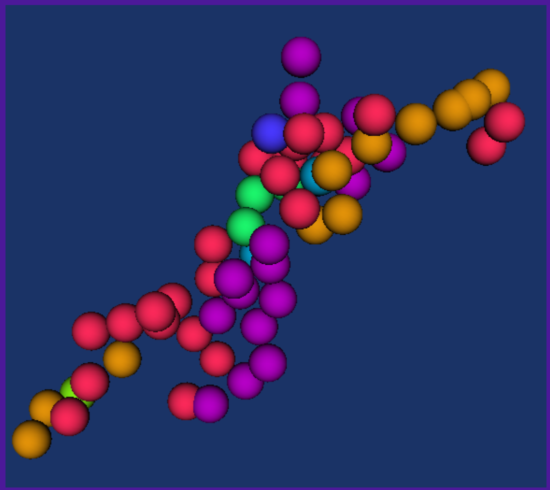
Self-Organized Criticality Below The Glass Transition

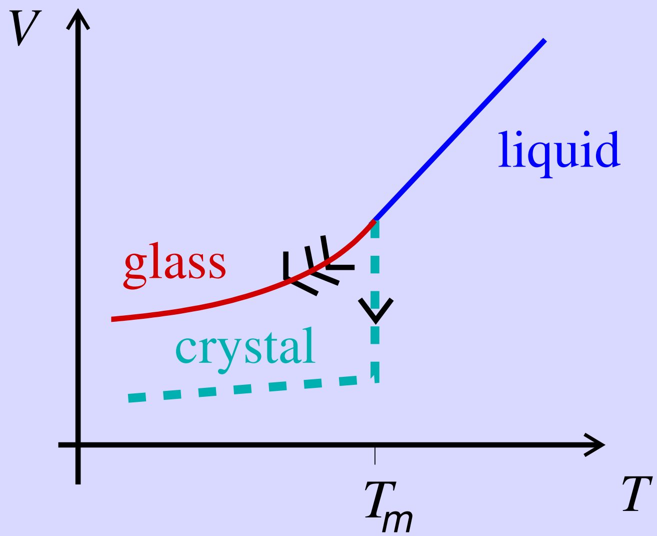
Katharina Vollmayr-Lee, Bucknell University

October 15, 2009



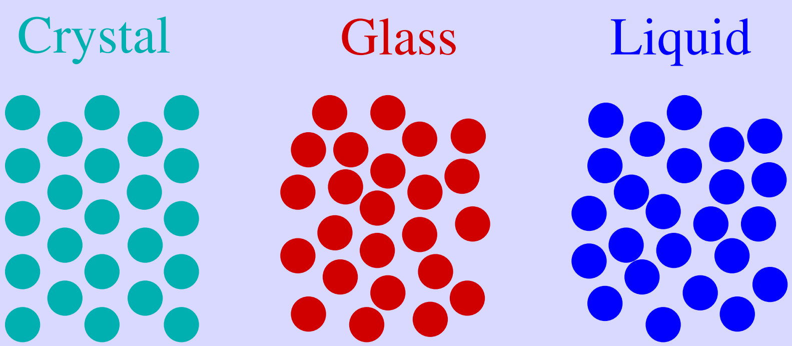
Thanks: E. A. Baker, A. Zippelius, K. Binder, and J. Horbach

Introduction: Glass



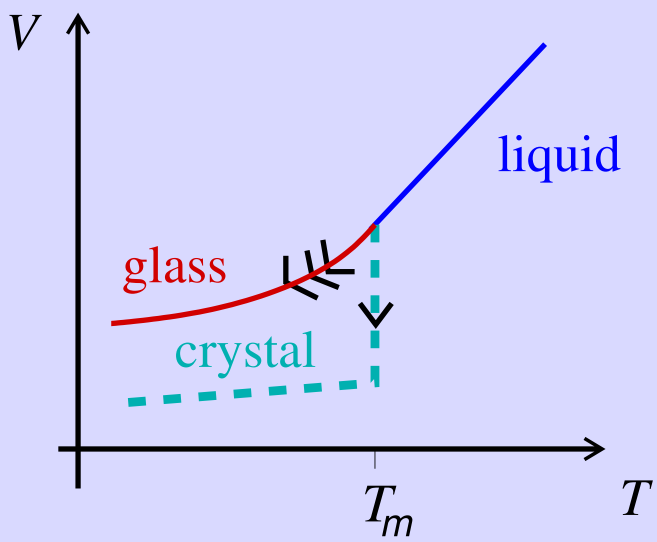
Glass:

→ system falls out of equilibrium



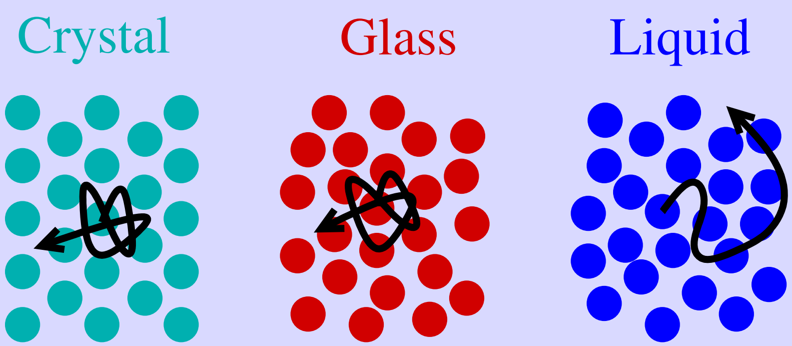
Structure: discordered

Introduction: Glass



Glass:

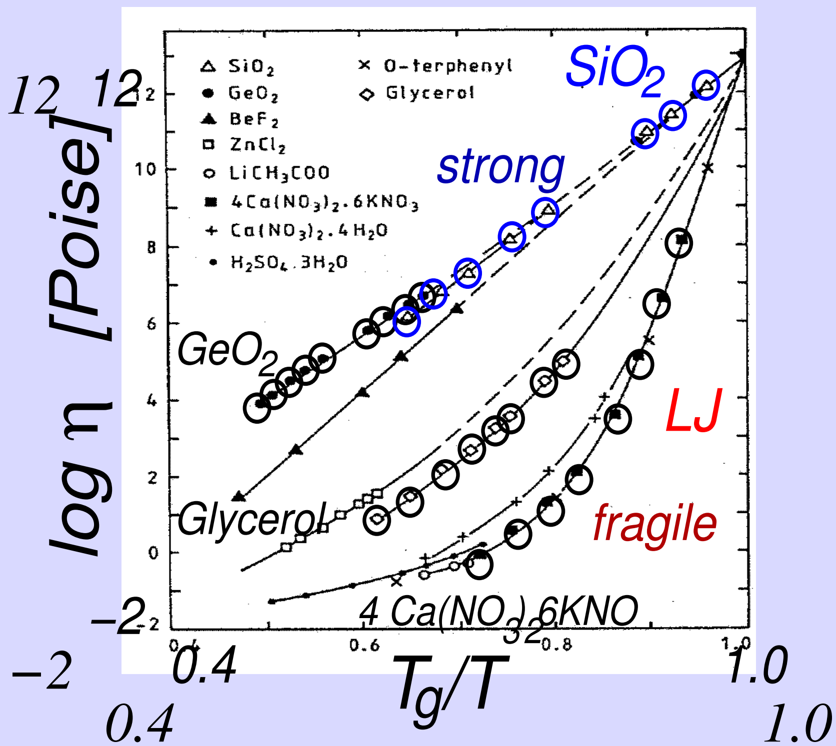
→ system falls out of equilibrium



Structure: discordered

Dynamics: frozen in

Introduction: Dynamics



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

- ⟶ slowing down of many decades
- ⟶ strong and fragile glass formers
- ⟶ SiO_2 strong glass former (end of talk)
- ⟶ LJ fragile glass (here)

Model

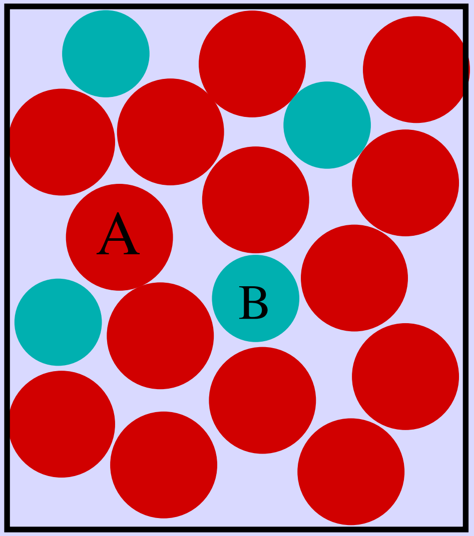
Binary Lennard-Jones System

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

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

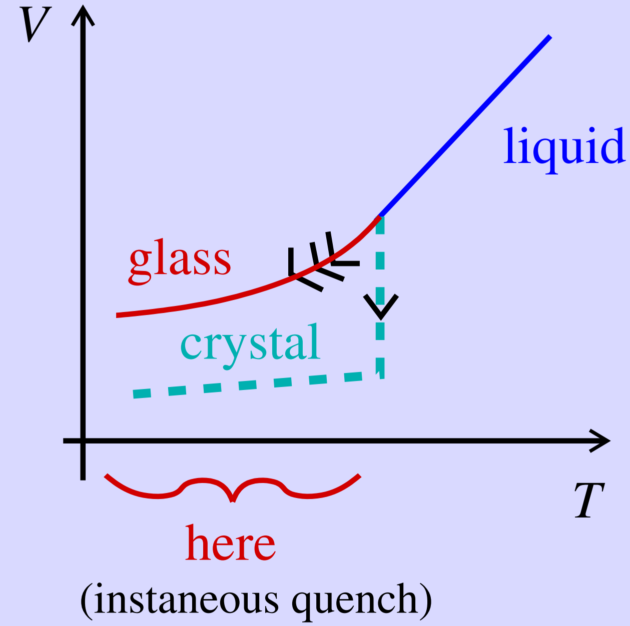
$\epsilon_{\mathsf{AA}} = 1.0 \quad \epsilon_{\mathsf{AB}} = 1.5 \quad \epsilon_{\mathsf{BB}} = 0.5$

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



800 A and 200 B

Simulations



Molecular Dynamics Simulations

Velocity Verlet

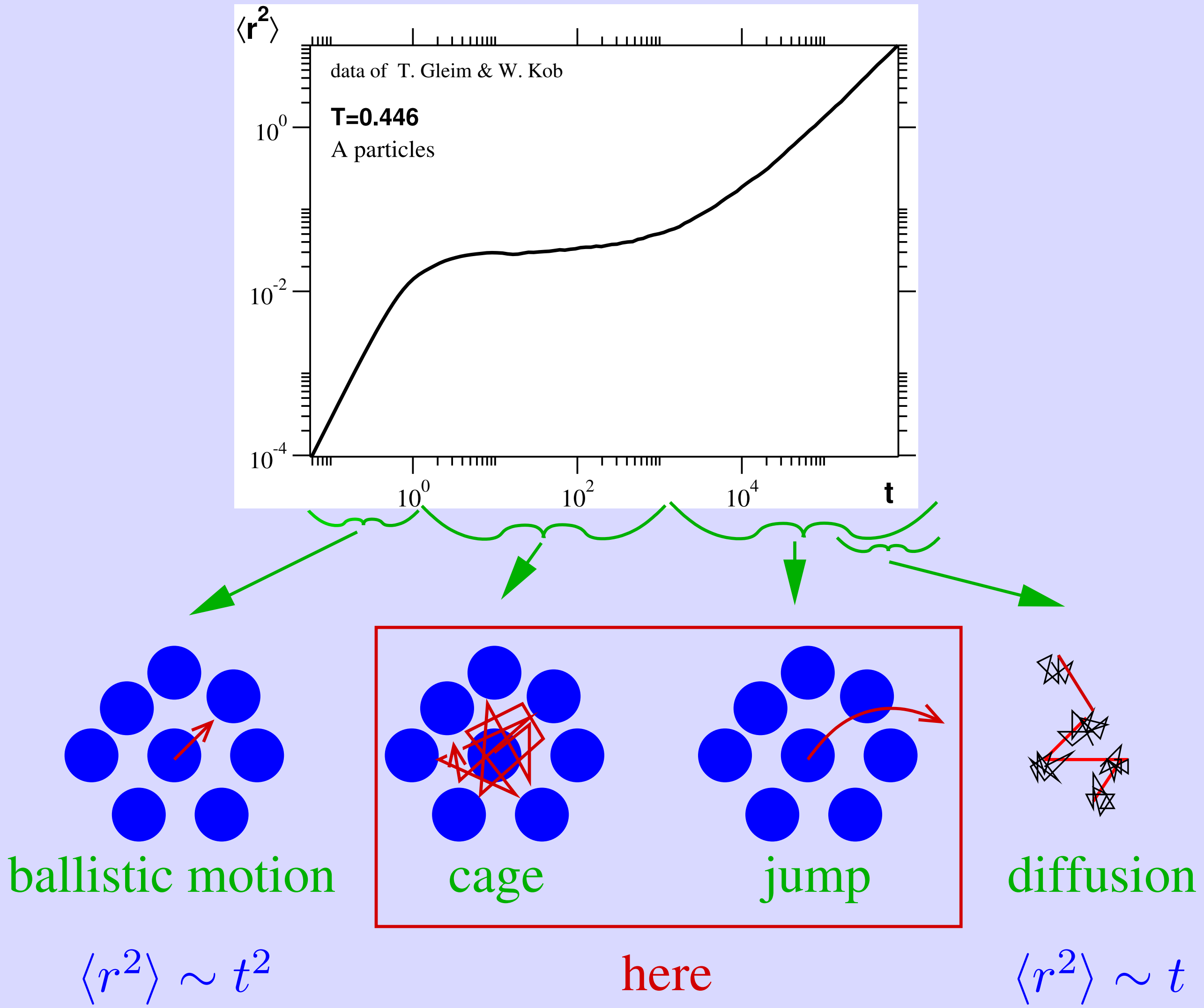
below glass transition:

$T = 0.15 - 0.43$

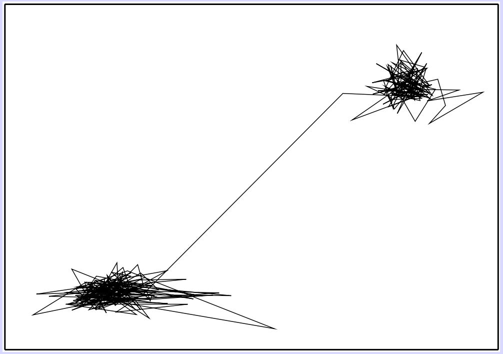
MCT: $T_{\mathrm{c}} = 0.435$ [W. Kob et al., PRL 73 (1994)]

Cage-Picture

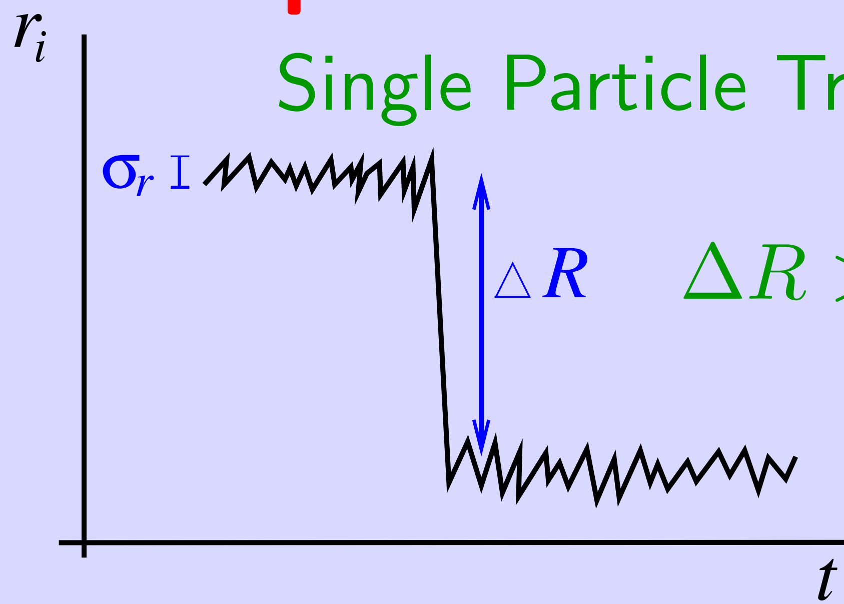
Mean-Squared Displacement: $\langle r^2 \rangle(t) = \left\langle \frac{1}{N} \sum_{i=1}^{N} \left(\underline{r}_i(t) - \underline{r}_i(0)\right)^2 \right\rangle$



Definition: Jump Occurrence

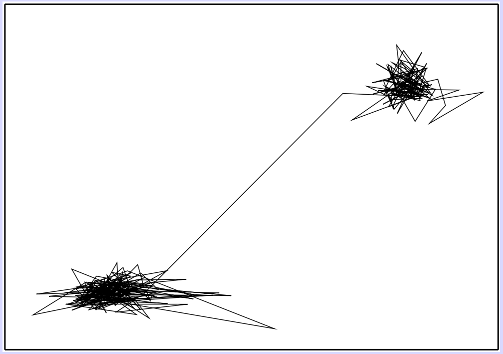


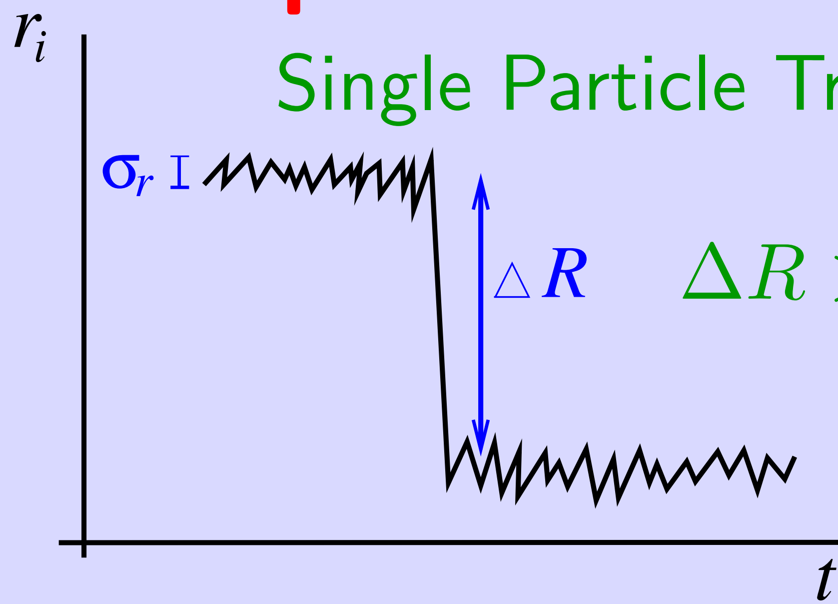
Single Particle Trajectory



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

Definition: Jump Occurrence



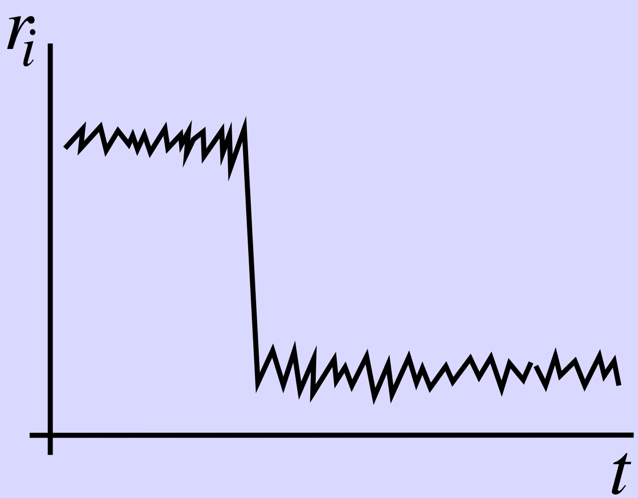


Single Particle Trajectory

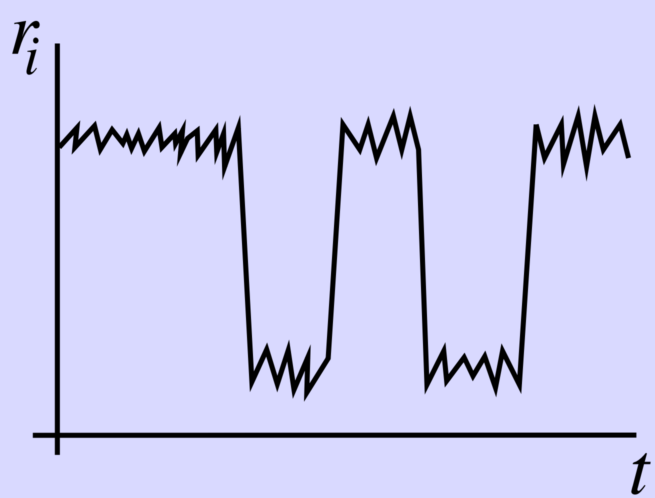
$$\Delta R > \sqrt{20}\,\sigma_r$$

Definition: Jump Type

Irreversible Jump



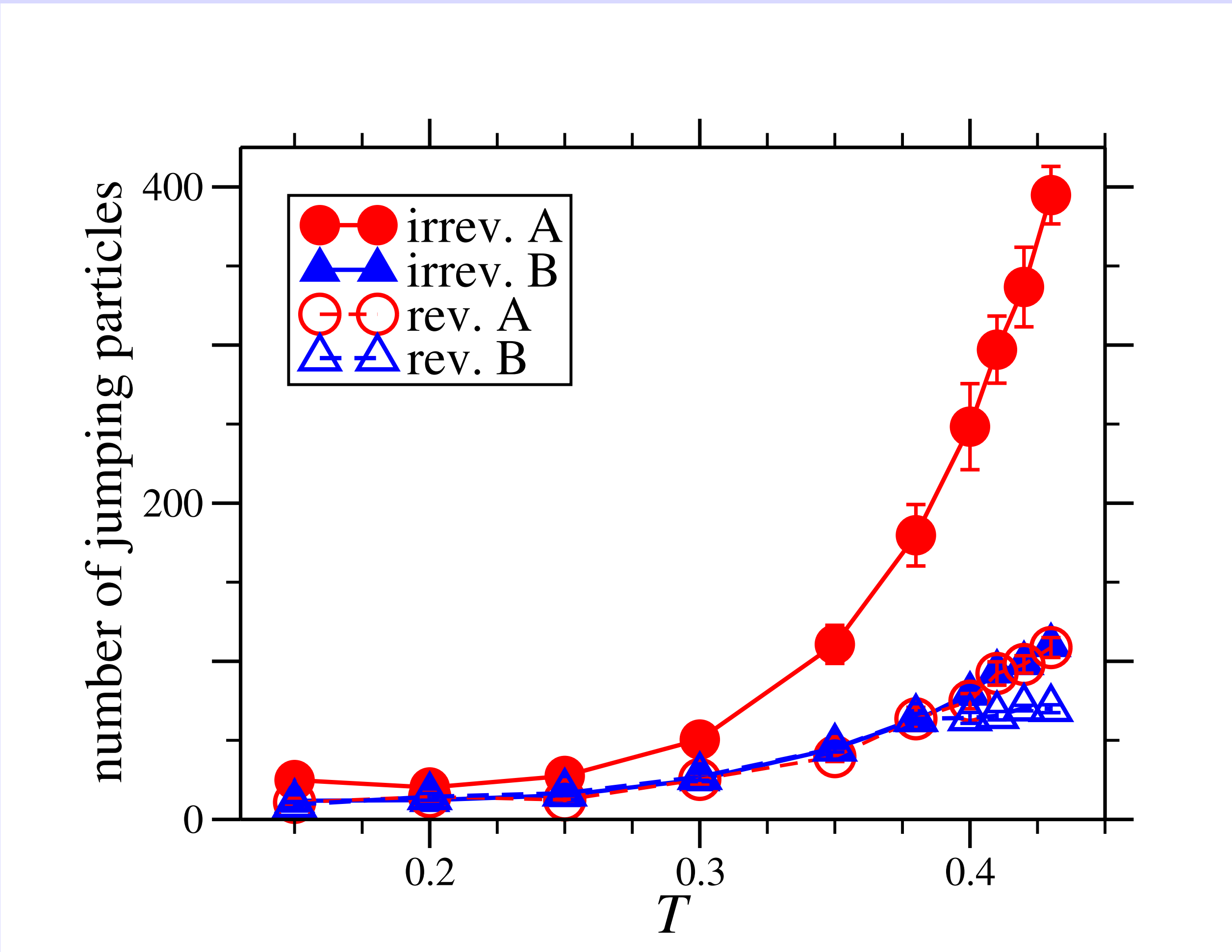
Reversible Jump



Outline

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

Number of Jumping Particles

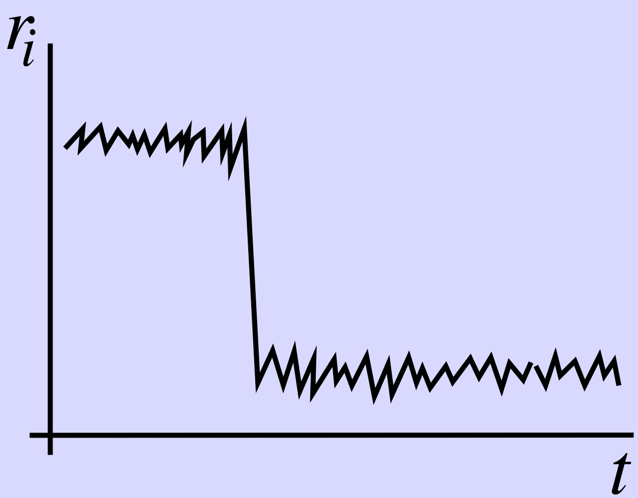


- ⟹ increasing with increasing T
- ⟹ both A & B particles jump
- ⟹ irrev. & reversible jumps at all temperatures T

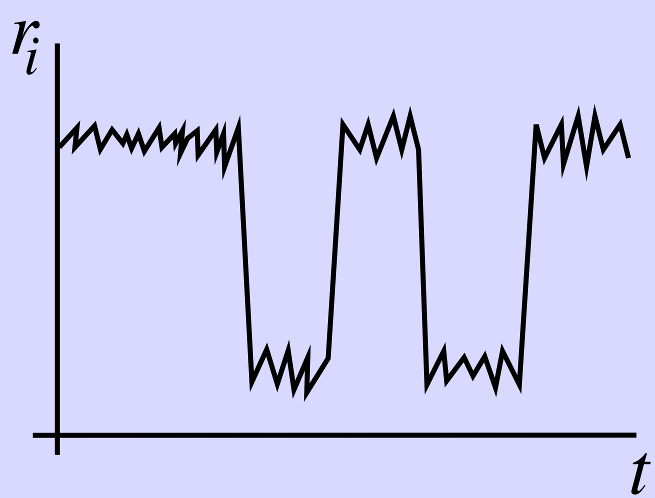
Fraction of Irreversibly Jumping Particles

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

Irreversible Jump

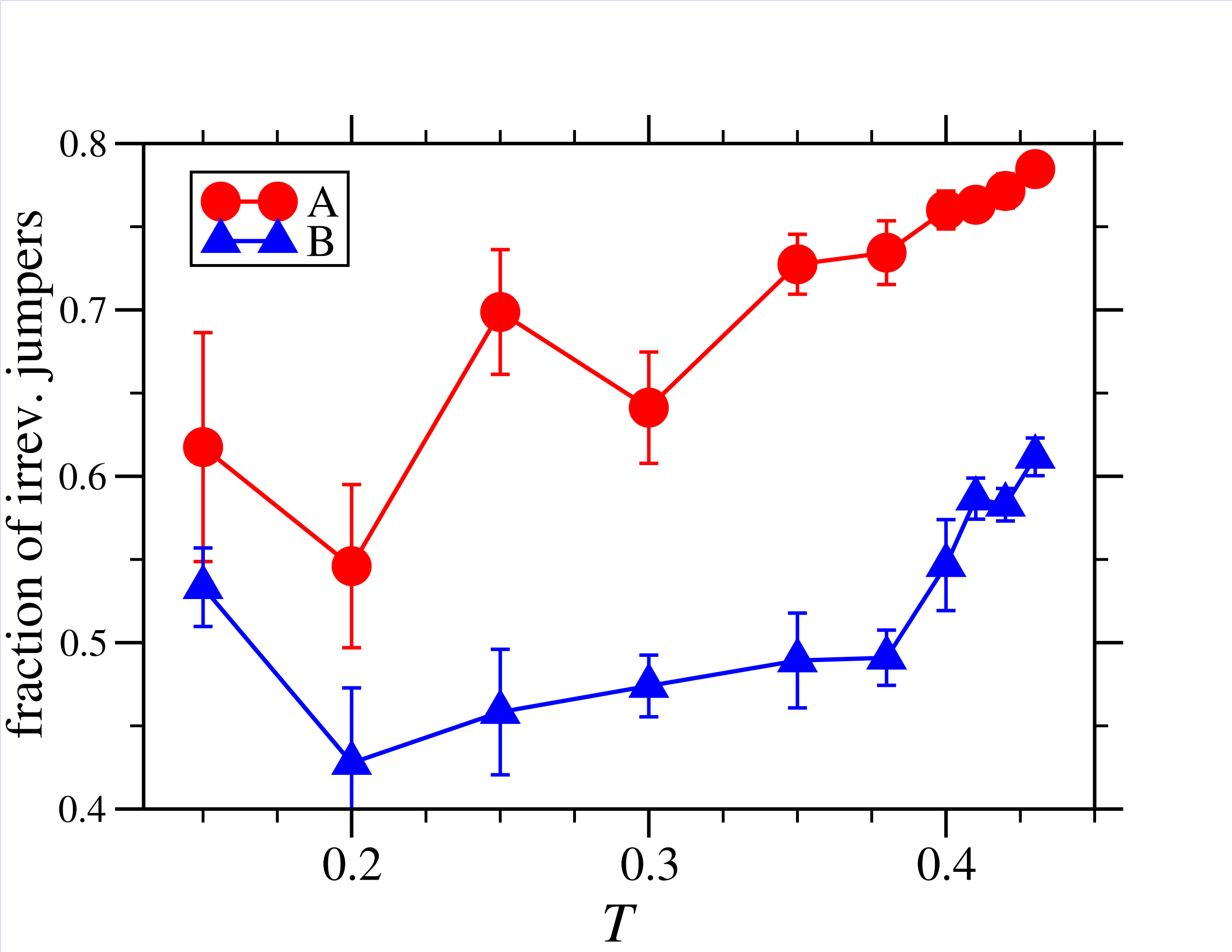


Reversible Jump



Fraction of Irreversibly Jumping Particles

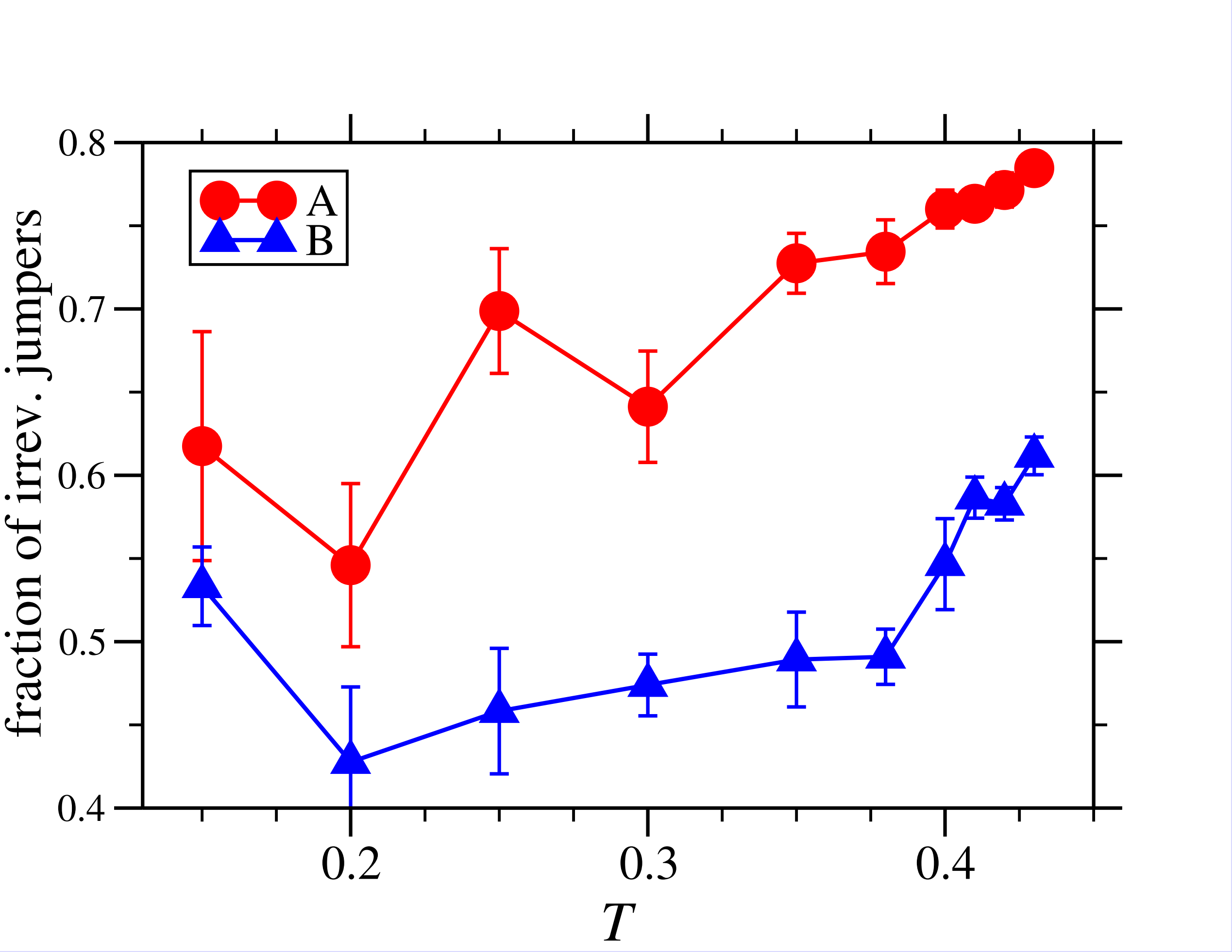
$$\text{fraction of irrev. jumpers} = \frac{\text{number of irrev. jump. part.}}{\text{number of jump. part.}}$$



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

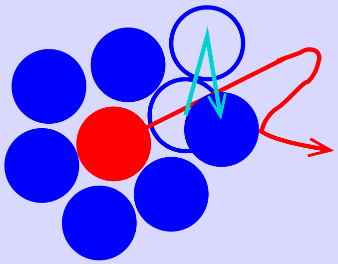
Fraction of Irreversibly Jumping Particles

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

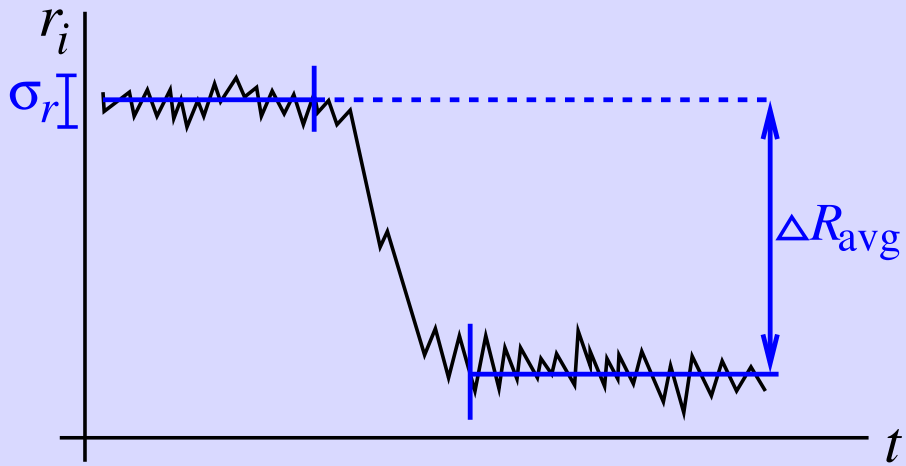


$\Longrightarrow$ fraction of irrev. jumpers increases with increasing T

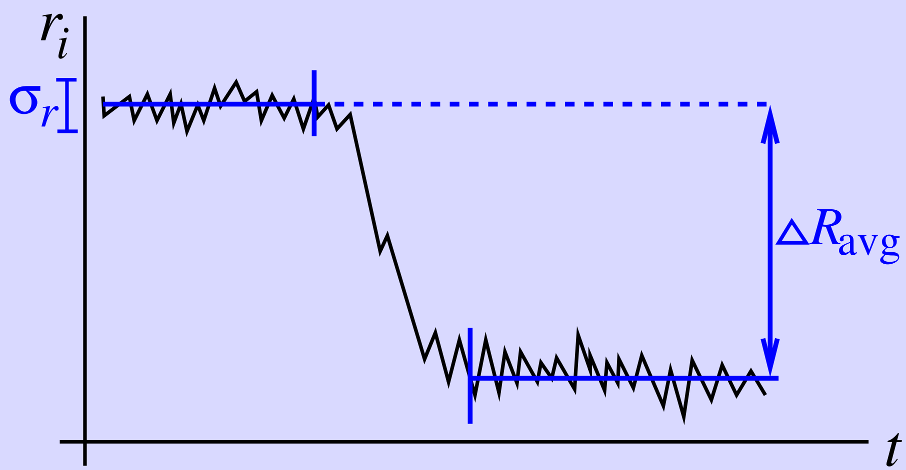
interpretation: door closing

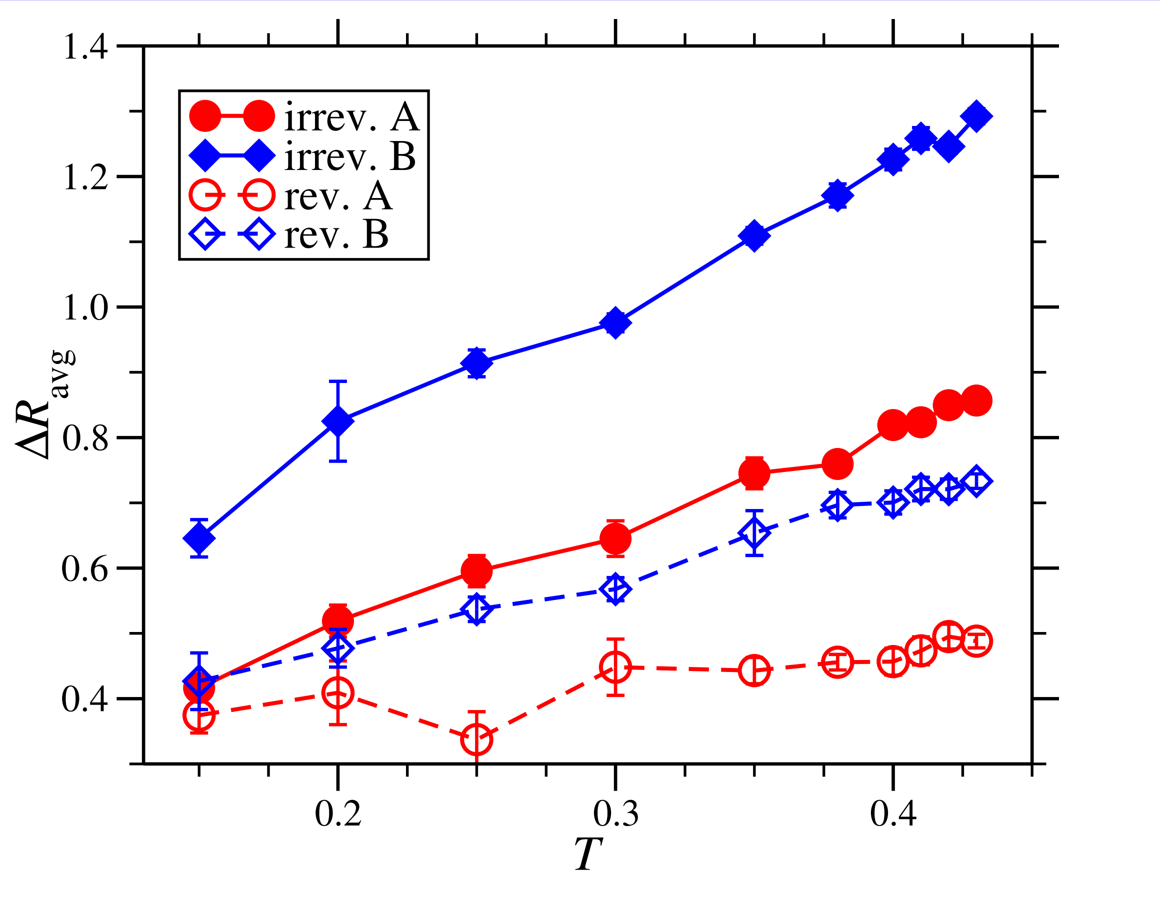


Jump Size



Jump Size



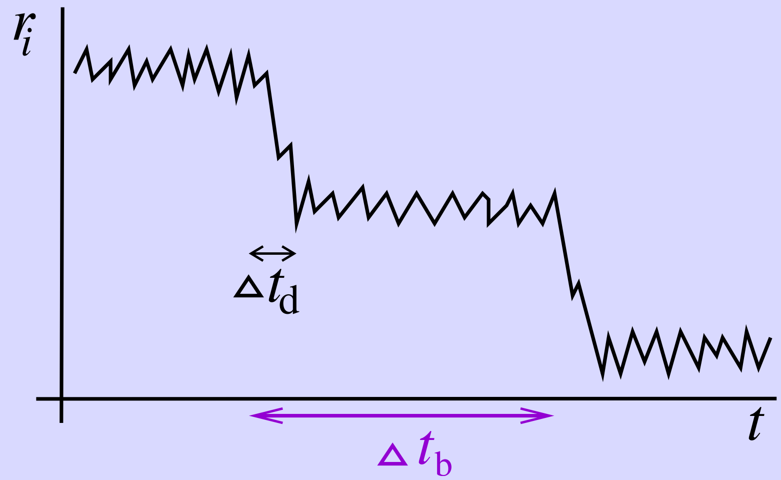


$\Longrightarrow$ increasing with increasing T

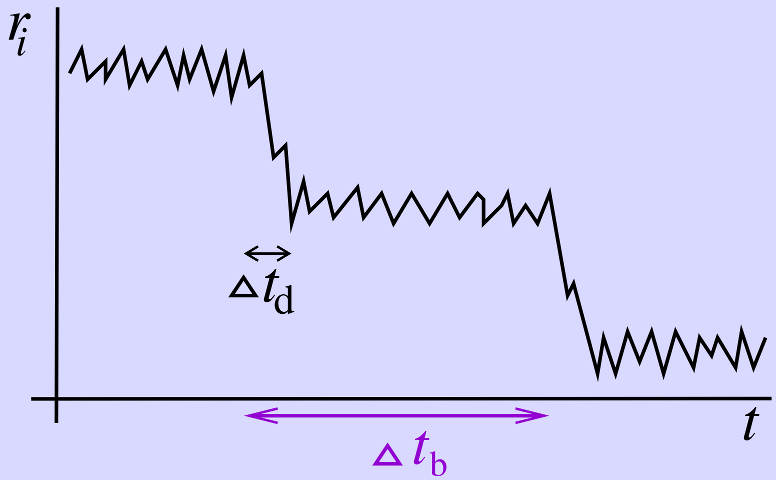
$\Longrightarrow$ (smaller) B-particles jump farther

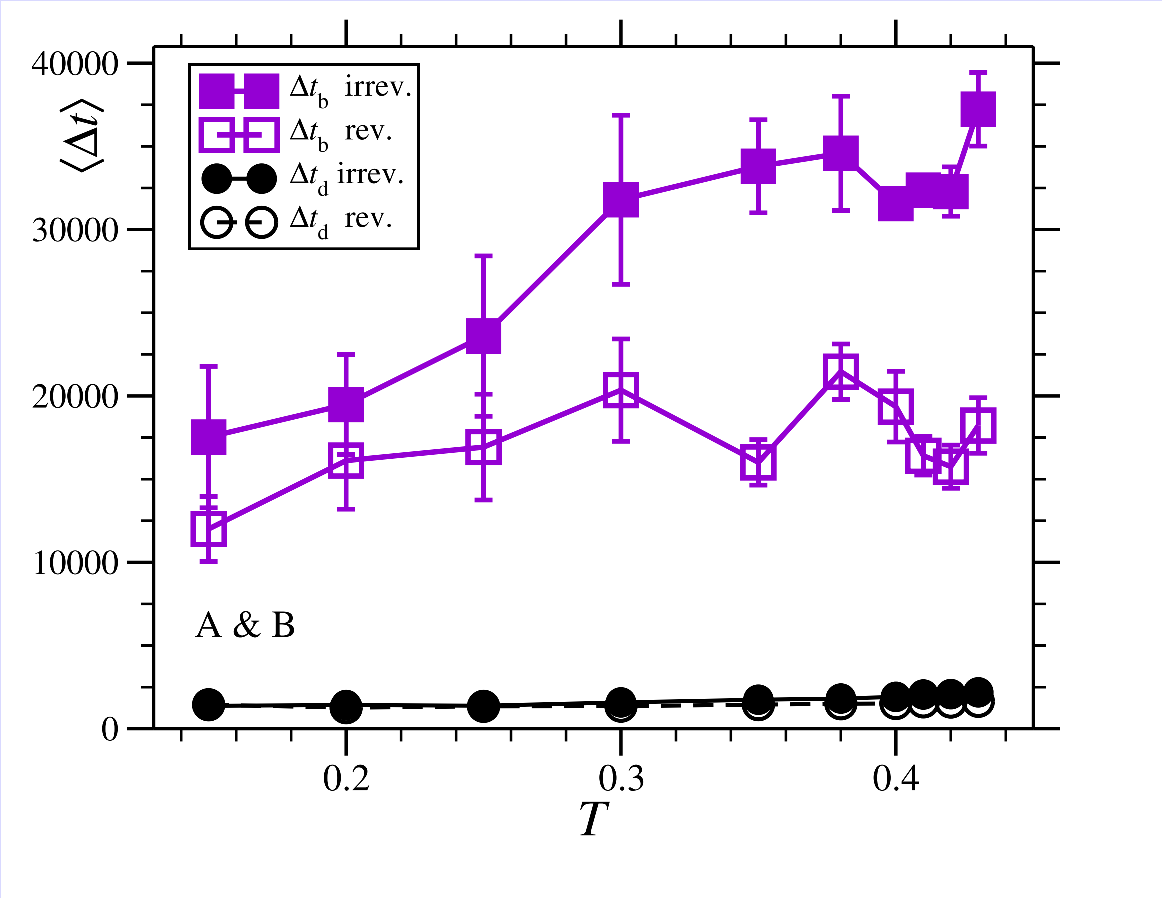
$\Longrightarrow$ irreversible jumps farther

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

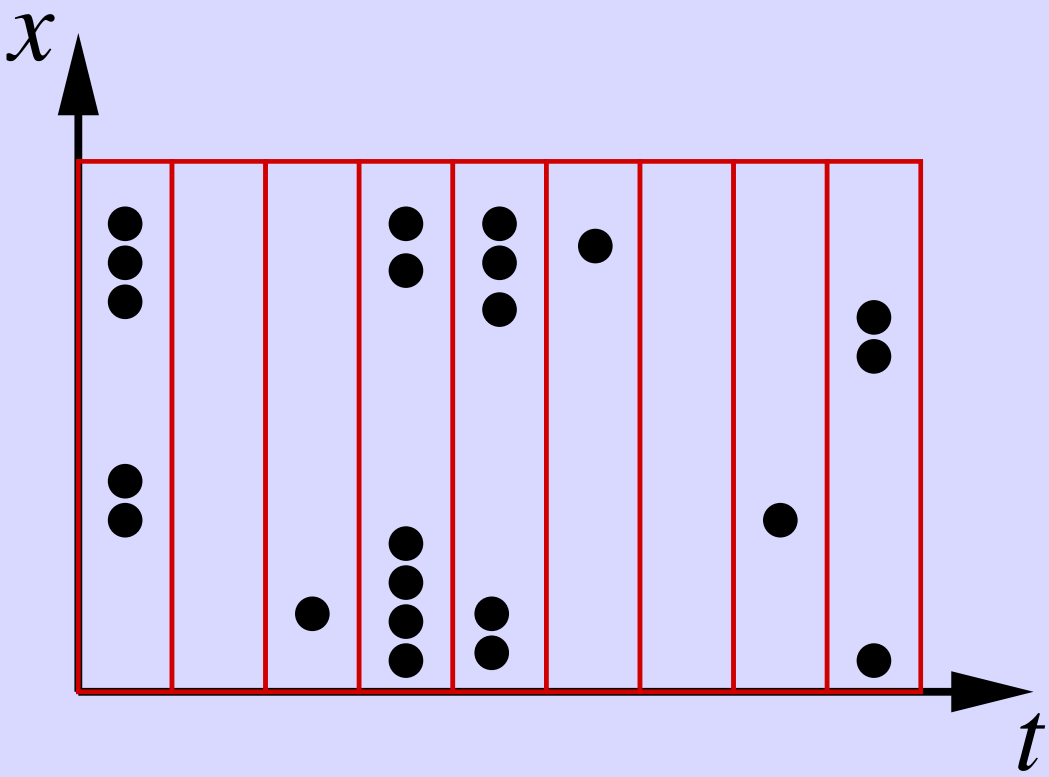
[J. Chem. Phys. **121**, 4781 (2004)]

Outline

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

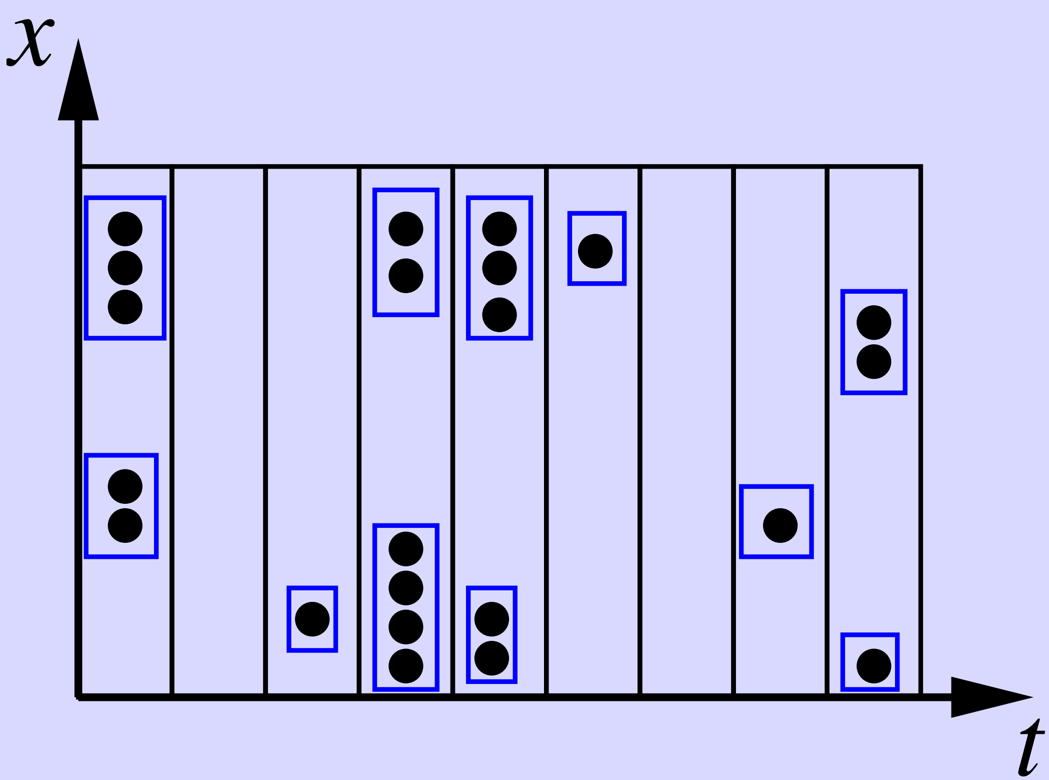
Simultaneously Jumping Particles

Definition: Correlated in Time & Space



Simultaneously Jumping Particles

Definition: Correlated in Time & Space

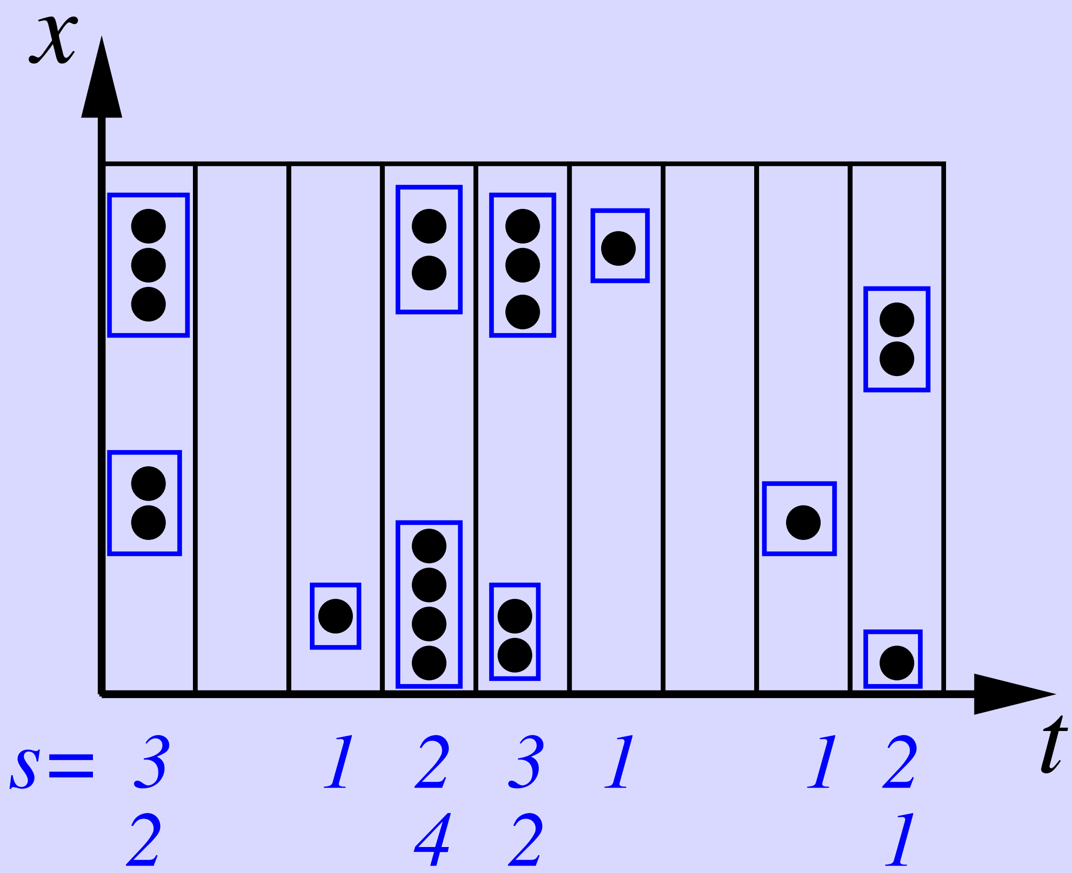


Cluster:

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

Simultaneously Jumping Particles

Cluster Size $=$ number of particles in cluster

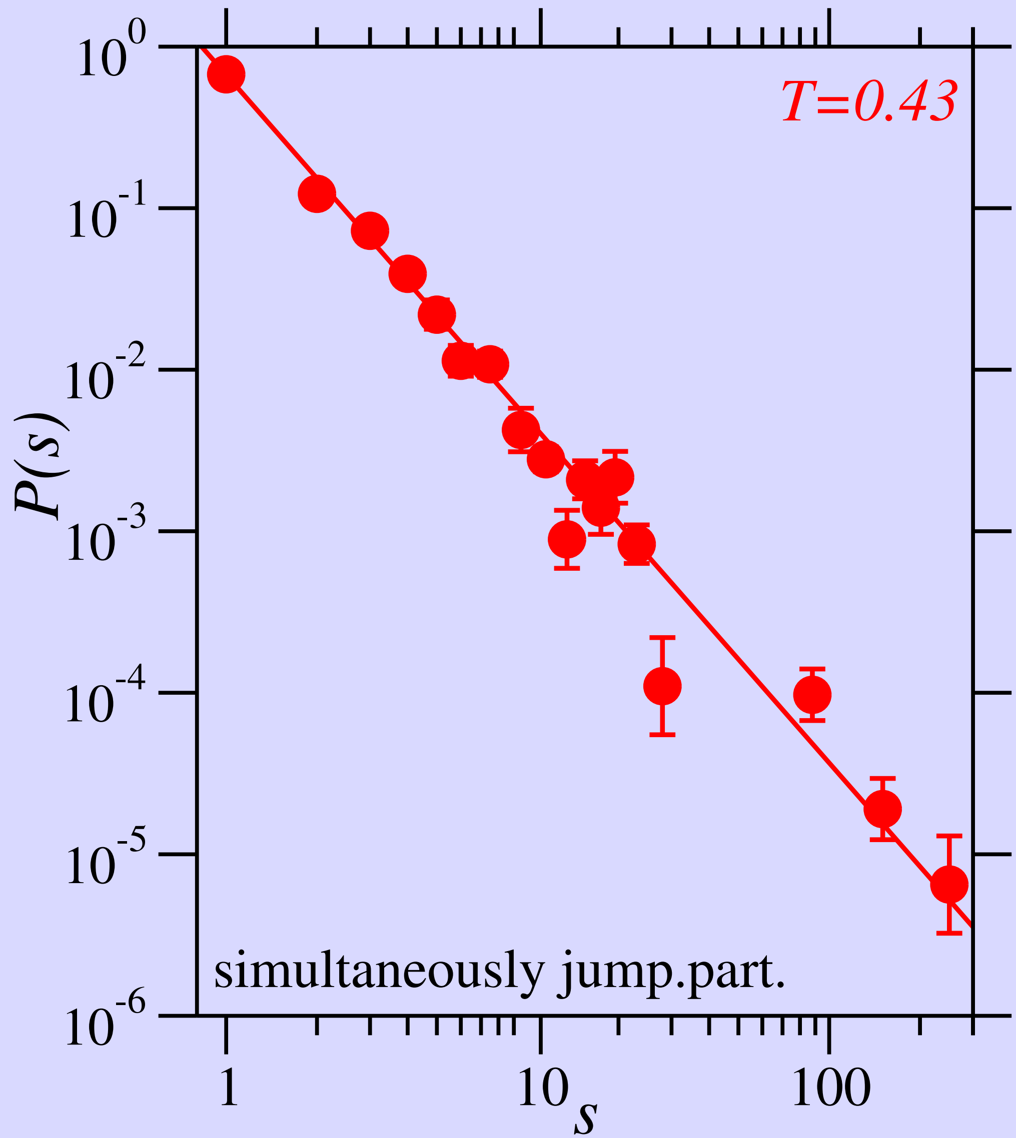


Cluster:

nearest neighbor connections

Cluster Size Distribution

of Simultaneously Jumping Particles



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

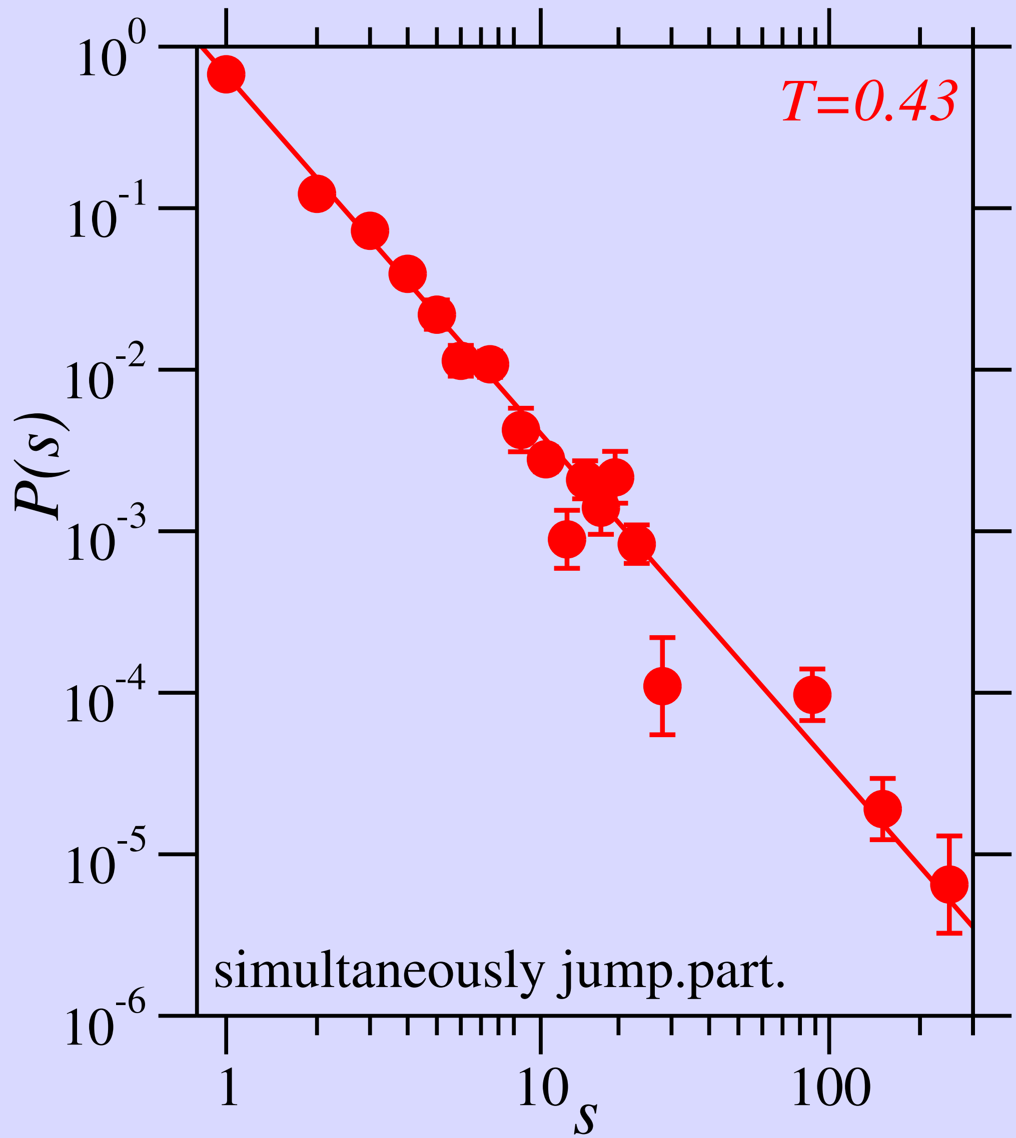
$\Longrightarrow P(s) \sim s^{-\tau}$

$\tau = 1.89 \pm 0.03$

$\Longrightarrow$ critical behavior

Cluster Size Distribution

of Simultaneously Jumping Particles



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

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

$\tau = 1.89 \pm 0.03$

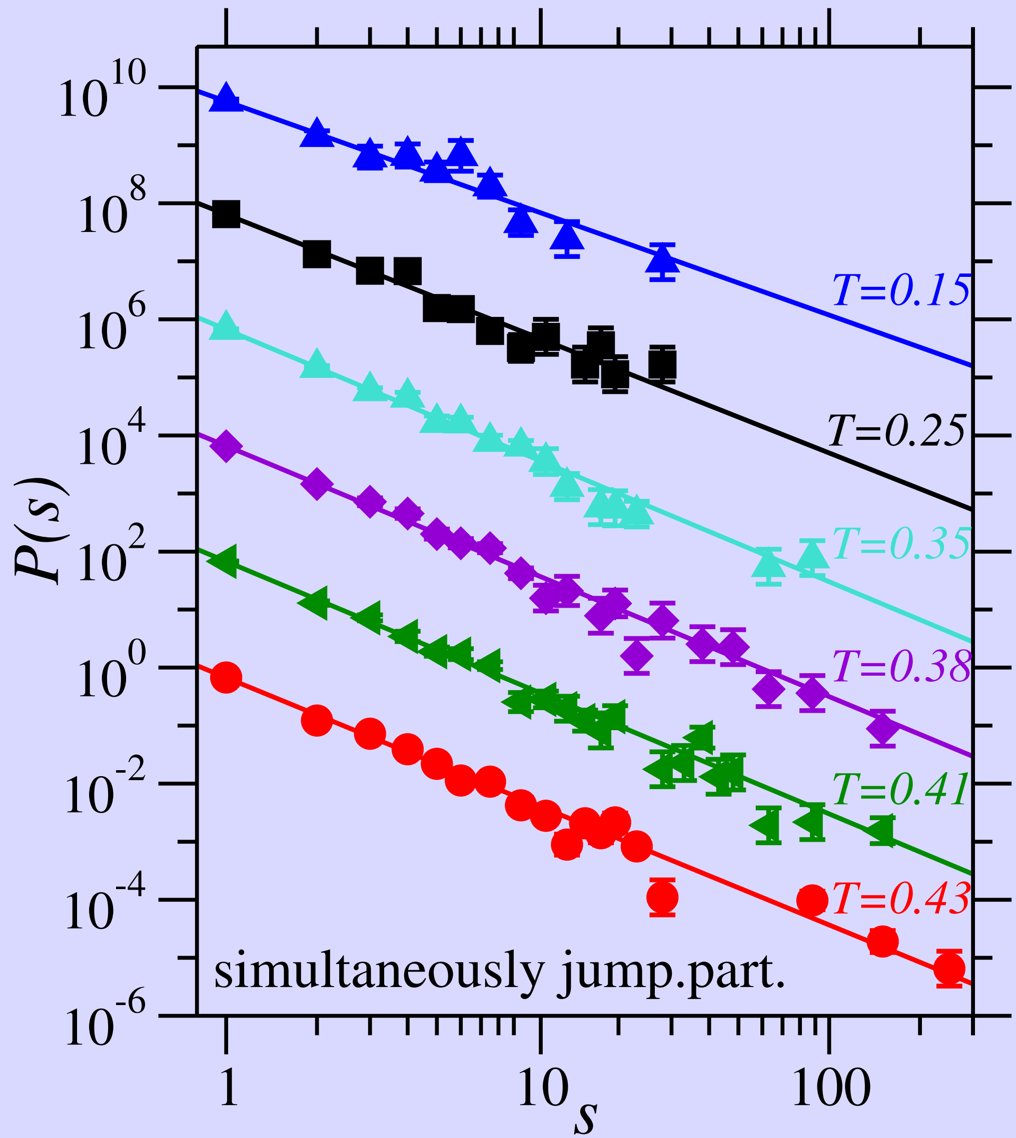
$\Longrightarrow$ critical behavior

$\Longrightarrow$ Percolation?

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

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**

$\tau(T)$

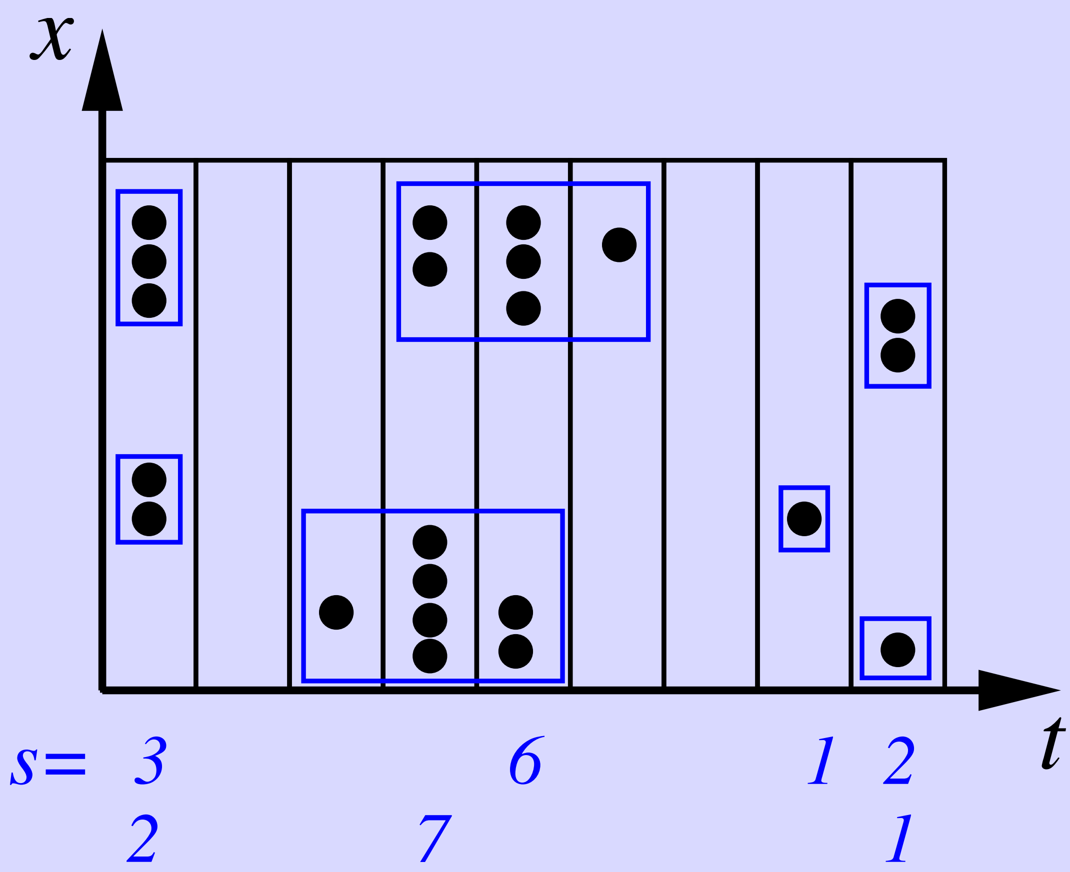
Self-Organized Criticality: Similarities

- 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

Outline

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

Temporally Extended Cluster



Definition:

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

connected if:

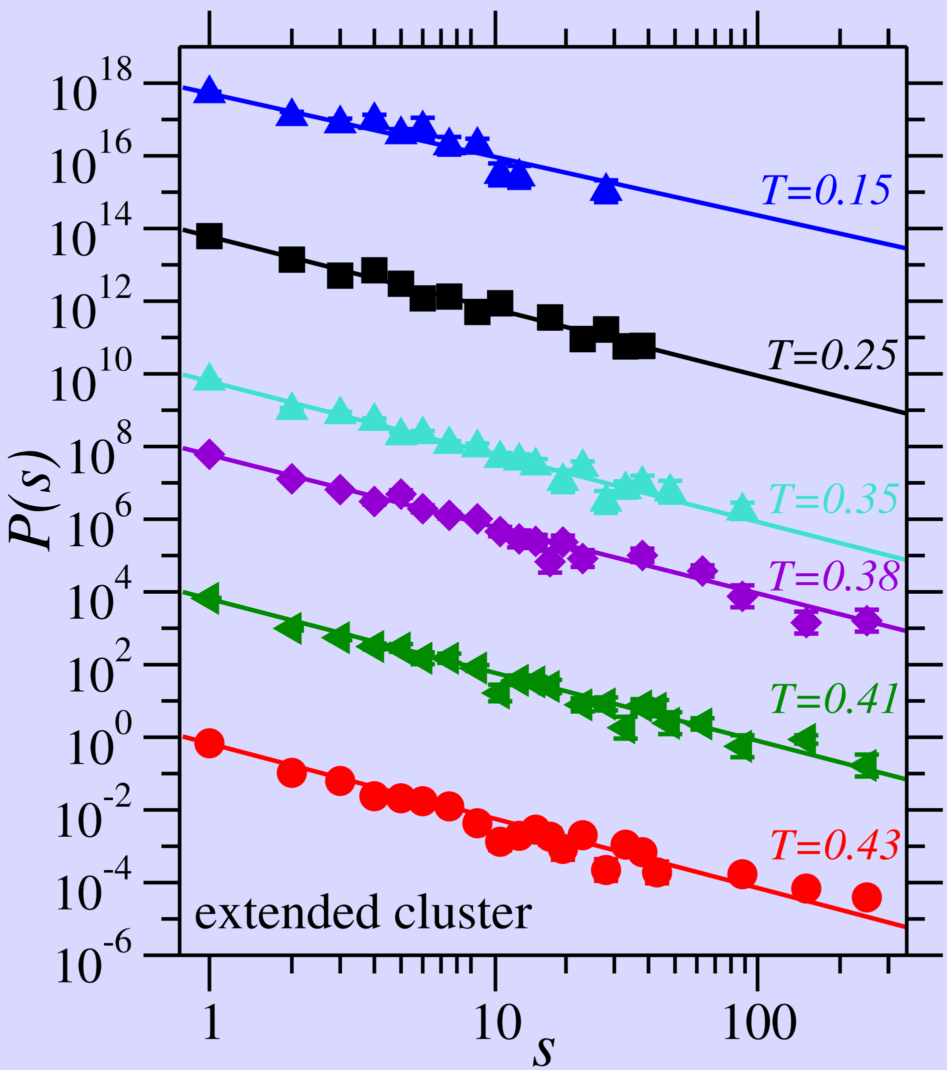
$$\Delta r \; < \; r_{\text{cutoff}} \quad \text{and}$$

$$\Delta t \; < \; t_{\text{cutoff}}$$

quantifies avalanche

Cluster Size Distribution

of Temporally Extended Clusters

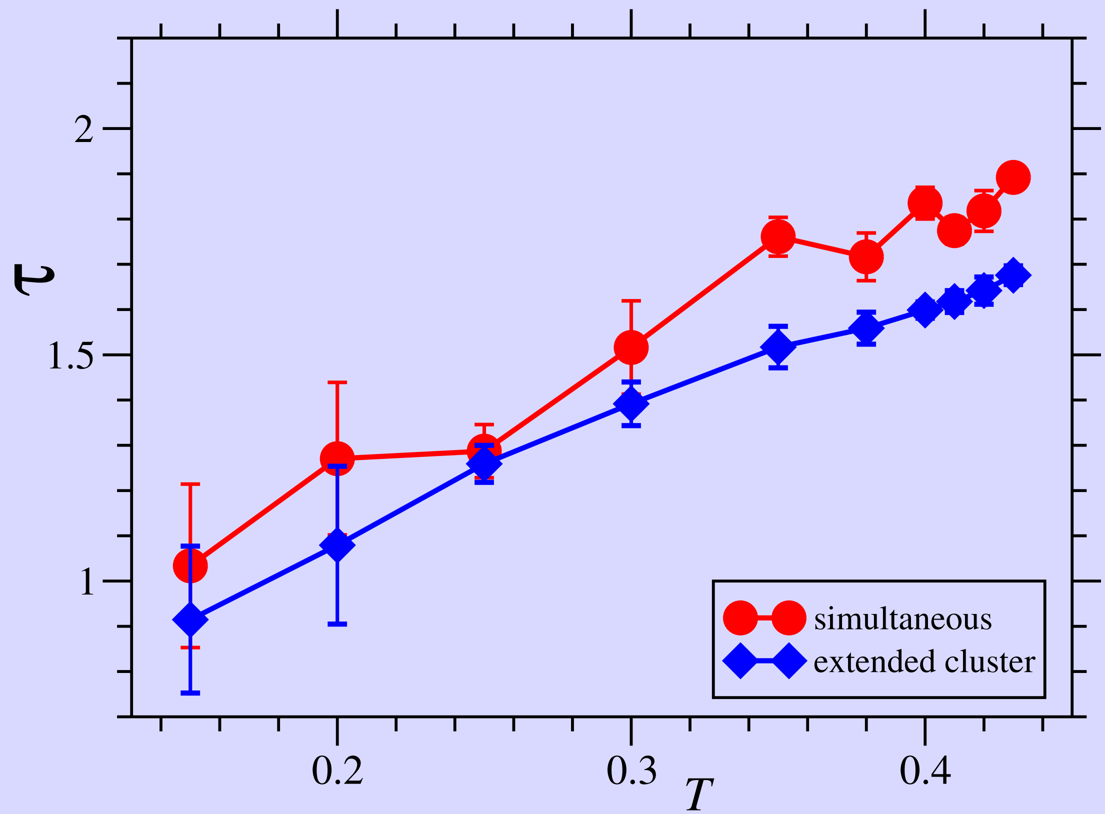


$\Longrightarrow P(s) \sim s^{-\tau}$

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

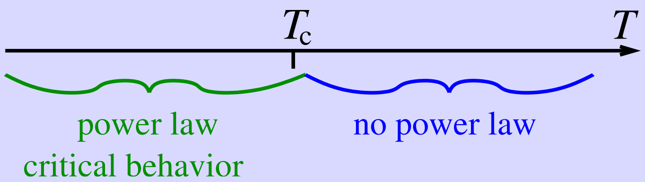
Exponent $\tau(T)$

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



slightly above T_c $\tau \approx 1.86$

[Donati et al. 1999]



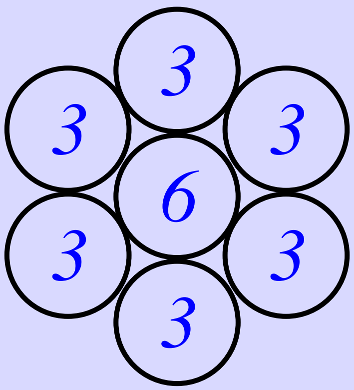
P simult.

Shape of Clusters

z = number of nearest neighbors within cluster

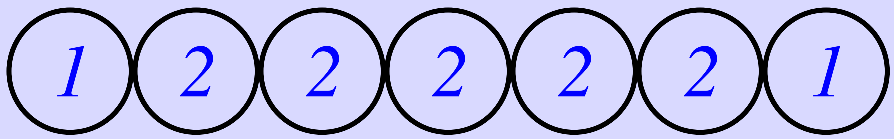
s = number of particles (cluster size)

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



s=7

$\langle z \rangle$=3.4



s=7

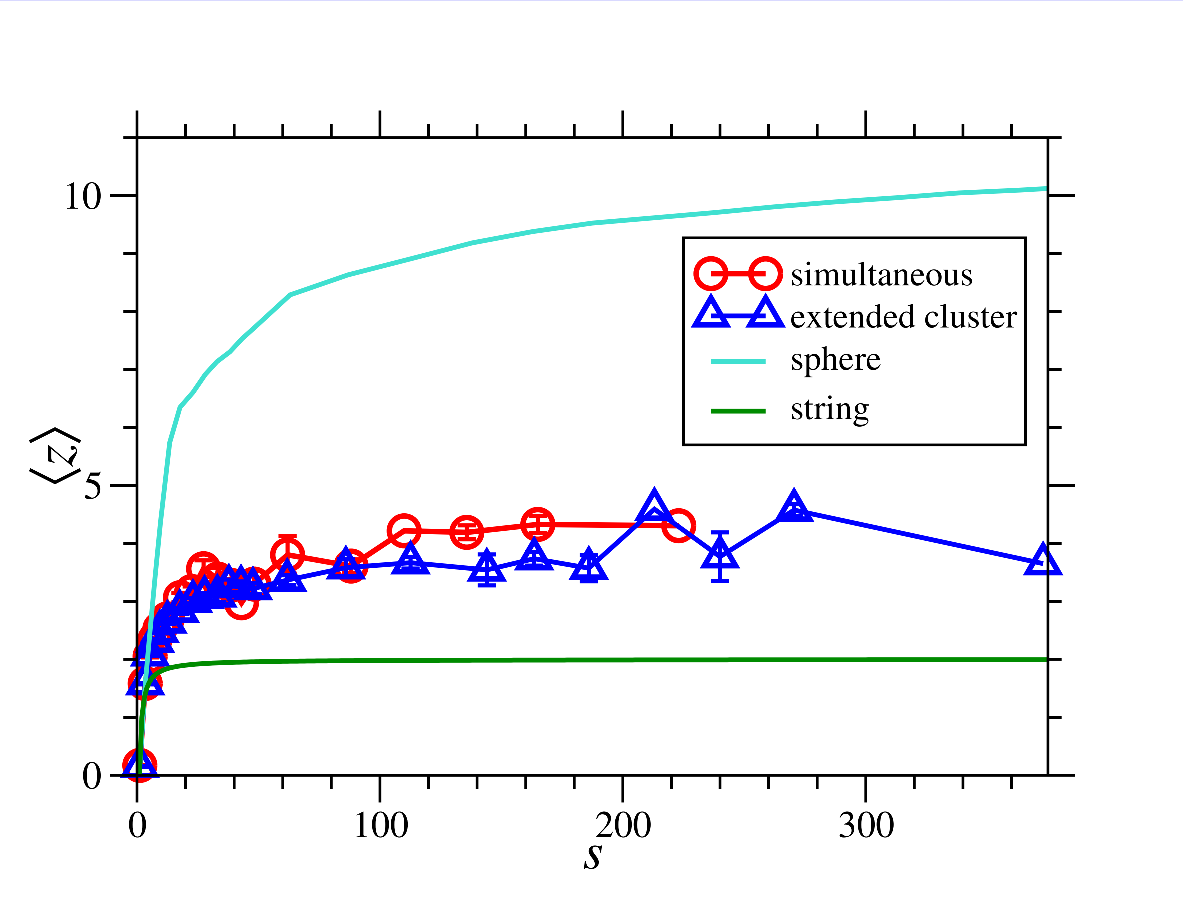
$\langle z \rangle$=1.7

Shape of Clusters

z = number of nearest neighbors within cluster

s = number of particles (cluster size)

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



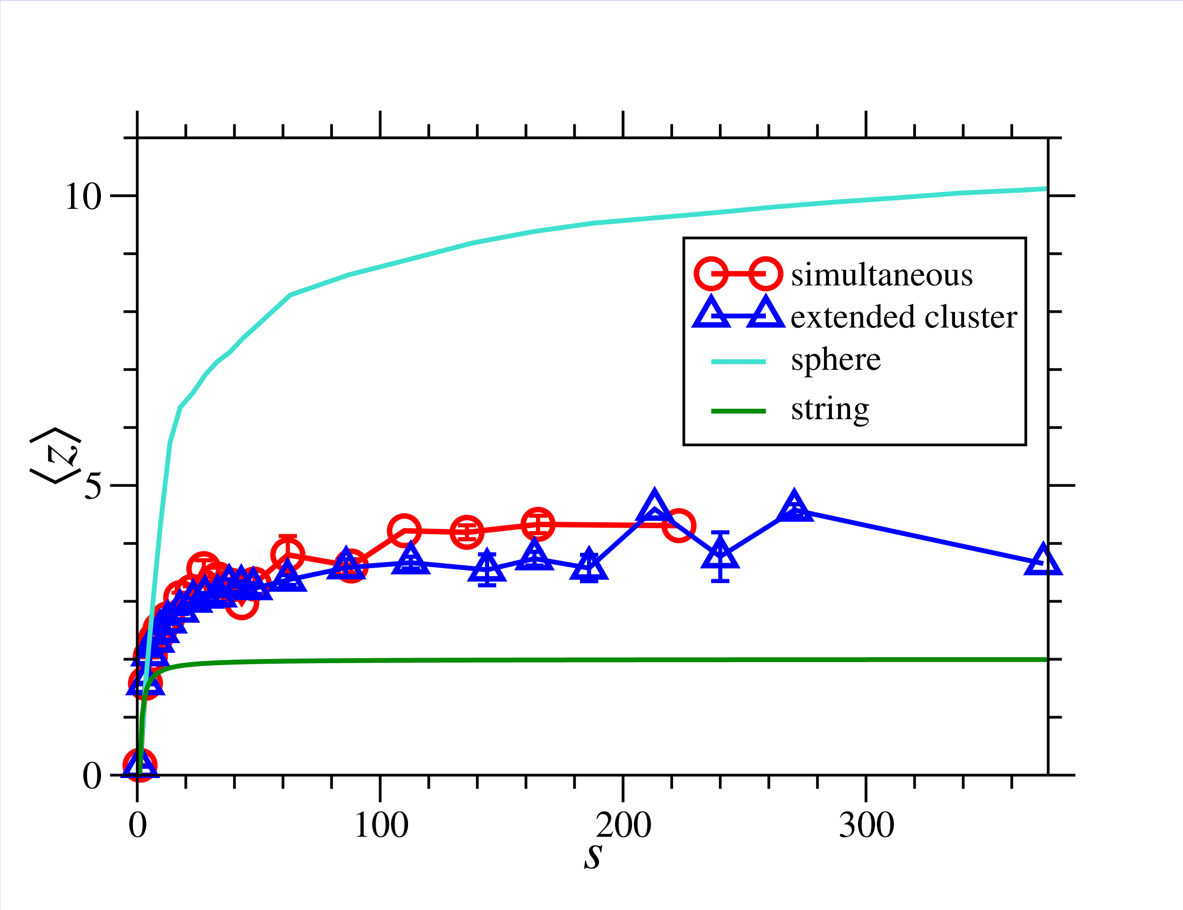
$\Longrightarrow$ string-like clusters

Shape of Clusters

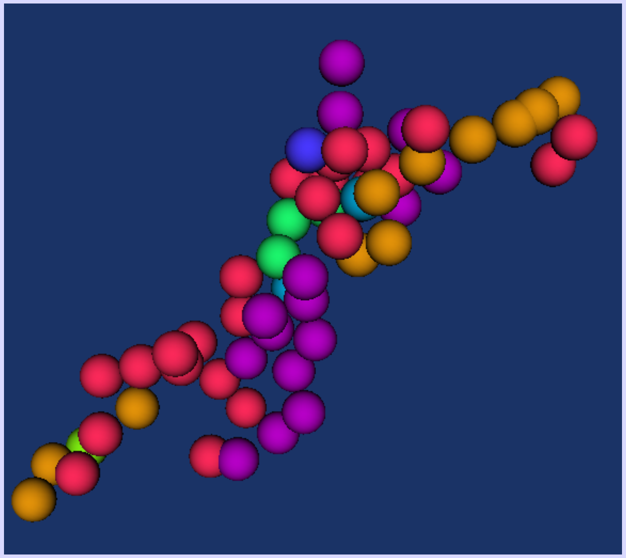
z = number of nearest neighbors within cluster

s = number of particles (cluster size)

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



$\Longrightarrow$ string-like clusters

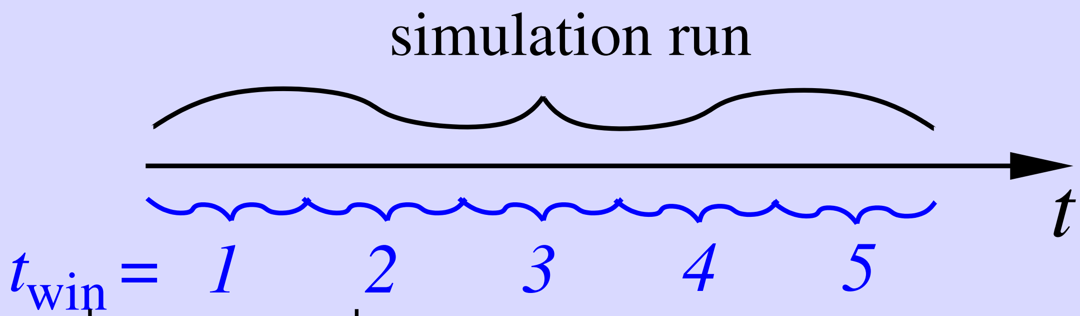


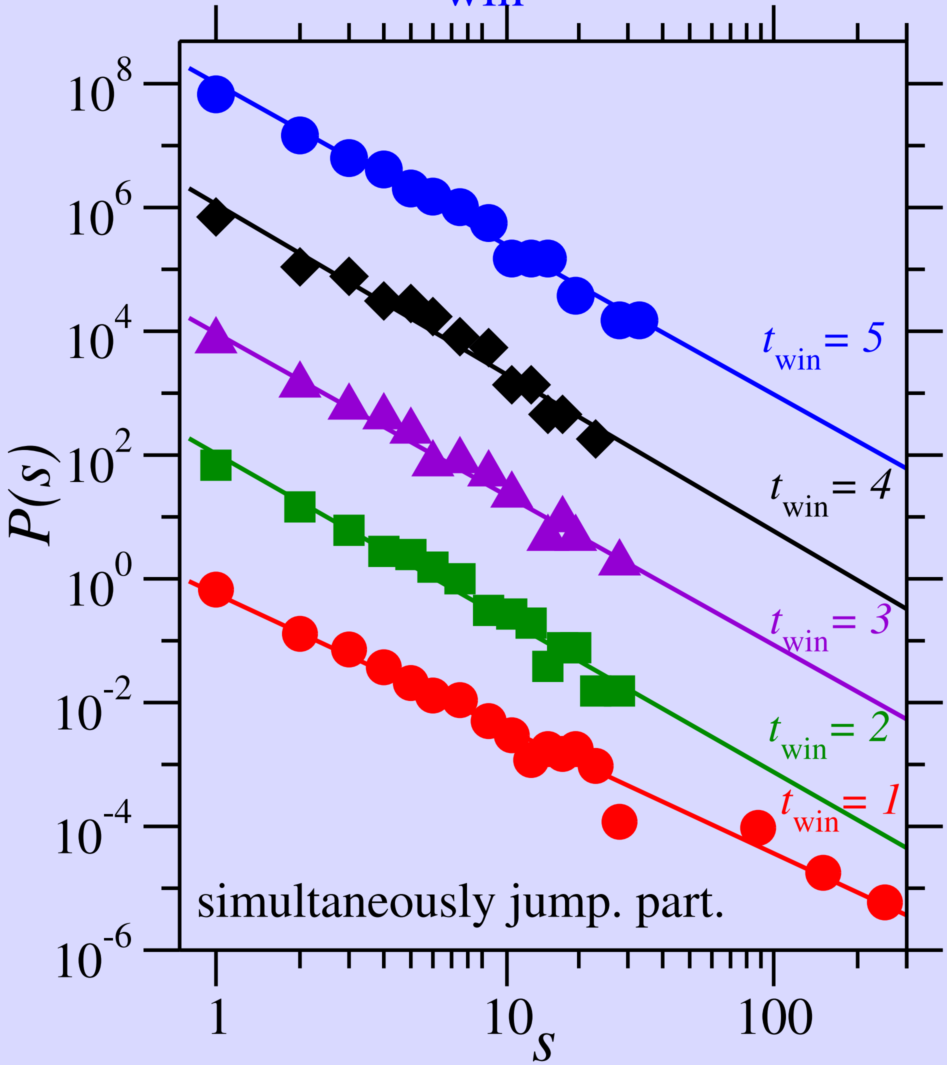
same color = same time

Outline

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

History Dependence





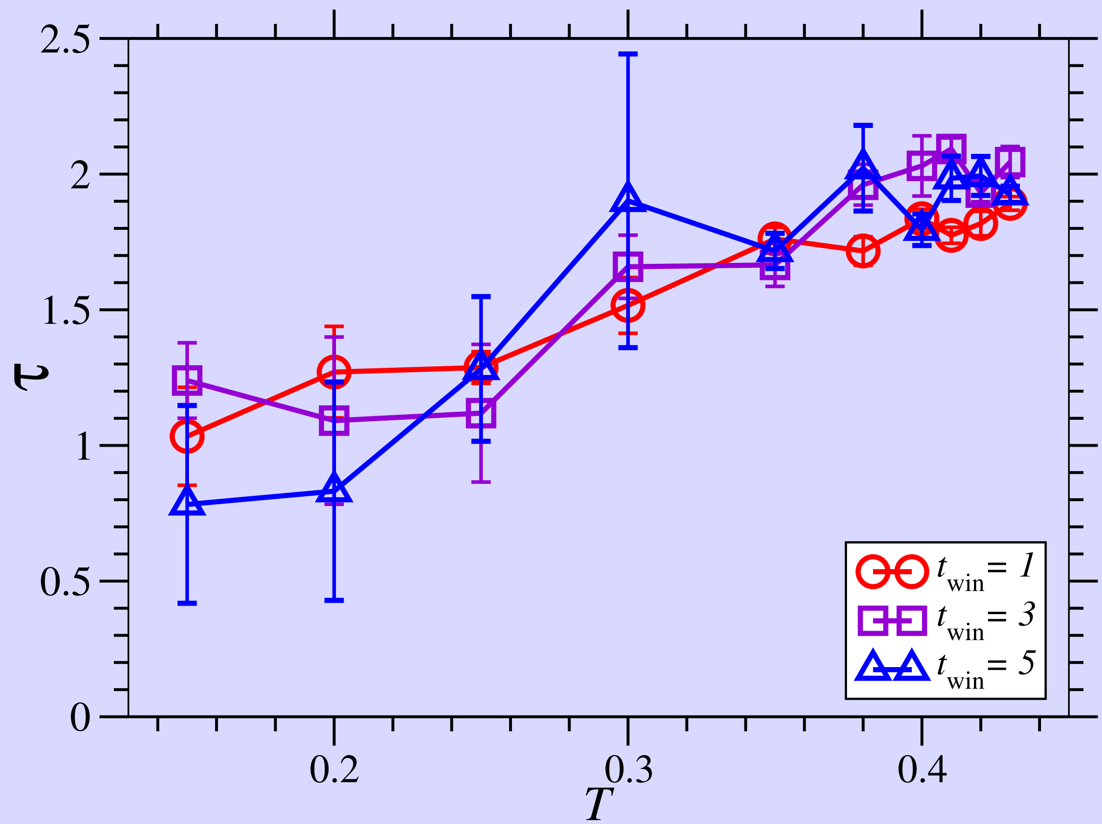
Power Law

(Simultan. Jump. Part.)

$\Longrightarrow$ aging independent

Exponent $\tau(T)$

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



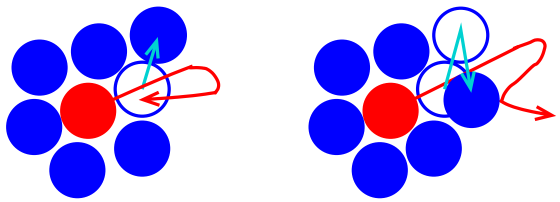
$\Longrightarrow$ aging independent

Outline

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

Summary: Jump Statistics

reversible and irreversible jumps:

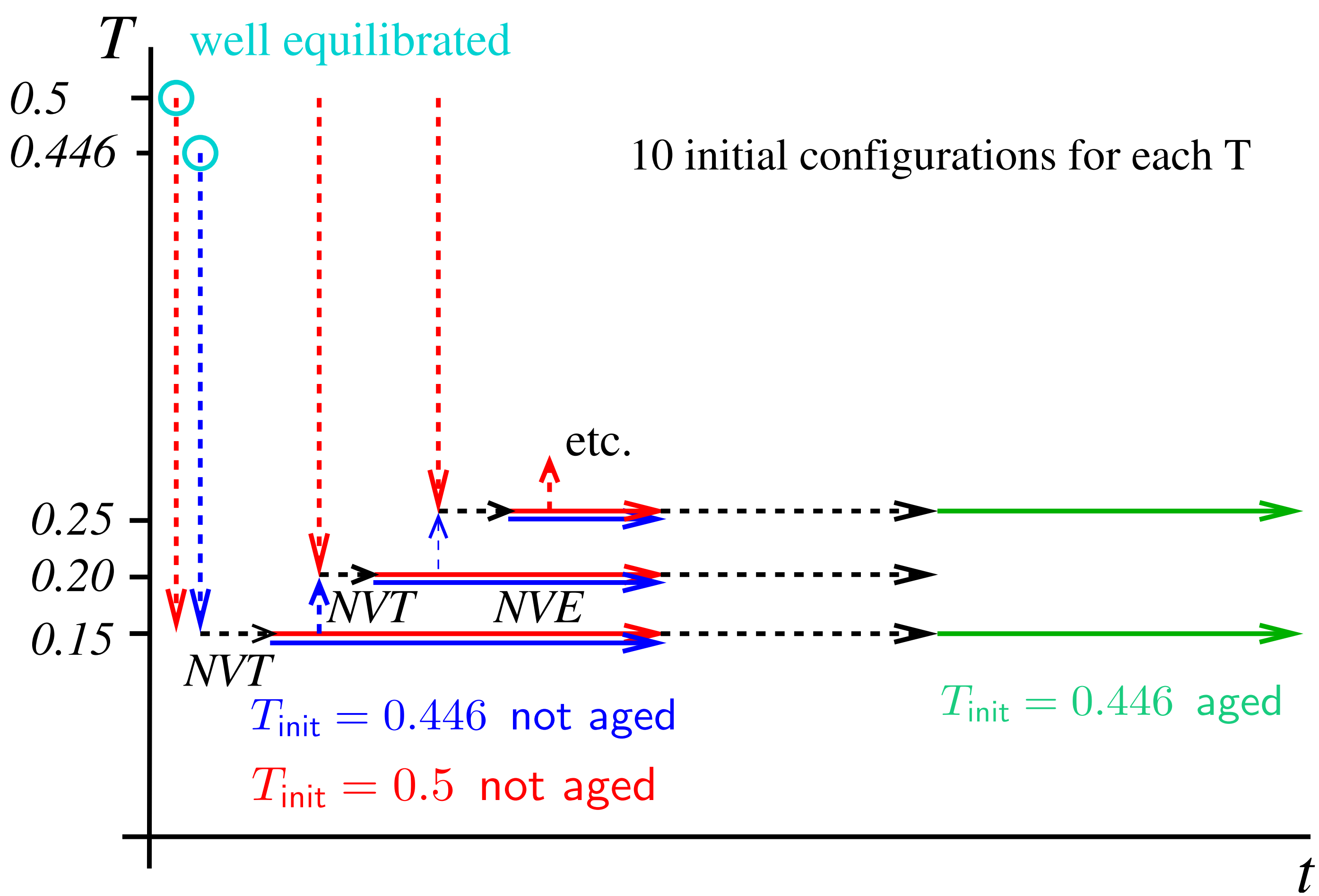


reversible jump   irreversible jump

At larger temperature relaxation:

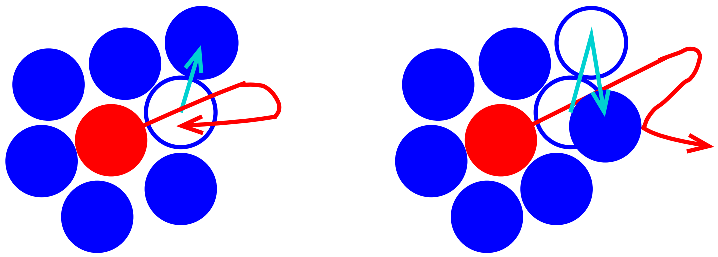
- via more jumping particles
- via larger jumpsizes
- not via Δt_{b} (indep. of T)

History of Production Runs



Summary: Jump Statistics

reversible and irreversible jumps:



reversible jump irreversible jump

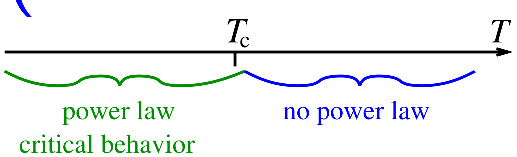
At larger temperature relaxation:

- 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:

- aging to equilibrium [to be submitted to PRE]
  (J. A. Roman & J. Horbach)
- local incoherent intermediate scattering function
  (A. Parsaeian & H. E. Castillo)
- jumps
  (R. A. Bjorkquist, L. M. Chambers)

granular media: (T. Aspelmeier & A. Zippelius)

Acknowledgments

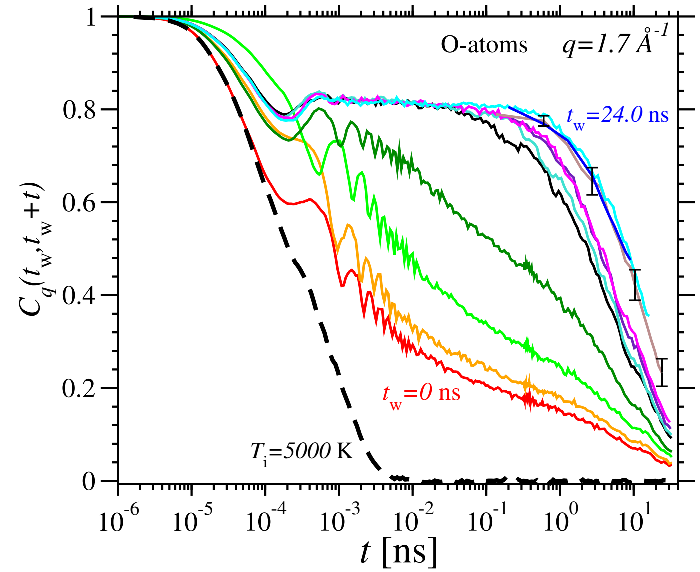
A. Zippelius, K. Binder, E. A. Baker, J. Horbach

Inst. of Theor. Physics, Univ. Göttingen, SFB 262 and DFG Grant No. Zi 209/6-1

SiO_2: Aging to Equilibrium

$C_q(t_{\rm w}, t_{\rm w}+t)$ and $\Delta r^2(t_{\rm w}, t_{\rm w}+t)$:

Three $t_{\rm w}$ Ranges:

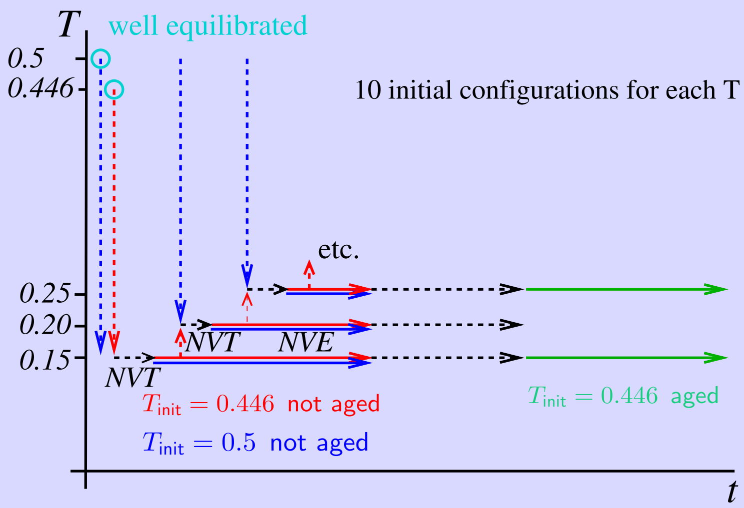


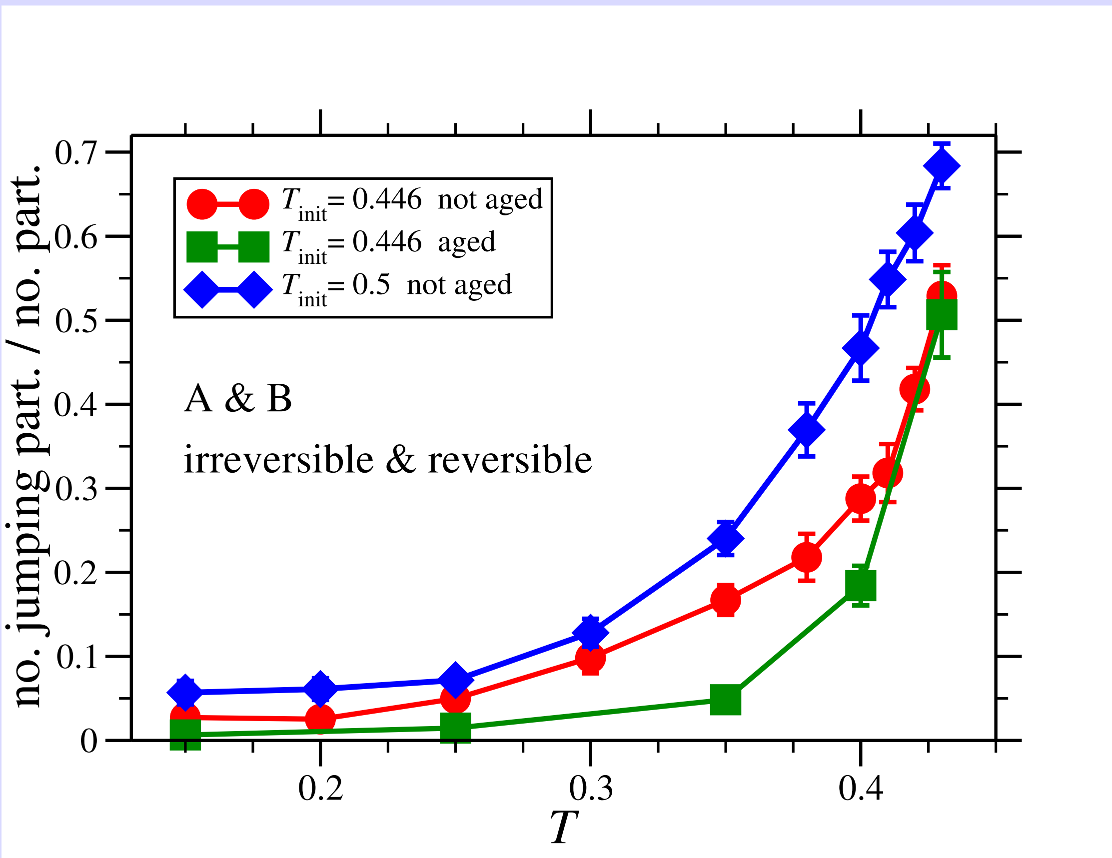
- $t_{\rm w}$ **small:**
  - ◇ $t_{\rm w} = 0$ and t small: $T_{\rm i}$ good approx.
  - ◇ dependent on $t_{\rm w}$, $T_{\rm i}$, $T_{\rm f}$
- $t_{\rm w}$ **intermediate:**
  - ◇ plateau indep. of $t_{\rm w}$ and T_i
  - ◇ C_q time superposition (not Δr^2)
  - ◇ $C_q^{\rm AG} = C(q, z(t_{\rm w}, t))$
- $t_{\rm w}$ **large:**
  - ◇ indep. of $t_{\rm w}$ and $T_i \longrightarrow$ equilibrium
  - ◇ for C_q equilibrium included in superposition

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

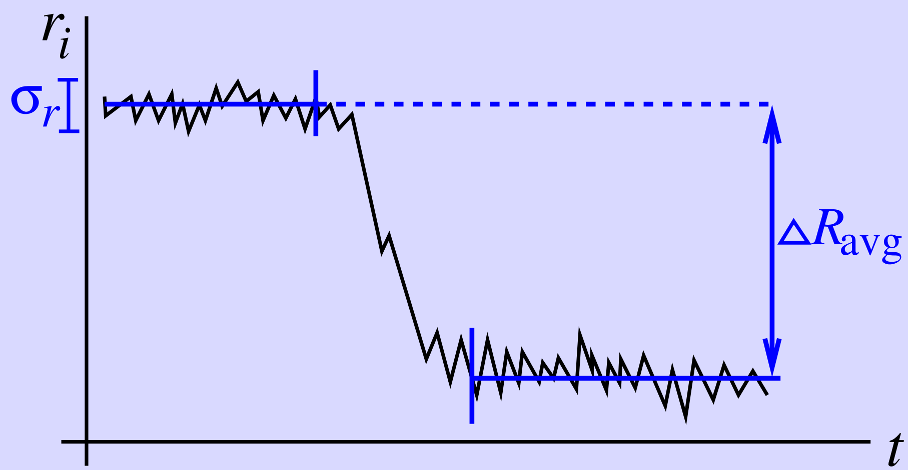


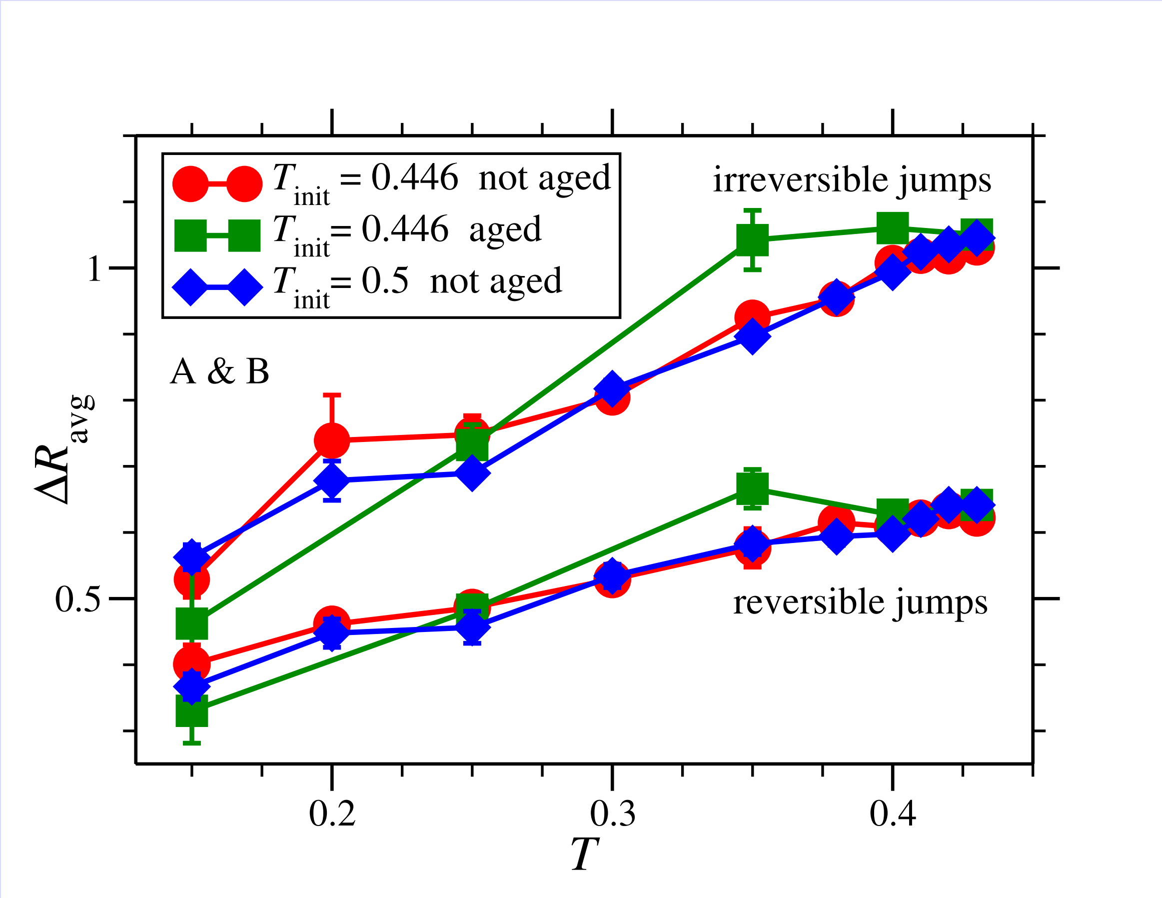


Number of Jump. Part.

$\Longrightarrow$ history dependent

History Dependence

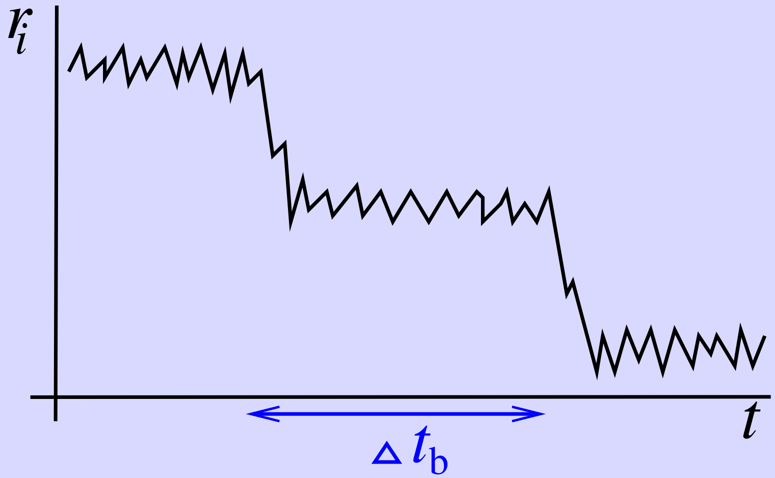


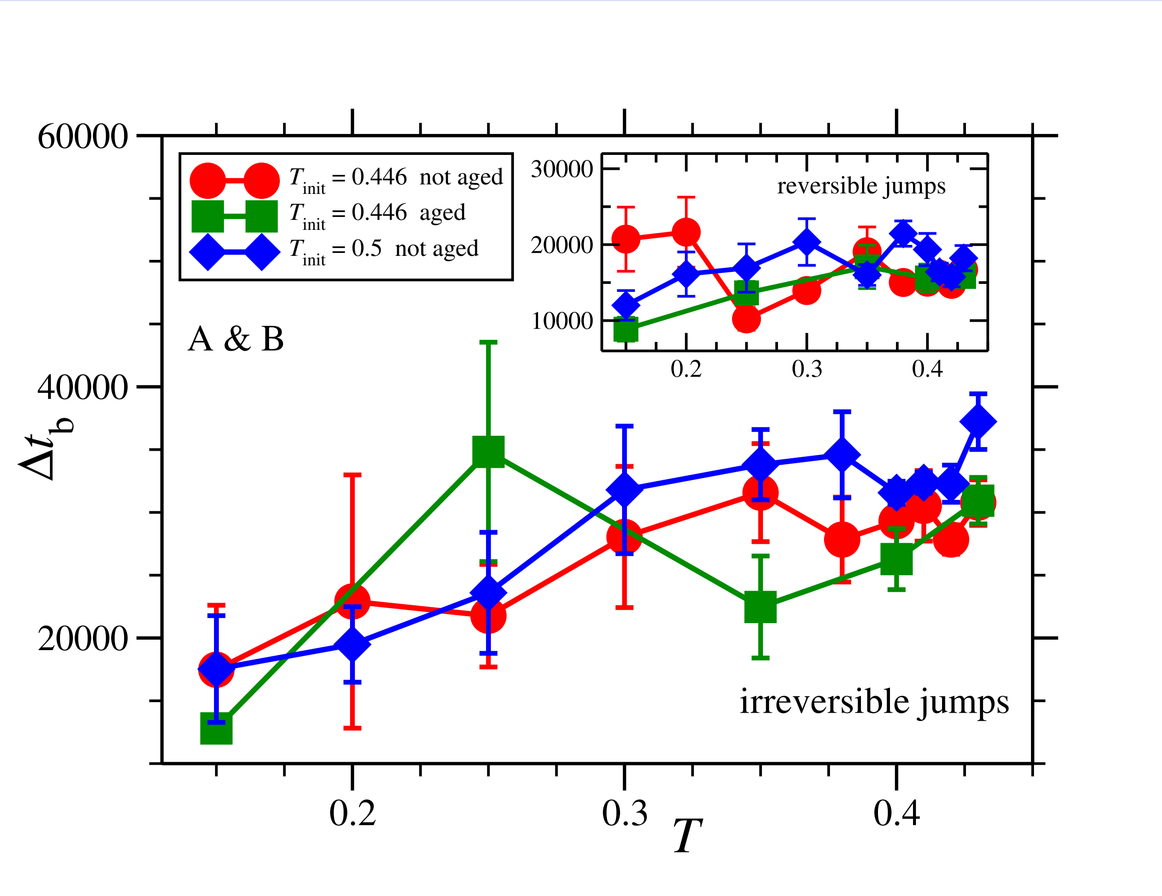


Jump Size

$\Longrightarrow$ history independent

History Dependence



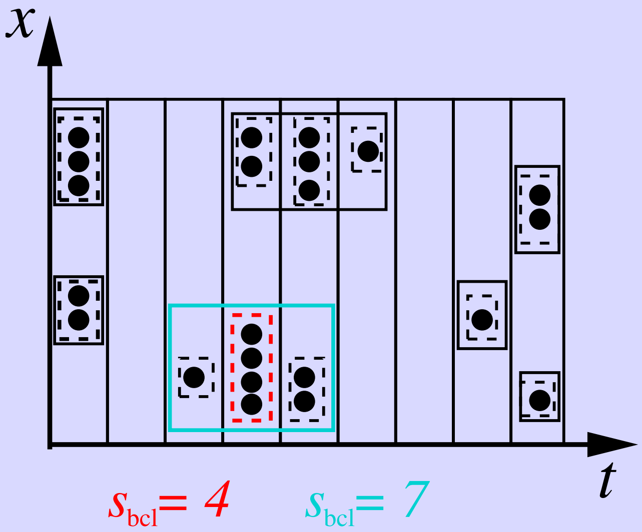


Time Between Jumps

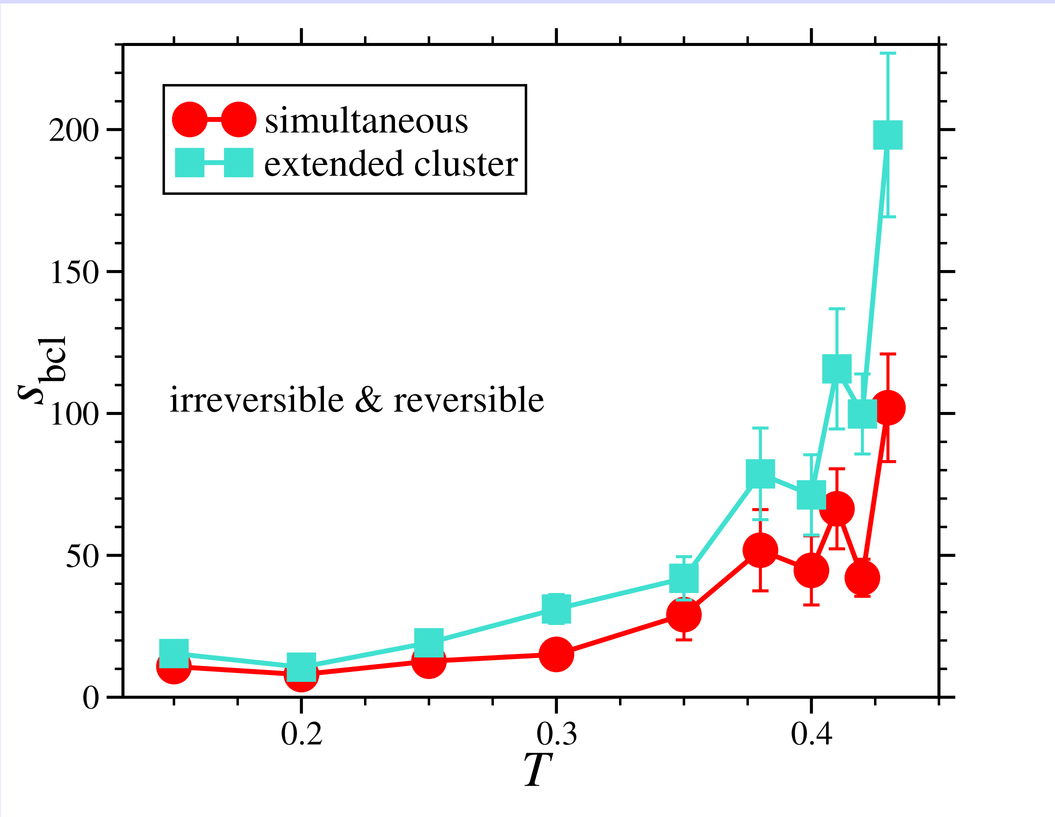
$\Longrightarrow$ history independent

Summary: Jump Statistics

Most Cooperative Processes



s_{bcl} = largest cluster size



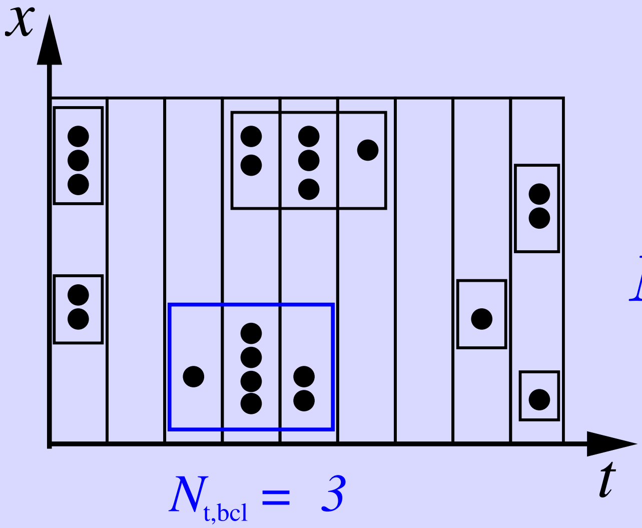
$\Longrightarrow$ highly correlated

single particle

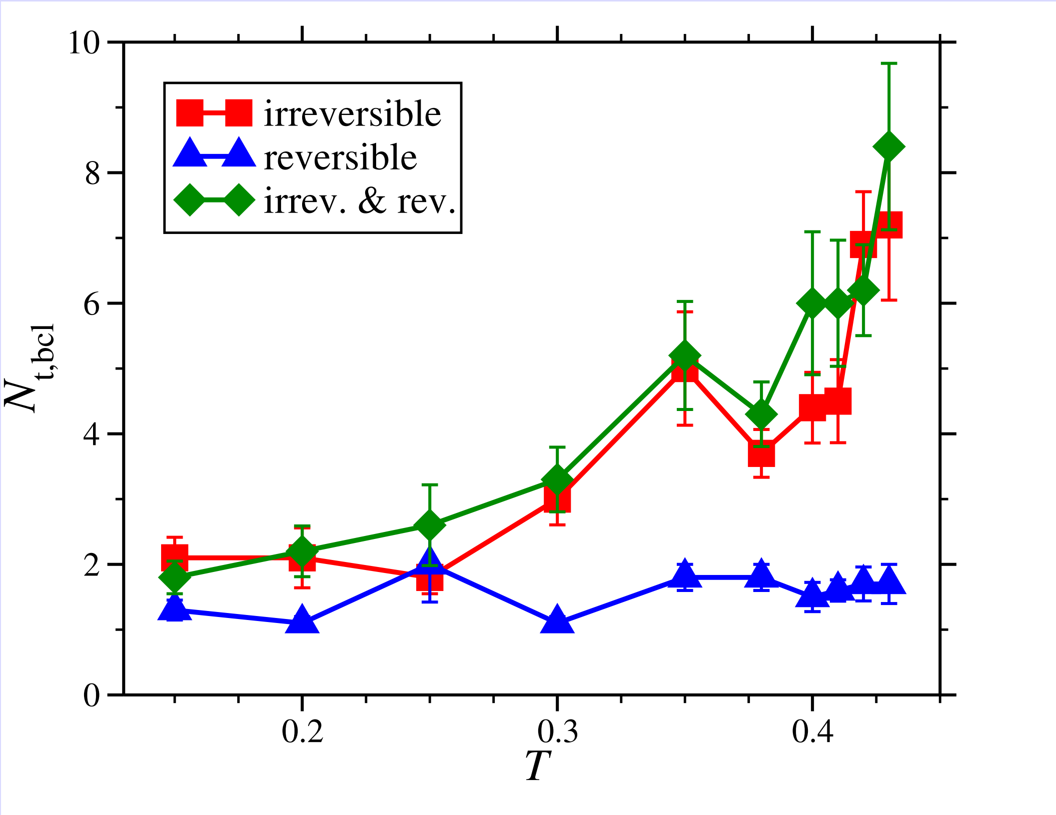
jumps

- many particles

Most Cooperative Processes



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

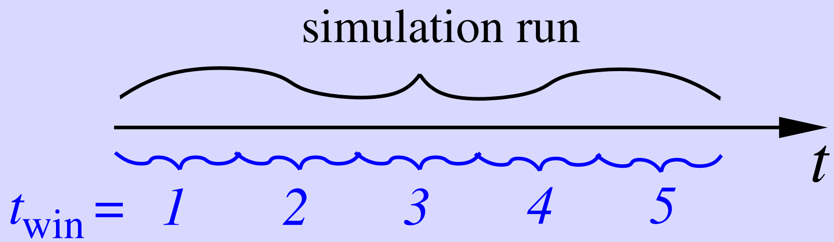


$\Longrightarrow$ highly correlated single particle jumps

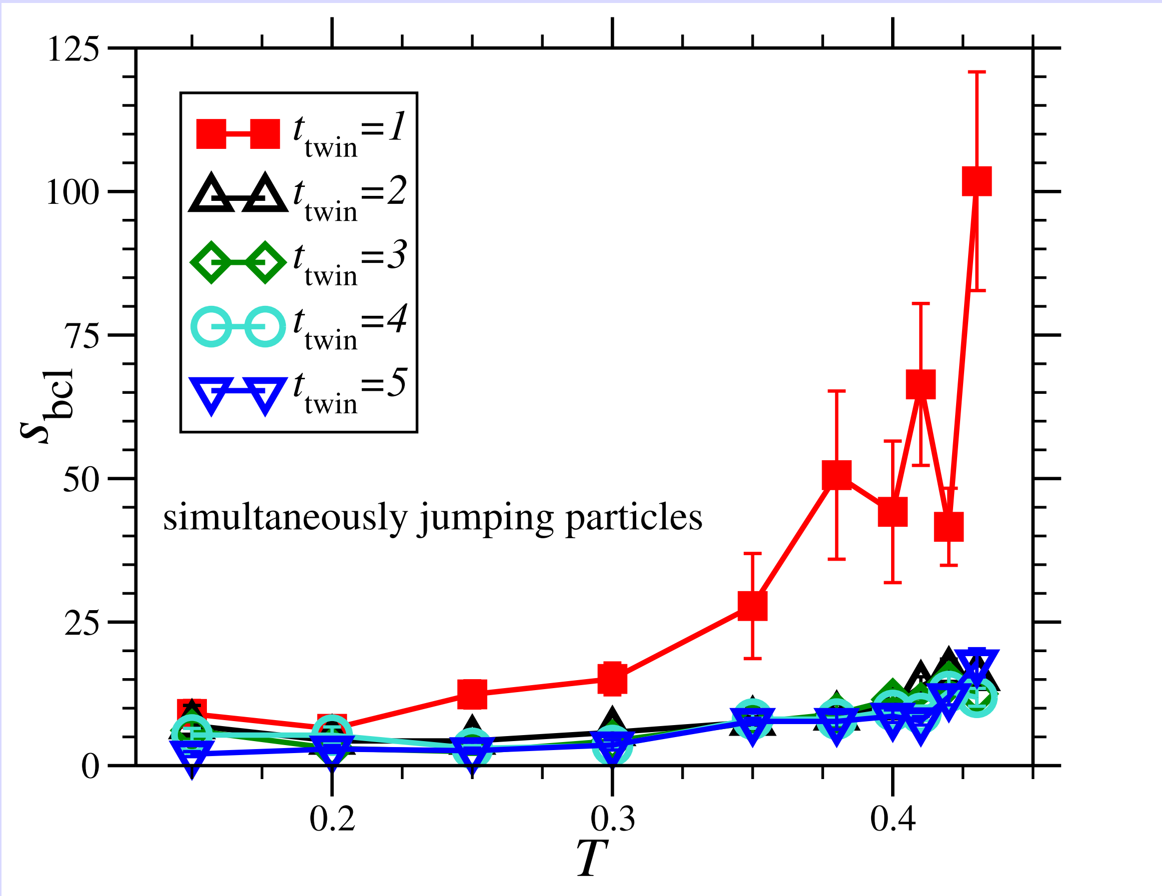
- many particles
- many time bins

(maximum = 125)

History Dependence



s_{bcl} = largest cluster size



⟹ aging dependent

- 1st t-window:

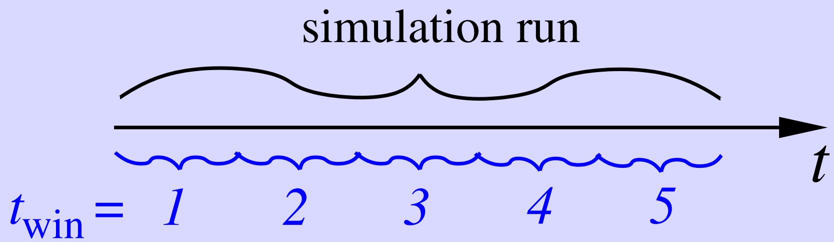
  highly cooperative

- 2nd - 5th t-window:

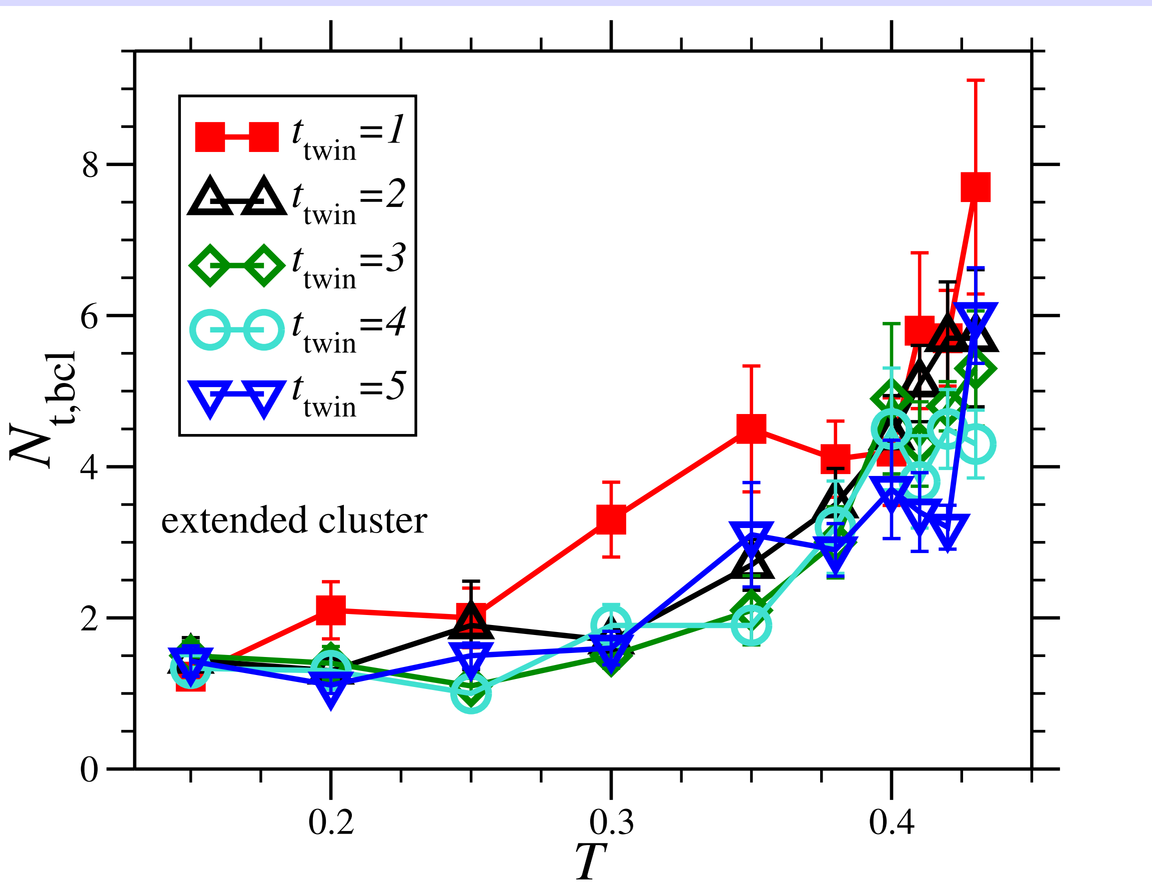
  same, cooperative

s_{bcl} extended cluster

History Dependence



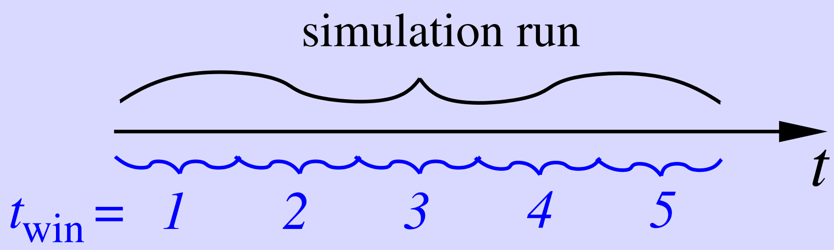
$N_{\mathrm{t,bcl}} =$ no. of t-bins of largest cluster

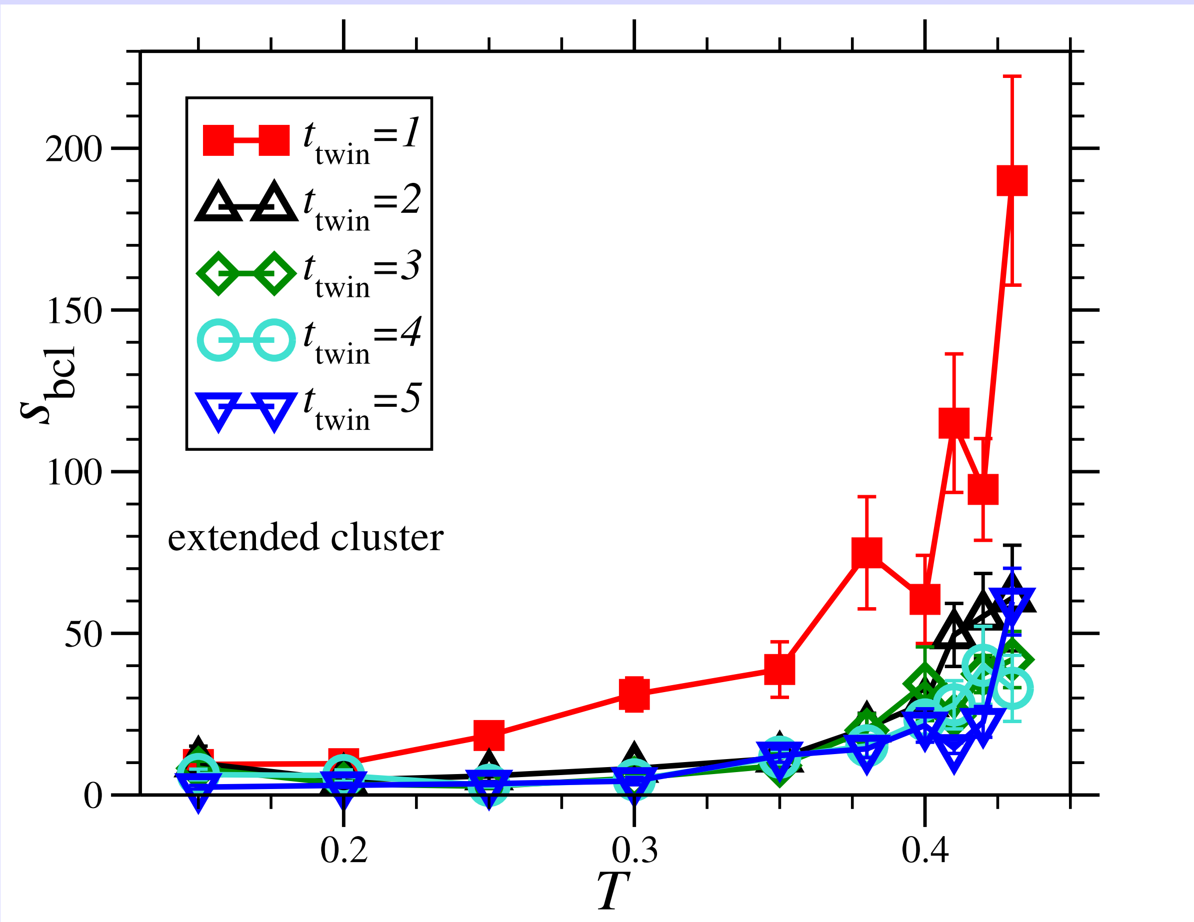


⟹ less aging dependent

⟹ highly cooperative

History Dependence





$\Longrightarrow$ aging dependent

- 1st t-window:

  highly cooperative

- 2nd - 5th t-window:

  same, cooperative

s_{bcl} simult. jump.

Molecular Dynamics Simulation

Initialize:

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

particles $i=1,\ldots,N$

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: (Velocity Verlet)

$$\vec{x}_i(t+\Delta t)=\vec{x}_i(t)+\vec{v}_i(t)\Delta t+\vec{a}_i(t)(\Delta t)^2/2$$

$$\vec{v}_i(t+\Delta t)=\vec{v}_i(t)+(\vec{a}_i(t)+\vec{a}_i(t+\Delta t))\,\Delta t/2$$

$$\vec{a}_i(t)=\vec{F}_i(t)/m_i=-\vec{\nabla}_i\,U(t)/m_i$$

Critical Behavior: power law ⟷ 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)]