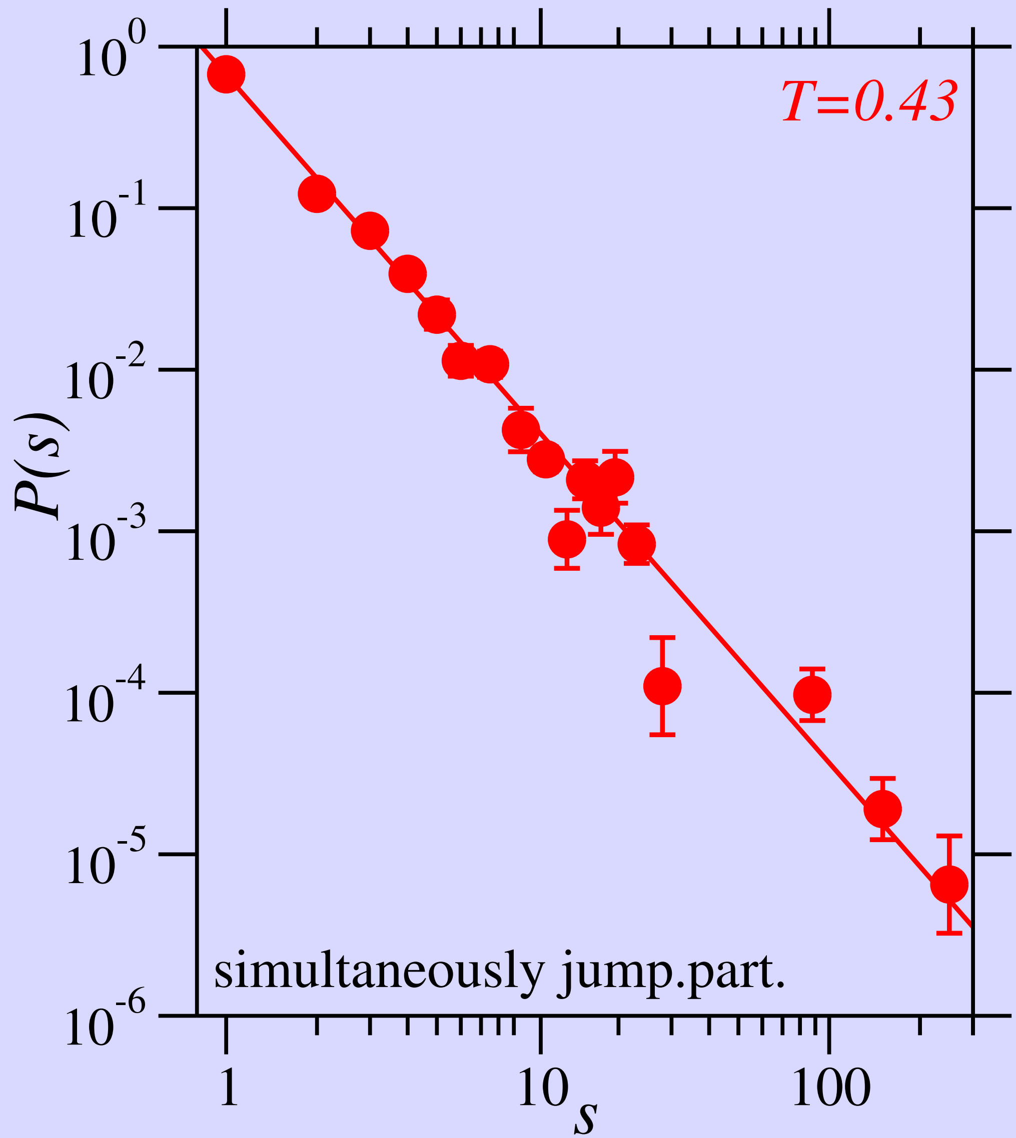


Cluster:

nearest neighbor connections

Cluster Size Distribution

of Simultaneously Jumping Particles



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

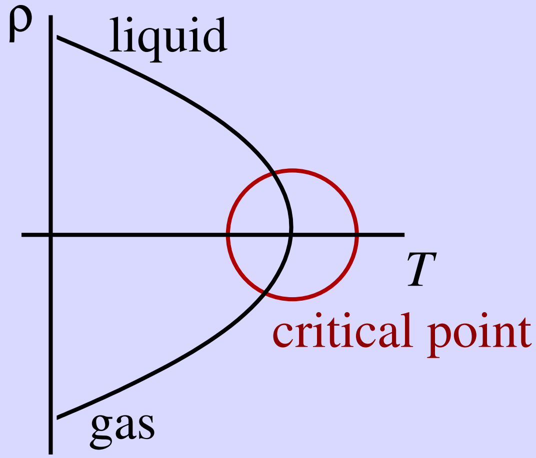
$\Longrightarrow P(s) \sim s^{-\tau}$

$\tau = 1.89 \pm 0.03$

$\Longrightarrow$ critical behavior

Critical Behavior *(Phase Transition)*

Example: Liquid ⟷ Gas



At Critical Point:

powerlaws ⟷ scale invariance

$f(x) = x^{\alpha}$

$f(\lambda x) = \lambda^{\alpha} x^{\alpha} = \lambda^{\alpha} f(x)$

rescale x–axis   rescale y–axis

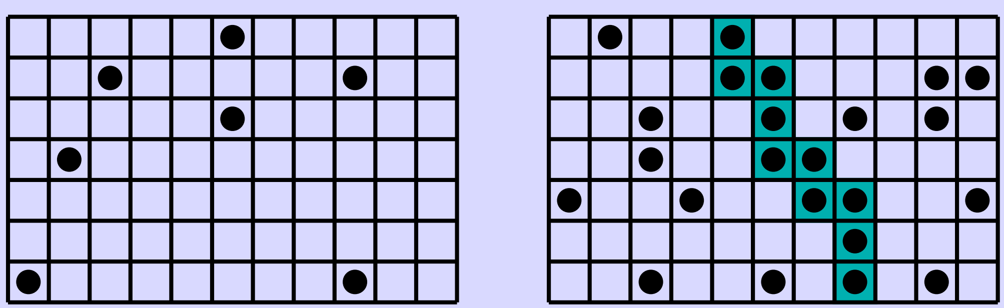
⟶ looks same from any distance

⟶ lack of specific length scale

⟶ large fluctuations

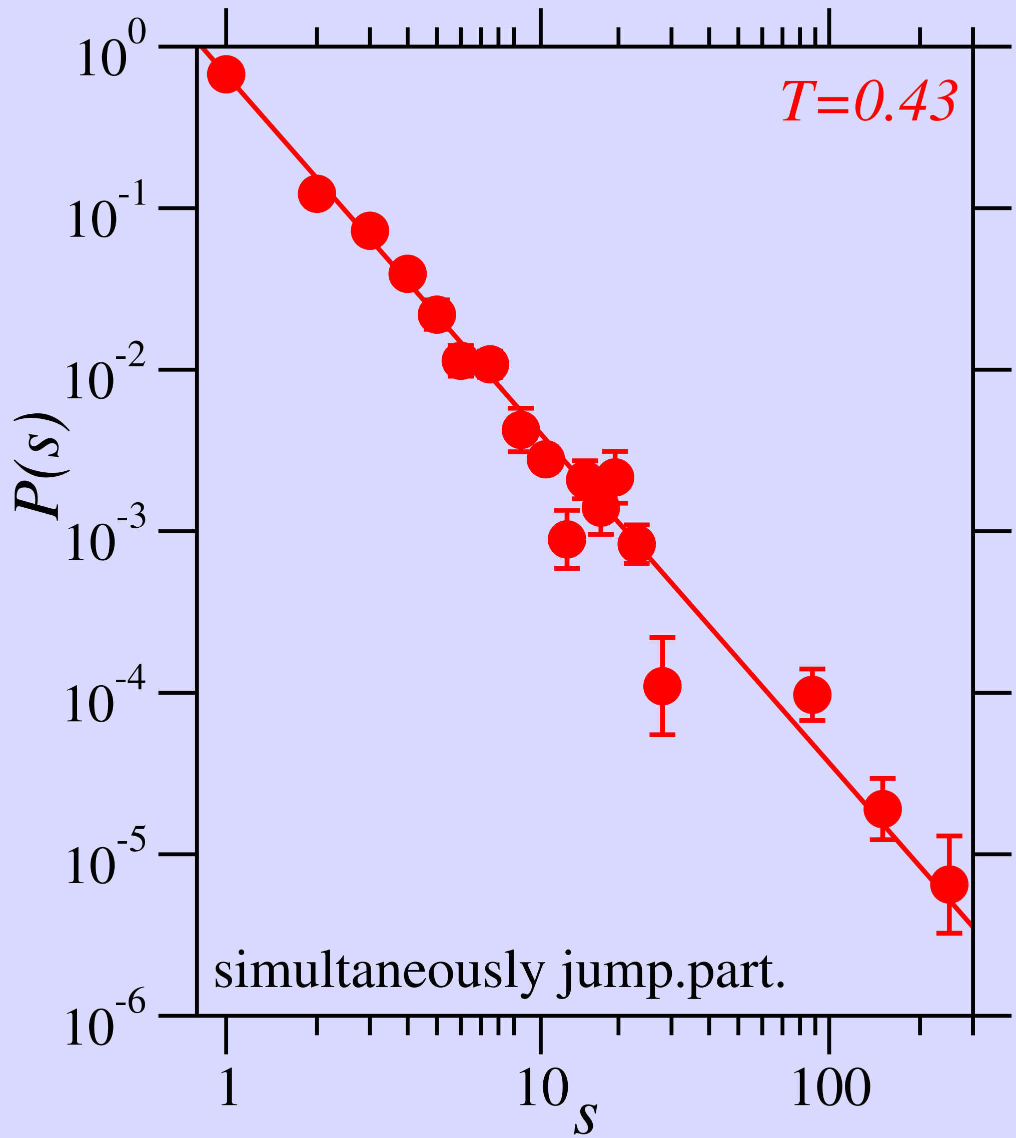
Other Examples:

- Magnet (Ising Model)
- Synchronization
- Percolation



Cluster Size Distribution

of Simultaneously Jumping Particles



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

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

$\tau = 1.89 \pm 0.03$

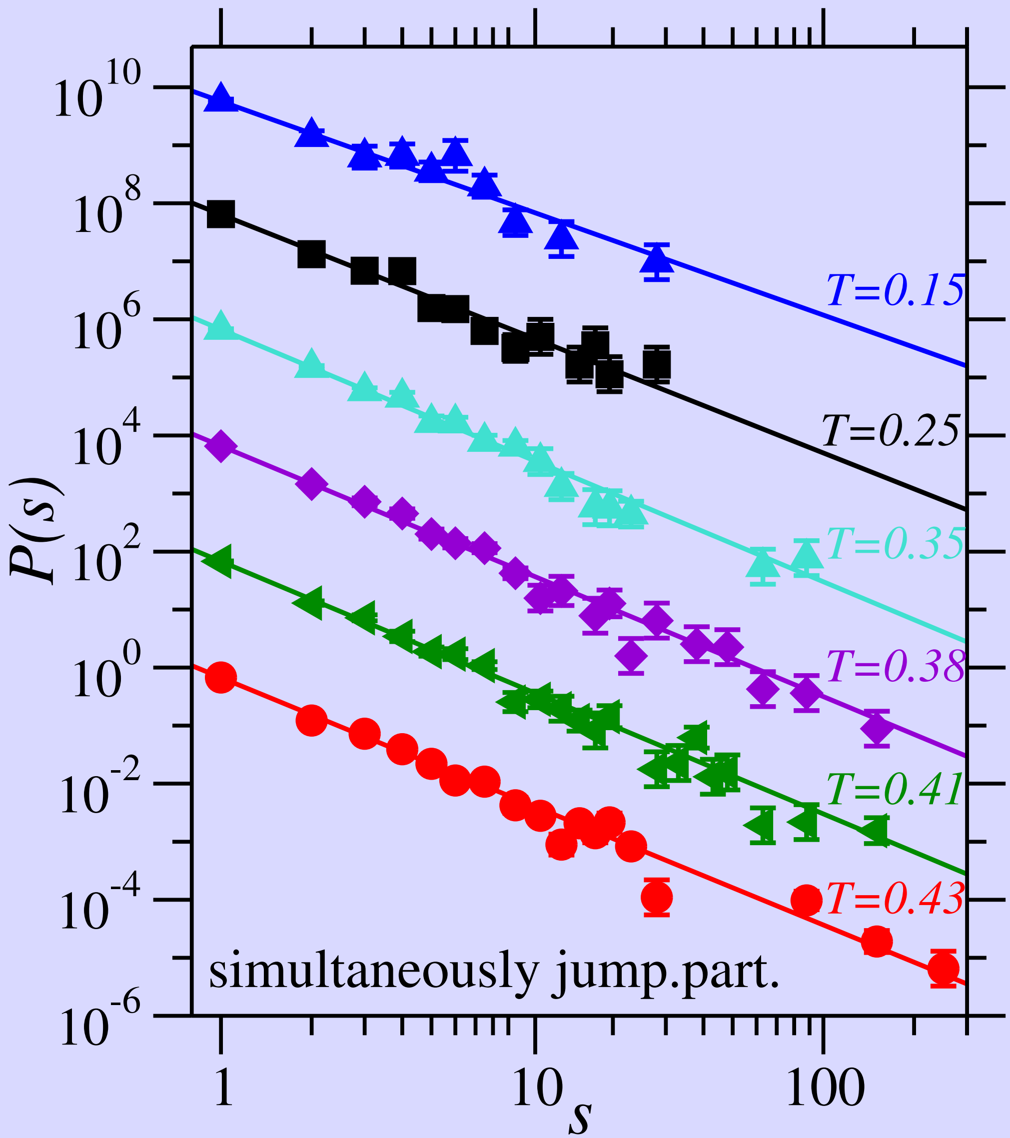
$\Longrightarrow$ critical behavior

$\Longrightarrow$ Percolation?

$\tau_{\mathrm{MF}} = 2.5 \qquad \tau_{3\mathrm{d}} = 2.2$

Cluster Size Distribution

of Simultaneously Jumping Particles



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

percolation?

NO because

$\Longrightarrow$ power law for **all** temperatures

$\Longrightarrow$ **self-organized criticality**

$\tau(T)$

Self-Organized Criticality

powerlaw not only at critical point but independent of details of external parameters

Examples: sandpile avalanches, forest fire, earth quakes

Similarities here:

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

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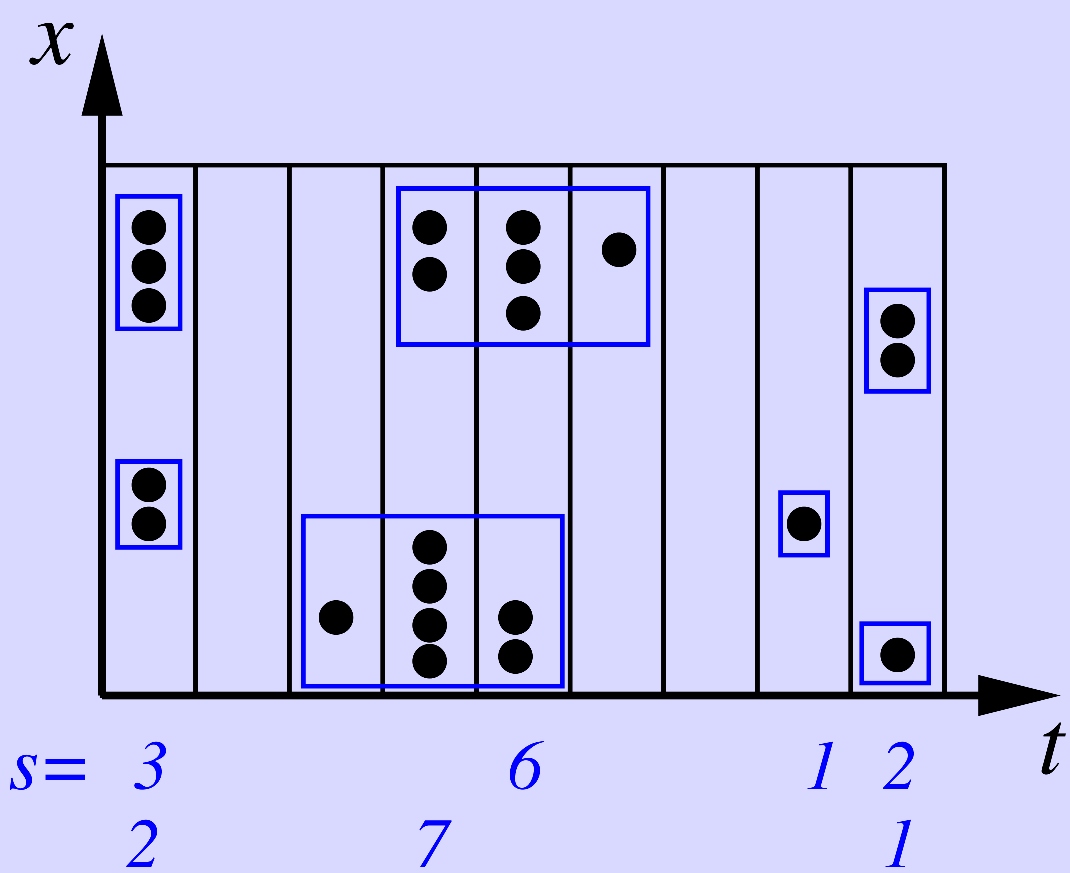
Temporally Extended Cluster



Definition:

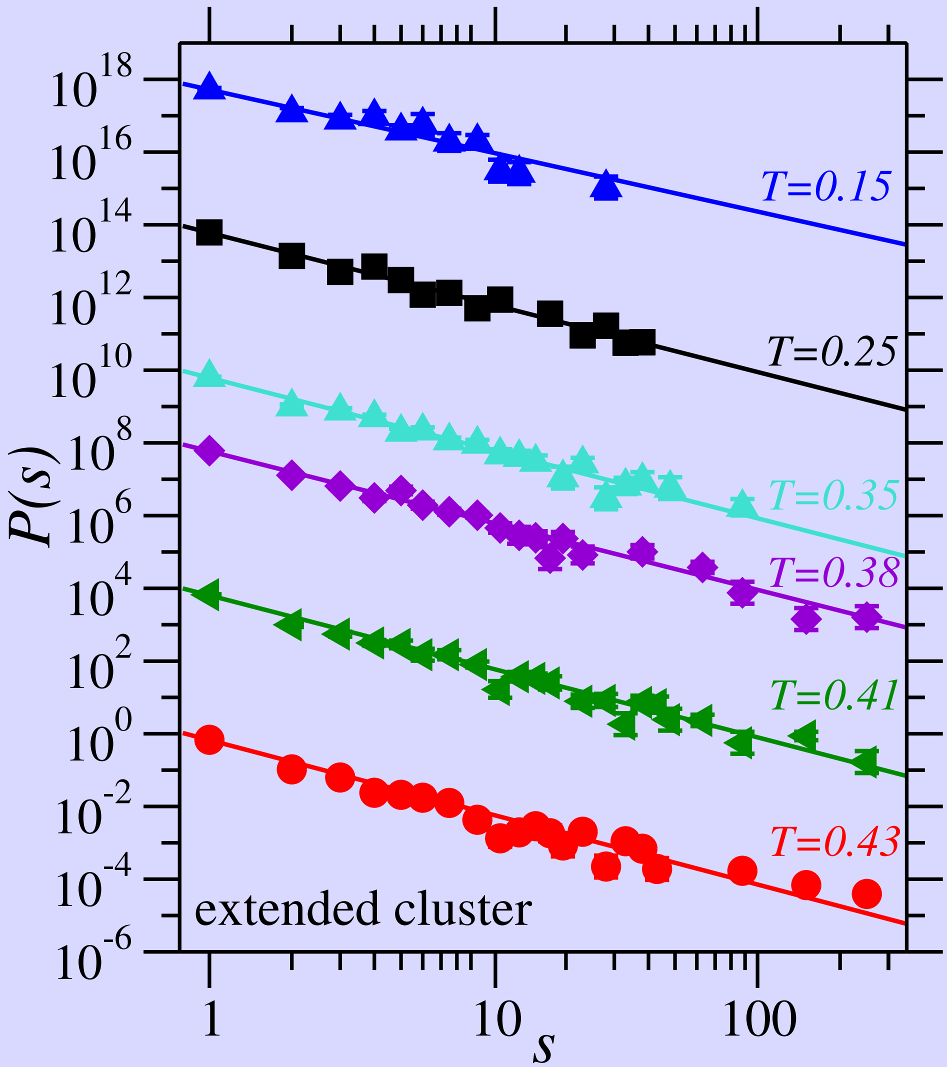
cluster of events $(\mathbf{r}_i, t_i)$

connected if:

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

Cluster Size Distribution

of Temporally Extended Clusters

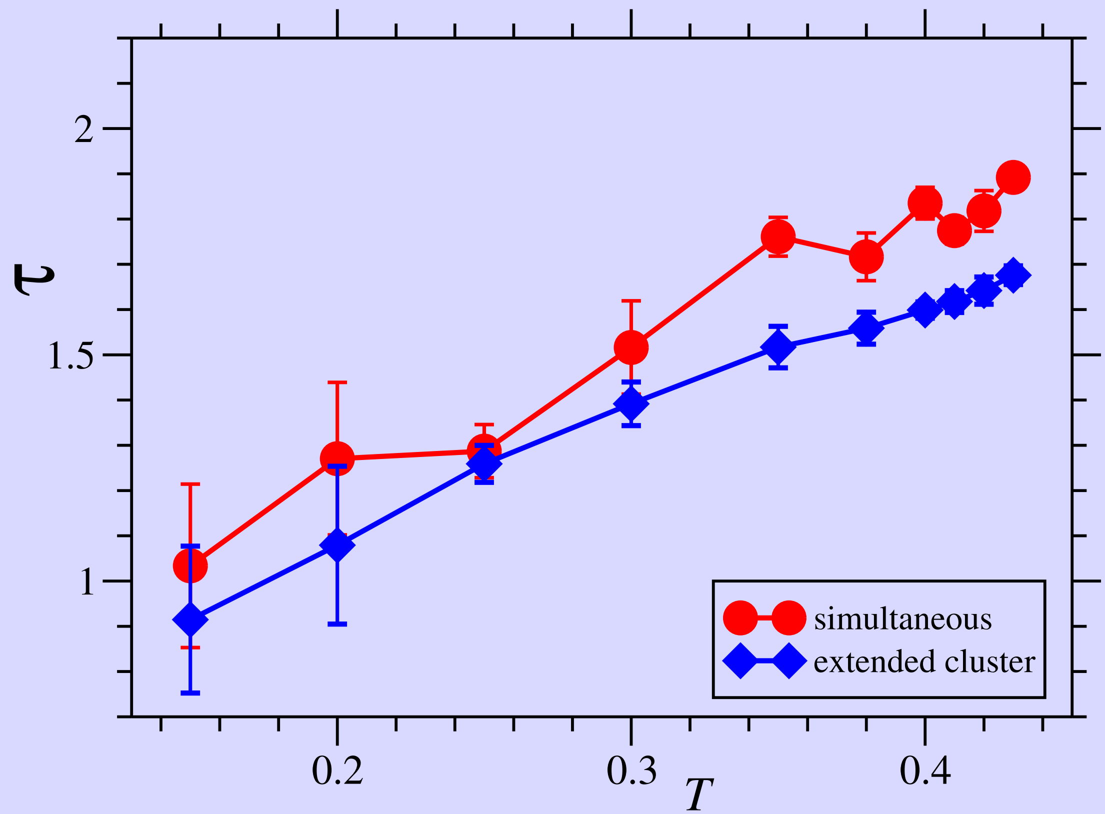


$\Longrightarrow P(s) \sim s^{-\tau}$

$\Longrightarrow$ for all temperatures (self-organized crit.)

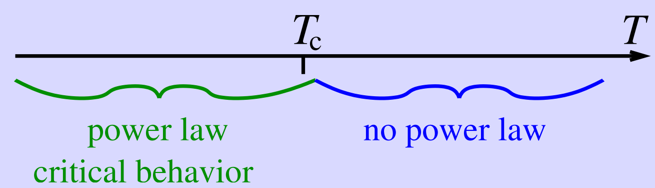
Exponent $\tau(T)$

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



slightly above T_c $\tau \approx 1.86$

[Donati et al. 1999]



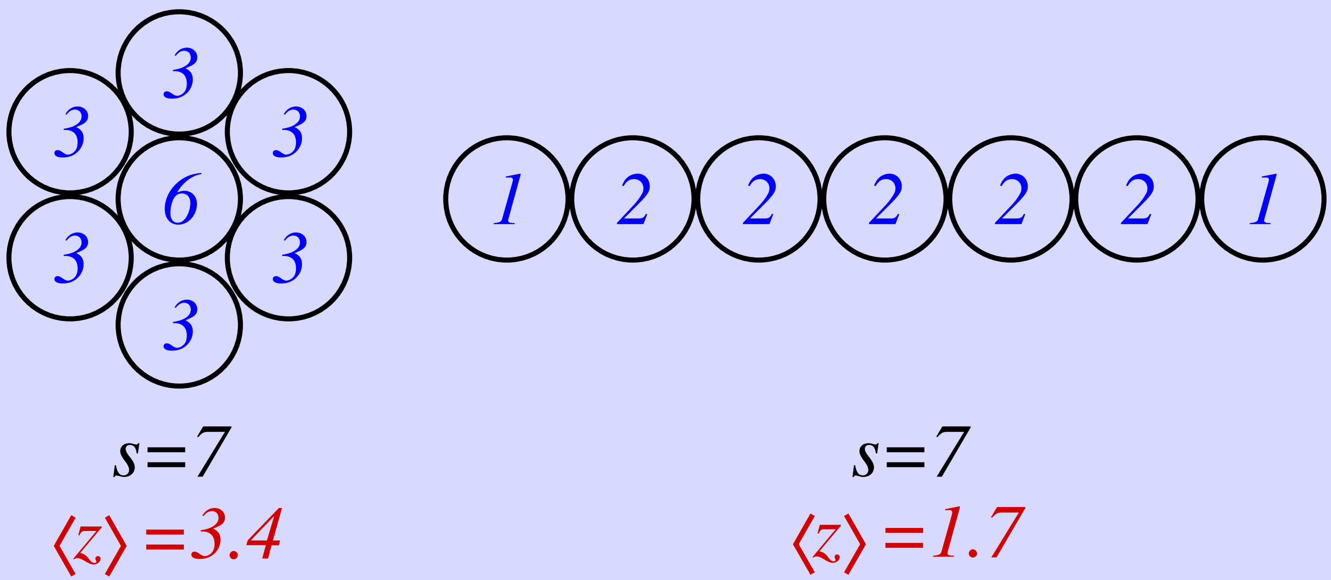
P simult.

Shape of Clusters

z = number of nearest neighbors within cluster

s = number of particles (cluster size)

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



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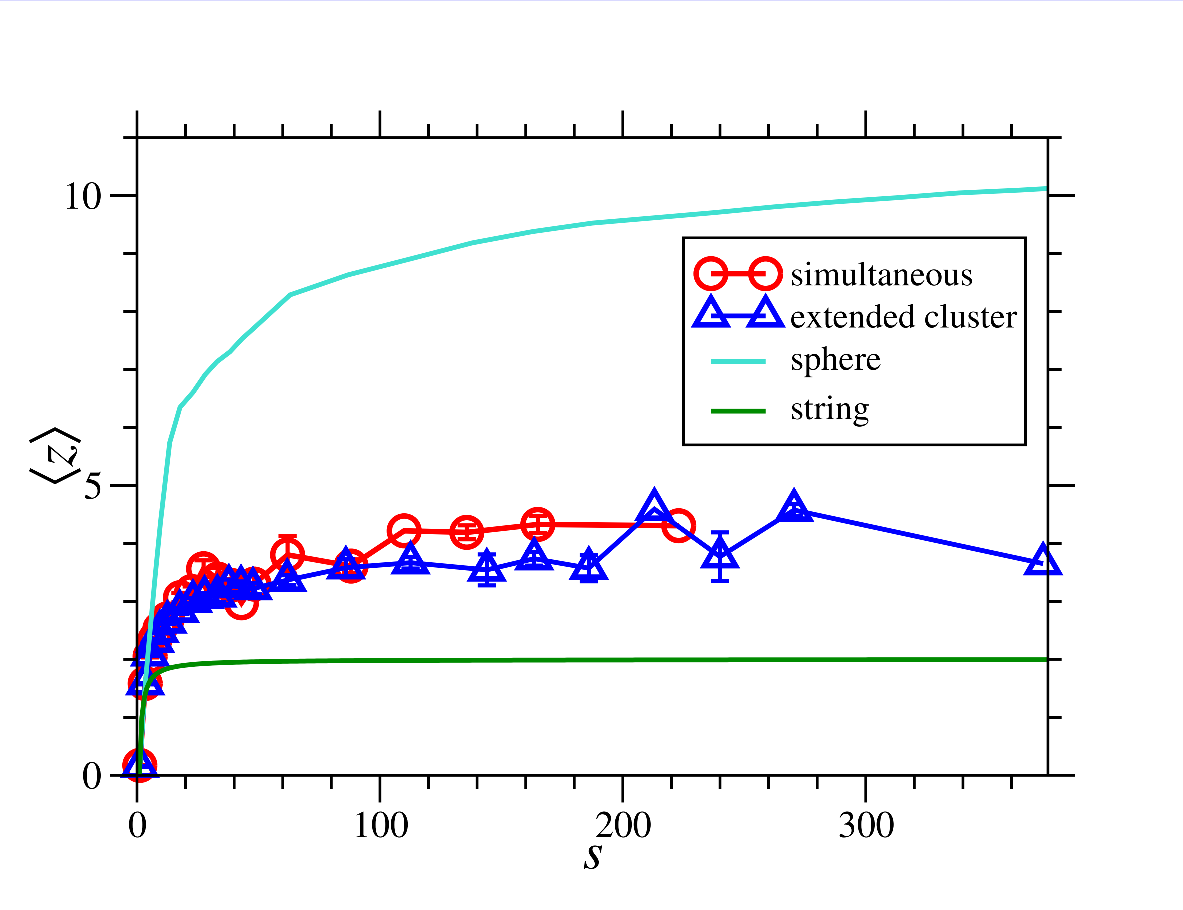

$\Longrightarrow$ string-like clusters

Shape of Clusters

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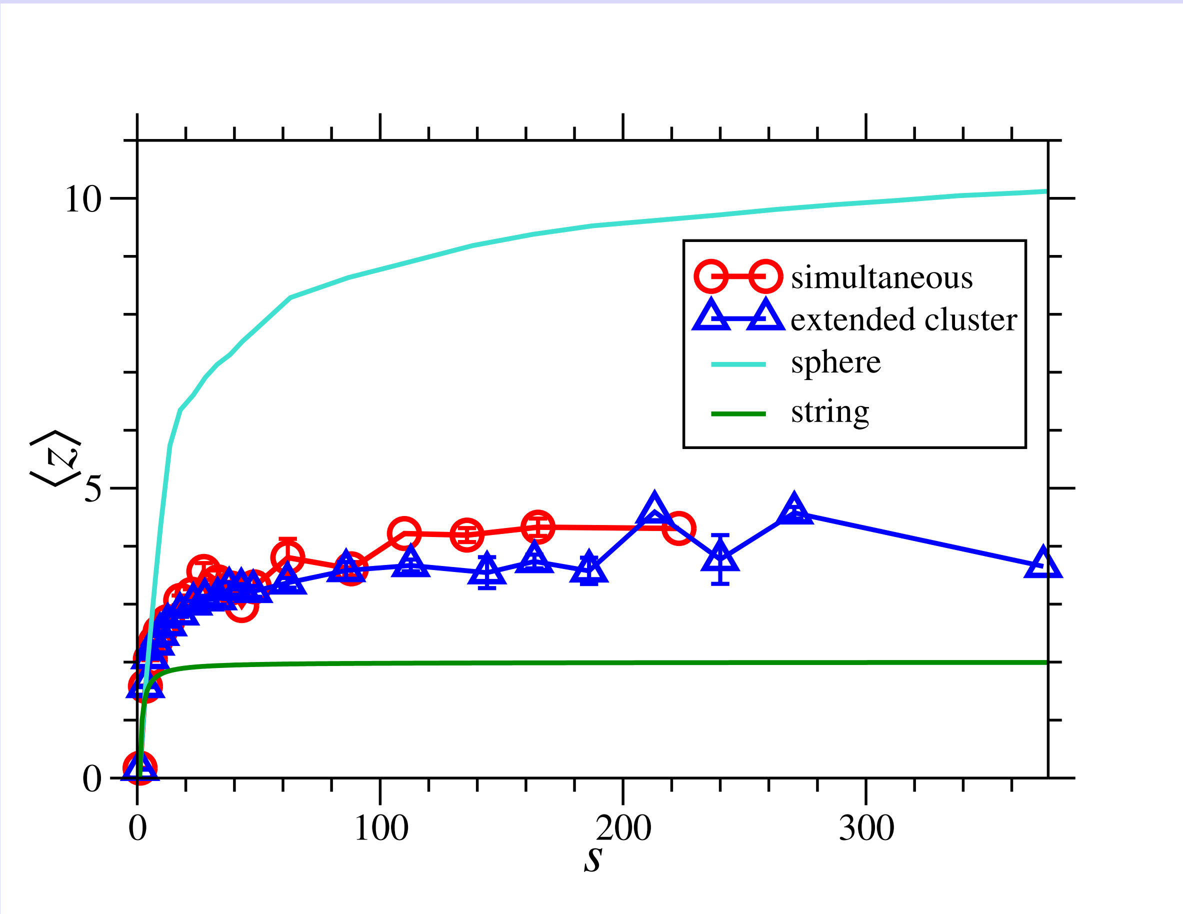
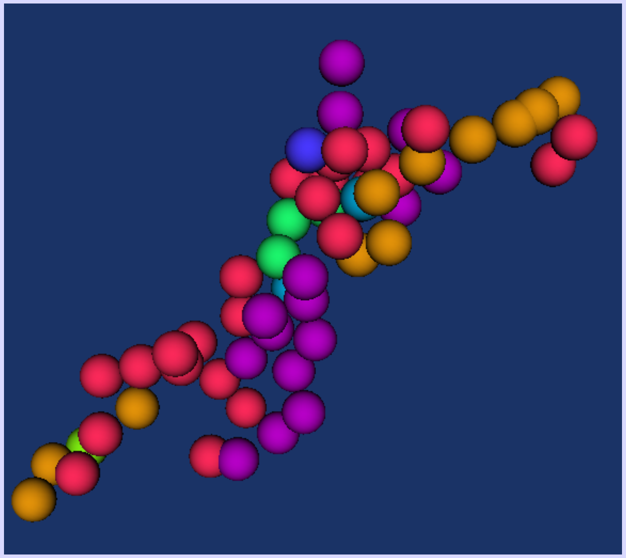


$\Longrightarrow$ string-like clusters



same color = same time

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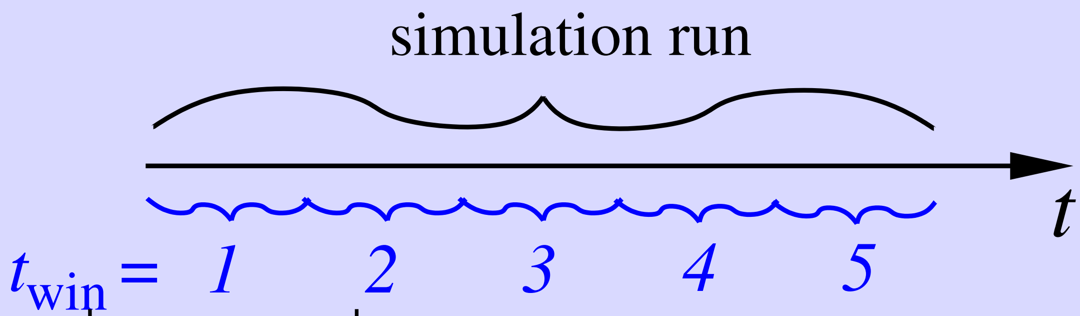
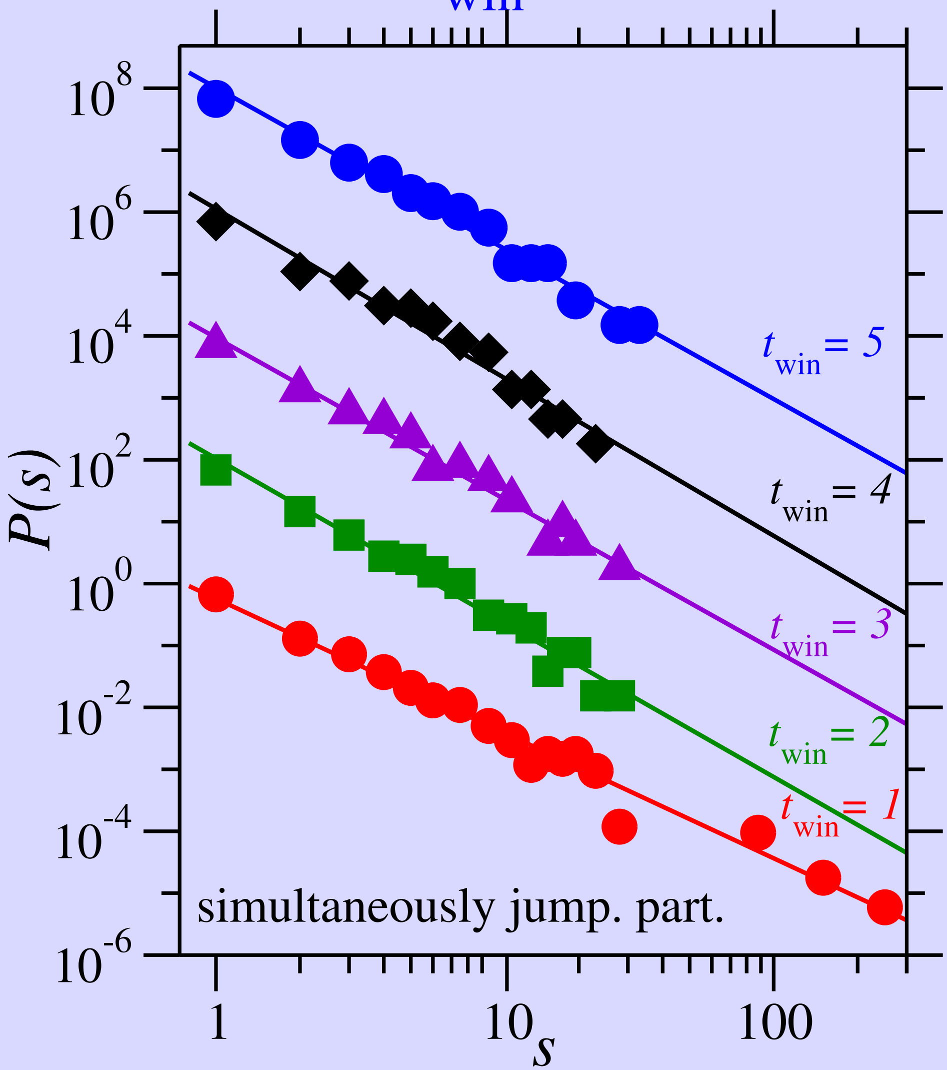
History Dependence





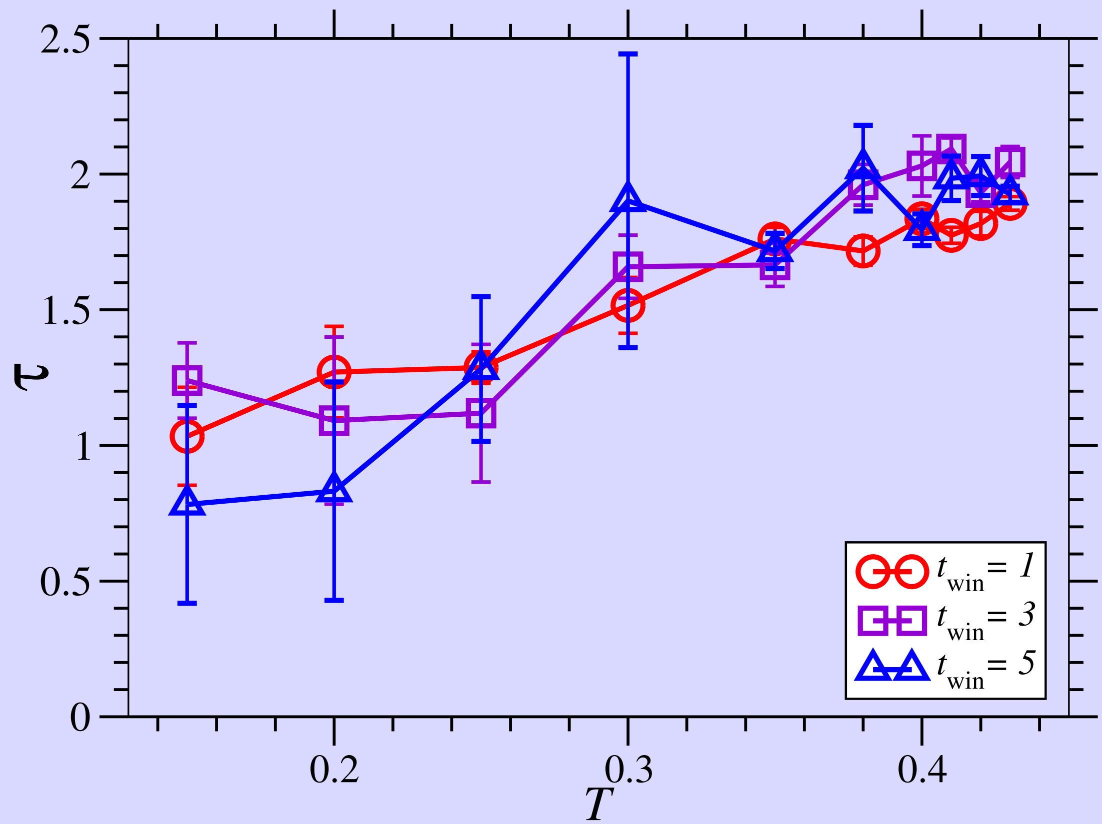
Power Law

(Simultan. Jump. Part.)

$\Longrightarrow$ aging independent

Exponent $\tau(T)$

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



$\Longrightarrow$ aging independent

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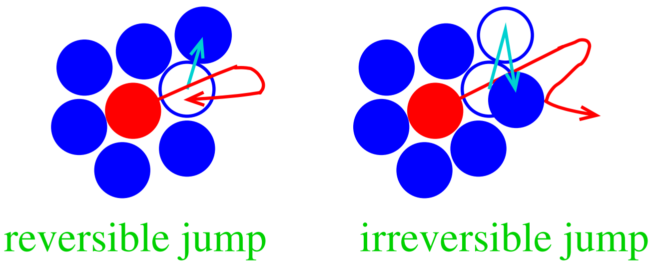
Summary: Jump Statistics

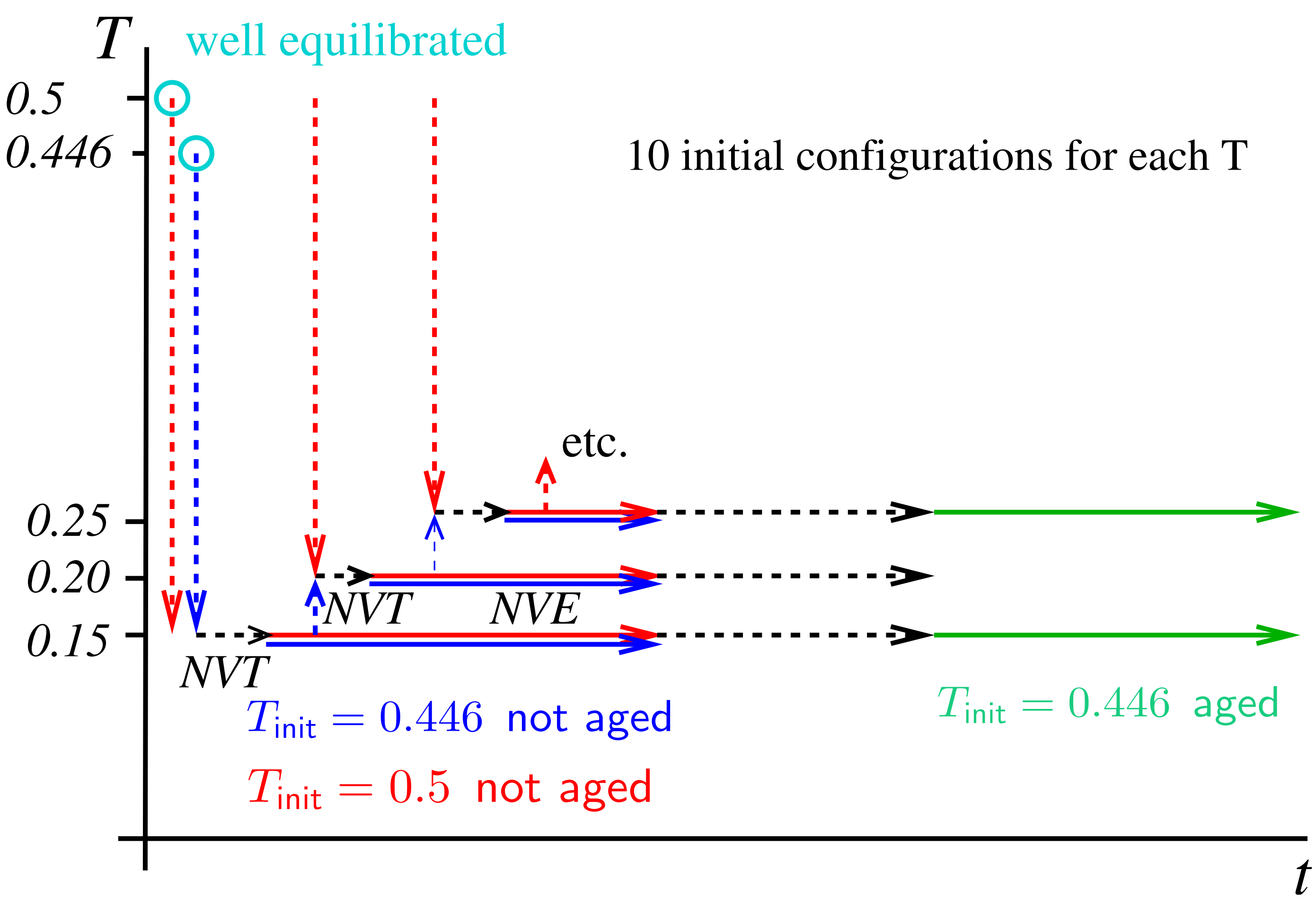
reversible and irreversible jumps:



At larger temperature relaxation:

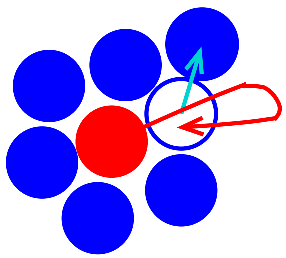
- via more jumping particles
- via larger jumpsizes
- not via Δt_{b} (indep. of T)

History of Production Runs

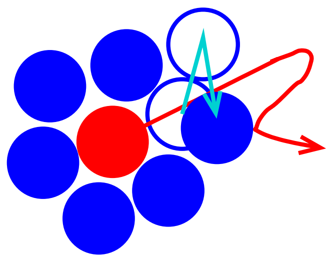


Summary: Jump Statistics

reversible and irreversible jumps:



reversible jump



irreversible jump

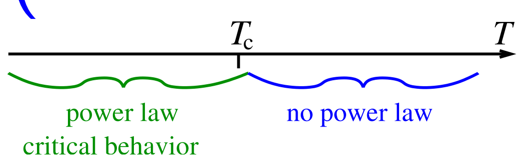
At larger temperature relaxation:

• 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

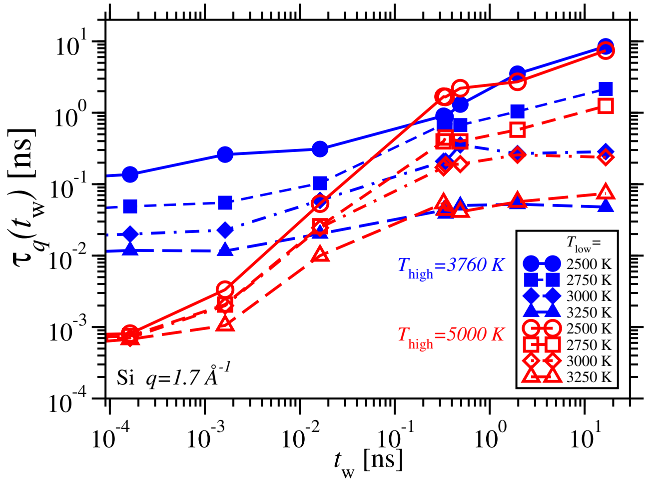
A. Zippelius, K. Binder, E. A. Baker, J. Horbach

Support from Institute of Theoretical Physics, University Göttingen,

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

Out-of-Equilibrium to In-Equilibrium: SiO_2

- jump statistics
- intermediate incoherent scattering function

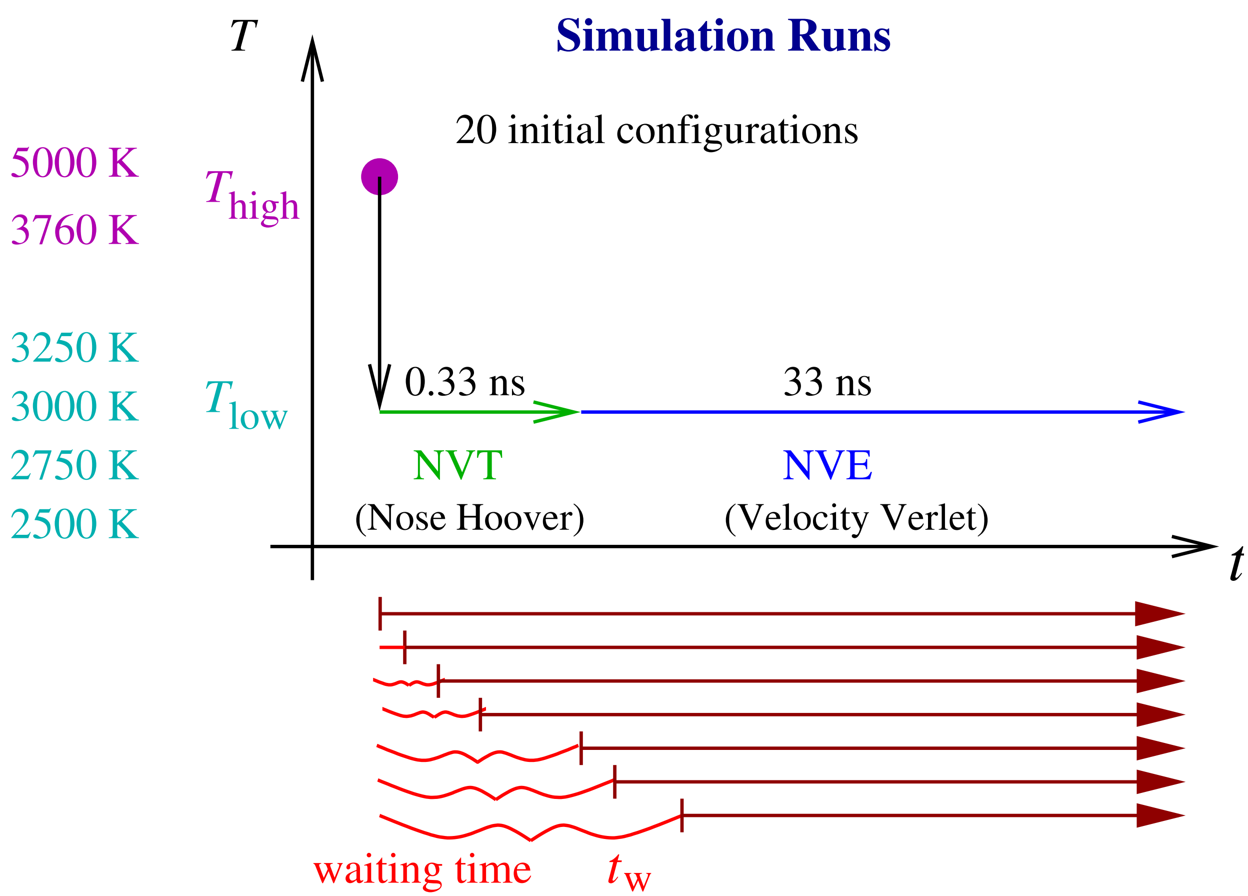


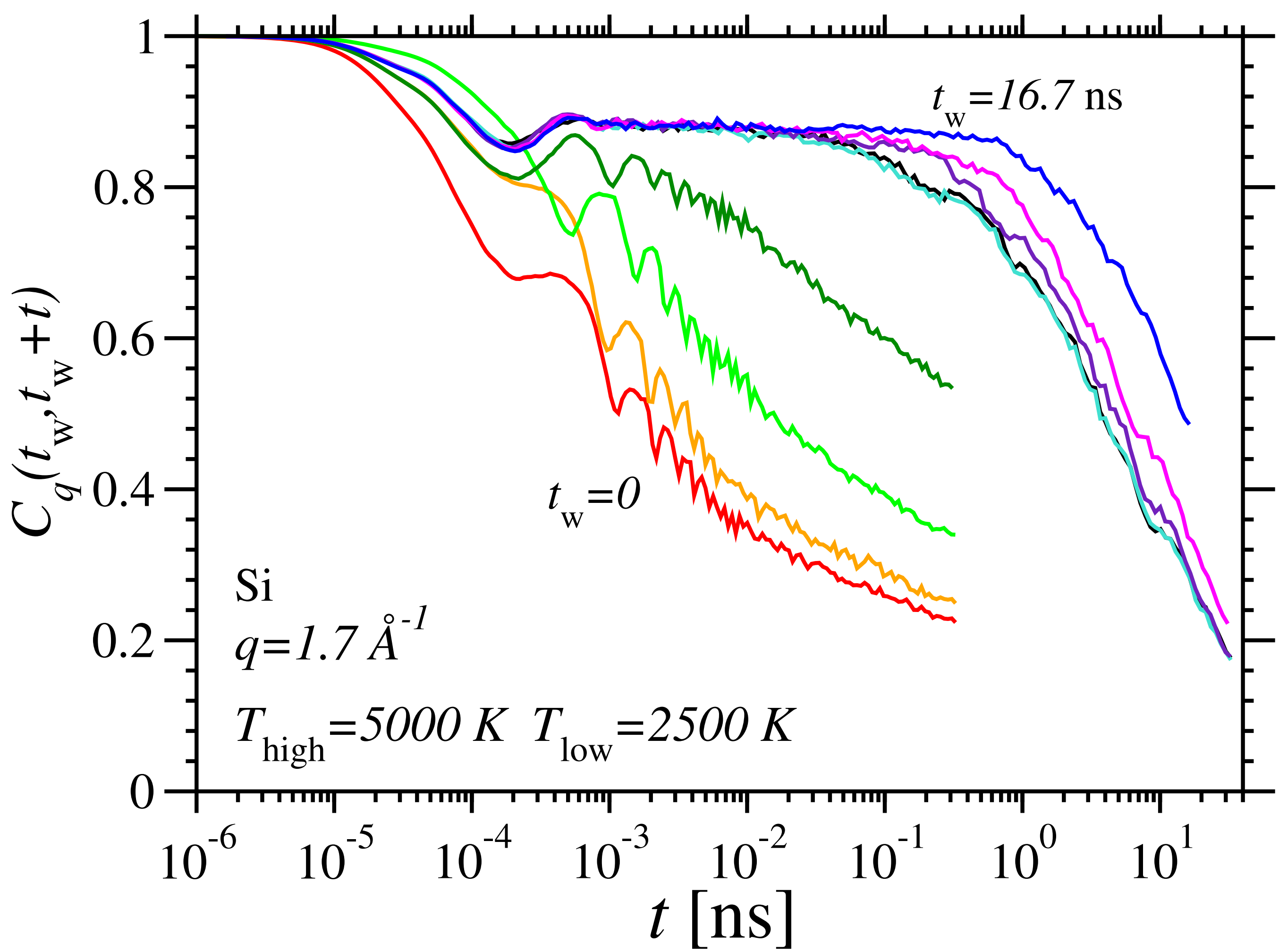
three t_w ranges:

t_w too small: aging regime: equilibrium

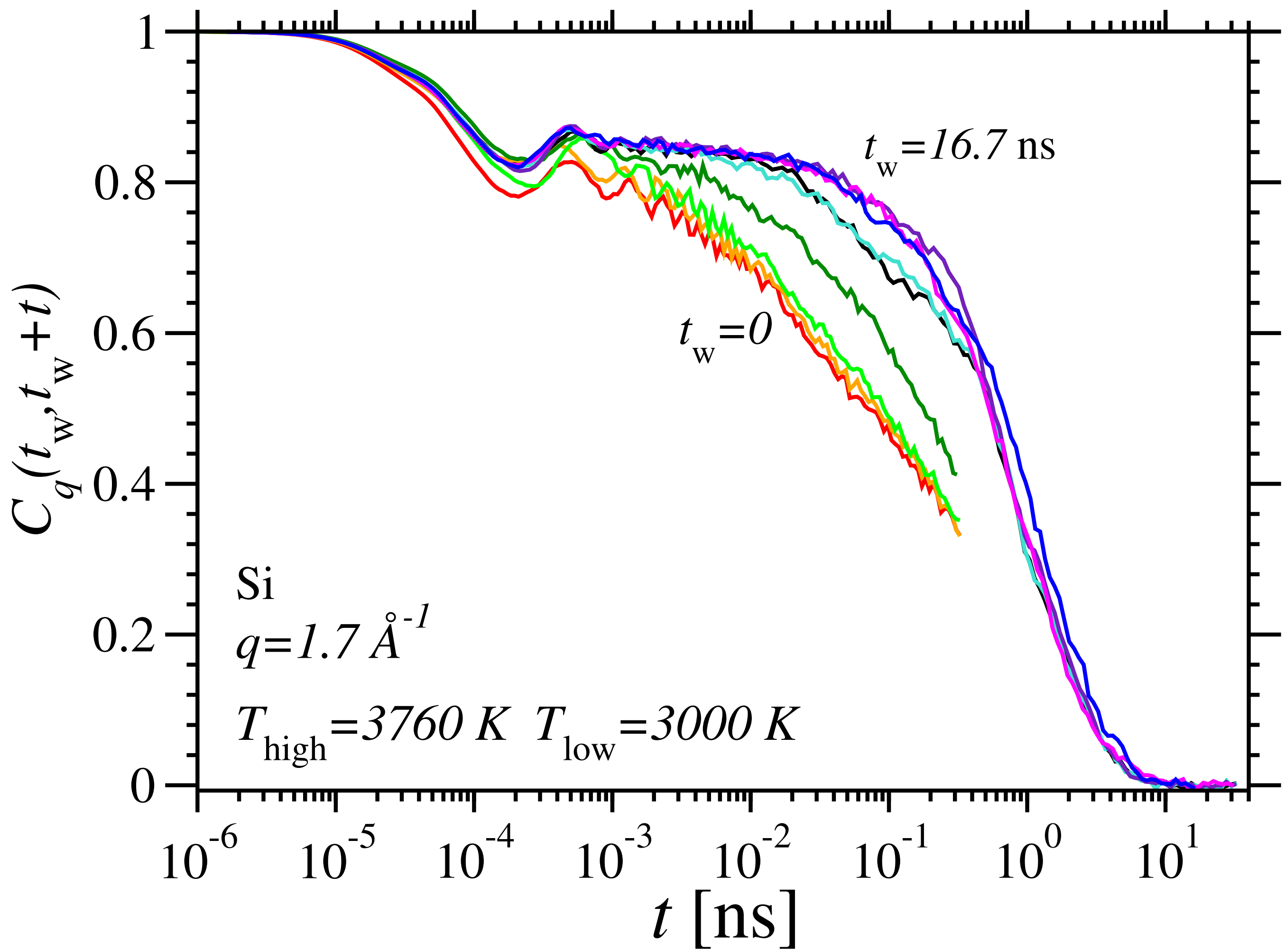
$C_q^{AG}(t/\tau)$

$C_q^{AG}(h(t_w+t)/h(t_w))$

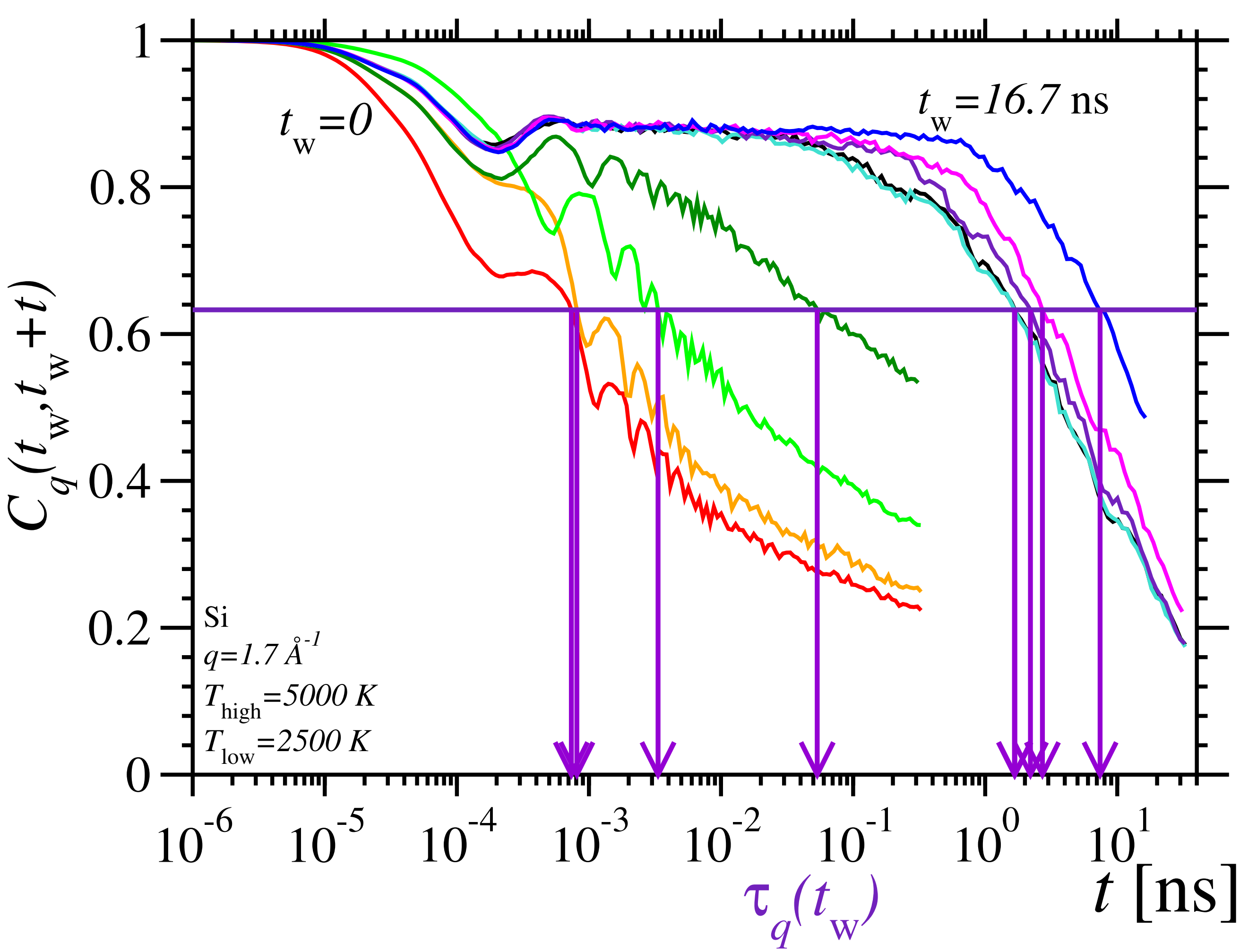

Simulation Runs
T
20 initial configurations
5000 K
3760 K
T_{high}
3250 K
3000 K
2750 K
2500 K
T_{low}
0.33 ns
33 ns
NVT
(Nose Hoover)
NVE
(Velocity Verlet)
t
waiting time
t_w



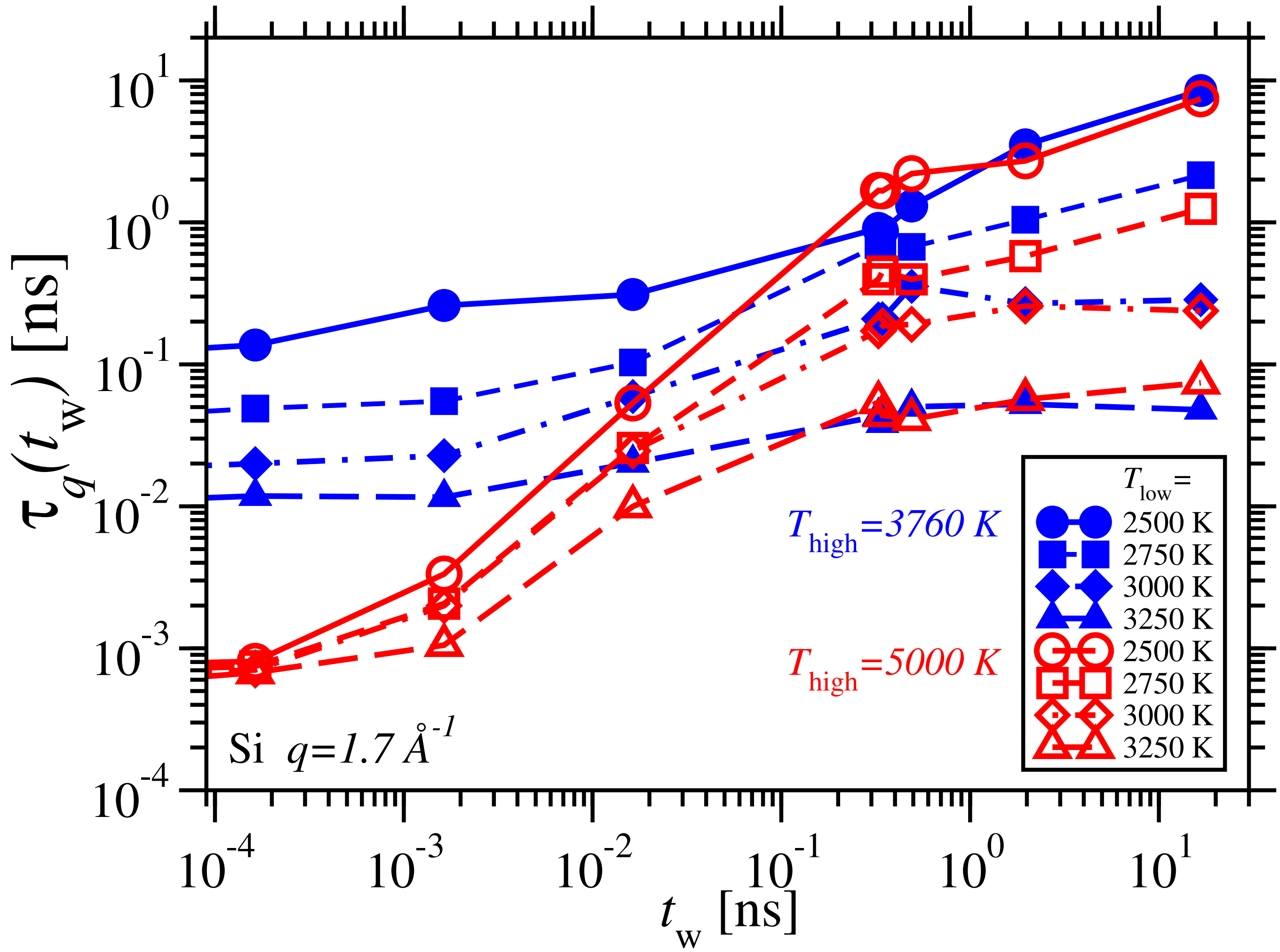
1
0.8
0.6
0.4
0.2
0
$C_q(t_w,t_w+t)$
t_w=16.7 ns
t_w=0
Si
q=1.7 Å^{-1}
T_{high}=5000 K T_{low}=2500 K
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
t [ns]



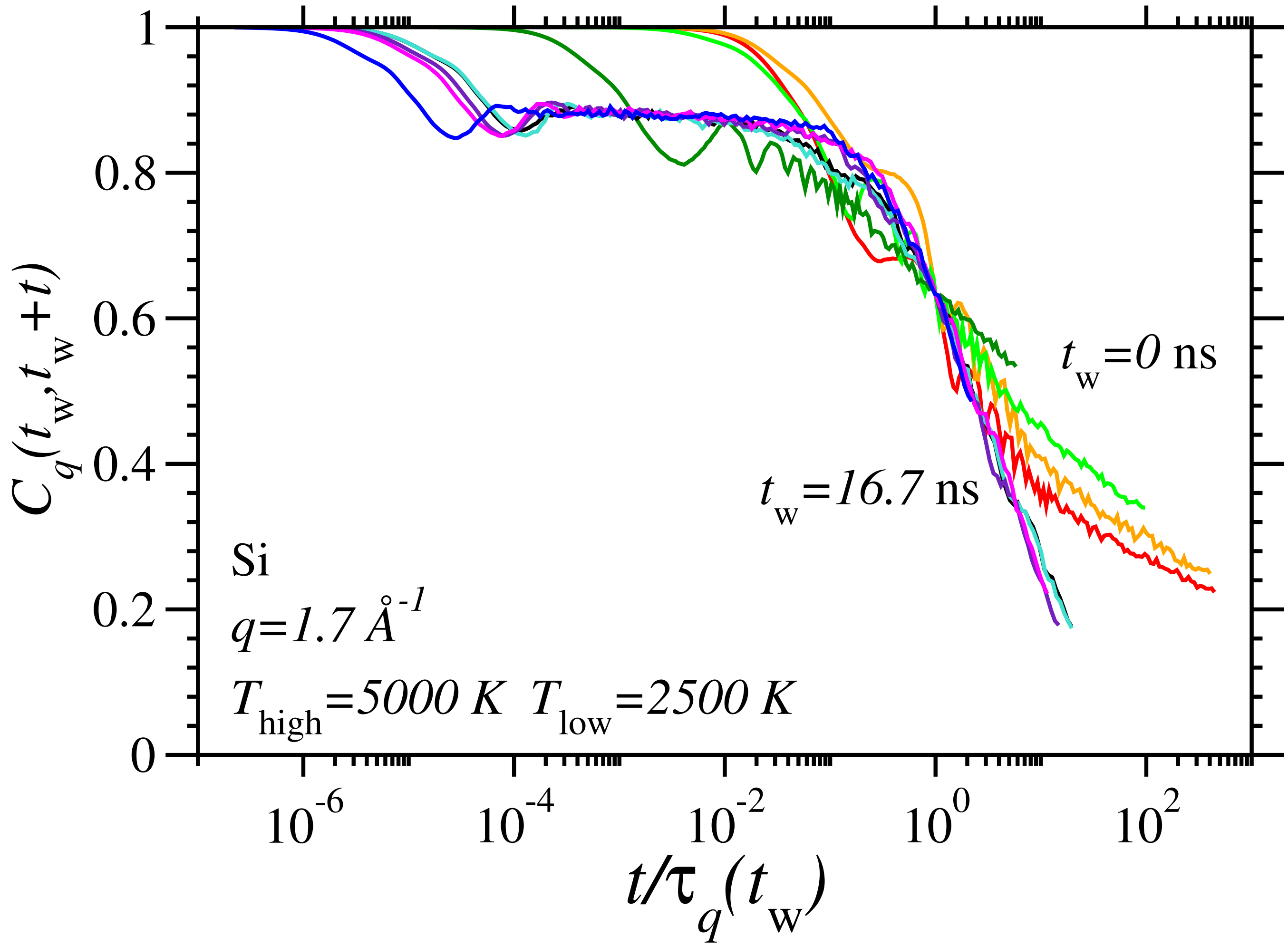
$C_q(t_w,t_w+t)$
t_w=16.7 ns
t_w=0
Si
q=1.7 Å^{-1}
T_{high}=3760 K T_{low}=3000 K
t [ns]



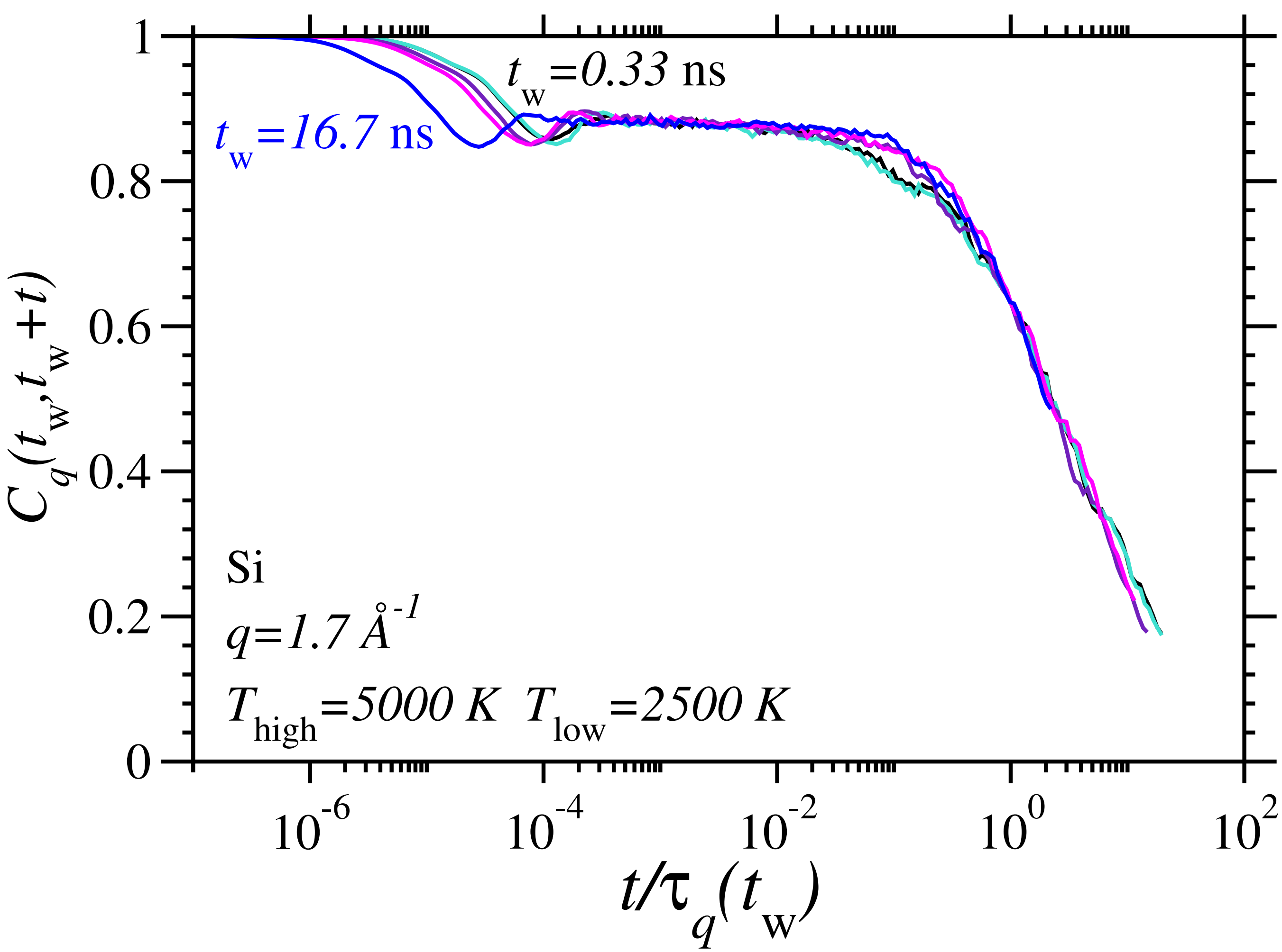
t_w=0
t_w=16.7 ns
$C_q(t_w,t_w+t)$
Si
q=1.7 Å^{-1}
T_{high}=5000 K
T_{low}=2500 K
t [ns]
$\tau_q(t_w)$



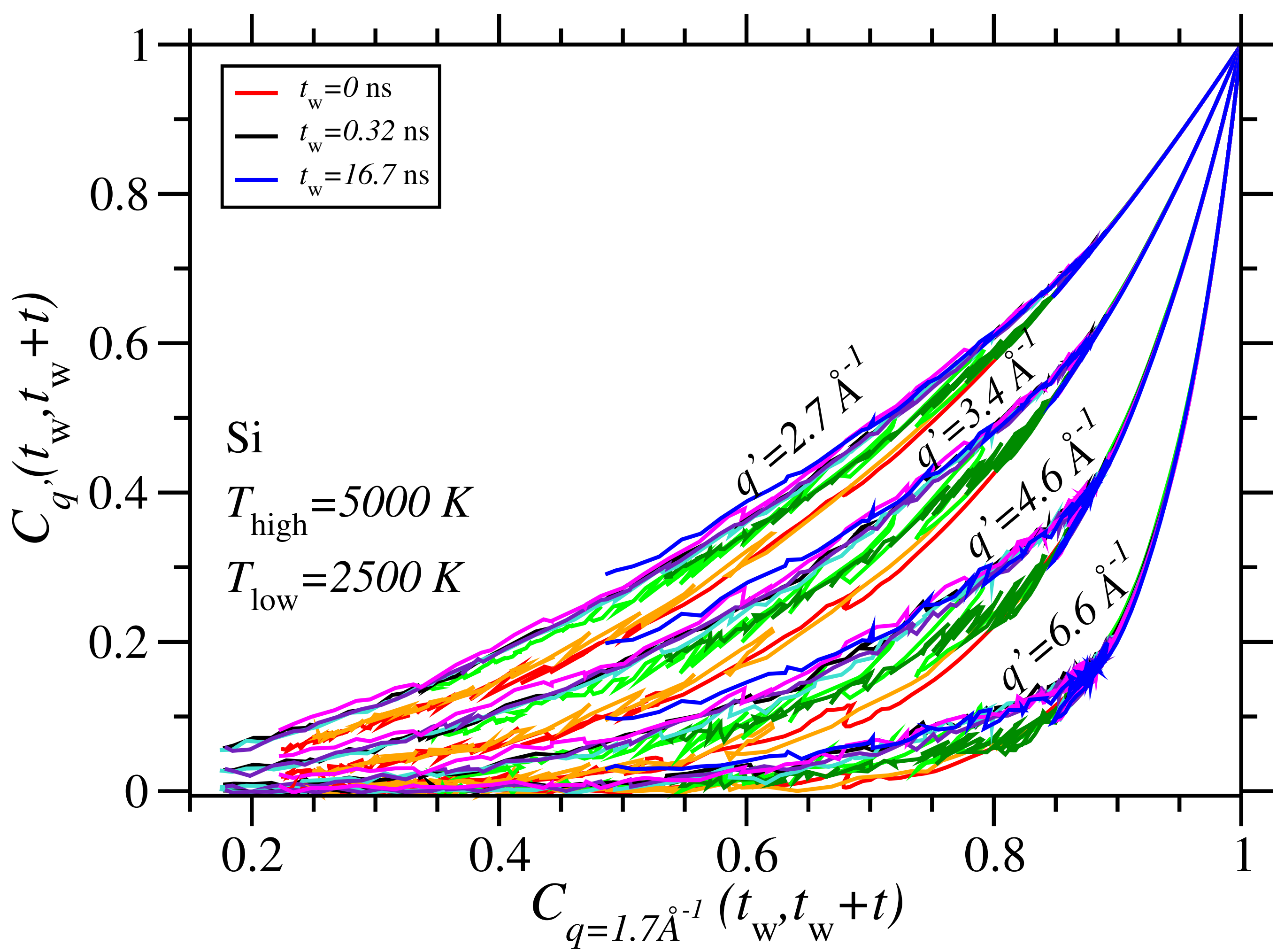
$\tau_q(t_w)$ [ns]
t_w [ns]
T_{high}=3760 K
T_{high}=5000 K
T_{low}=
2500 K
2750 K
3000 K
3250 K
2500 K
2750 K
3000 K
3250 K
Si q=1.7 Å^{-1}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}



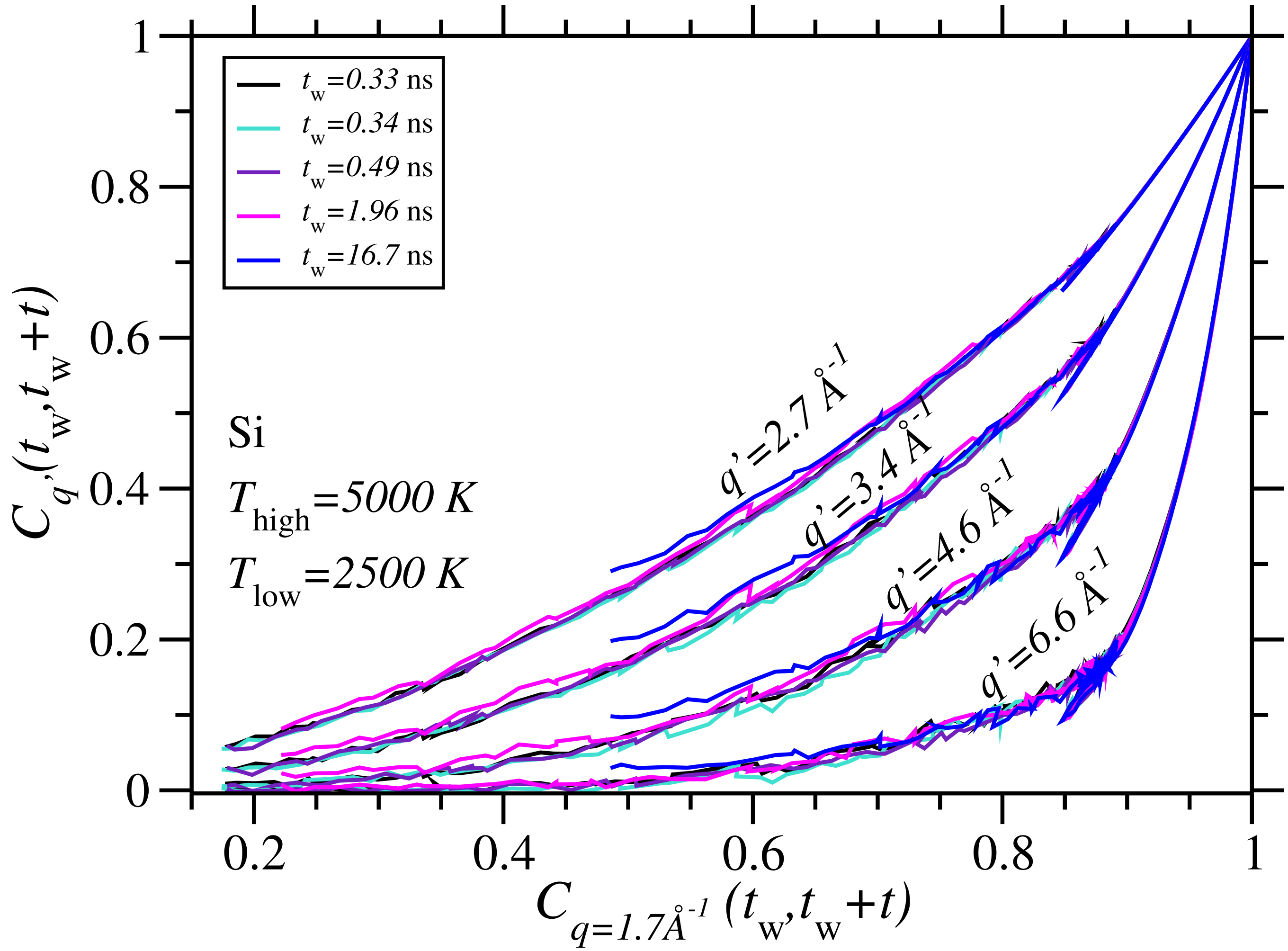
1
0.8
0.6
0.4
0.2
0
$C_q(t_w, t_w+t)$
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
$t/\tau_q(t_w)$
t_w=0 ns
t_w=16.7 ns
Si
q=1.7 Å^{-1}
T_{high}=5000 K T_{low}=2500 K



t_w=0.33 ns
t_w=16.7 ns
Si
q=1.7 Å^{-1}
T_{high}=5000 K T_{low}=2500 K
$C_q(t_w,t_w+t)$
$t/\tau_q(t_w)$
1
0.8
0.6
0.4
0.2
0
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}



t_w=0 ns
t_w=0.32 ns
t_w=16.7 ns
Si
T_{high}=5000 K
T_{low}=2500 K
q'=2.7 Å^{-1}
q'=3.4 Å^{-1}
q'=4.6 Å^{-1}
q'=6.6 Å^{-1}
$C_{q'}(t_w,t_w+t)$
$C_{q=1.7Å^{-1}}(t_w,t_w+t)$
0
0.2
0.4
0.6
0.8
1

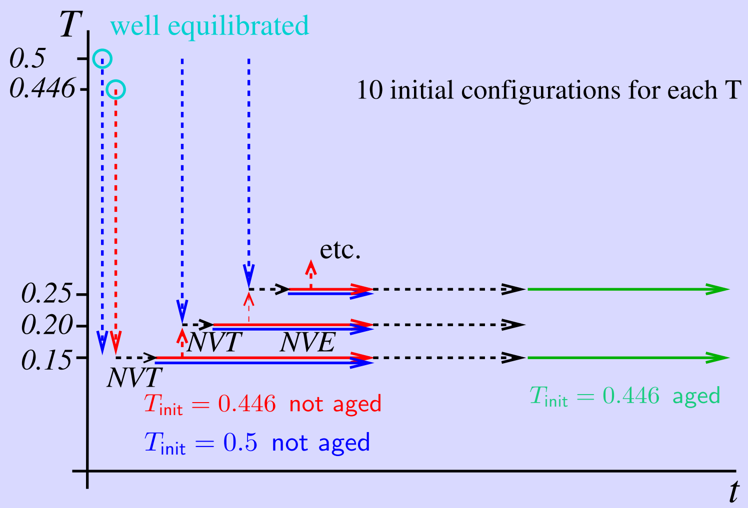


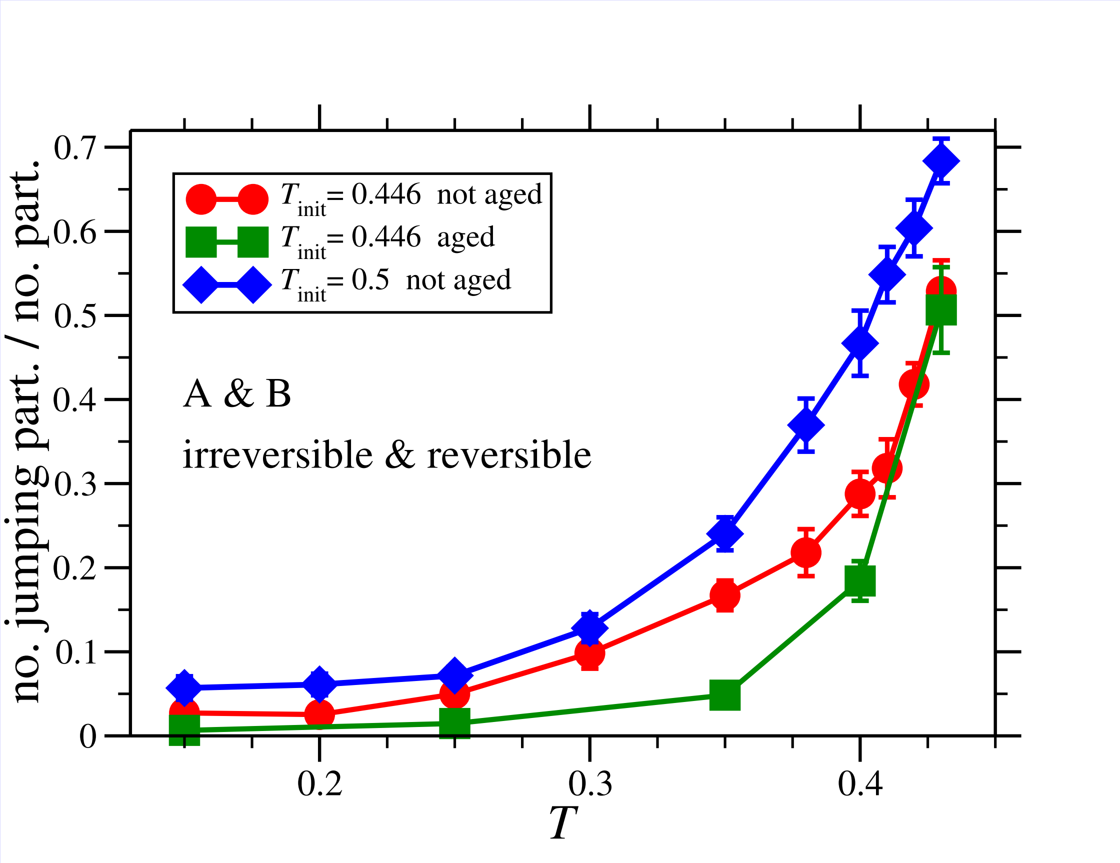
t_w=0.33 ns
t_w=0.34 ns
t_w=0.49 ns
t_w=1.96 ns
t_w=16.7 ns
Si
T_{high}=5000 K
T_{low}=2500 K
q'=2.7 Å^{-1}
q'=3.4 Å^{-1}
q'=4.6 Å^{-1}
q'=6.6 Å^{-1}
$C_{q'}(t_w,t_w+t)$
$C_{q=1.7Å^{-1}}(t_w,t_w+t)$
0
0.2
0.4
0.6
0.8
1

Time Scales

- one MD step: 0.02 time units, Ar: $3 \cdot 10^{-13}$s$\cdot 0.02 = 6$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

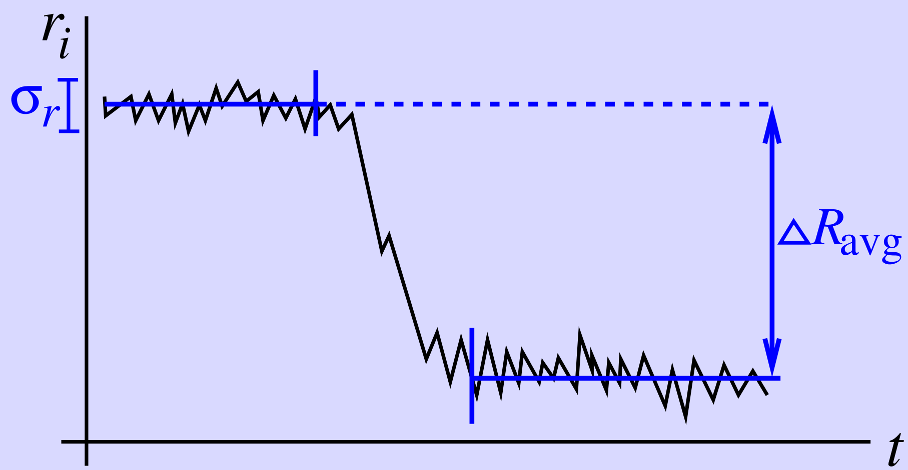


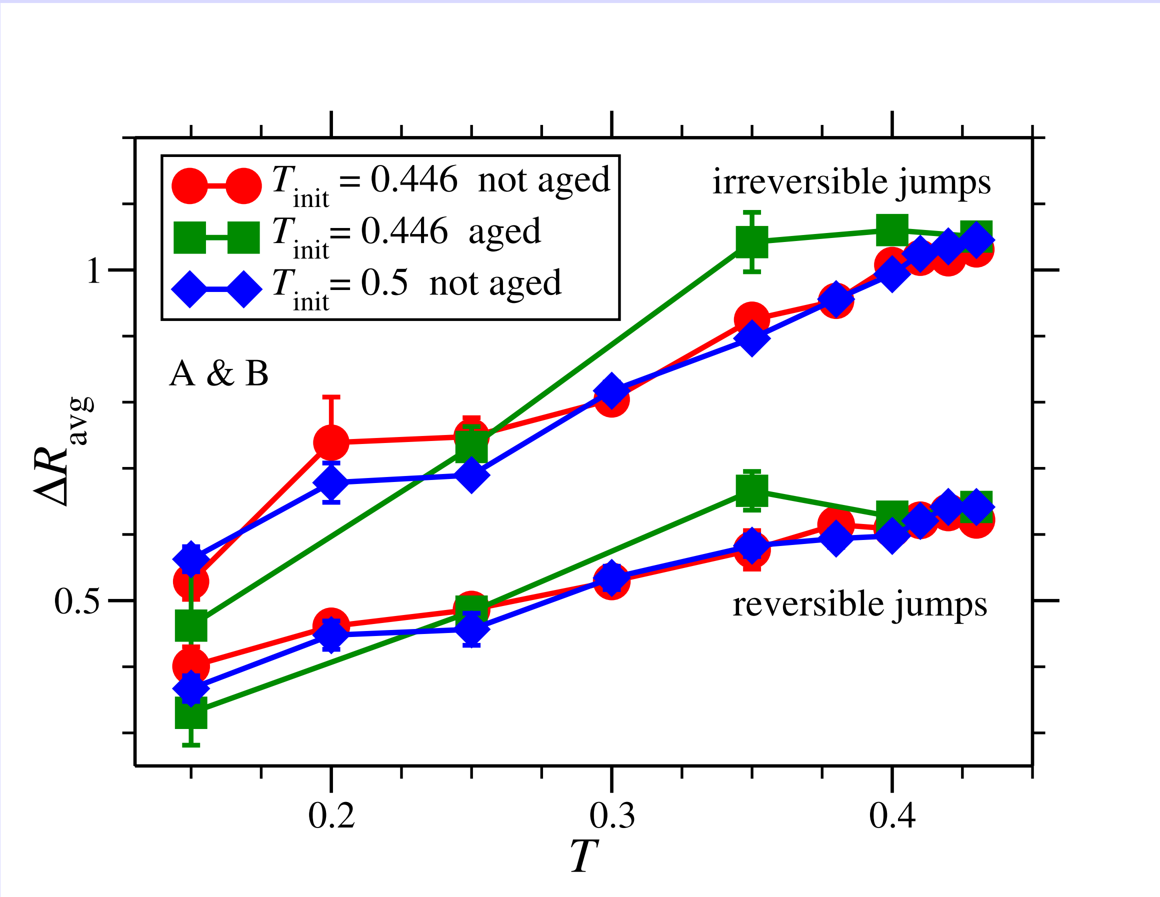


Number of Jump. Part

$\Longrightarrow$ history dependent

History Dependence

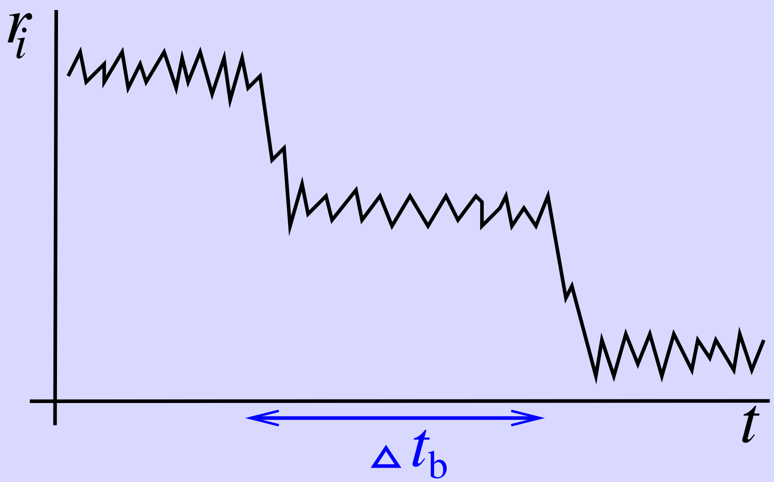


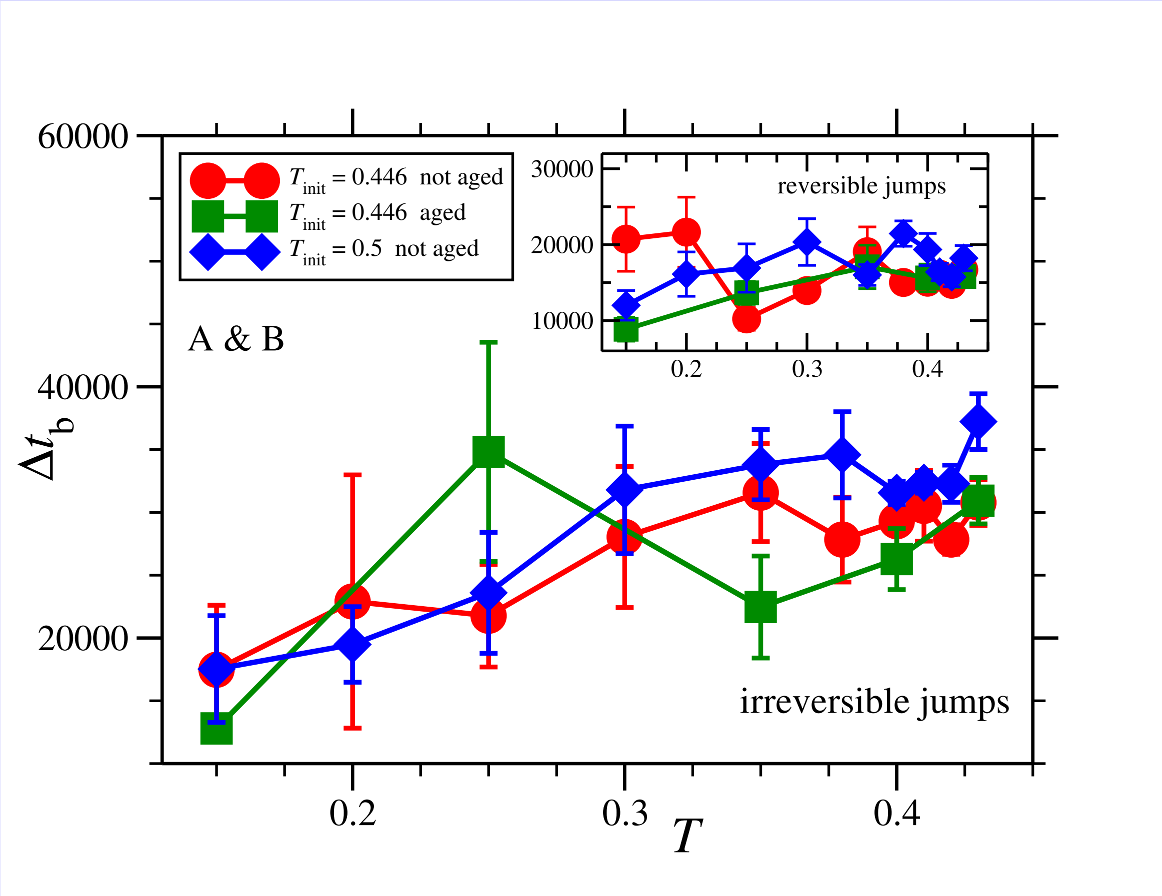


Jump Size

$\Longrightarrow$ history independent

History Dependence





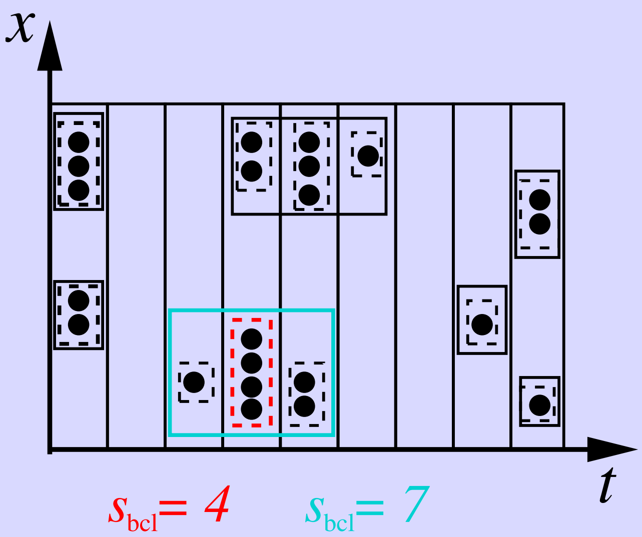
Time Between Jumps

$\Longrightarrow$ history independent

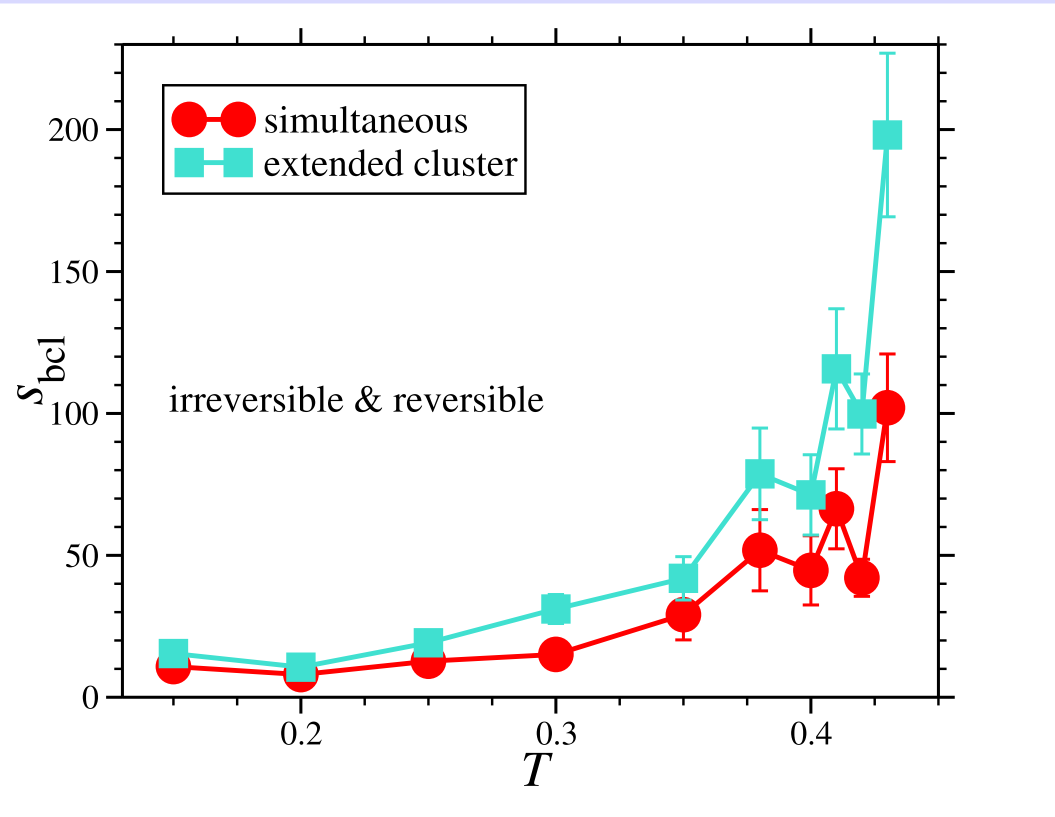
Summary: Jump Statistics

summary jump statistics

Most Cooperative Processes



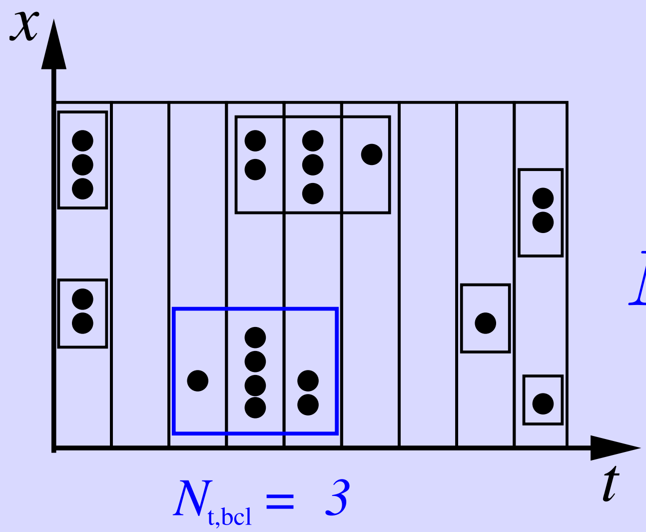
s_{bcl} = largest cluster size



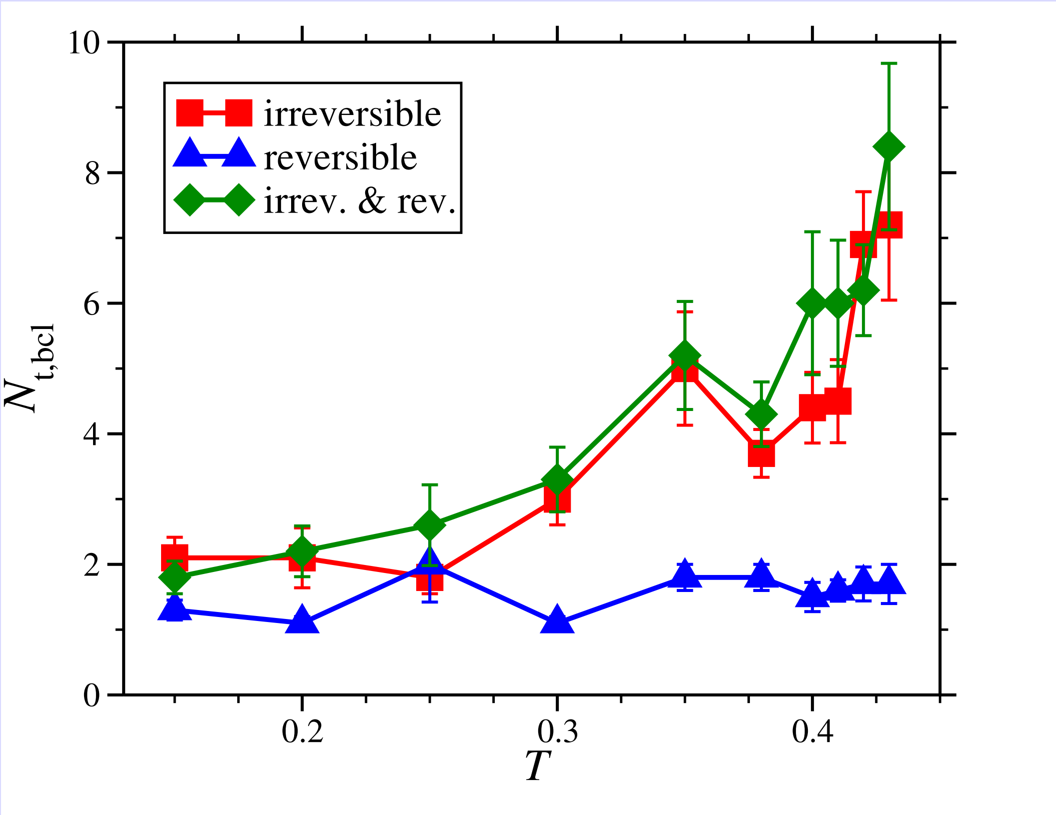
$\Longrightarrow$ highly correlated single particle jumps

- many particles

Most Cooperative Processes



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

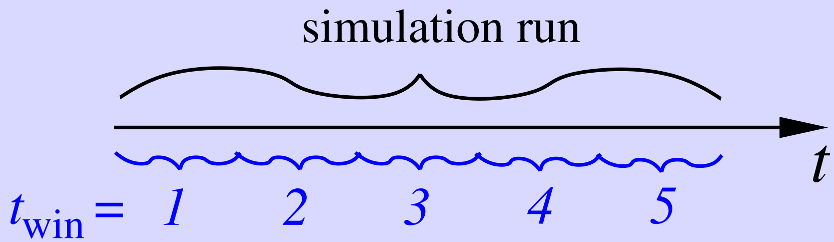


$\Longrightarrow$ highly correlated single particle jumps

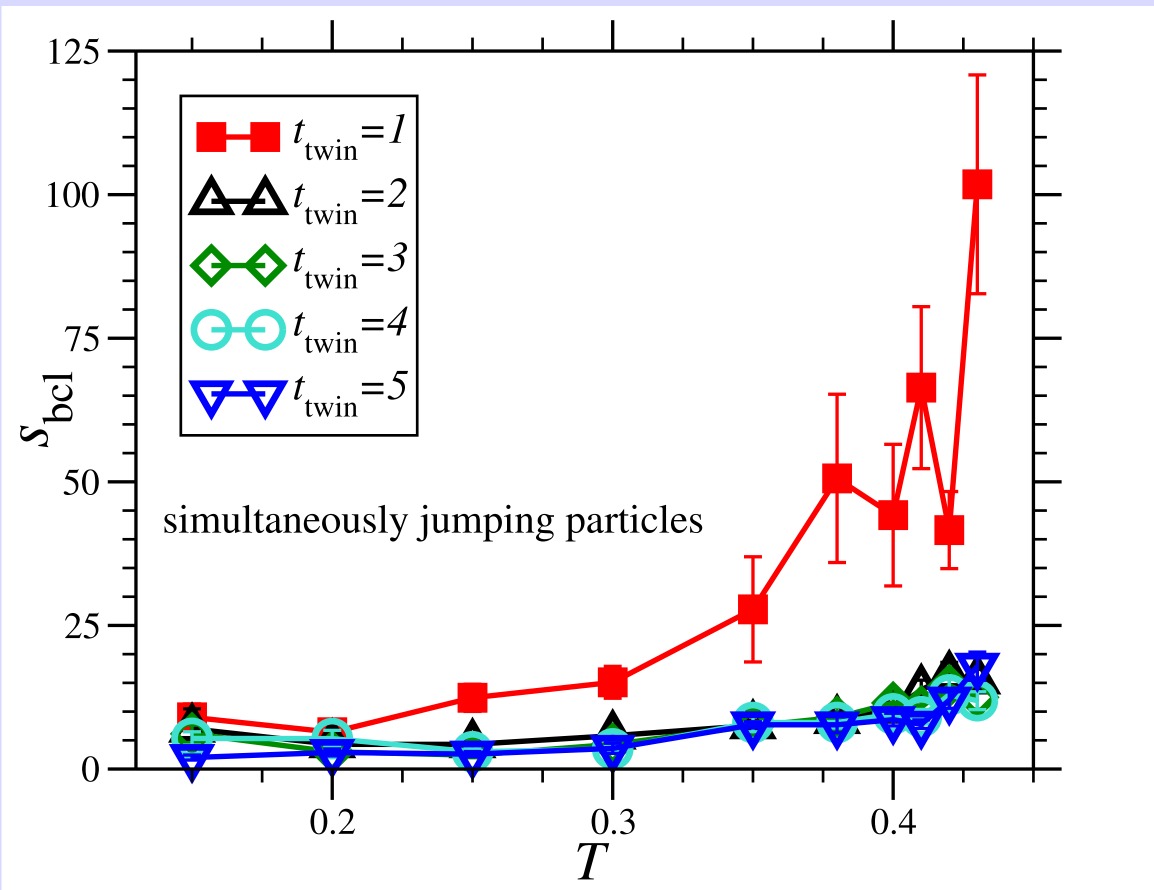
- many particles
- many time bins

(maximum = 125)

History Dependence



s_{bcl} = largest cluster size

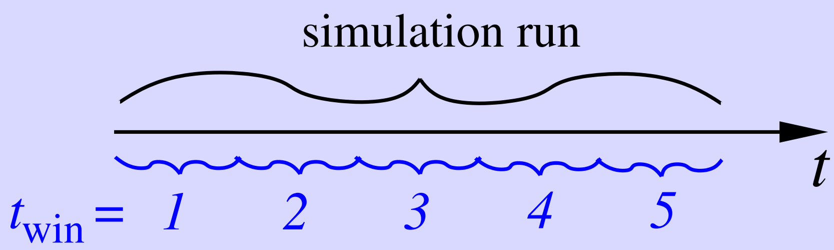


$\Longrightarrow$ aging dependent

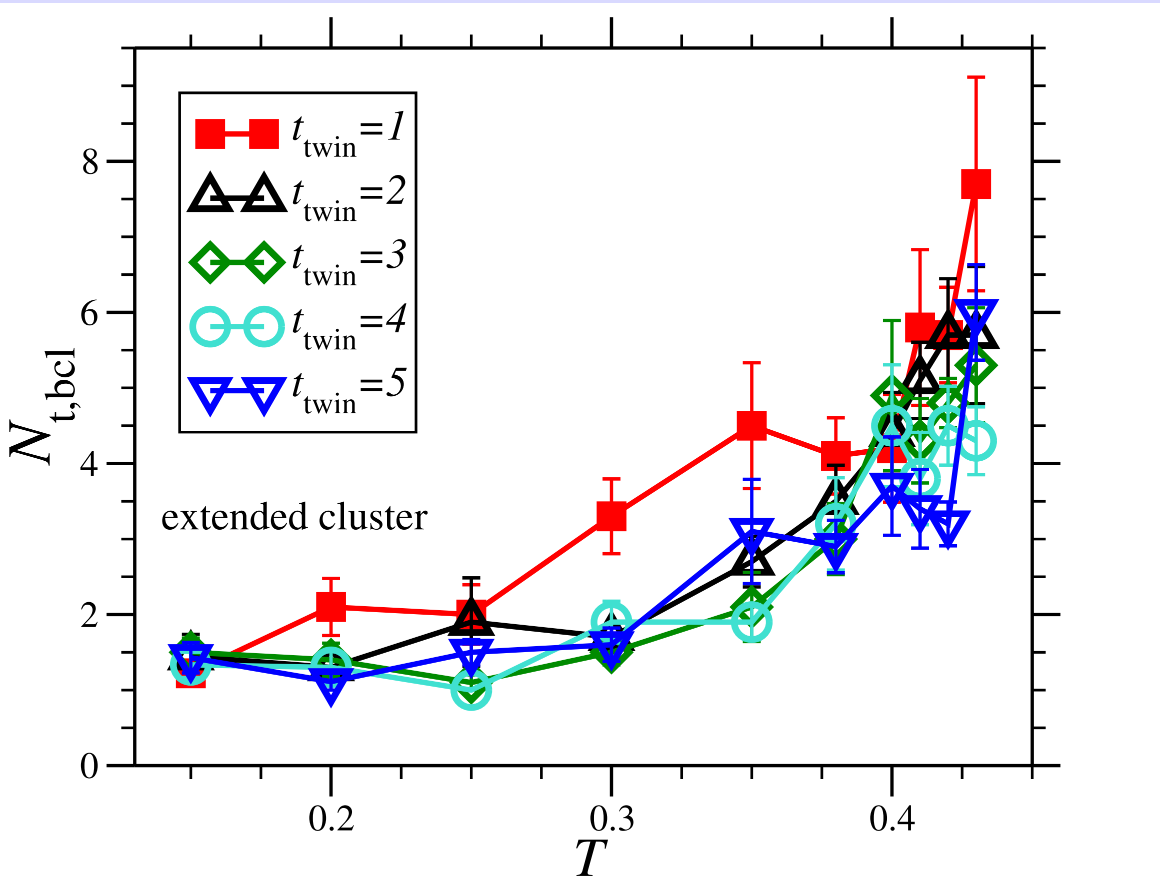
- 1st t-window:
  highly cooperative
- 2nd - 5th t-window:
  same, cooperative

s_{bcl} extended cluster

History Dependence



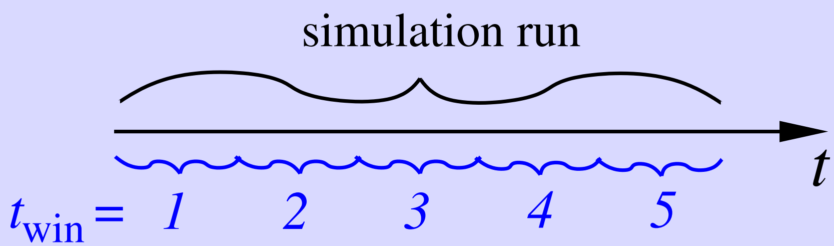
$N_{\mathrm{t,bcl}}$ = no. of t-bins of largest cluster

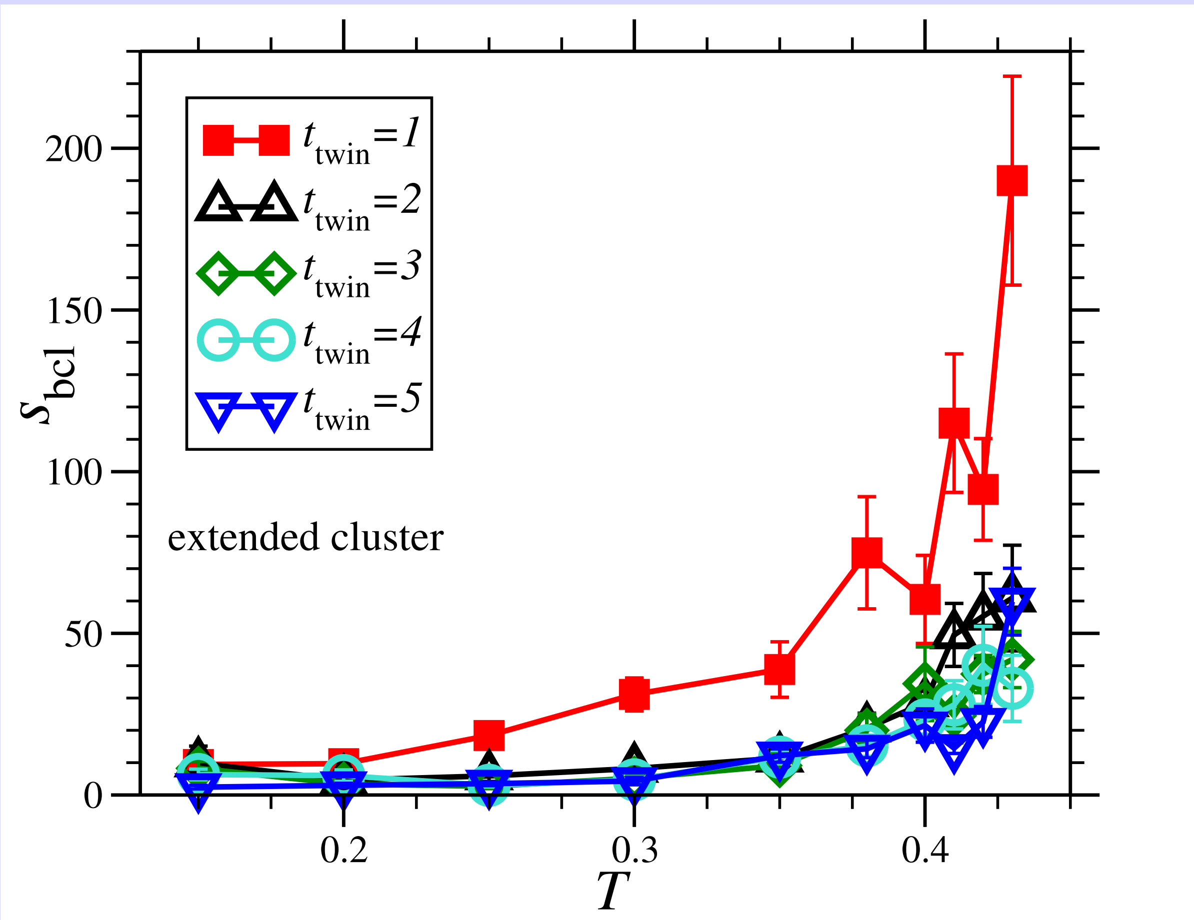


⟹ less aging dependent

⟹ highly cooperative

History Dependence

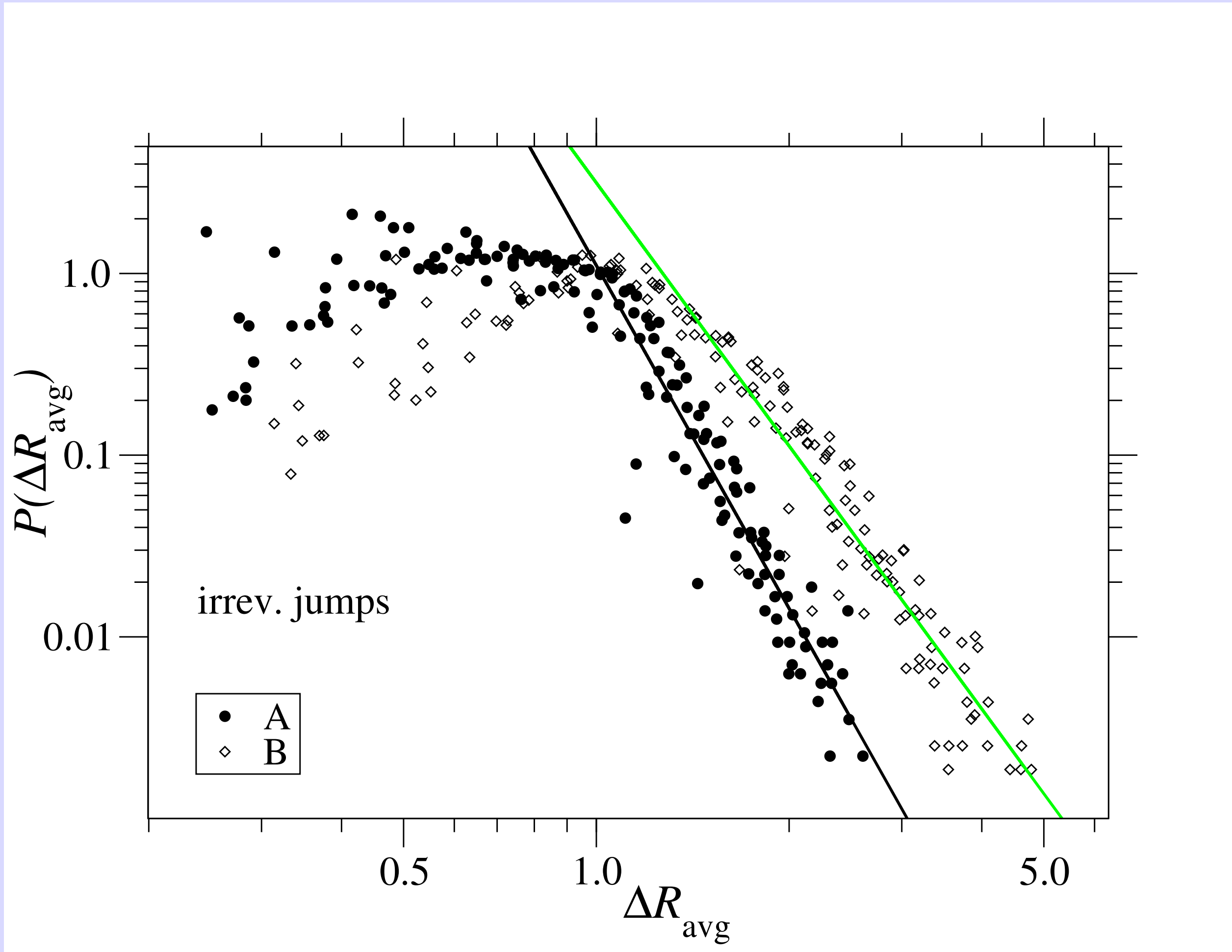




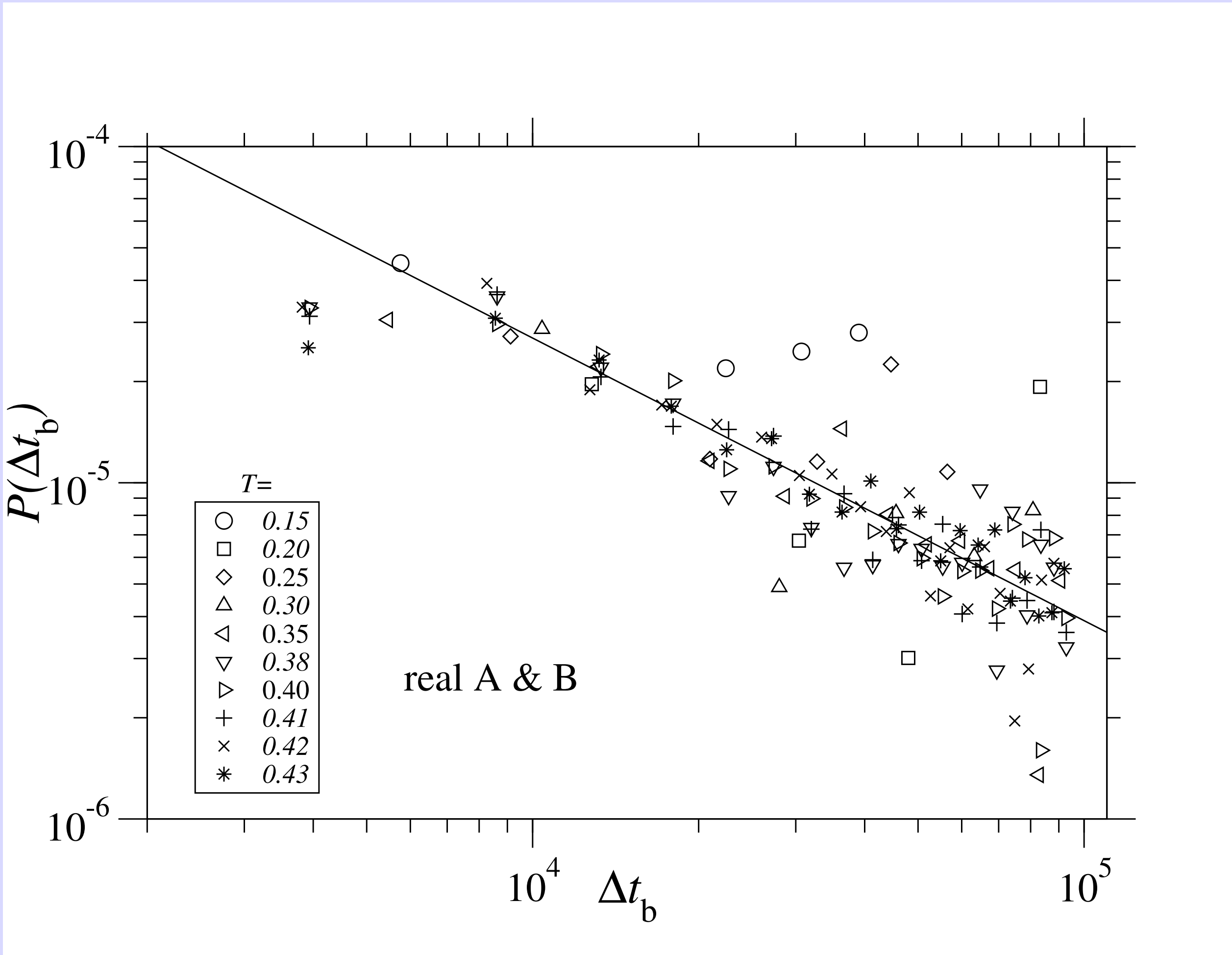
$\Longrightarrow$ aging dependent

- 1st t-window:
  highly cooperative
- 2nd - 5th t-window:
  same, cooperative

s_{bcl} simult. jump.



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



slopes -0.84 $\longrightarrow$ subdiffusive