Computer Simulation of Glasses: Jumps and Self-Organized Criticality

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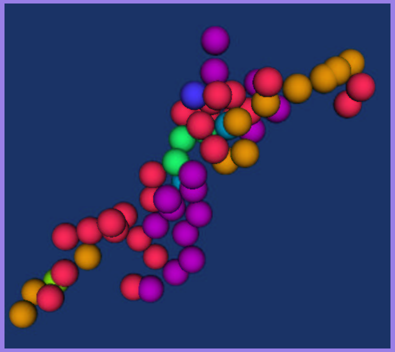
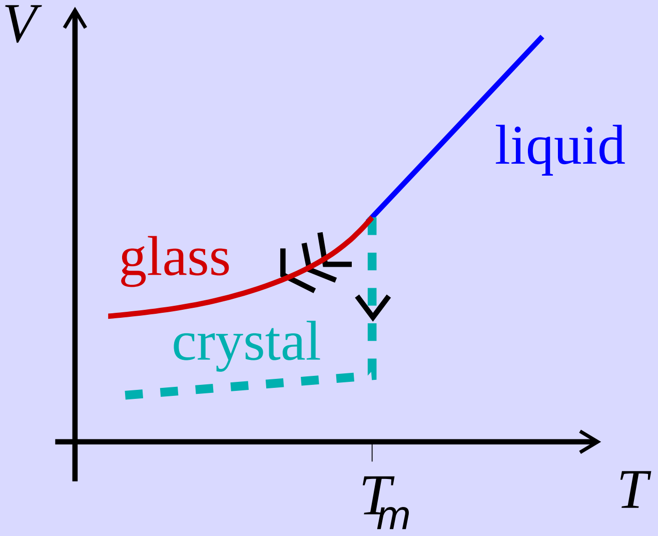


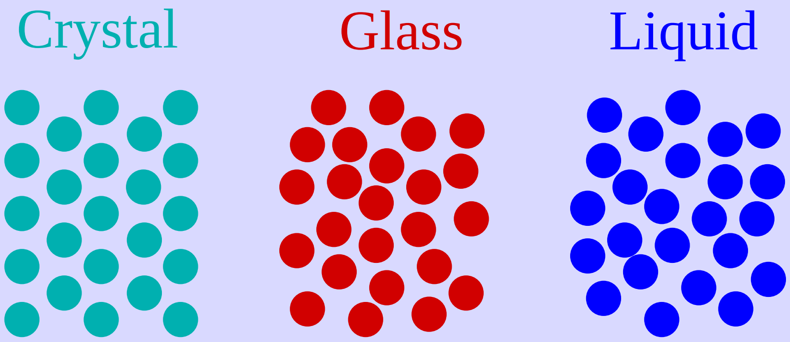
Thanks: E. A. Baker, A. Zippelius, K. Binder, and J. Horbach

Introduction



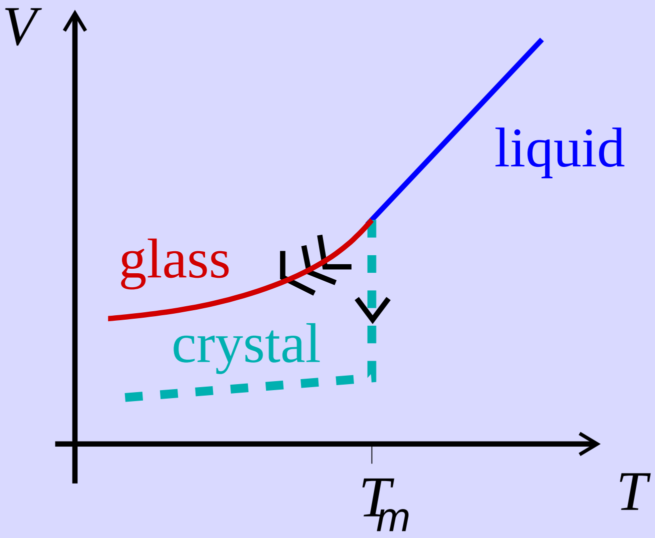
Glass:

→ system falls out of equilibrium



Structure: discordered

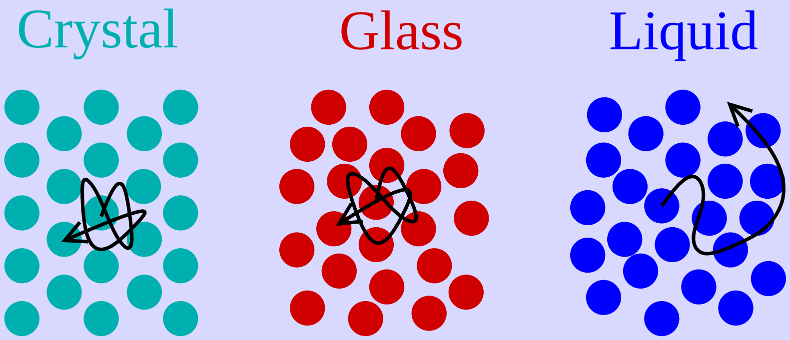
Introduction



Glass:

⟶ system falls

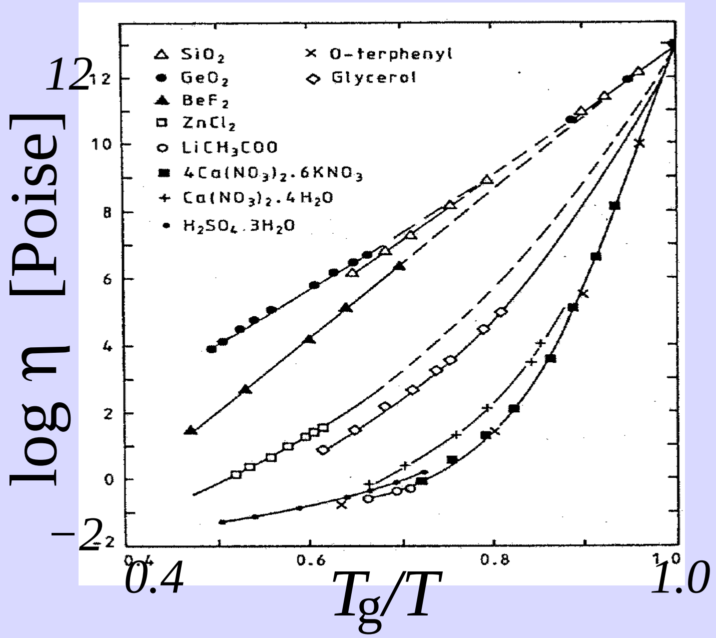
out of equilibrium



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

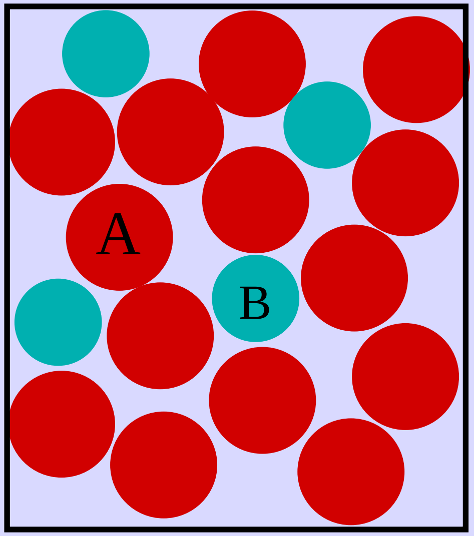
Binary Lennard-Jones System

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

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

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

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



800 A and 200 B

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

Initialize:

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

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

three dimensions

↓

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

↓

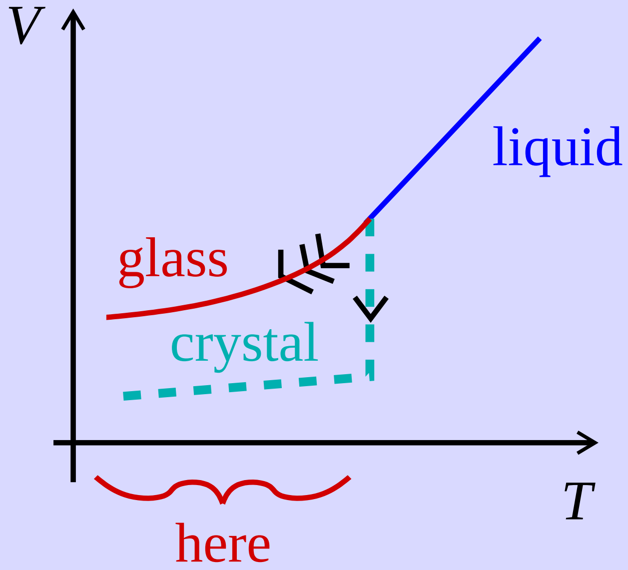
$\vec{x}_i(t_0+2\Delta t), \ \vec{v}_i(t_0+2\Delta t), \ \vec{a}_i(t_0+2\Delta t)$

↓ etc.

↓ = Iteration Step:

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

Simulations



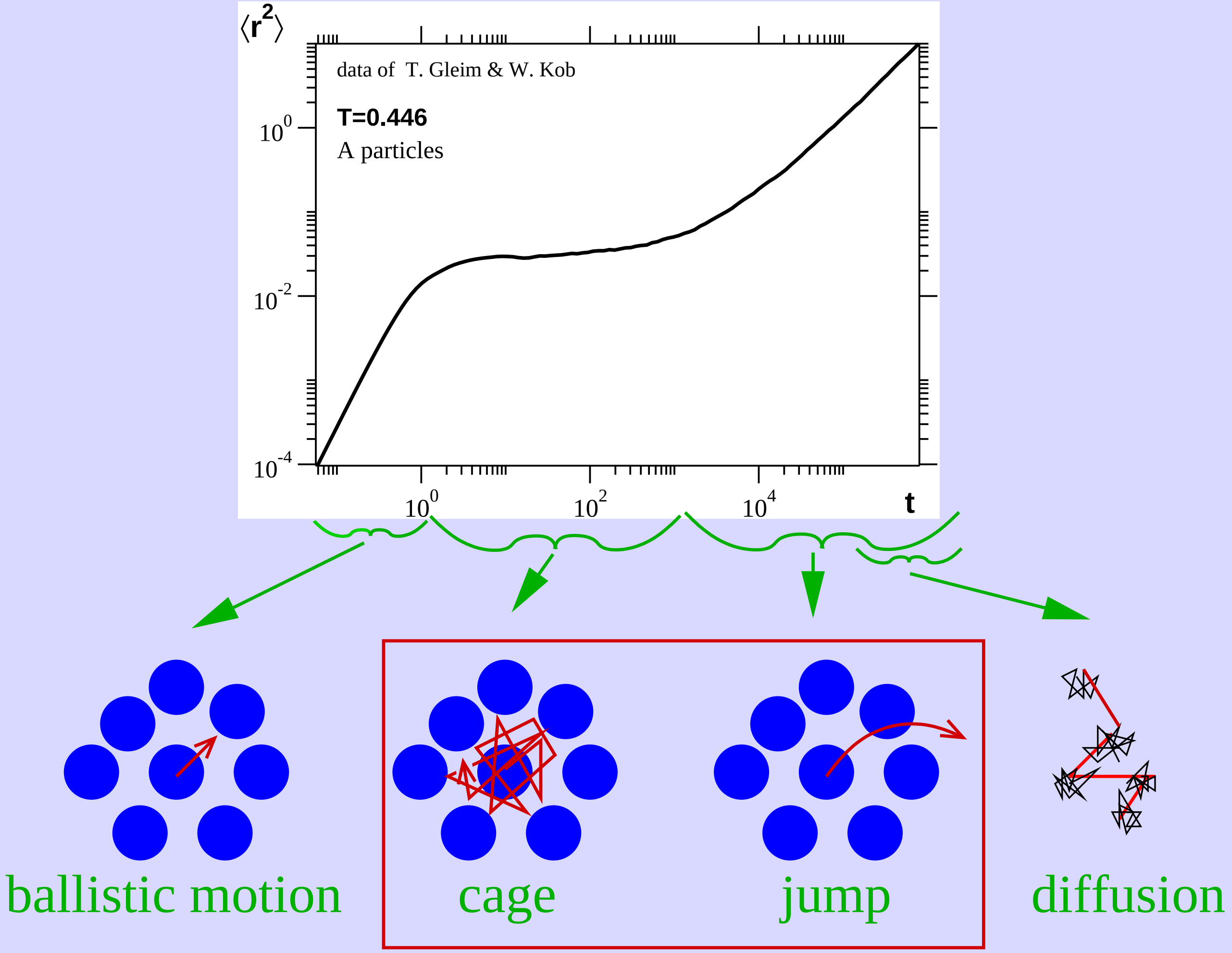
Dynamics

below glass transition:

$T = 0.15 - 0.43 \qquad T_{\mathsf{c}} = 0.435$

Cage-Picture

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



ballistic motion

cage

jump

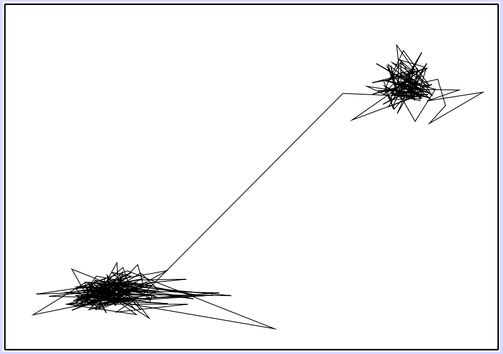
diffusion

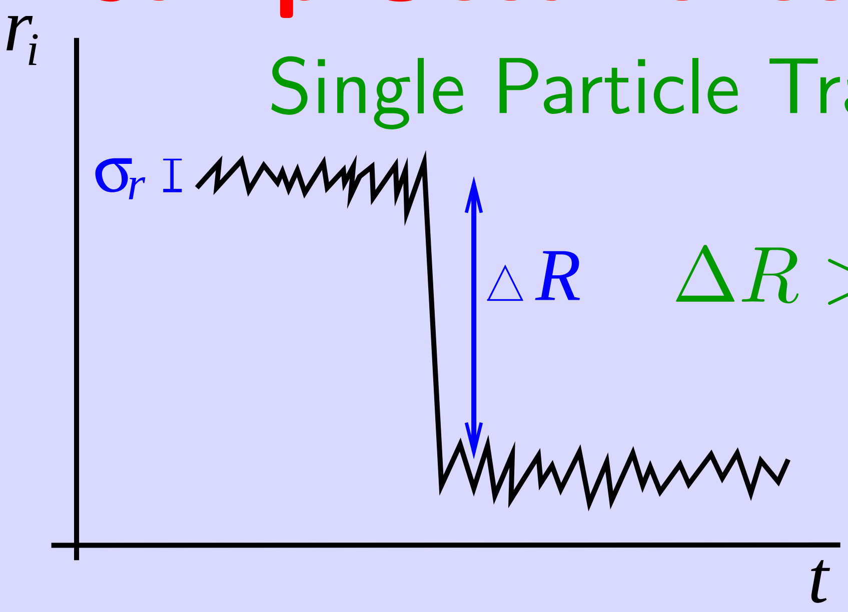
$\langle r^2 \rangle \sim t^2$

here

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

Definition: Jump Occurrence



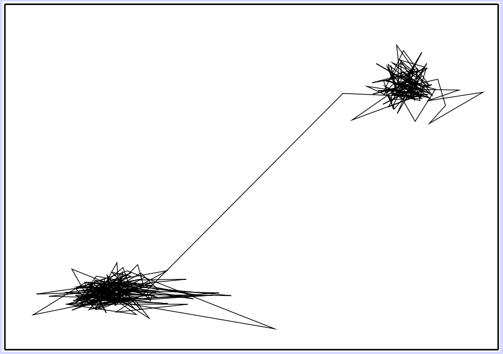


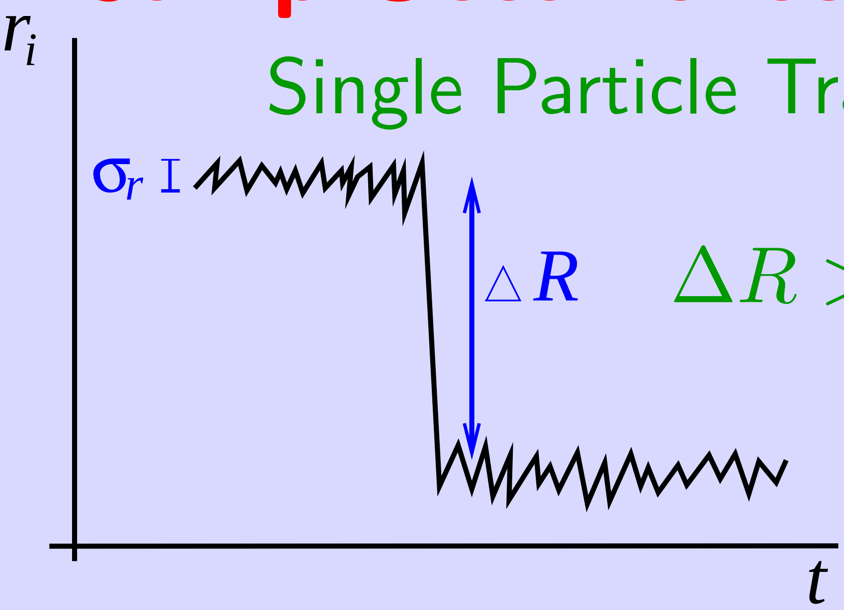
Single Particle Trajectory

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

Definition: Jump Occurrence

Single Particle Trajectory

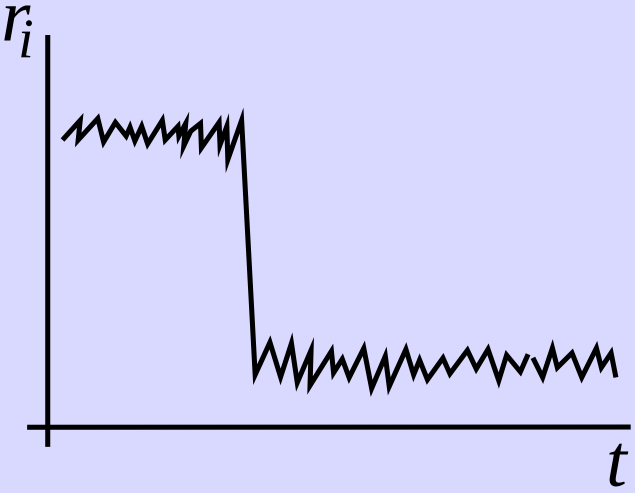




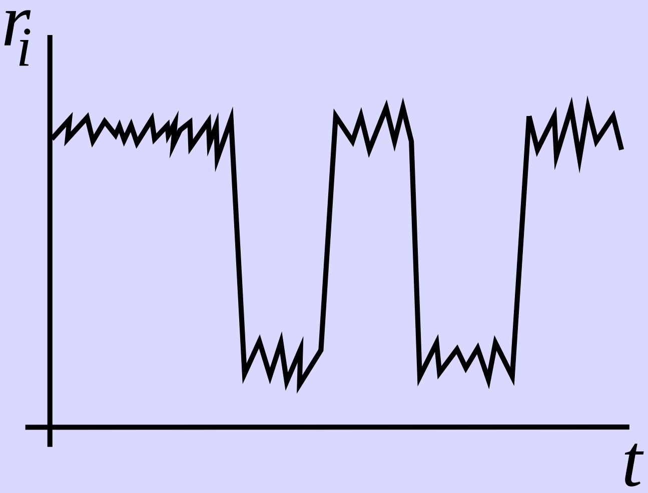
$$\Delta R > \sqrt{20}\,\sigma_r$$

Definition: Jump Type

Irreversible Jump



Reversible Jump



Outline

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- Correlated Single Particle Jumps
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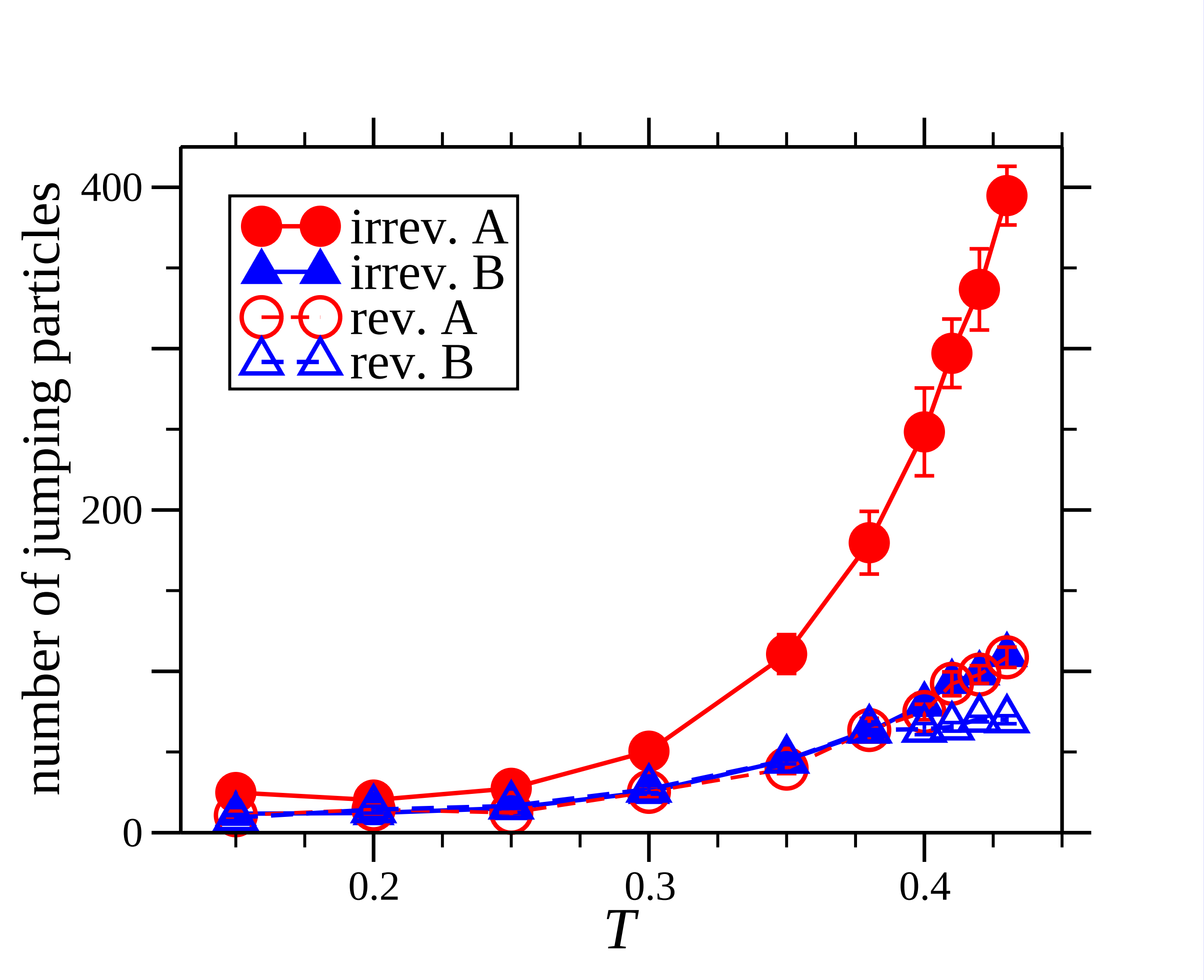
Number of Jumping Particles



$\Longrightarrow$ 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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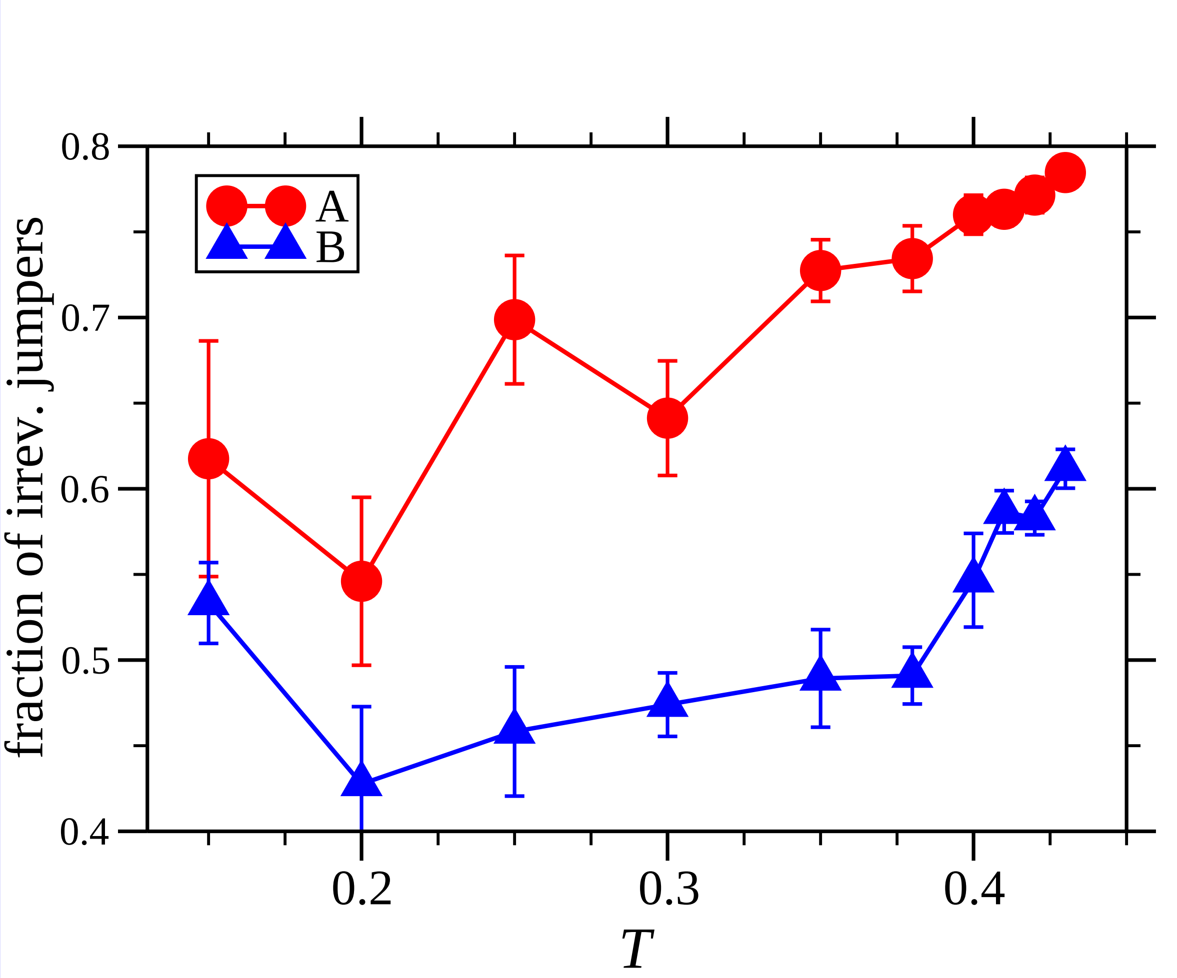
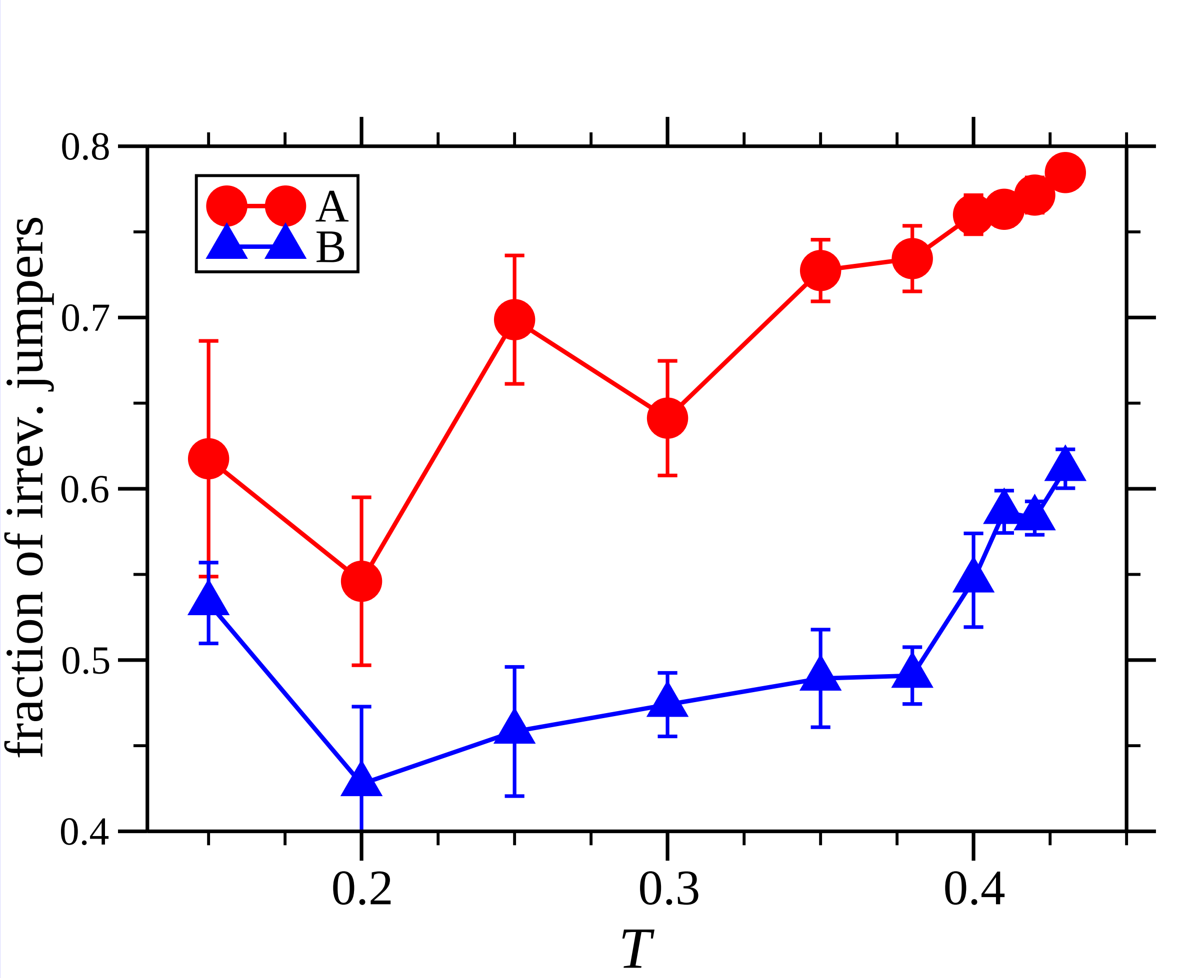


$\Longrightarrow$ fraction of irrev. jumpers increases with increasing T

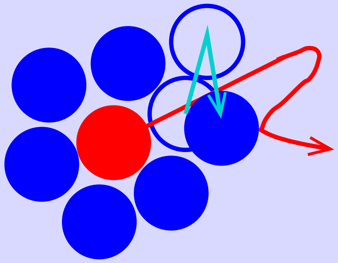
Fraction of Irreversibly Jumping Particles

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

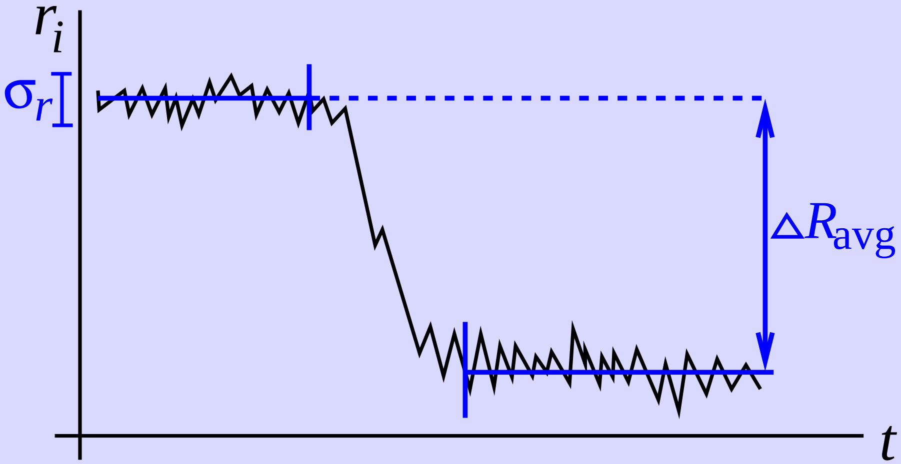


$\Longrightarrow$ fraction of irrev. jumpers increases with increasing T

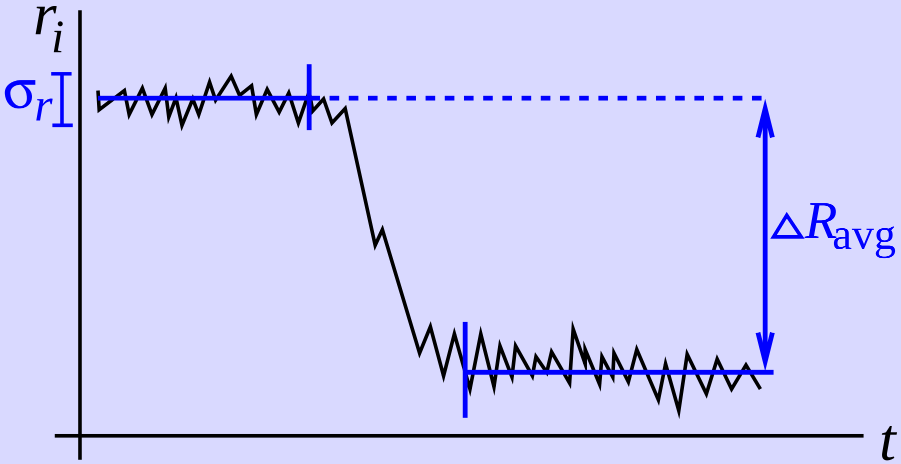
interpretation: door closing

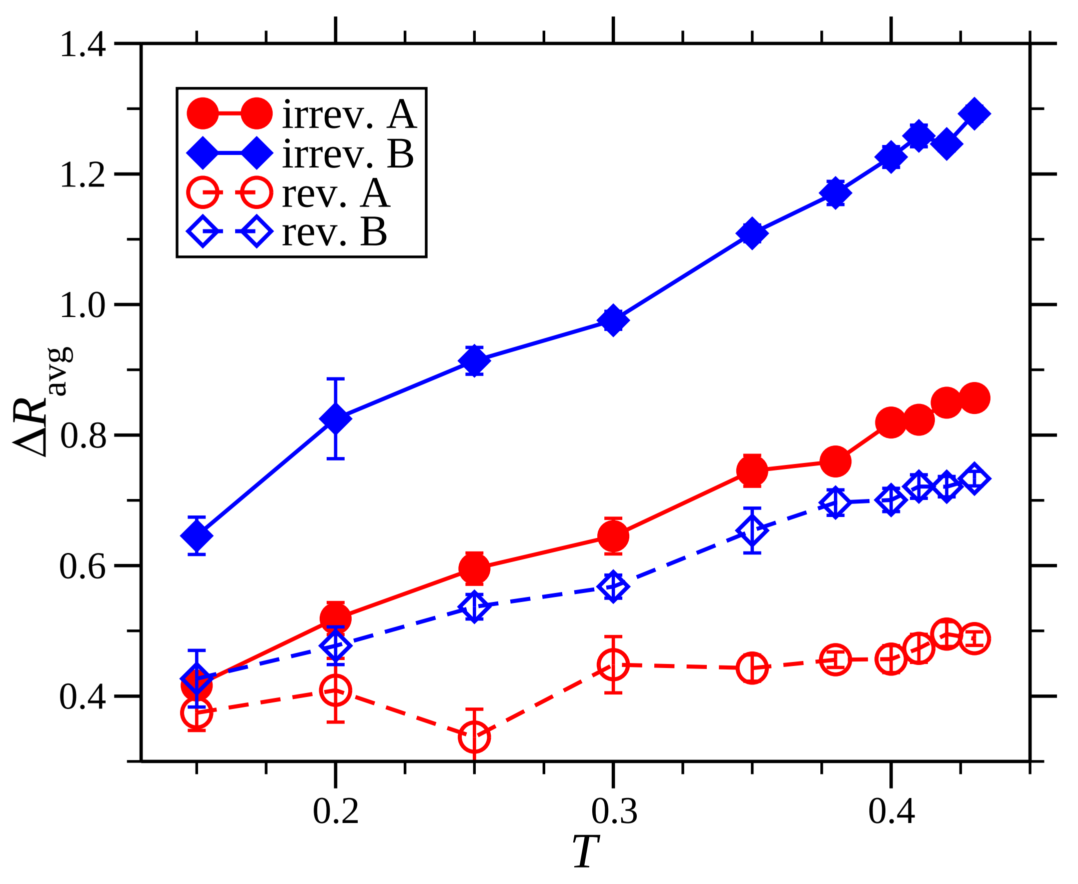


Jump Size



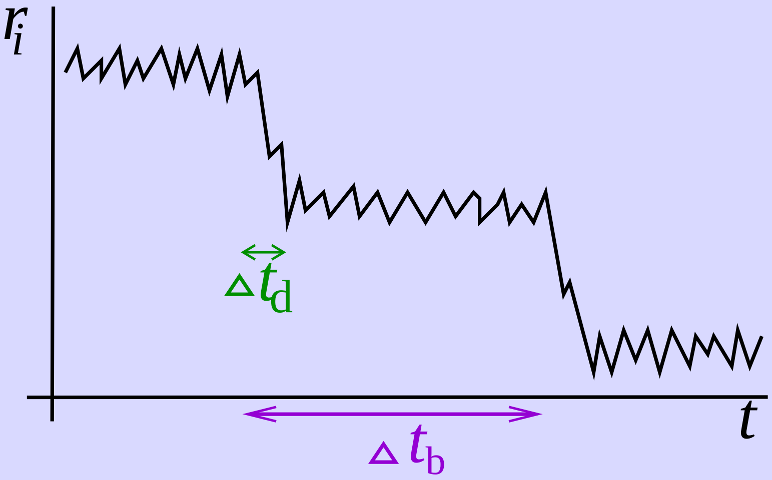
Jump Size



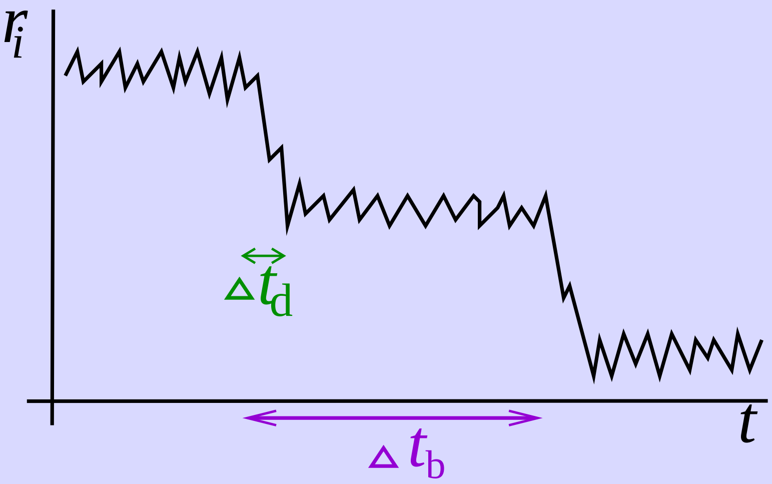


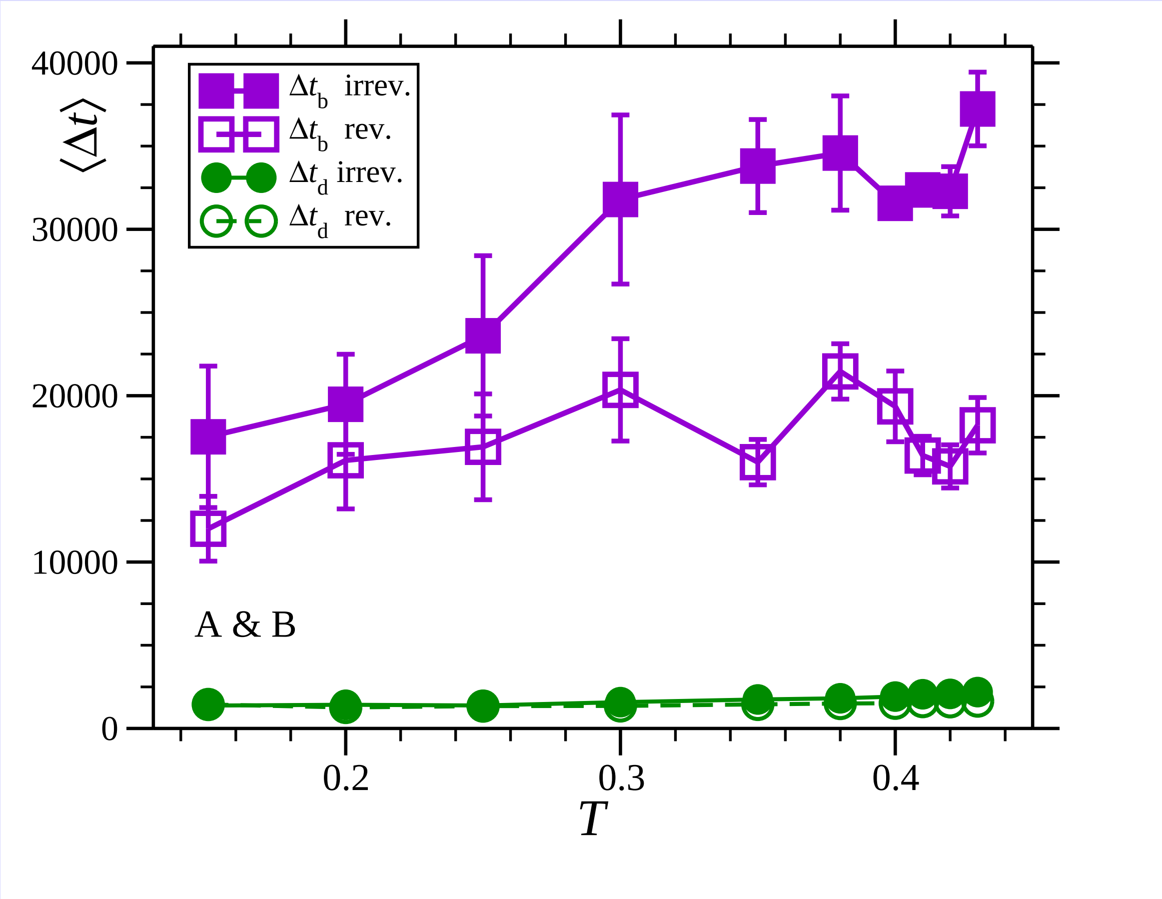
- $\Longrightarrow$ increasing with increasing T
- $\Longrightarrow$ (smaller) B-particles jump farther
- $\Longrightarrow$ irreversible jumps farther

Time Scale


r_i
$\overset{\leftrightarrow}{\vartriangle t_{\mathrm{d}}}$
t
$\vartriangle t_{\mathrm{b}}$

Time Scale





$\Longrightarrow \Delta t_\mathrm{b} \gg \Delta t_\mathrm{d}$

$\Longrightarrow \Delta t_\mathrm{b}$ independent of temperature

(whole simulation 10^5)

Time Scales Extra

Summary: Jump Statistics

At larger temperature relaxation:

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

Outline

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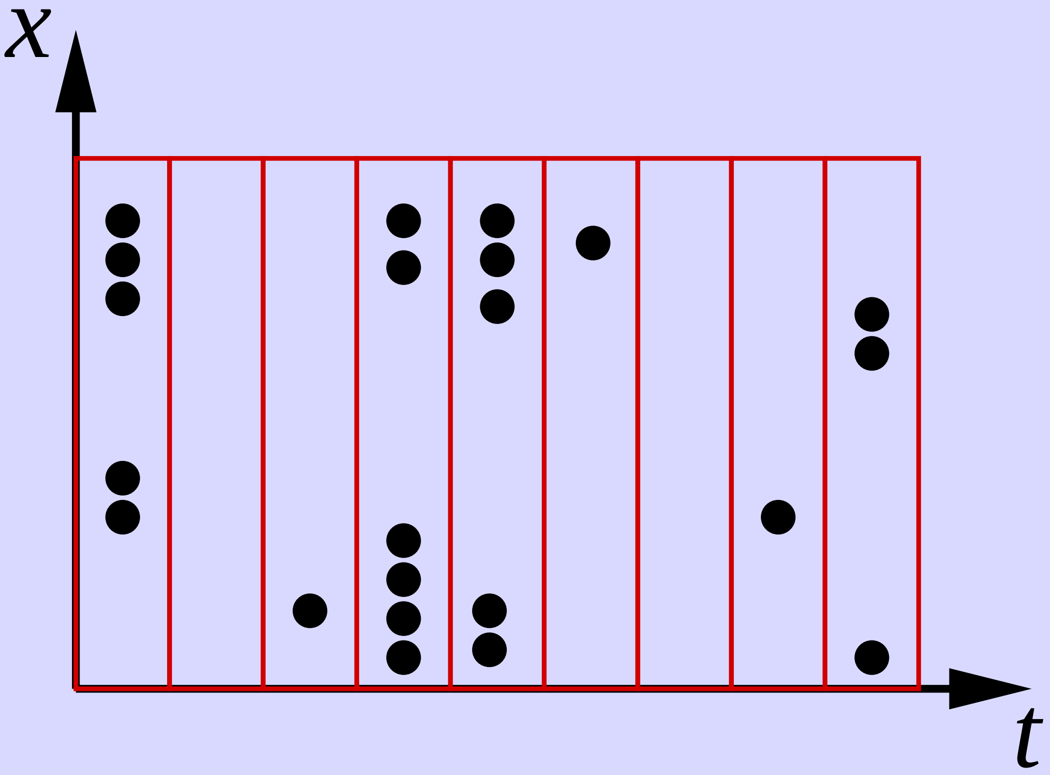
Simultaneously Jumping Particles

Definition: Correlated in Time & Space



Simultaneously Jumping Particles

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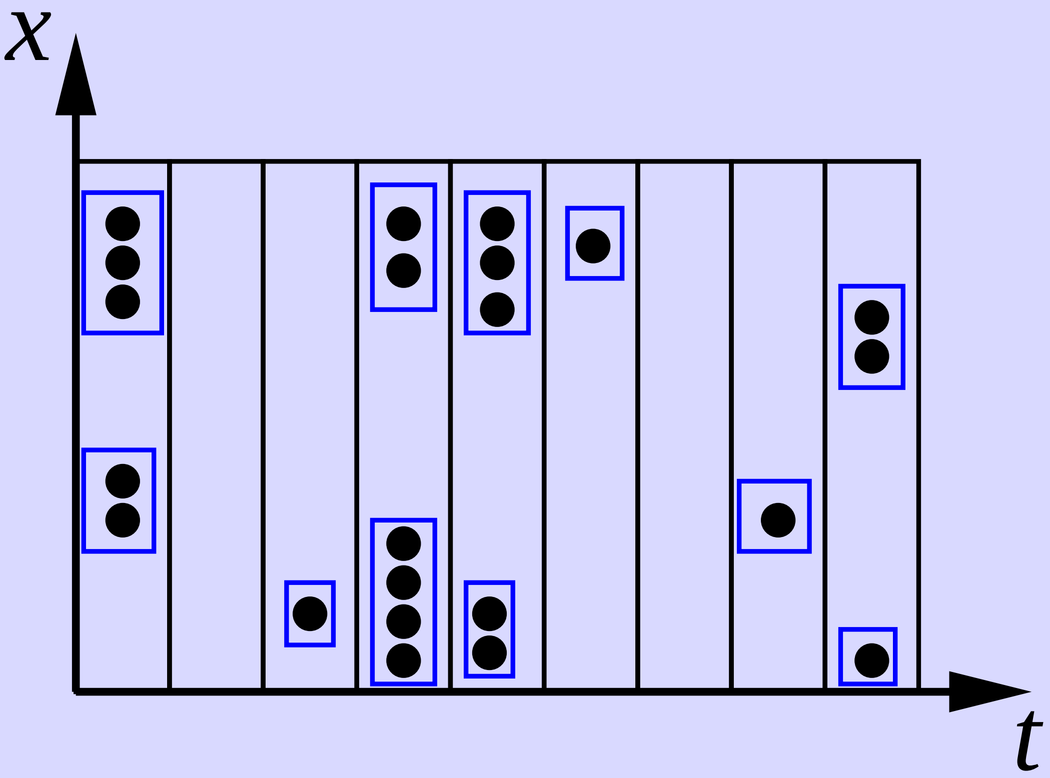
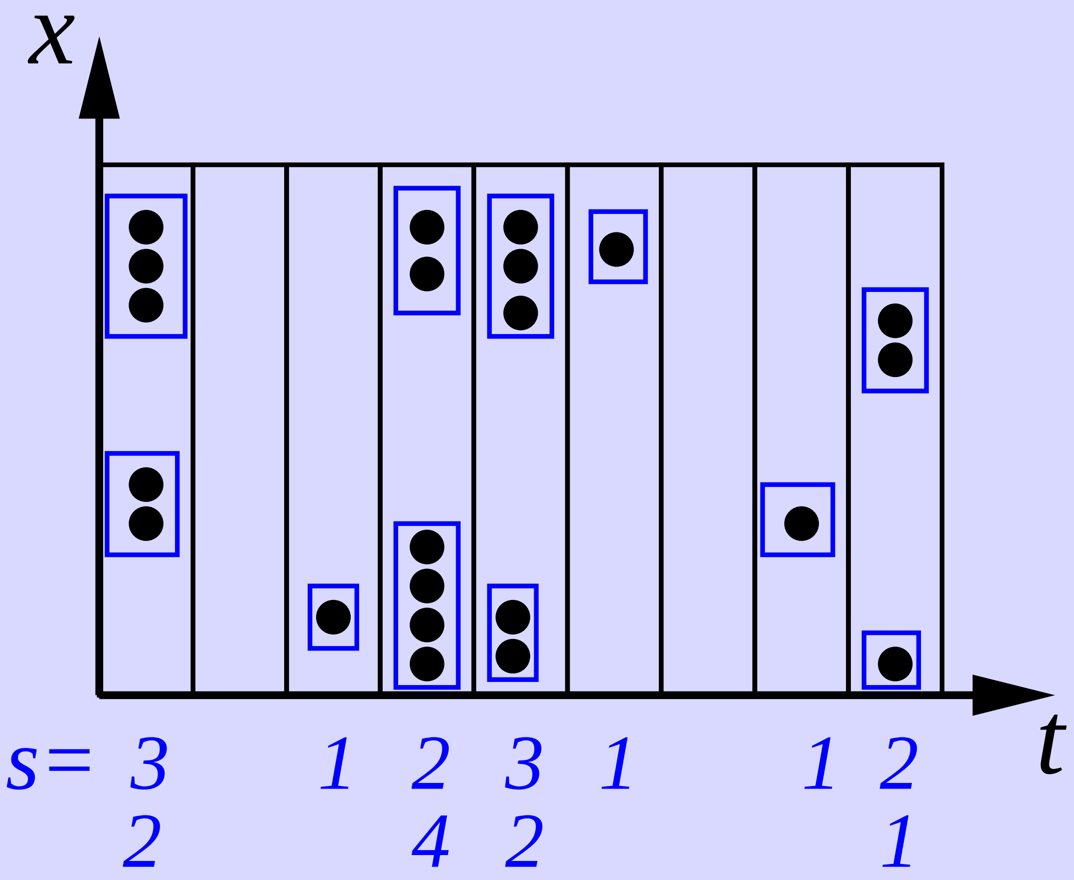


Cluster:

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

Simultaneously Jumping Particles

Cluster Size $=$ number of particles in cluster

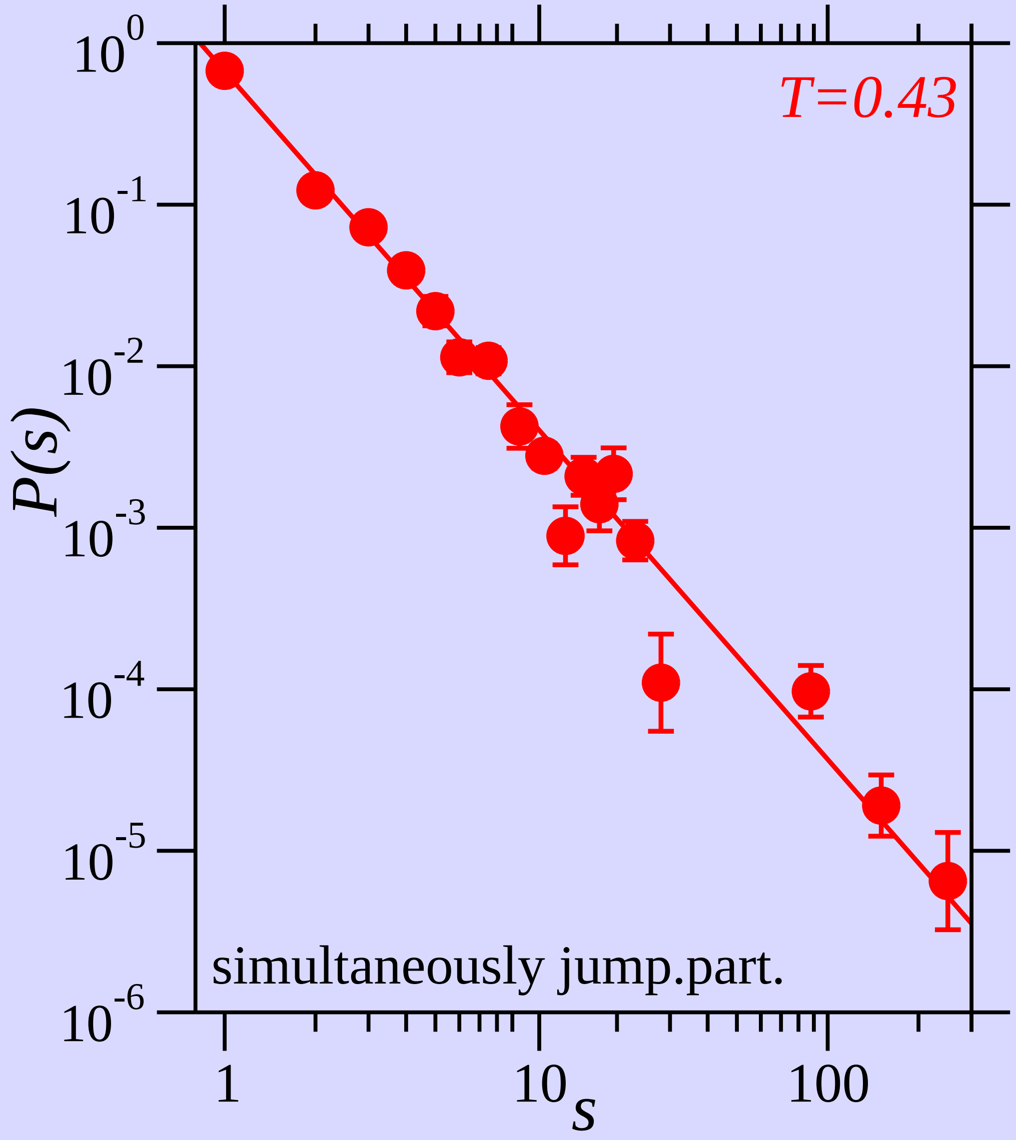


Cluster:

nearest neighbor connections

Cluster Size Distribution

of Simultaneously Jumping Particles



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

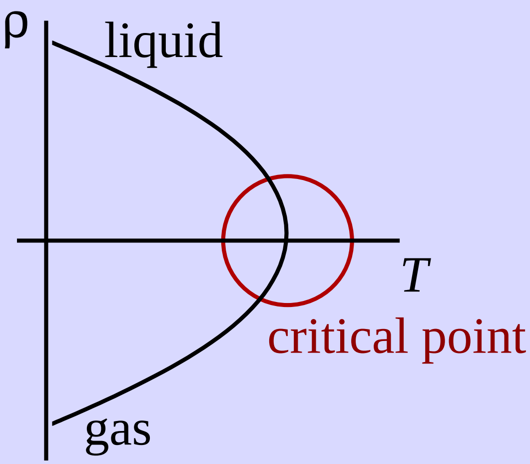
$$\Longrightarrow P(s) \sim s^{-\tau}$$

$$\tau = 1.89 \pm 0.03$$

$\Longrightarrow$ critical behavior

Critical Behavior *(Phase Transition)*

Example: Liquid ⟷ Gas



At Critical Point:

powerlaws ⟷ scale invariance

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

$$f(\underbrace{\lambda}_{\text{rescale x−axis}} x) = \lambda^{\alpha} x^{\alpha} = \underbrace{\lambda^{\alpha}}_{\text{rescale y−axis}} f(x)$$

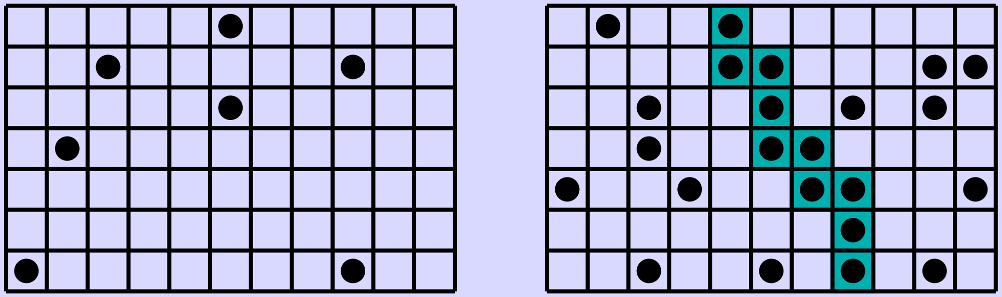
⟶ looks same from any distance

⟶ lack of specific length scale

⟶ large fluctuations

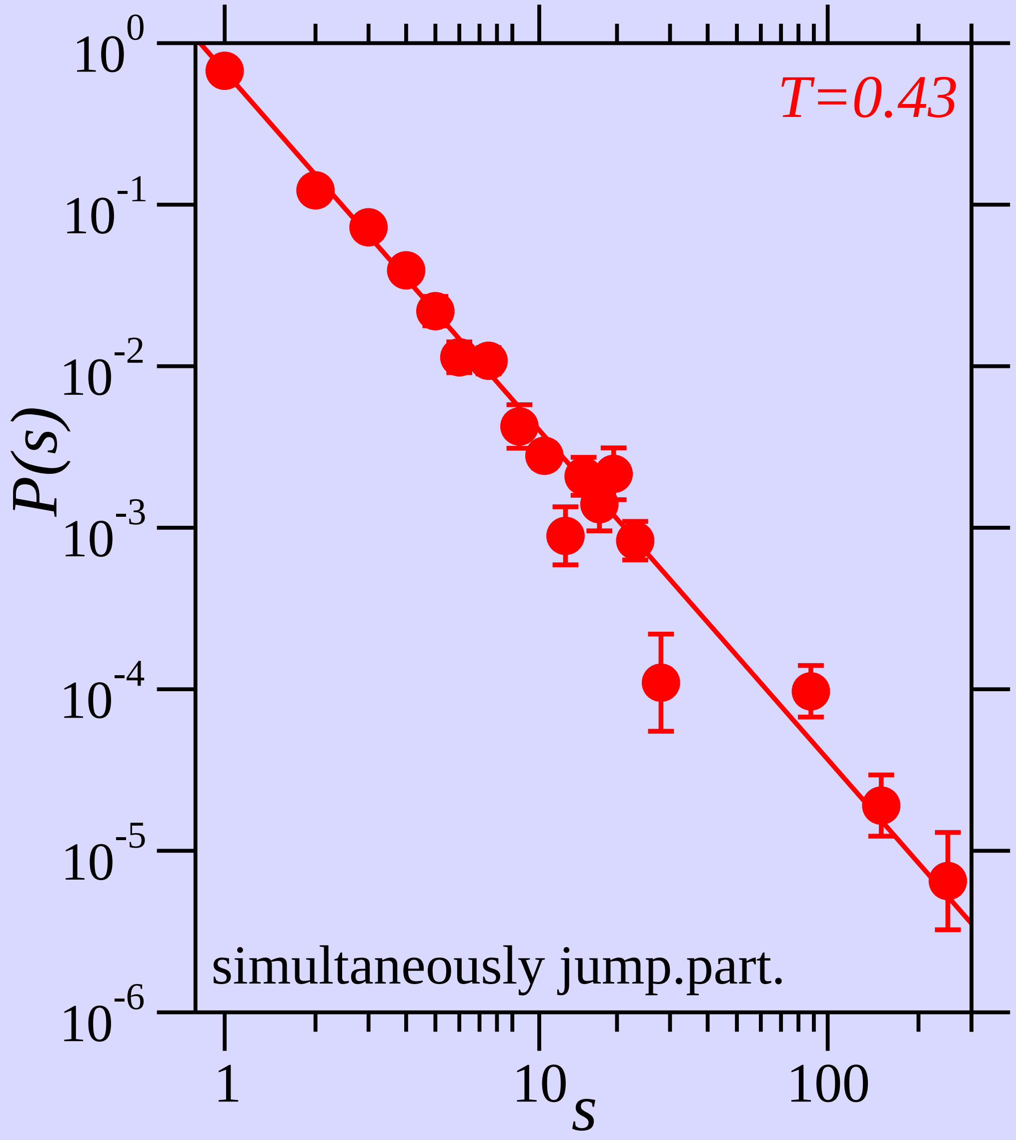
Other Examples:

- Magnet (Ising Model)
- Synchronization
- Percolation



Cluster Size Distribution

of Simultaneously Jumping Particles



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

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

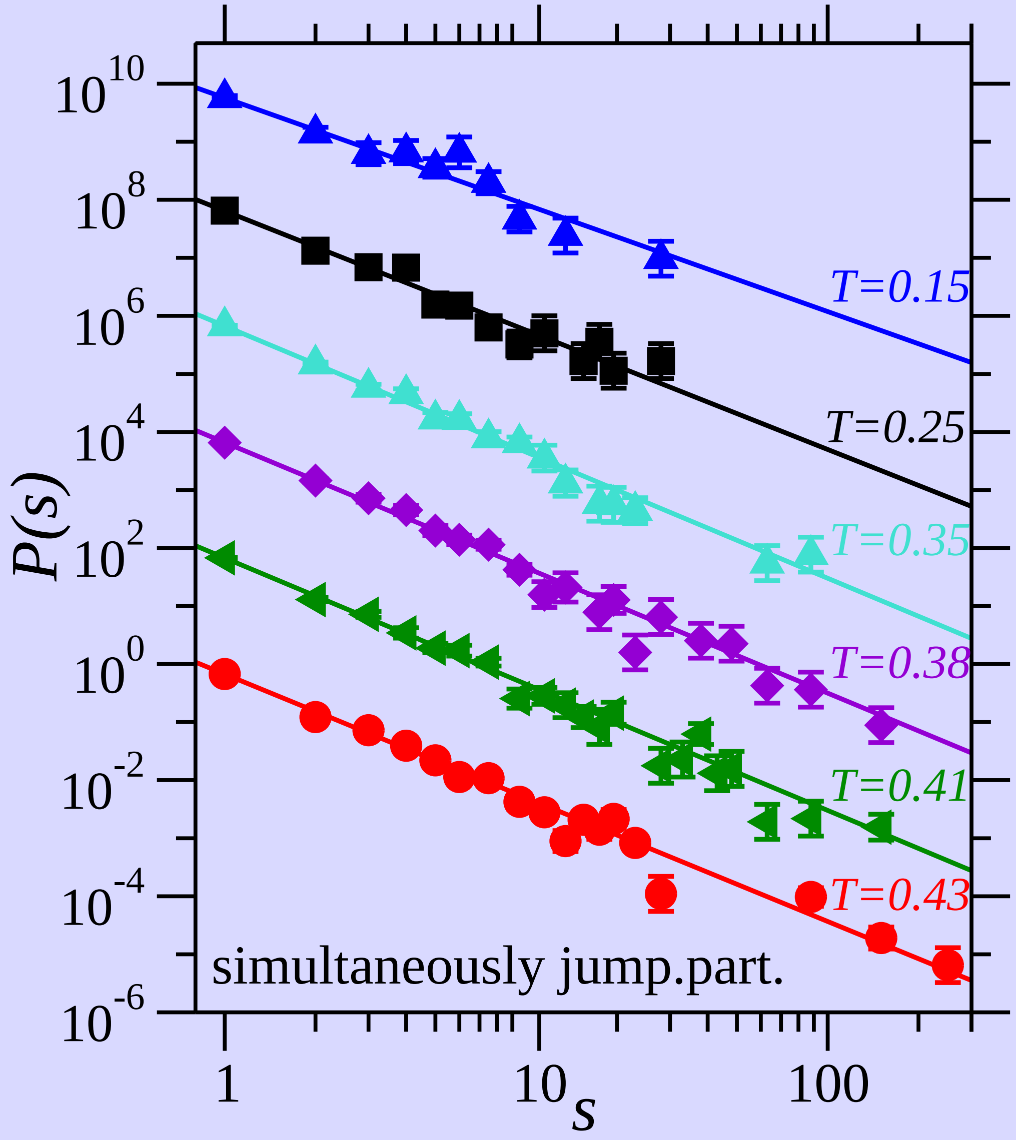
$$\tau = 1.89 \pm 0.03$$

$\Longrightarrow$ critical behavior

$\Longrightarrow$ Percolation?

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 paramters

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

Examples:

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

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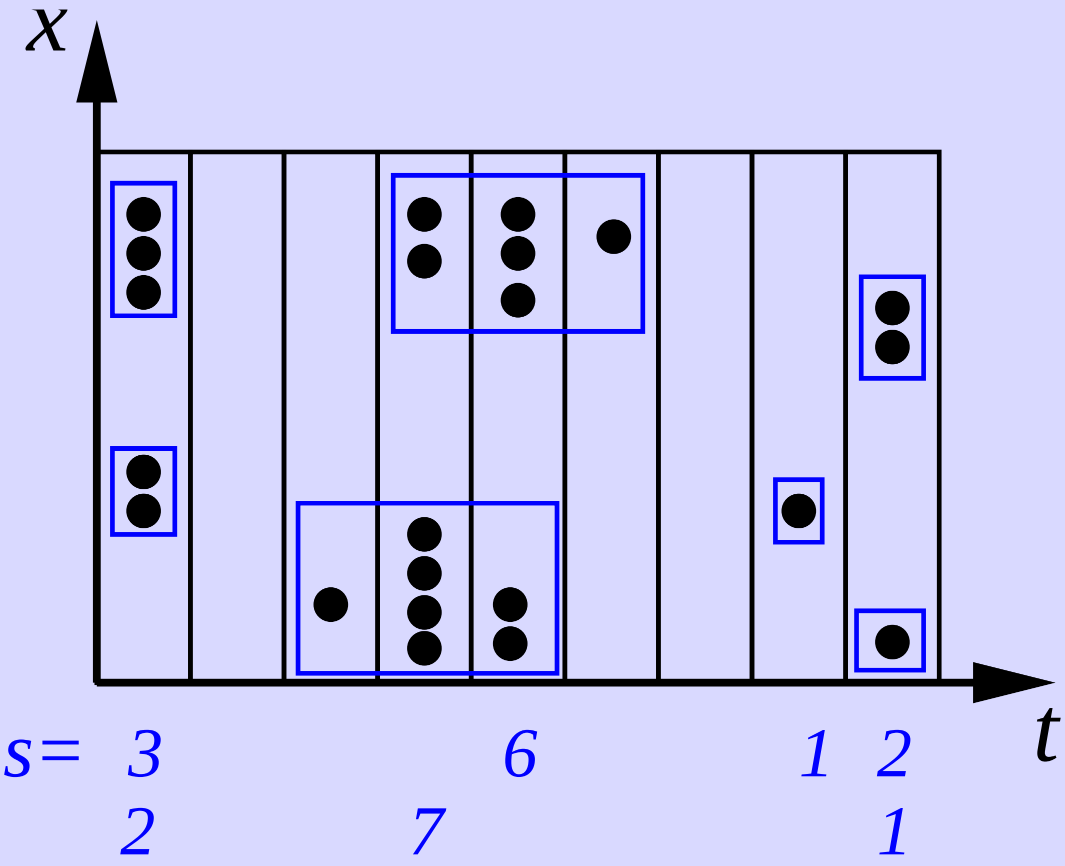
Temporally Extended Cluster



Definition:

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

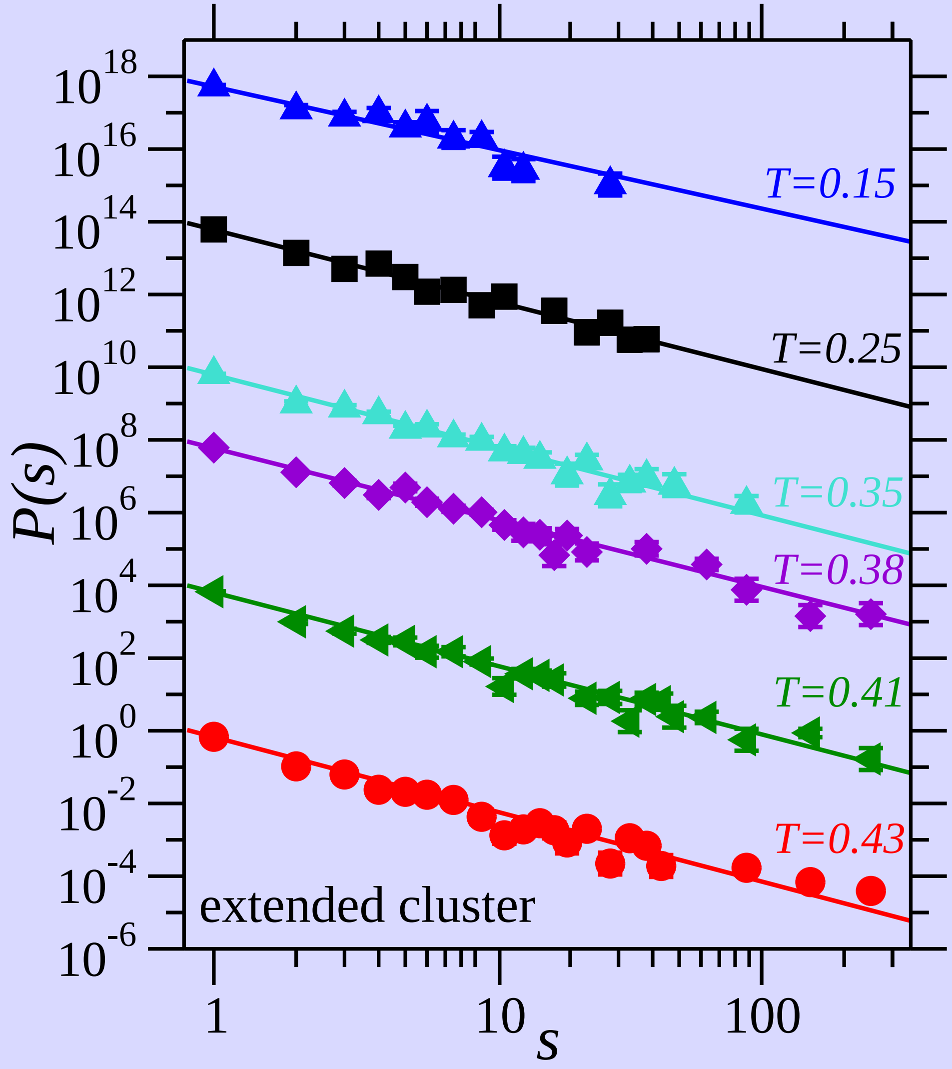
connected if:

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

$$\Delta t < t_{\mathsf{cutoff}}$$

Cluster Size Distribution

of Temporally Extended Clusters



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

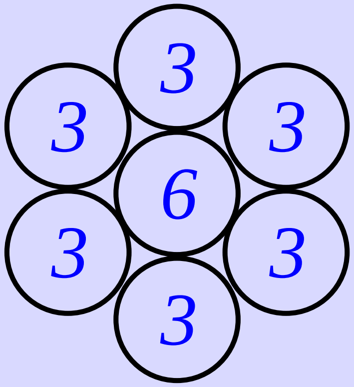
$\Longrightarrow$ for all temperatures (self-organized crit.)

Shape of Clusters

z = number of nearest neighbors within cluster

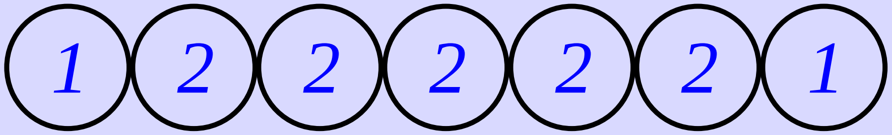
s = number of particles (cluster size)

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



s=7

$\langle z \rangle$ =3.4



s=7

$\langle z \rangle$ =1.7

Shape of Clusters

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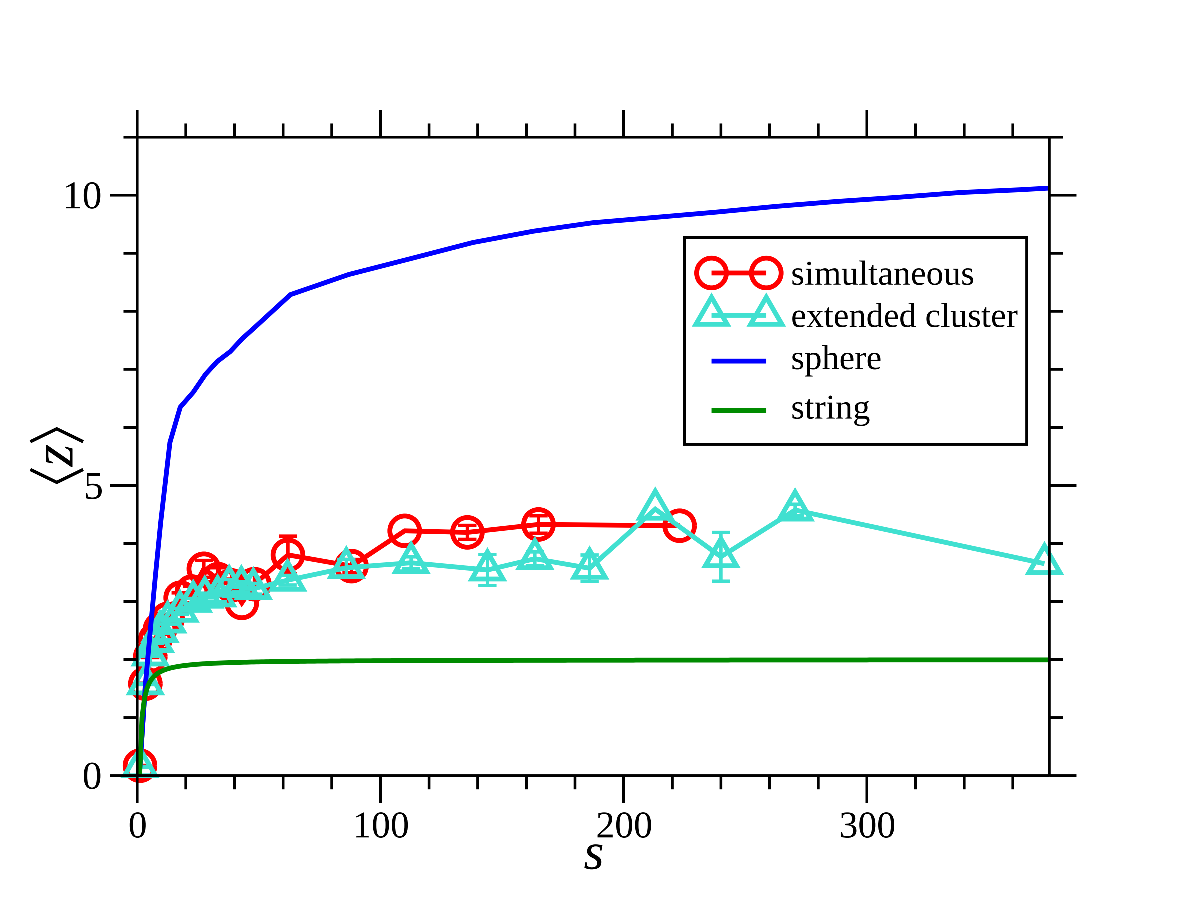

$\Longrightarrow$ string-like clusters

Shape of Clusters

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s = number of particles (cluster size)

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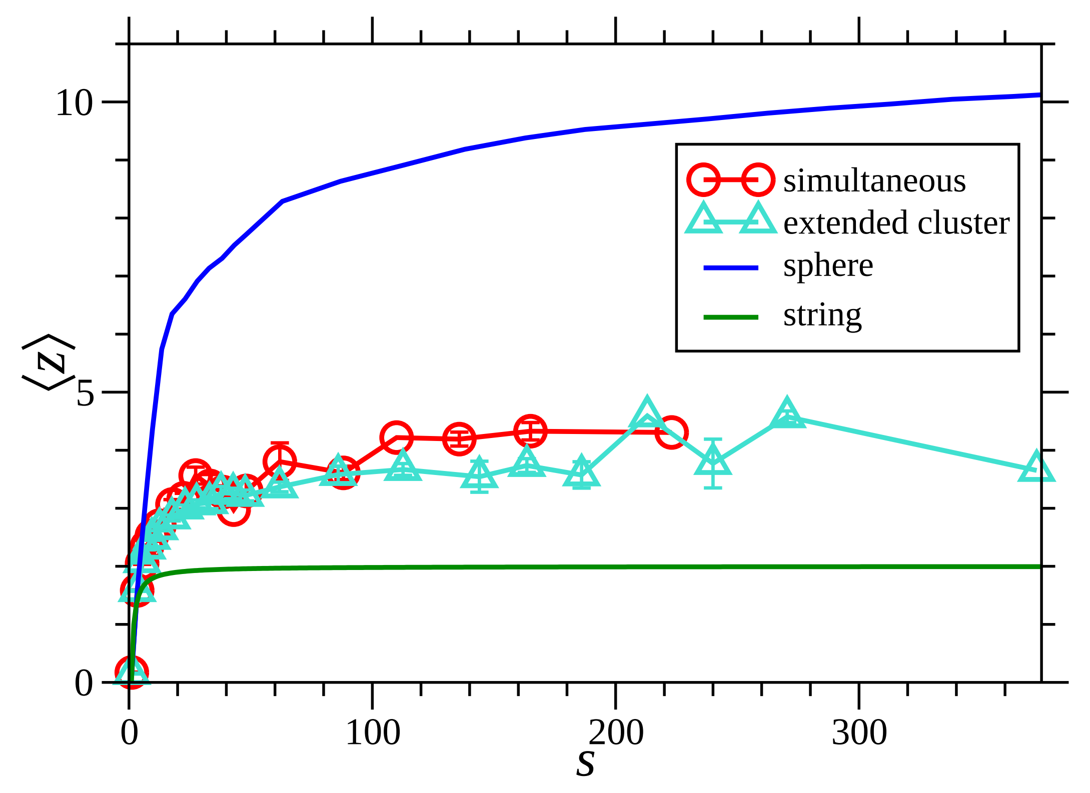
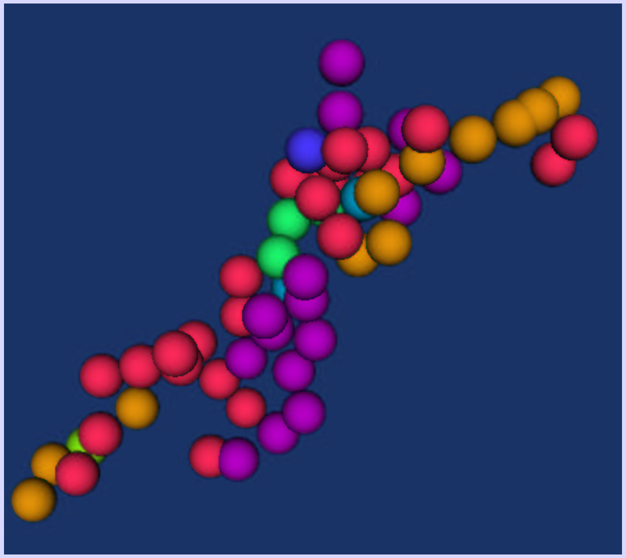


$\Longrightarrow$ string-like clusters



same color = same time

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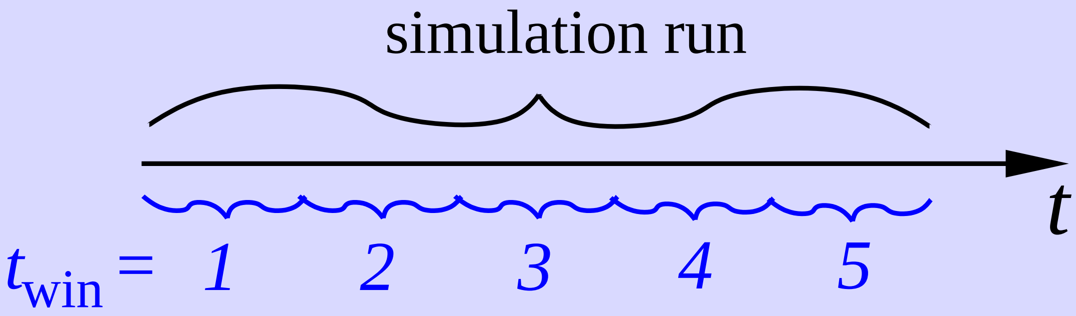
History Dependence

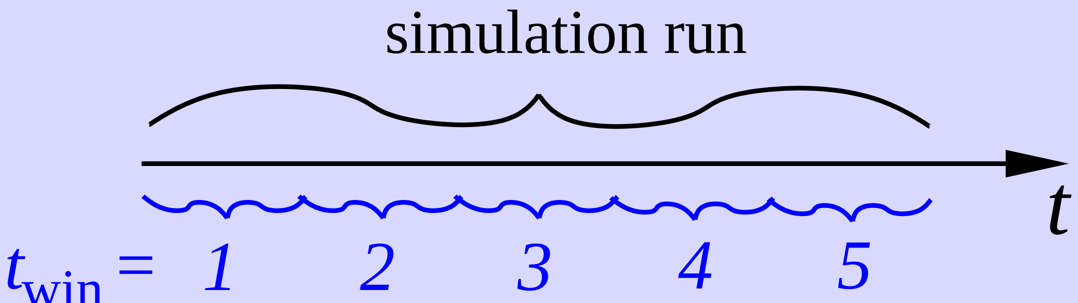


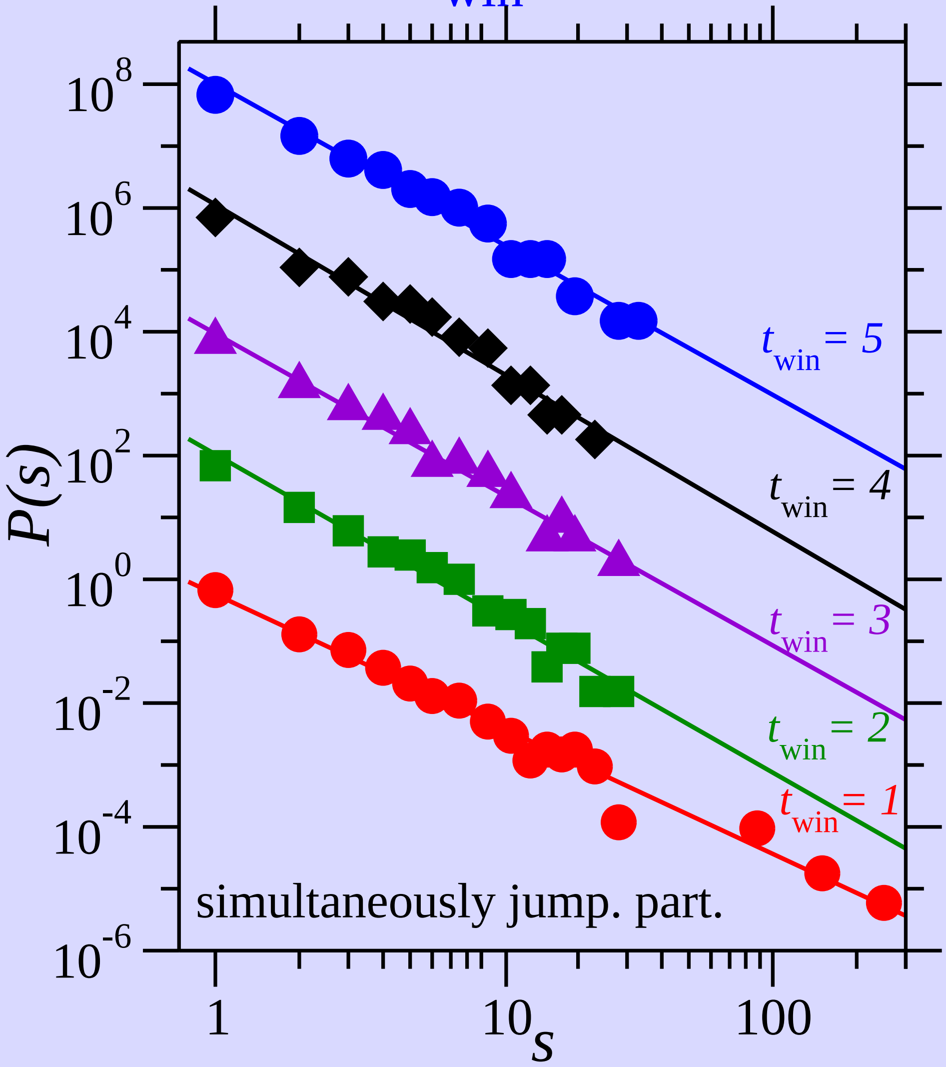
simulation run

t

$t_{\text{win}} =$ *1* *2* *3* *4* *5*

History Dependence





Power Law

(Simultan. Jump. Part.)

$\Longrightarrow$ aging independent

$\tau(T)$

Outline

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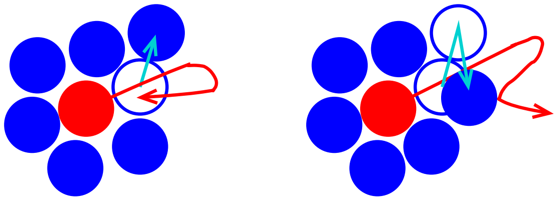
Summary: Jump Statistics

reversible and irreversible jumps:



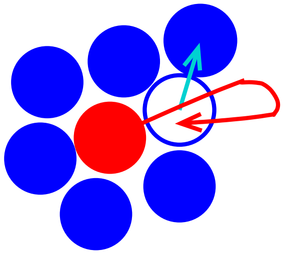
reversible jump irreversible jump

At larger temperature relaxation:

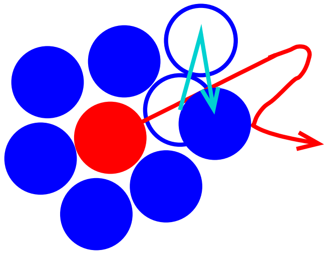
- via more jumping particles
- via larger jumpsizes
- not via Δt_{b} (indep. of T)

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

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

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

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

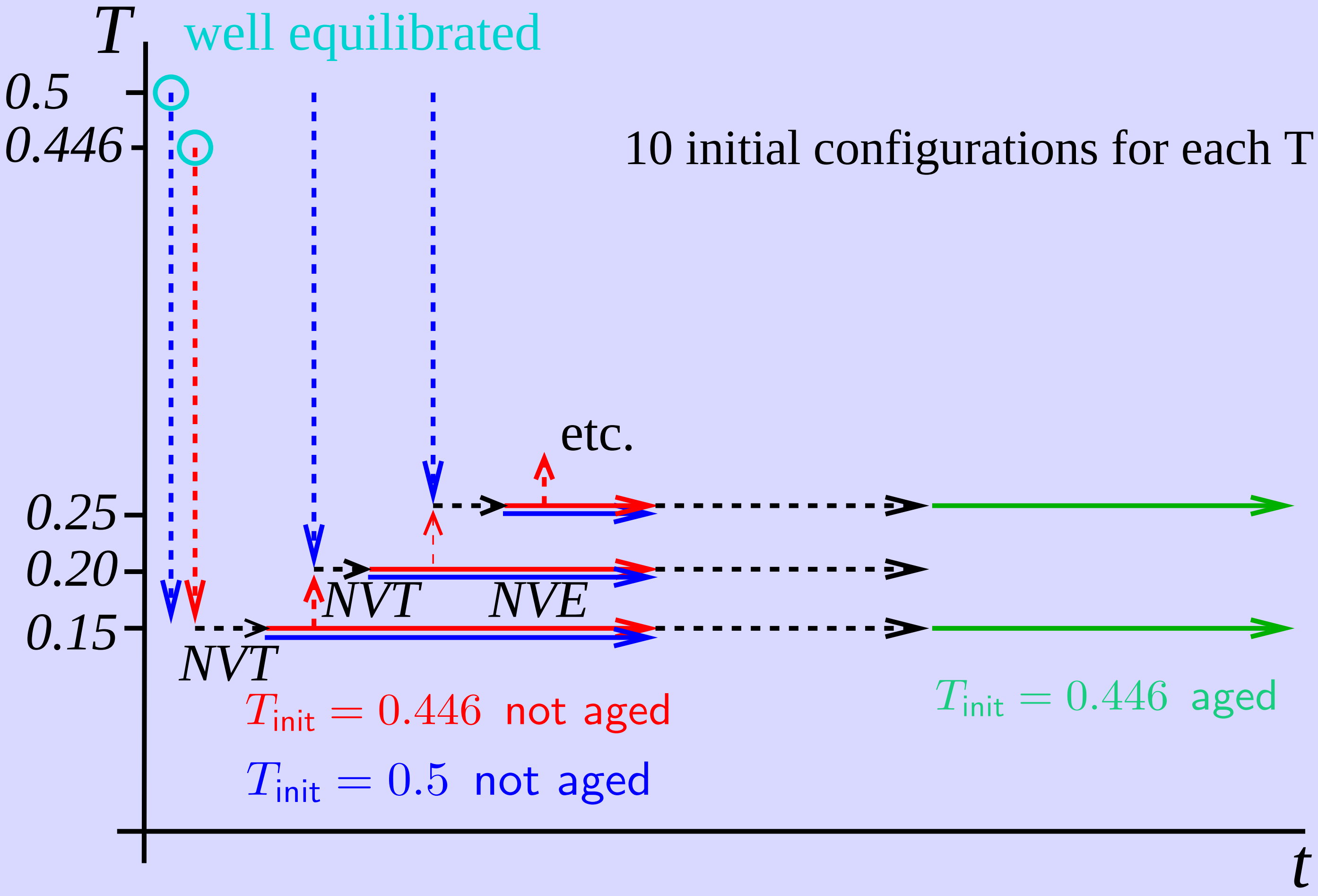
Time Scales

- 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

Time Scales

Cooperative Processes: $N_{\mathrm{t,bcl}}$

History of Production Runs



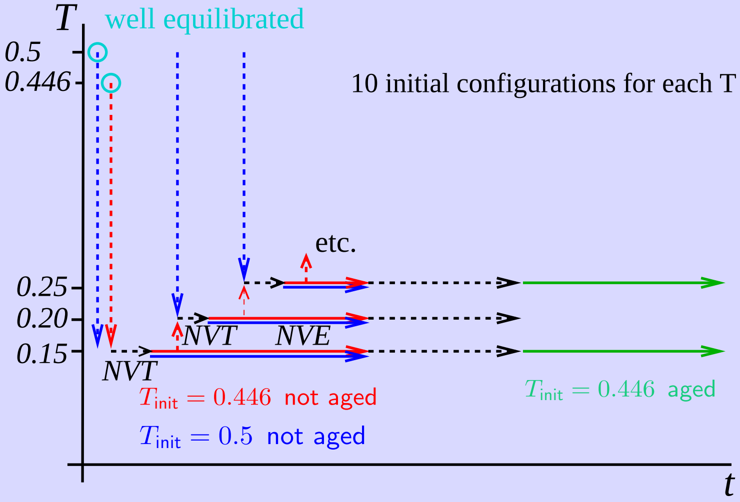
10 initial configurations for each T

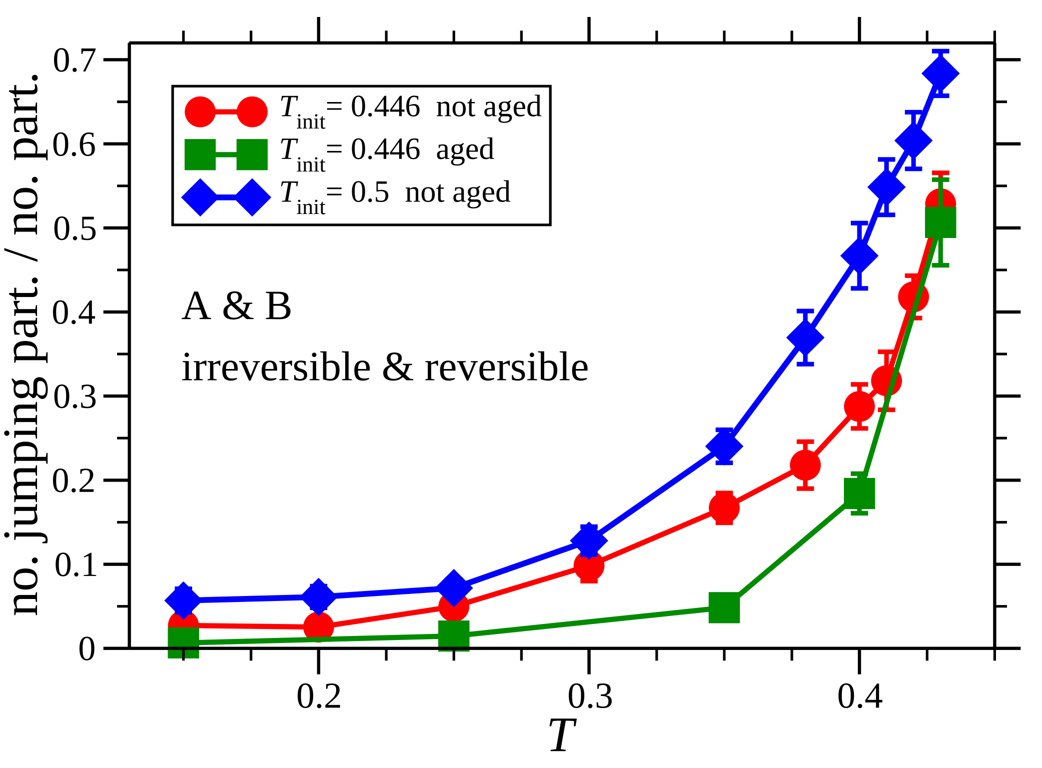
$T_{\text{init}} = 0.446$ not aged

$T_{\text{init}} = 0.5$ not aged

$T_{\text{init}} = 0.446$ aged

History Dependence

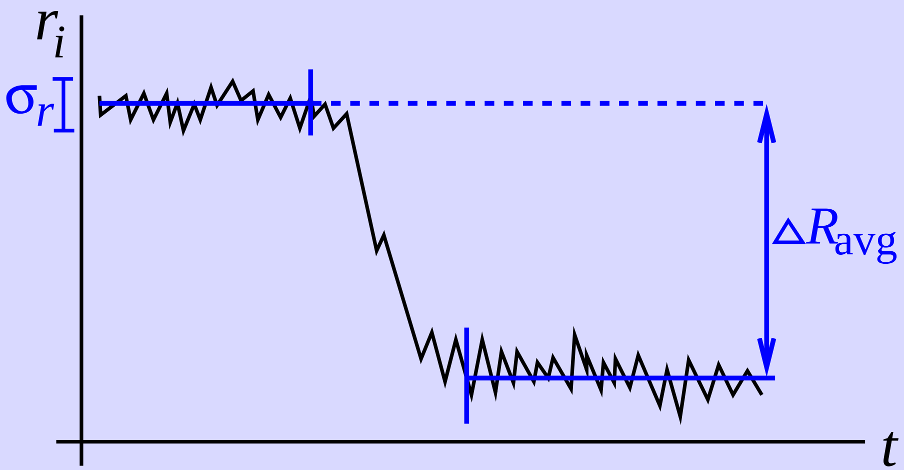


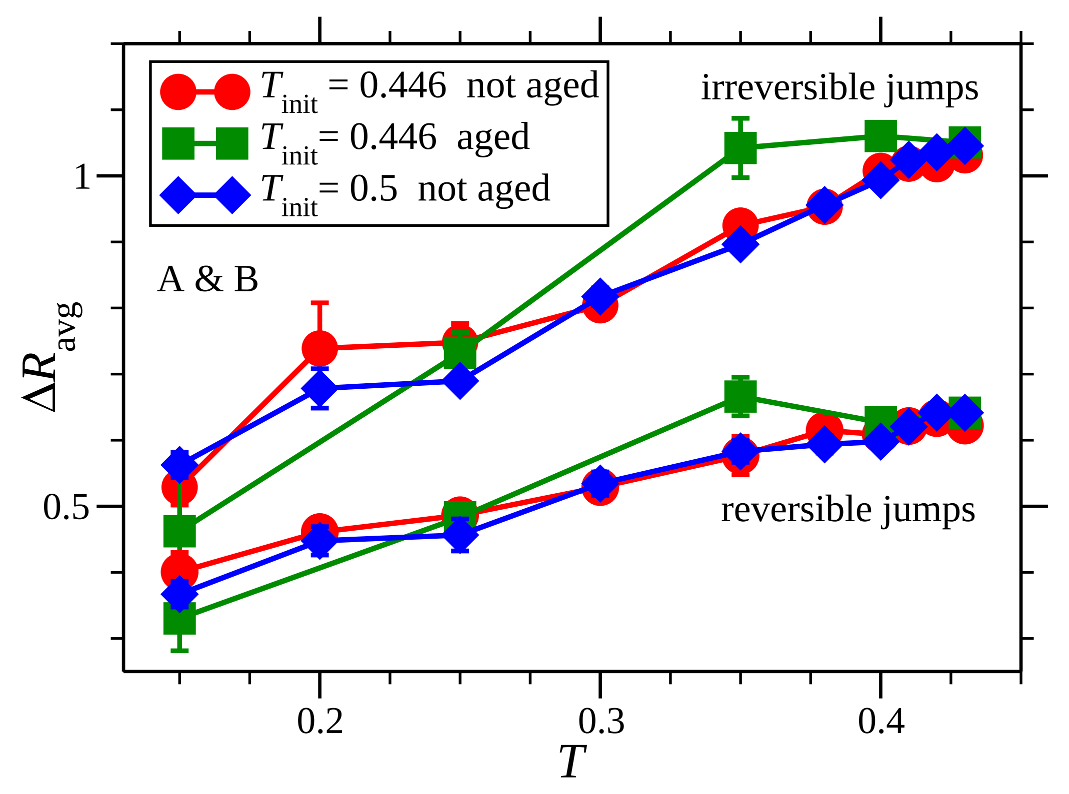


Number of Jump. Part.

$\Longrightarrow$ history dependent

History Dependence

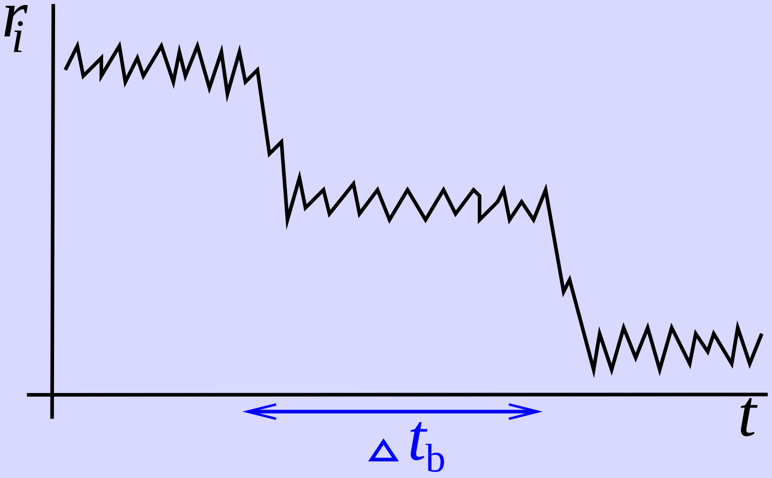


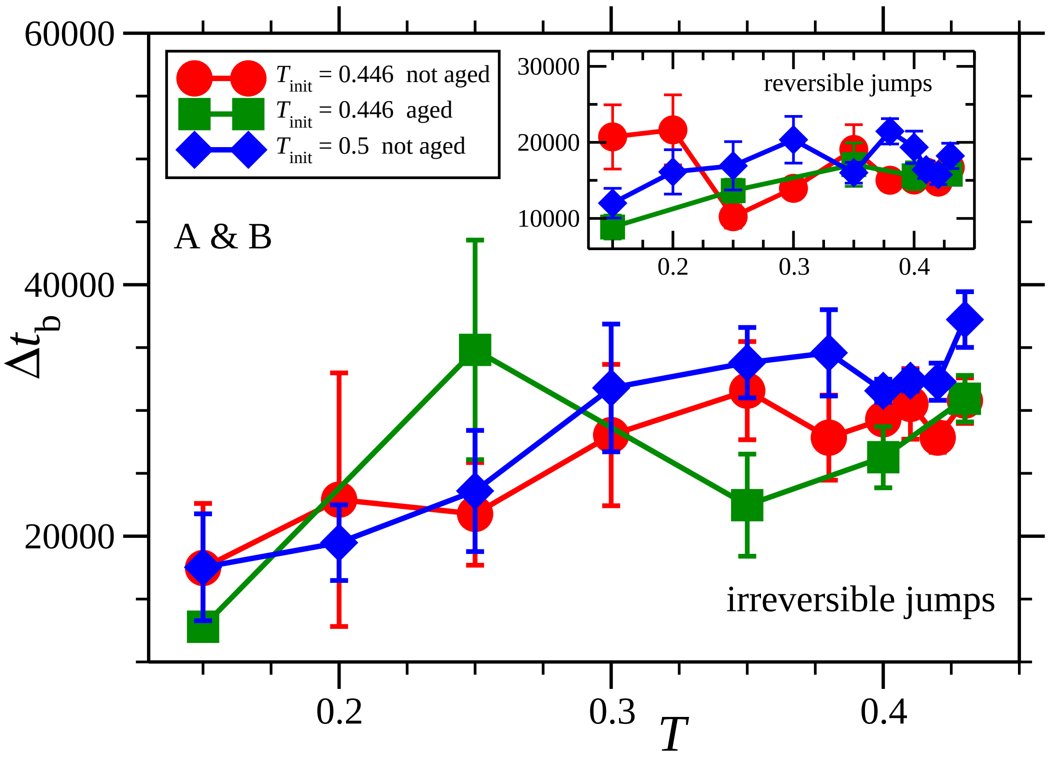


Jump Size

$\Longrightarrow$ history independent

History Dependence



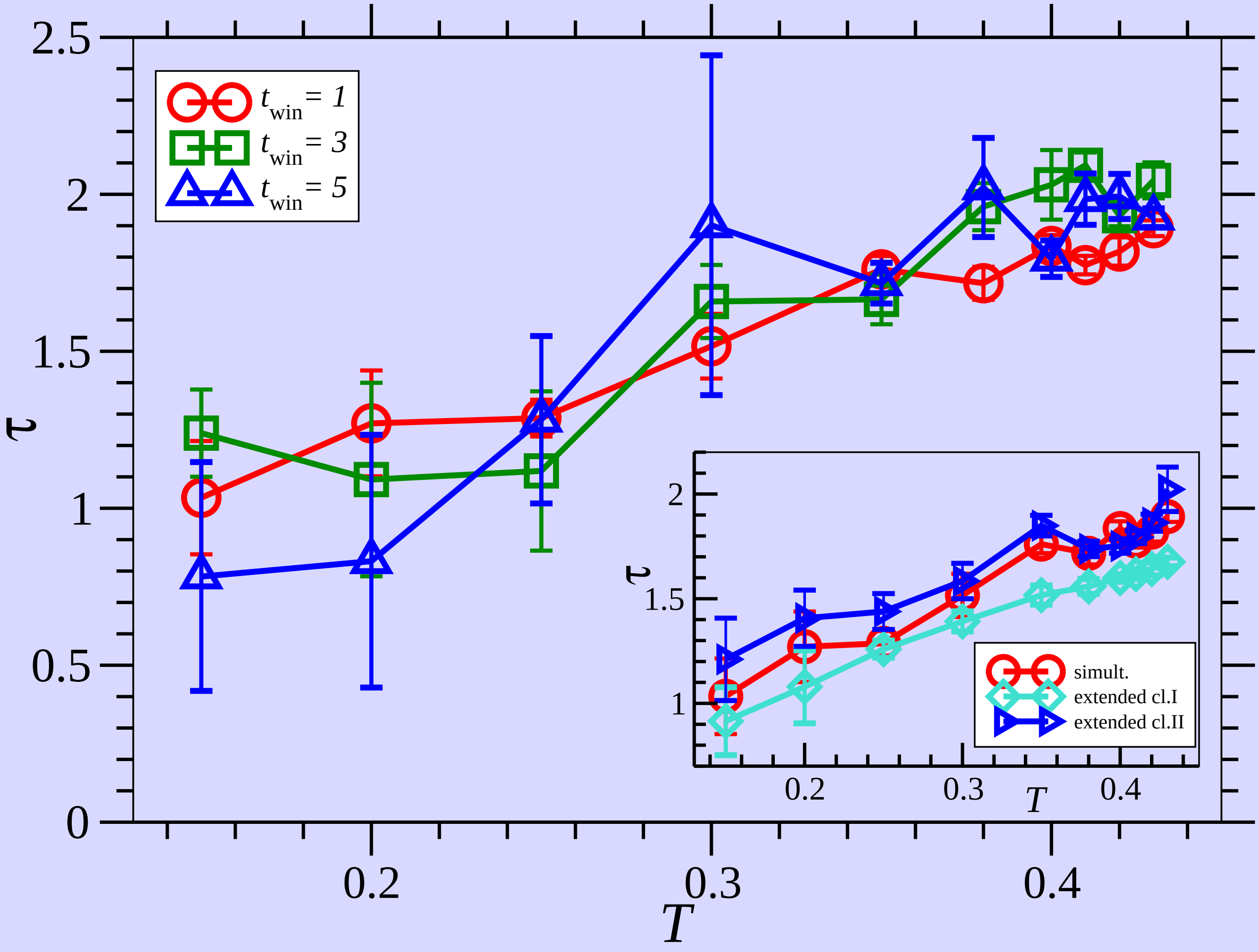


Time Between Jumps

$\Longrightarrow$ history independent

Summary: Jump Statistics

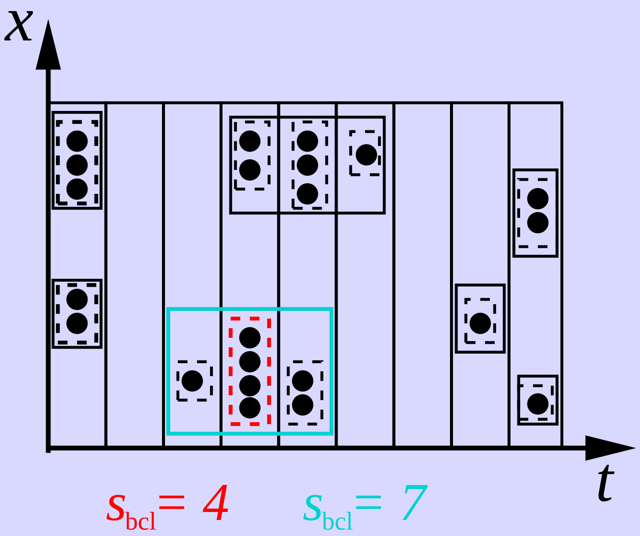
Exponent $\tau(T)$



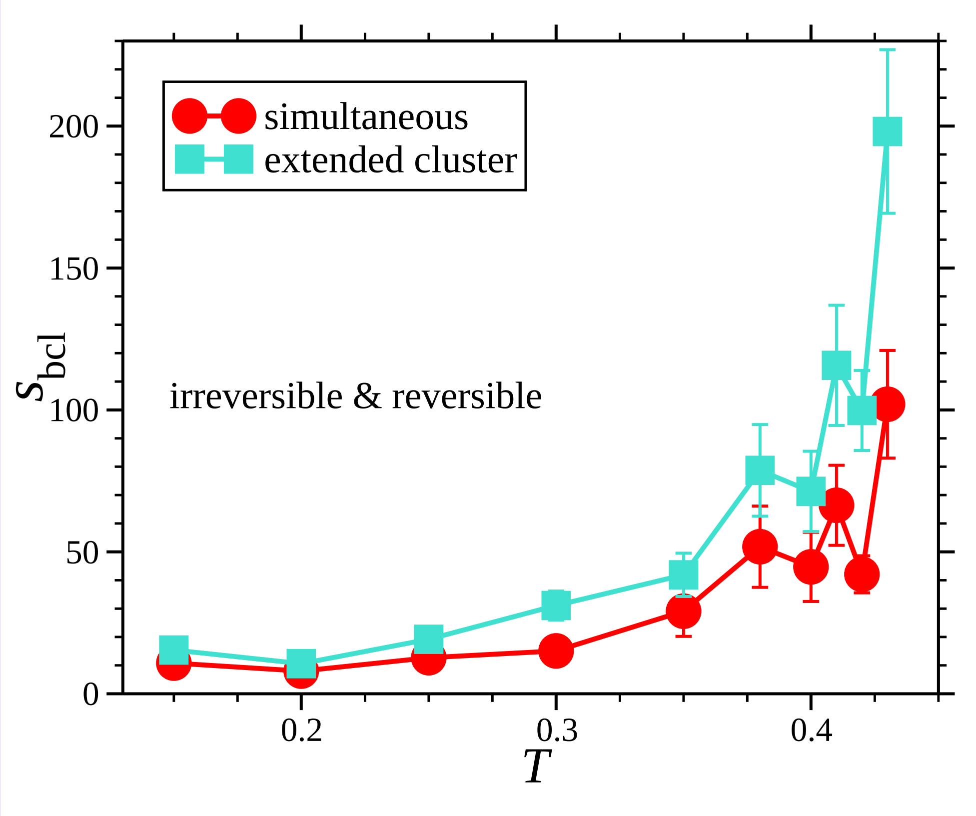
$P(s)_T$

$P(s)_{\text{twin}}$

Most Cooperative Processes



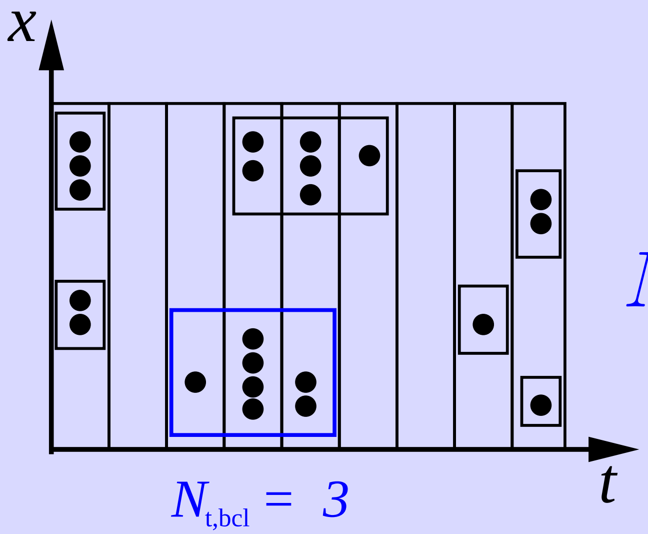
s_{bcl} = largest cluster size



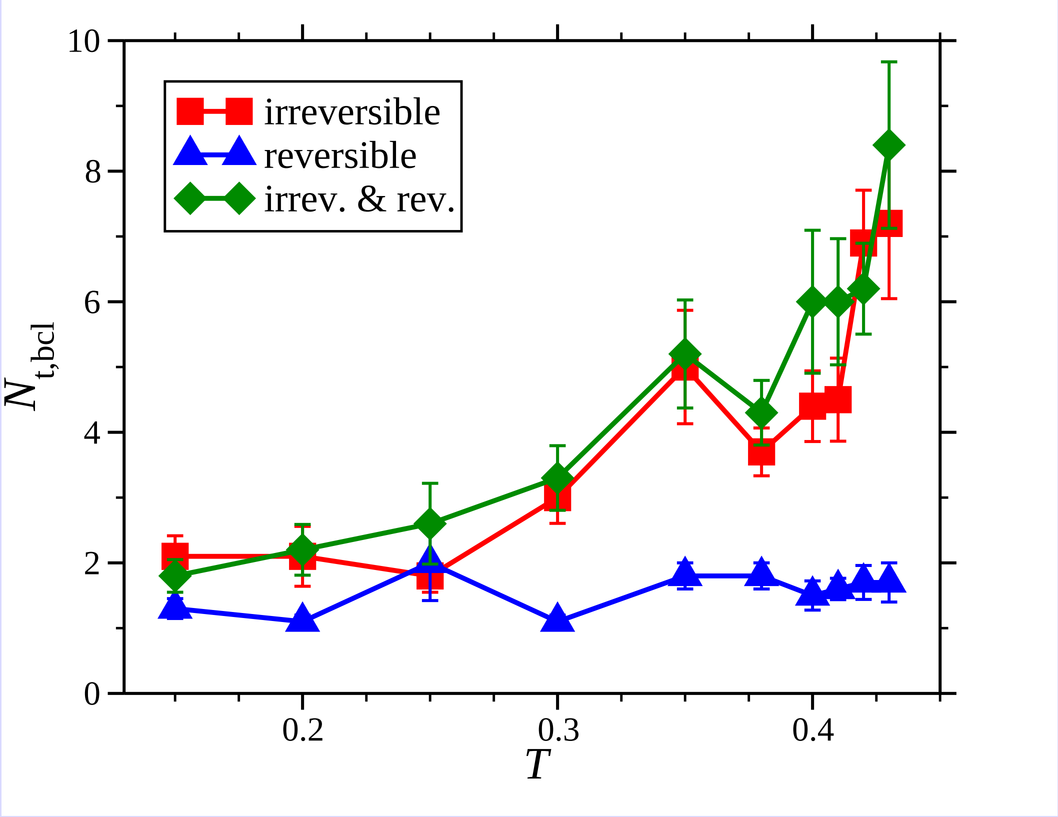
$\Longrightarrow$ highly correlated single particle jumps

- many particles

Most Cooperative Processes



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



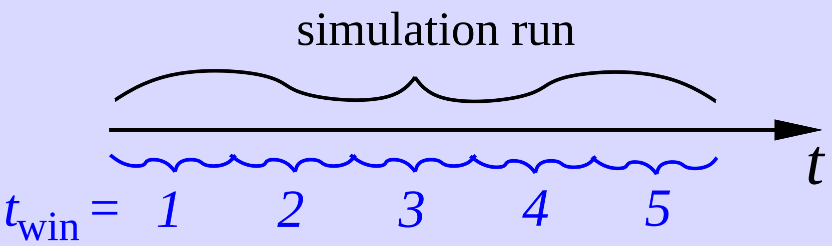
$\Longrightarrow$ highly correlated single particle jumps

- many particles
- many time bins

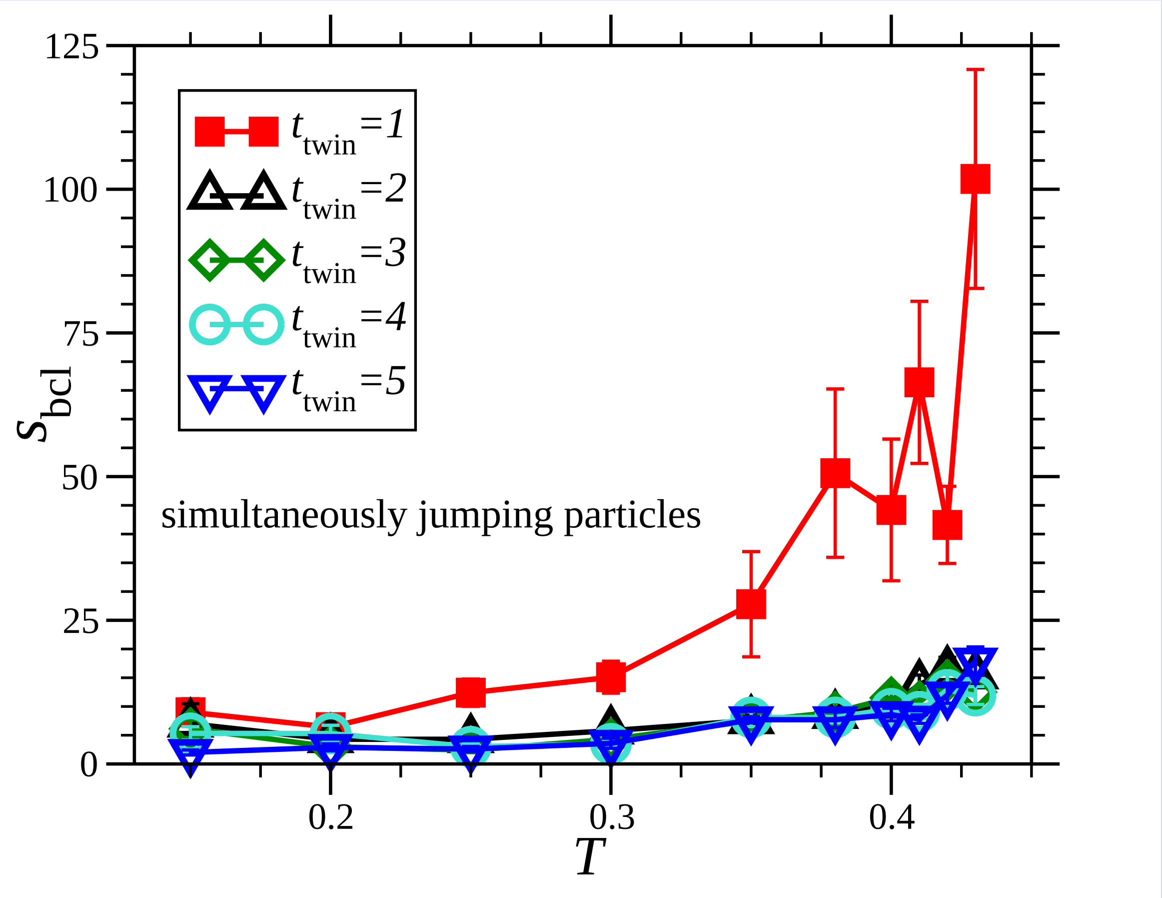
(maximum = 125)

Time Scales Extra

History Dependence



s_{bcl} = largest cluster size

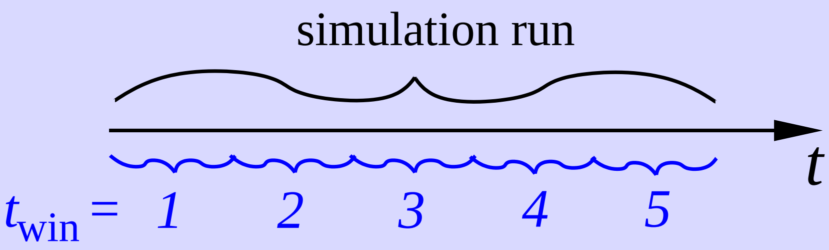


$\Longrightarrow$ aging dependent

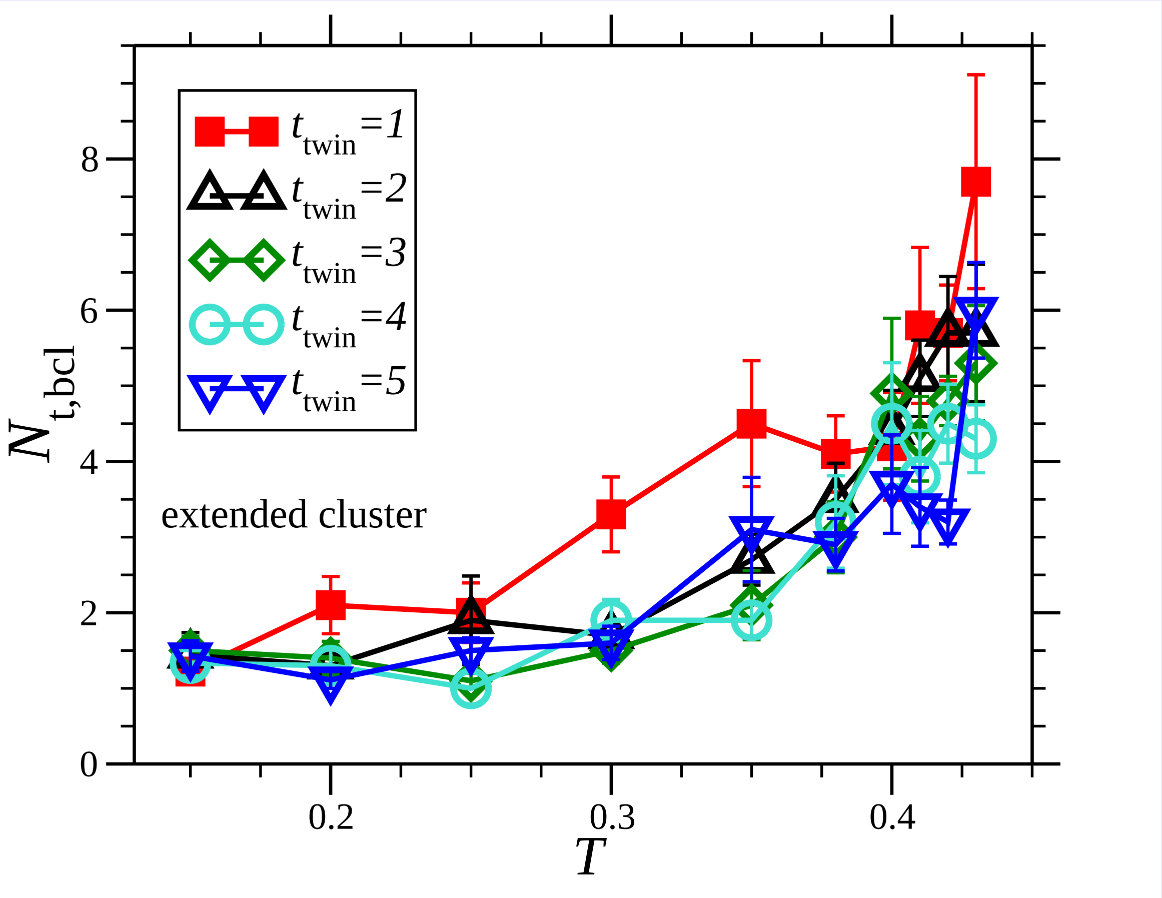
- 1st t-window:
  highly cooperative
- 2nd - 5th t-window:
  same, cooperative

s_{bcl} extended cluster

History Dependence



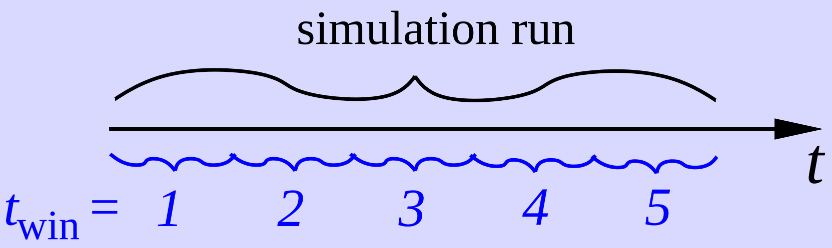
$N_{\mathsf{t,bcl}} =$ no. of t-bins of largest cluster

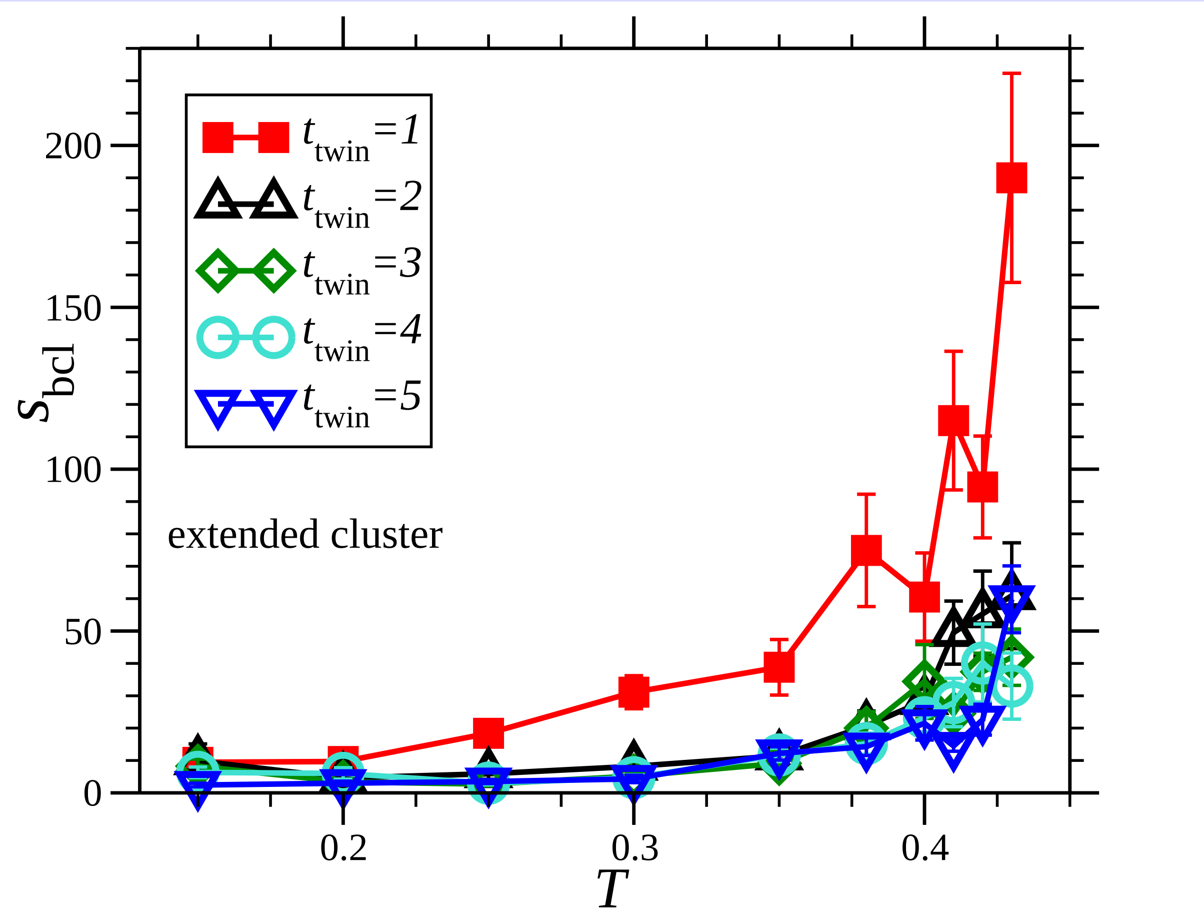


$\Longrightarrow$ less aging dependent

$\Longrightarrow$ highly cooperative

History Dependence



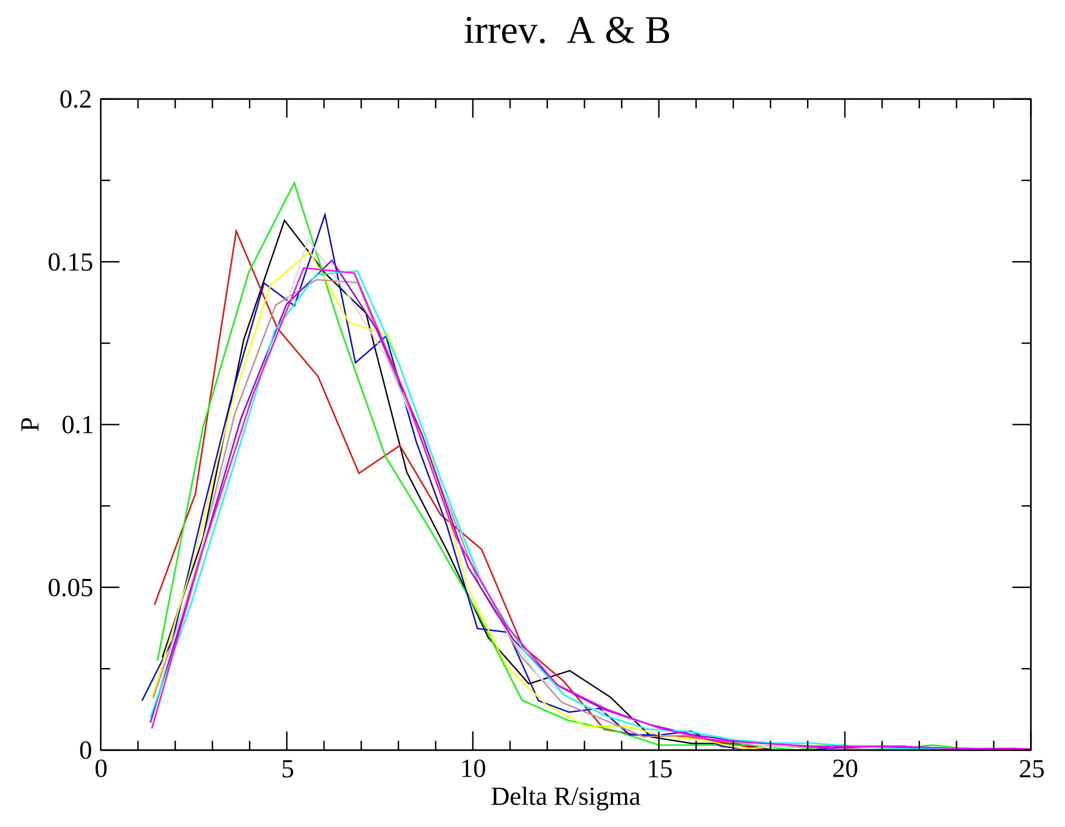


$\Longrightarrow$ aging dependent

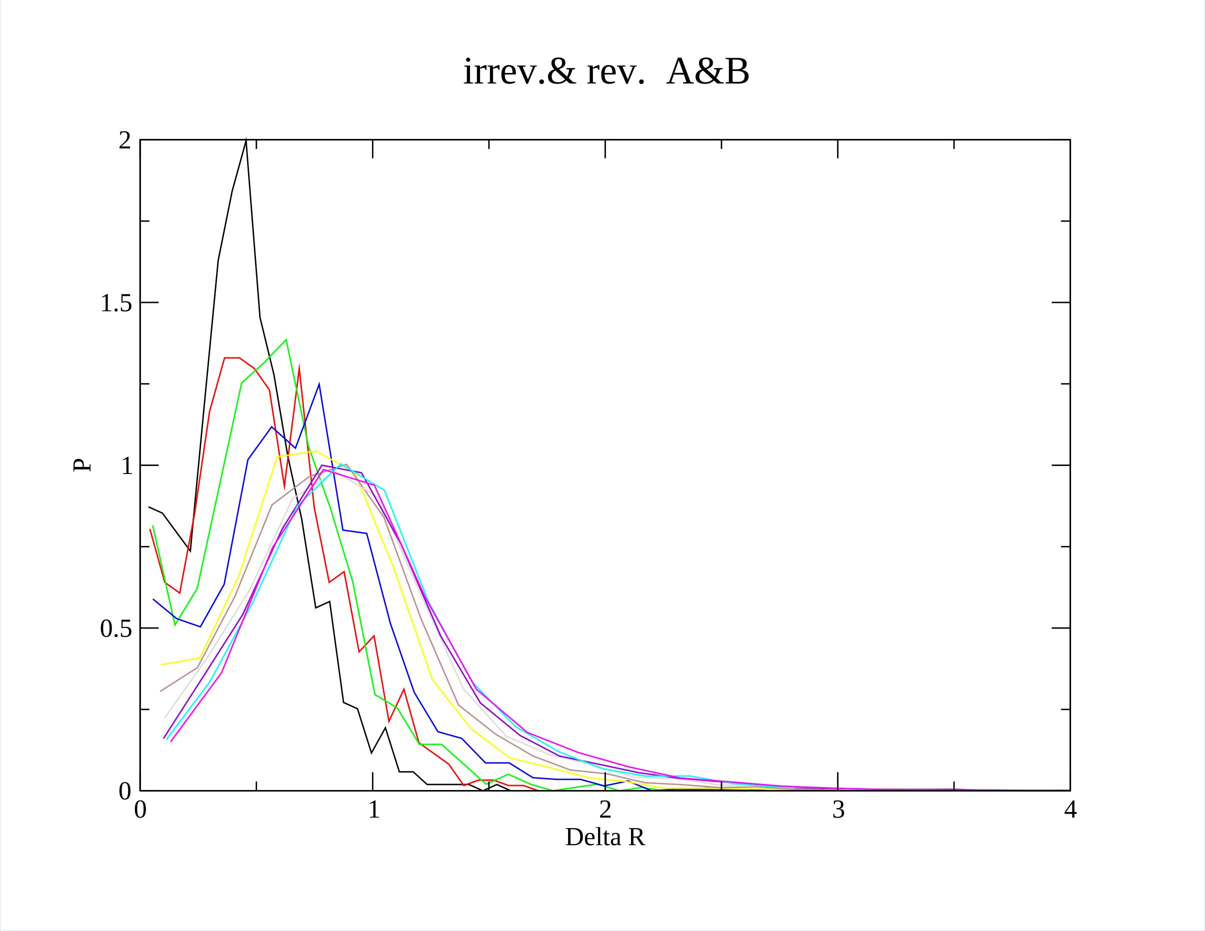
- 1st t-window:
  highly cooperative
- 2nd - 5th t-window:
  same, cooperative

s_{bcl} simult. jump.

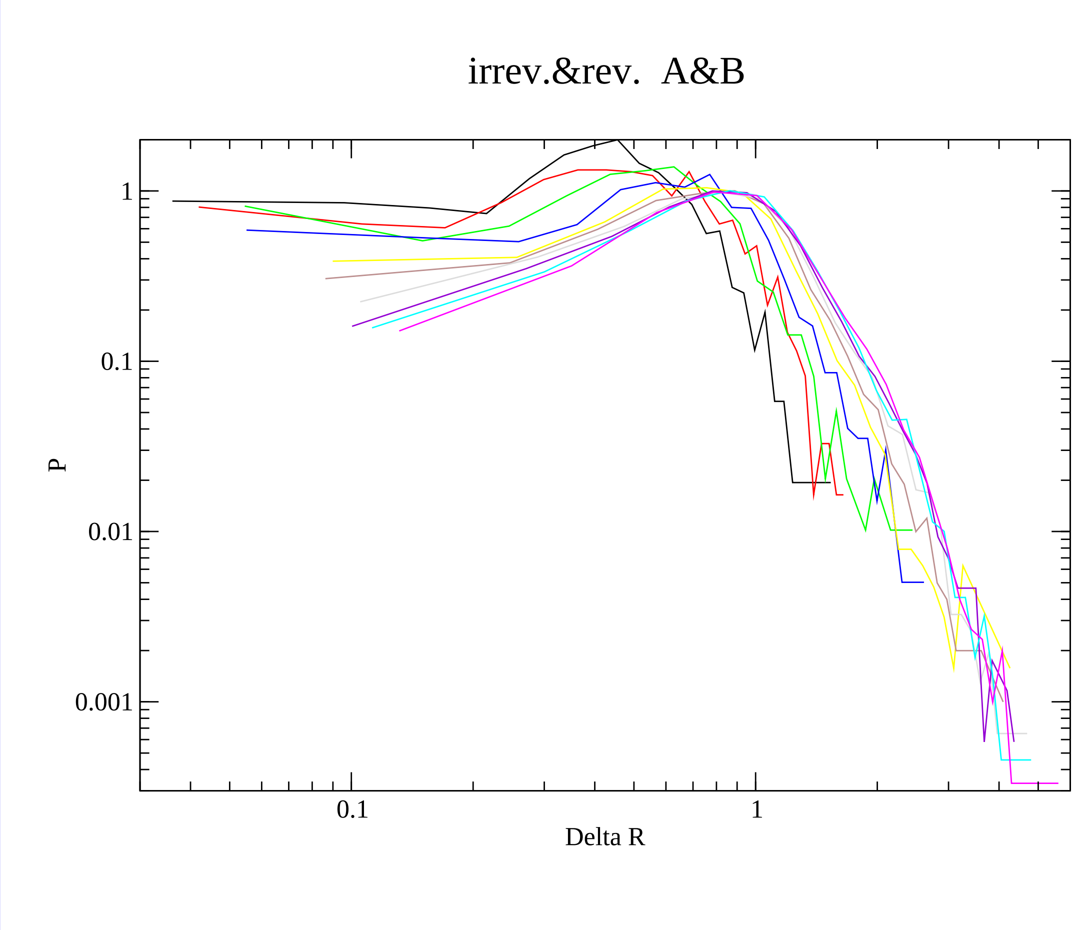
Normalized Jump Size Distribution



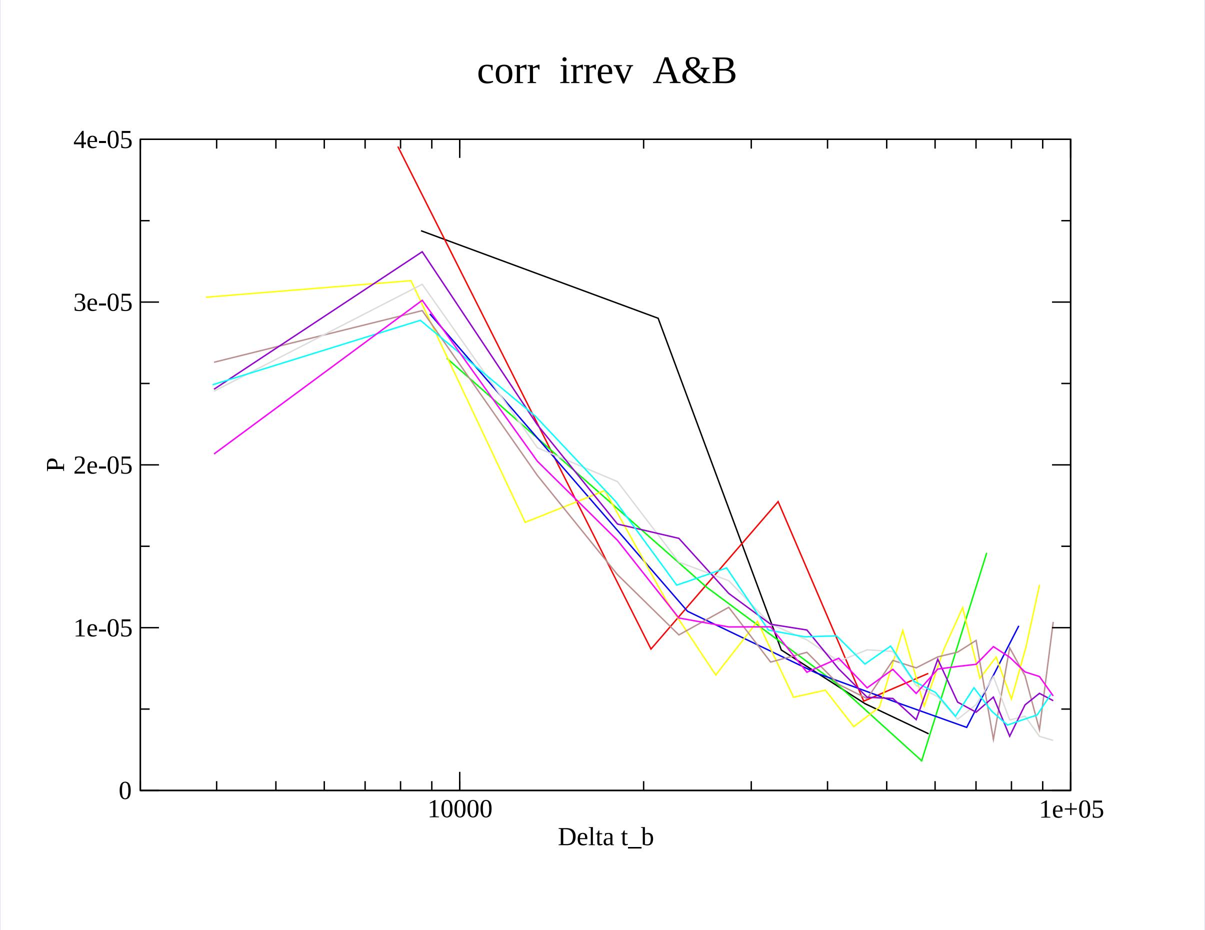
Jump Size Distribution



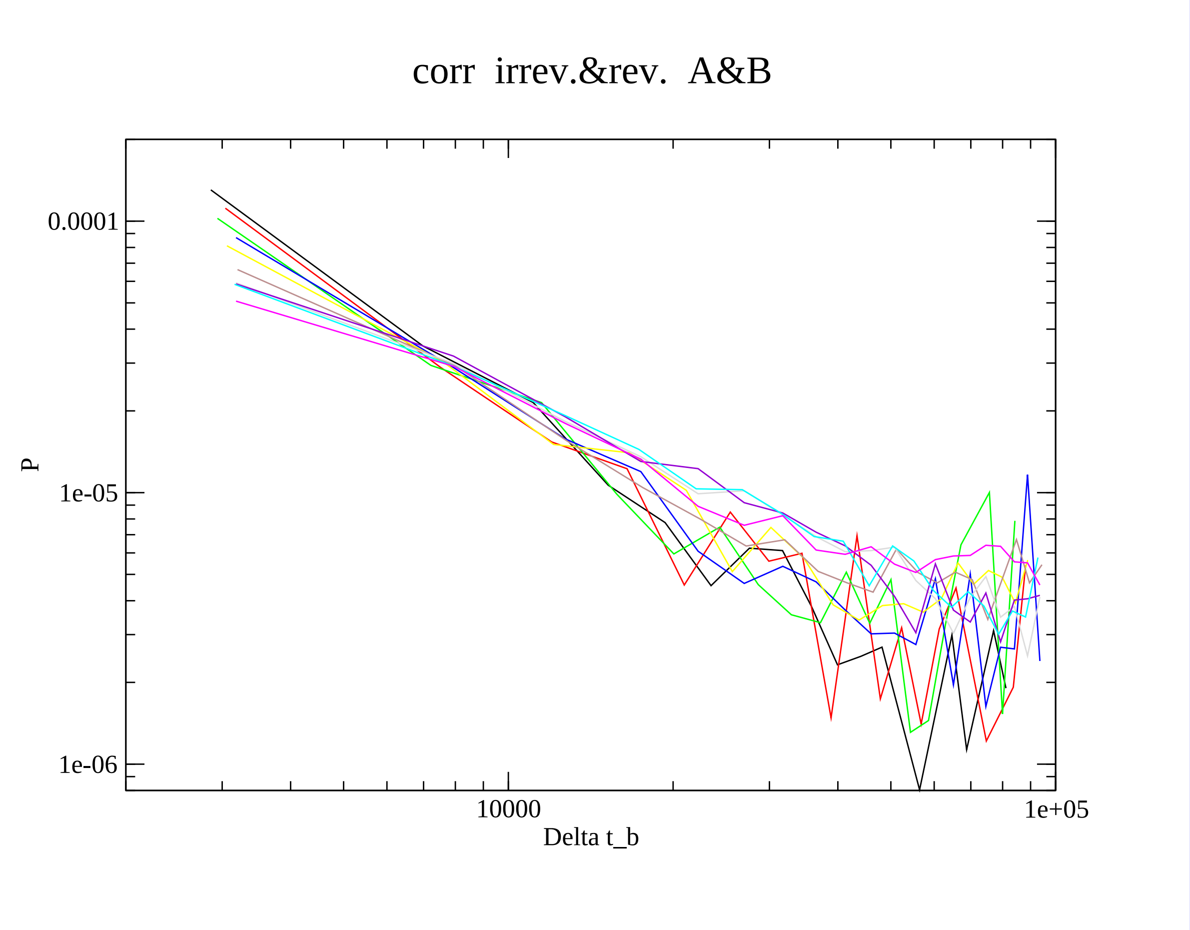
Jump Size Distribution



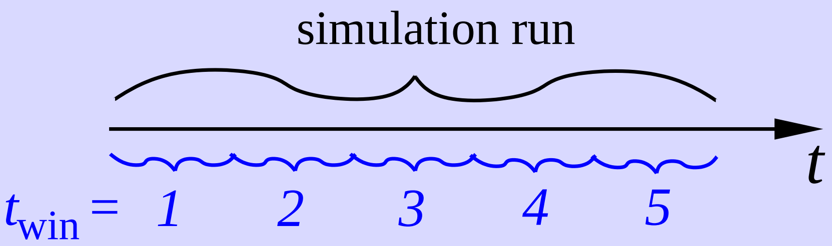
Distribution of Δt_{b}

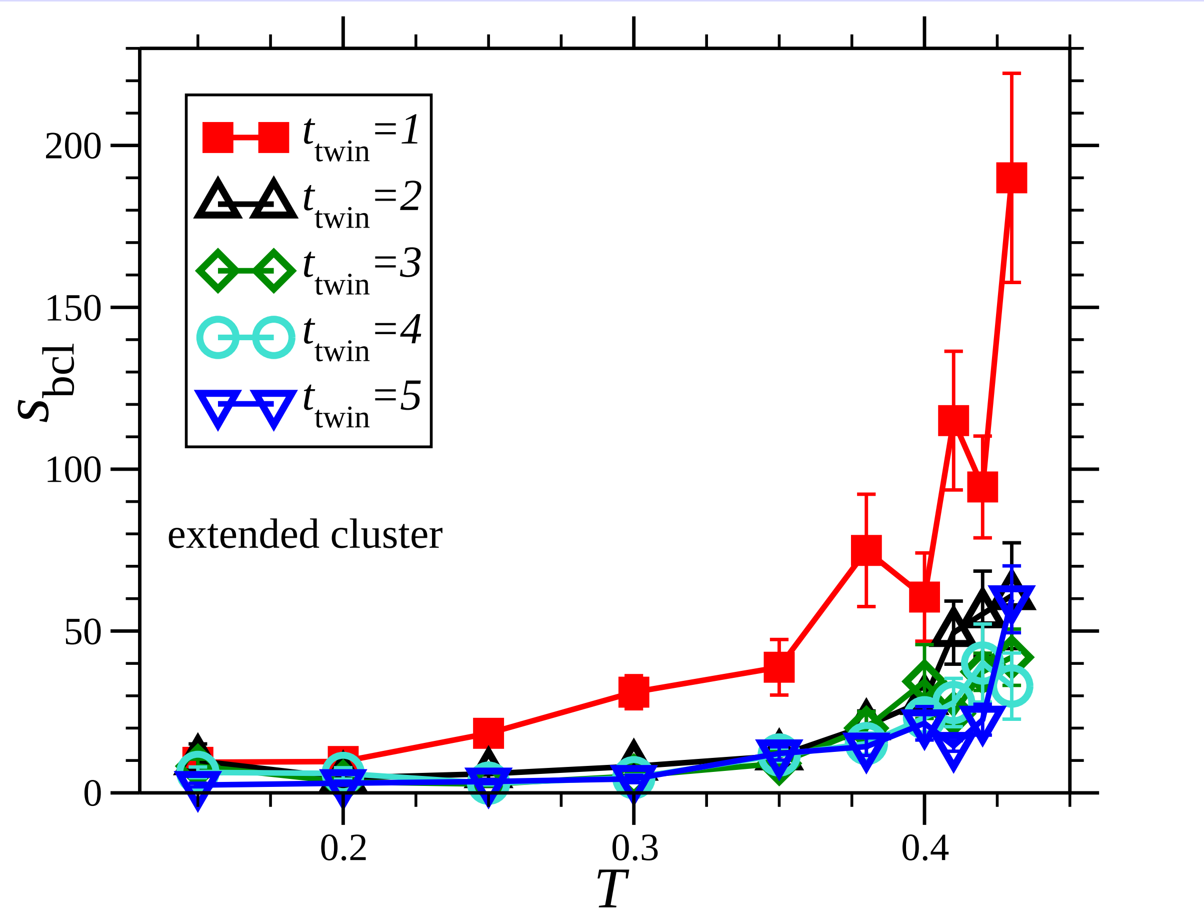


Distribution of Δt_b



History Dependence





$\Longrightarrow$ aging dependent

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

s_{bcl} simult. jump.

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

Time Scales

Cooperative Processes: $N_{\text{t,bcl}}$