# Exchange Monte Carlo: An efficient workhorse for optimization problems

ETH
Eidgenössische Technische Hochschule Zürich
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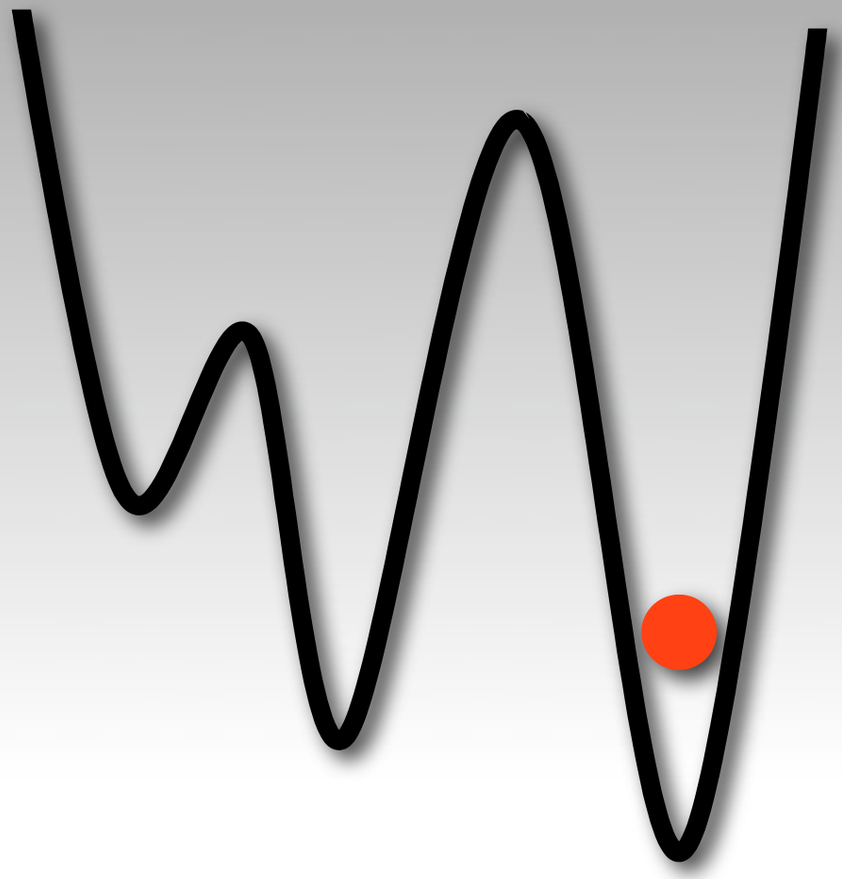

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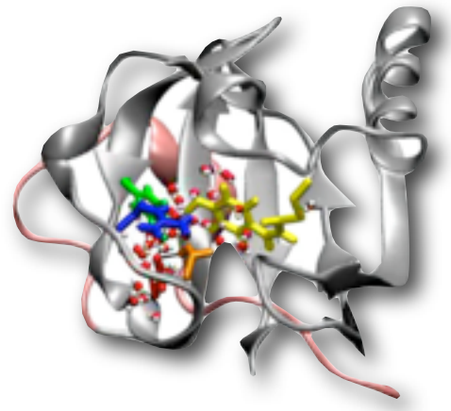
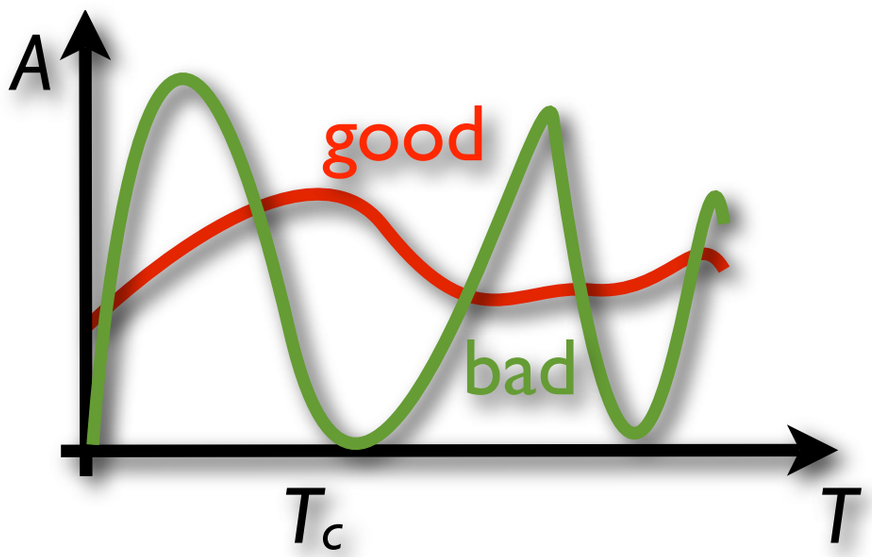
# Outline

- Brief overview of optimization problems:
  - Why do we need finite-temperature algorithms?



- Exchange (parallel tempering) Monte Carlo:
  - Advantages over simple Monte Carlo.
  - Algorithm description.


- Tuning the method:
  - Traditional vs feedback-optimized.
  - Some extensions and applications.

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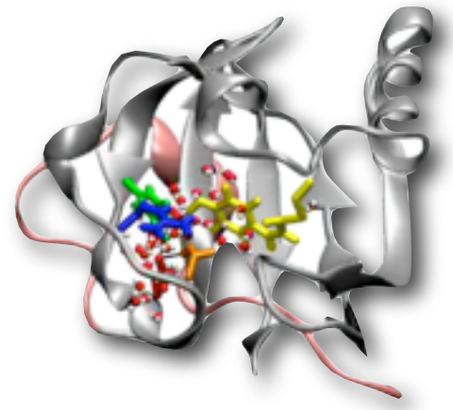

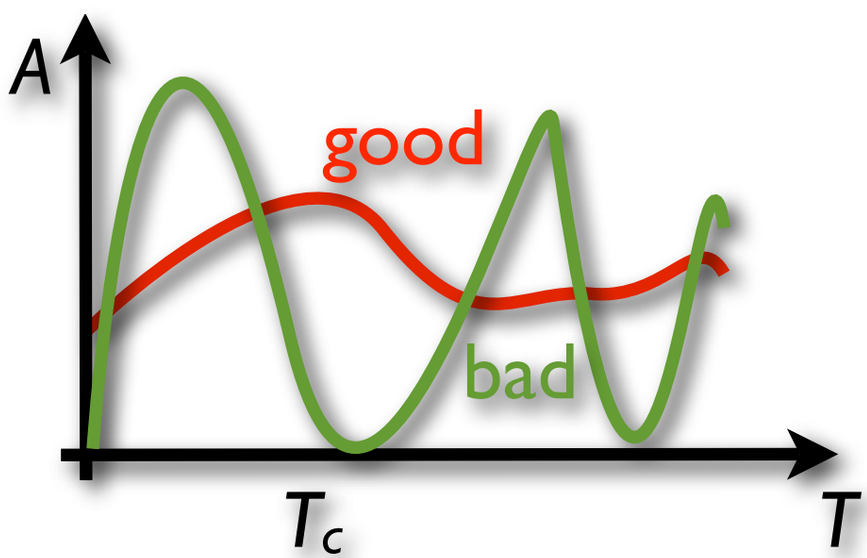

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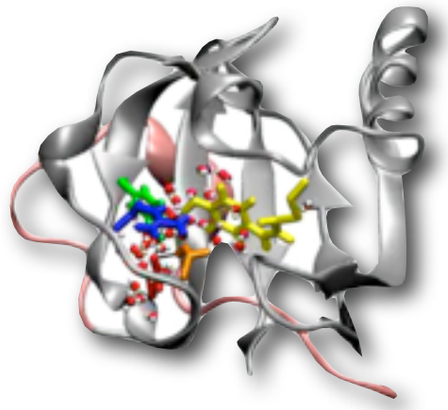

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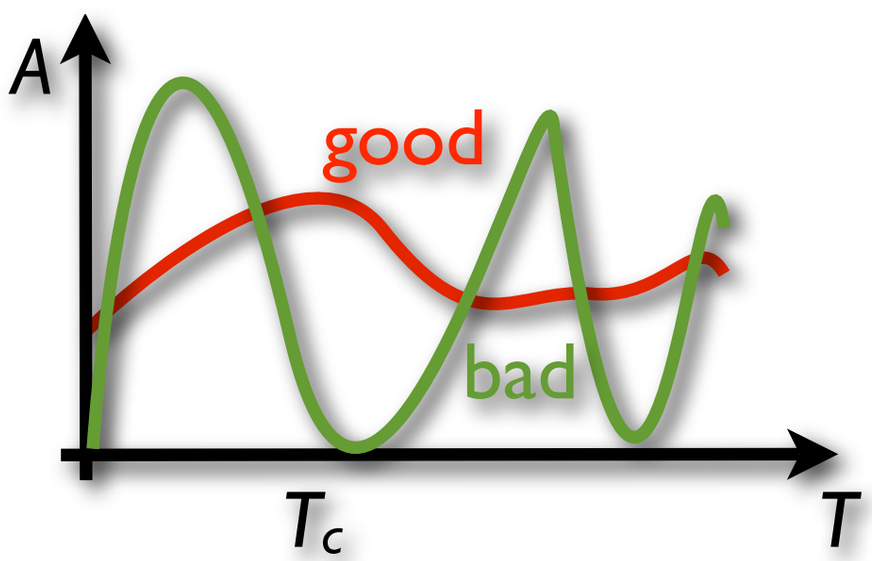


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# Exchange vs parallel tempering

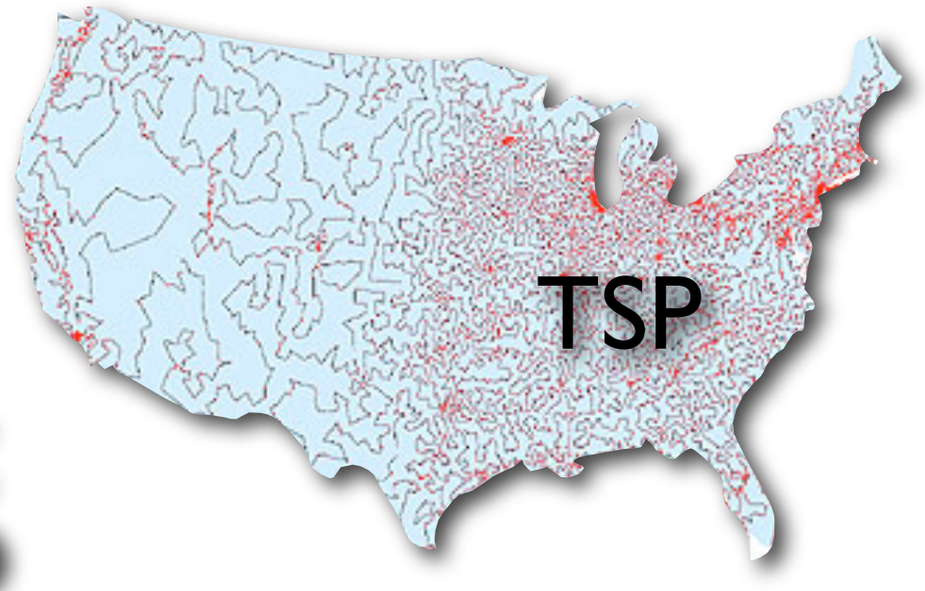
- History:
  - The method was developed in 1996 by Hukushima and Nemoto. They called it "exchange Monte Carlo."
  - Marinari & Parisi developed a similar method called simulated tempering and suggested a variation they dubbed "parallel tempering Monte Carlo".
  - Recently, I discovered that Geyer presented another version in 91 in a proceedings book. So far, I could not get my hands on it...

- Conundrum:
  - What should we call it?
  - Traditionally it is called "parallel tempering."
  - Politically correct probably "exchange Monte Carlo."

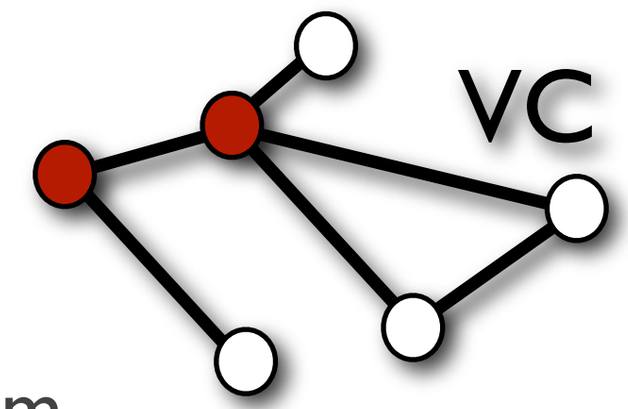
# Optimization problems

# Overview of optimization problems

- Typical goals one usually wants to tackle:
  - Minimize a cost function of a problem (e.g., calculate the ground-state energy of a system).
  - Compute an observable (e.g., energy, magnetization, ...) at low temperature.




- Typical optimization problems:
  - Physical, biological, chemical systems
  - *k*-SAT
  - NPP
  - Vertex cover problem
  - TSP, ...



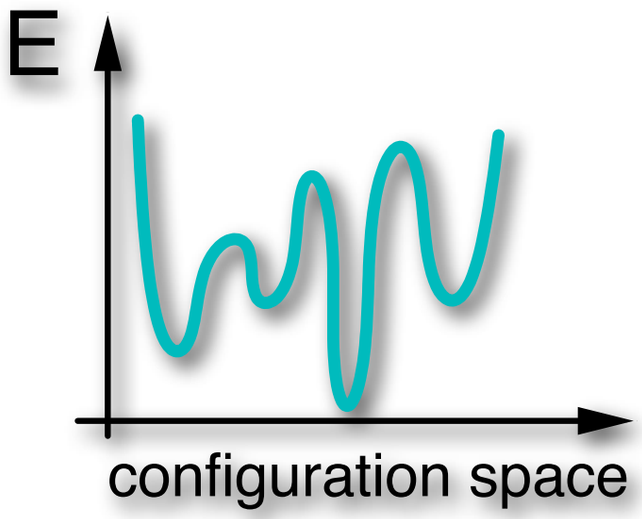

NPP $\sum_{i \in A_1} a_i = \sum_{i \in A_2} a_i$

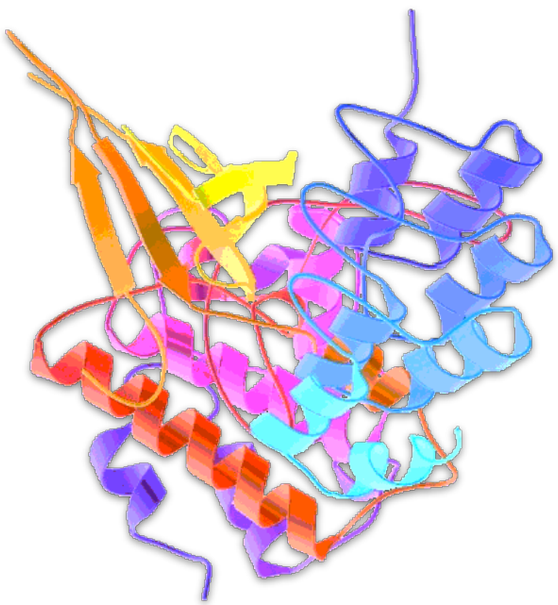
$A = \{a_1, a_2, \ldots a_n\} \rightarrow A_1 \cup A_2$

3-SAT $(x_{11}$ OR $x_{12}$ OR $x_{13})$ AND $(x_{21}$ OR $x_{22}$ OR $x_{23})$ AND...

# Optimization in physical systems

- Several physical problems which contain randomness can be classified as (often hard) optimization problems.
- Due to the randomness, one obtains competing interactions and thus a complex energy landscape.
- Examples:
  - Spin glasses: $\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j$ $\mathcal{P}(J_{ij})$ random
  - Structural glasses
  - Polymers in random media (interfaces)
  - Biomolecules (proteins, ...)



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  - Reconstruction of geological structures from seismic measurements, ...

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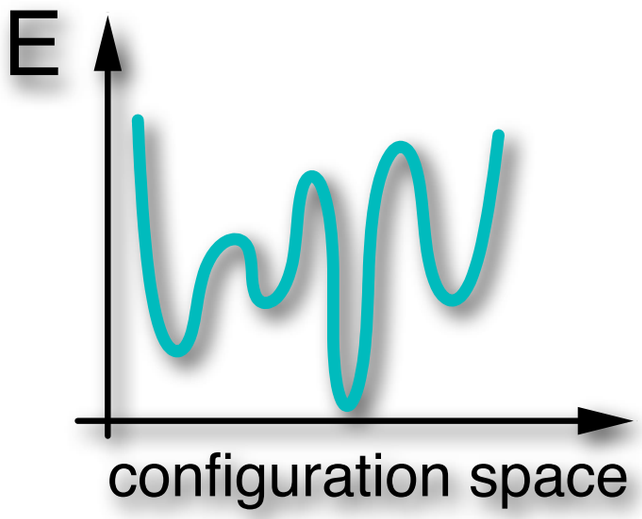
mañana

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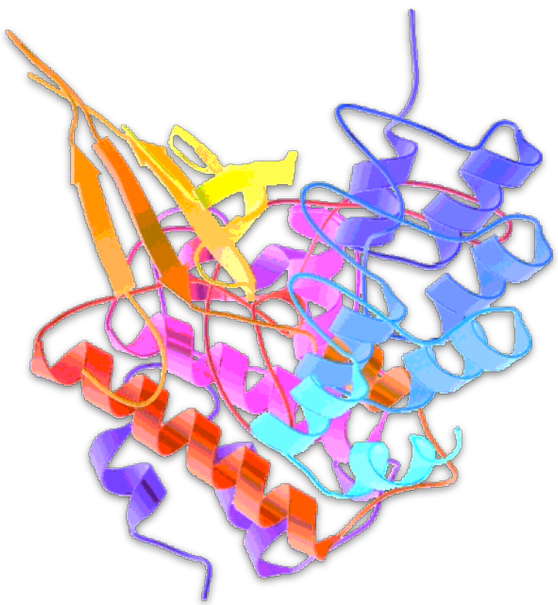

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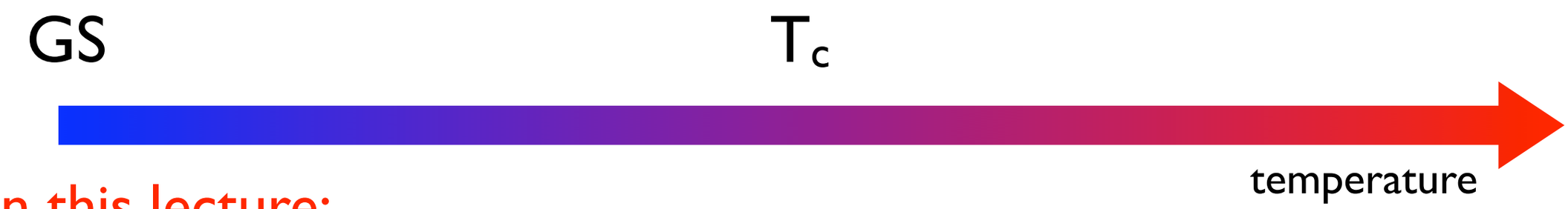
# What will be discussed here?

- So far:
  - Methods to compute ground states of complex systems (zero-temperature methods).
  - Methods to study phase transitions and overcome critical slowing down (for example cluster algorithms).
  - Methods to tackle systems which undergo first-order transitions (for example Wang-Landau algorithm).
  - Methods for infinite temperature (series expansions).

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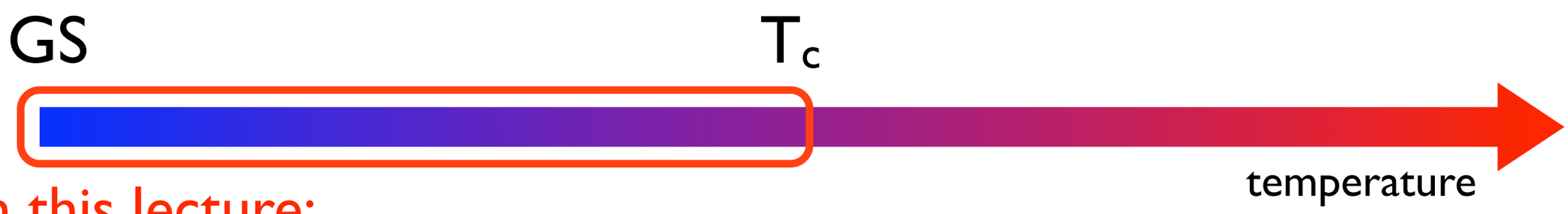


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# Simple benchmark model family

# Prototype for a magnet: the Ising model

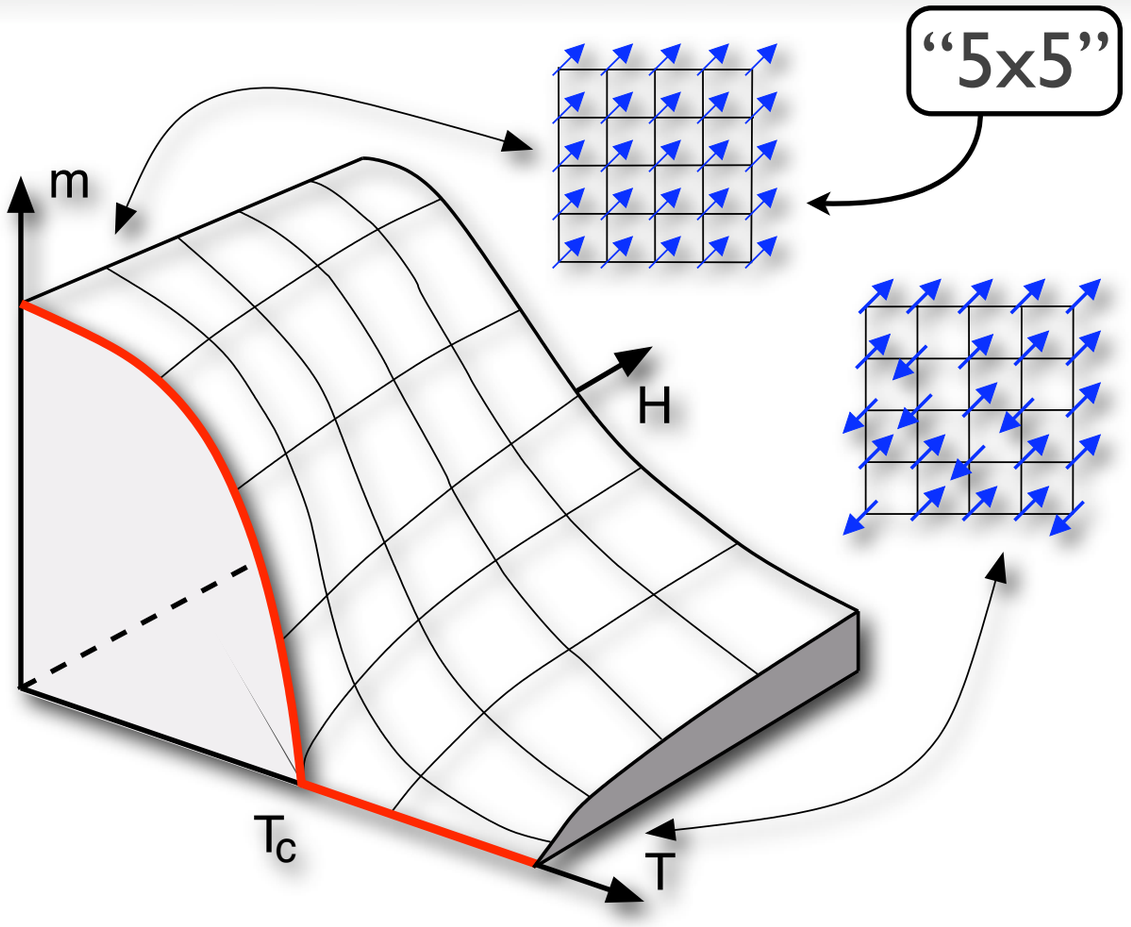
- Hamiltonian:

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - H \sum_i S_i$$

$$J_{ij} = 1 \;\; \forall i, j \quad i \neq j$$

- Order parameter:

$$m = \frac{1}{N} \sum_i S_i \quad \text{(magnetization)}$$




- Some properties:
  - Describes many magnetic systems (also other spin symmetries).
  - Exact solution in 2 space dimensions (Onsager).
  - Nearest-neighbor interactions, in 2D $T_c$ ~2.27.

# Adding frustration...

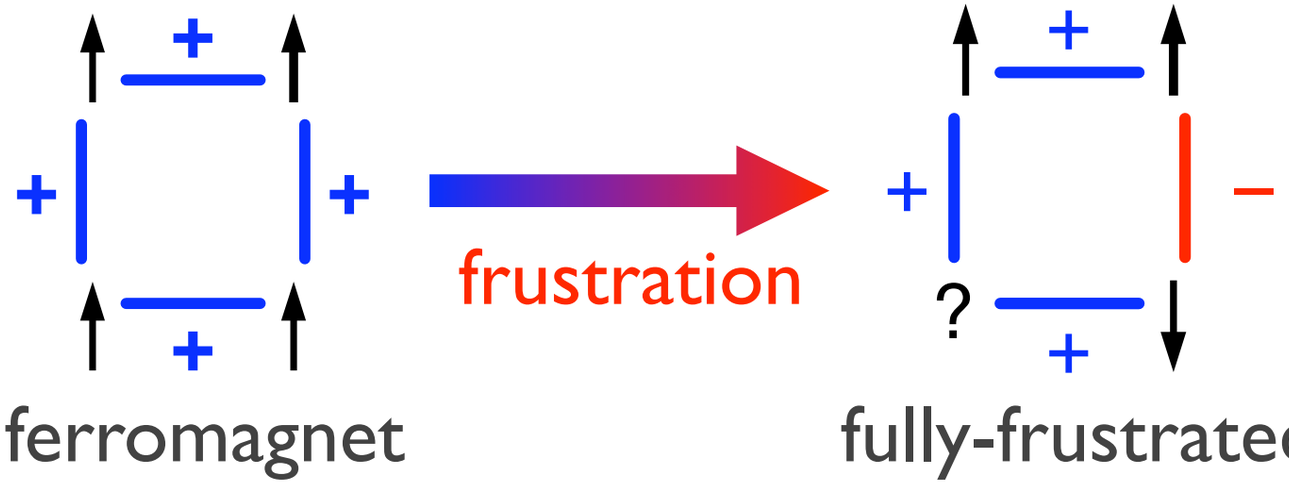
- General Hamiltonian:

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j$$

$+J$

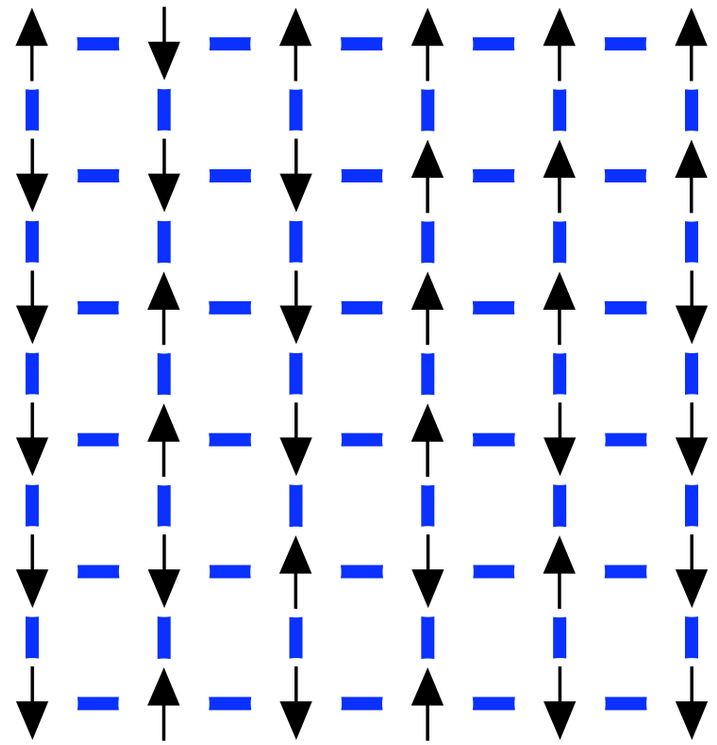
$-J$

- Introduce frustration between the spins:




ferromagnet

fully-frustrated



- Properties of the fully-frustrated Ising model:
  - Huge ground-state degeneracy and complex energy landscape.
  - $T_c = 0$ in 2D.
  - $\prod_{\square} J_{ij} < 0 \quad \forall\, i, j$
- What happens if we add randomness to the frustration?

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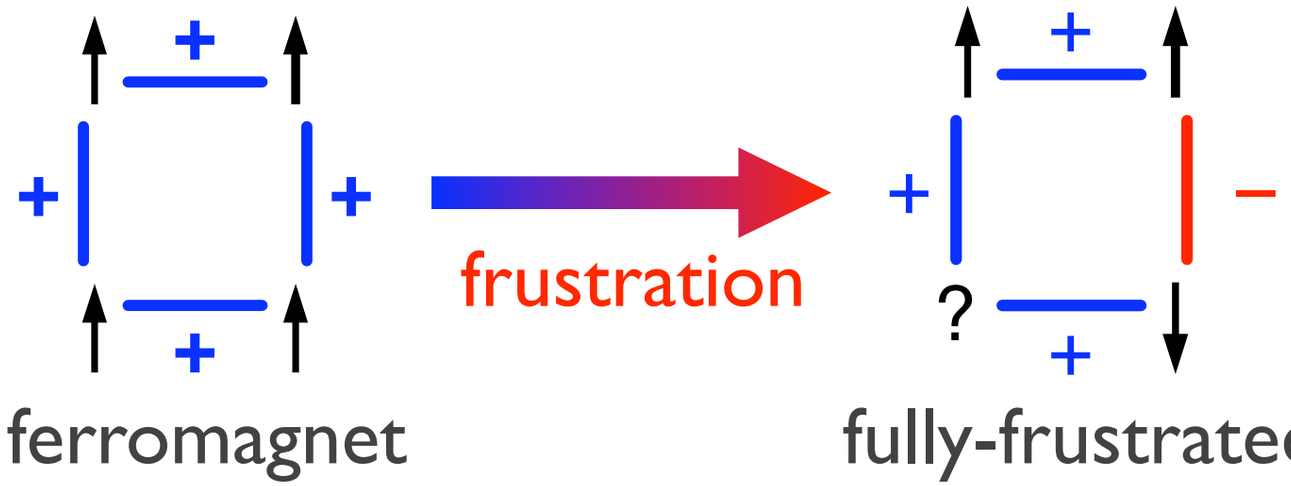


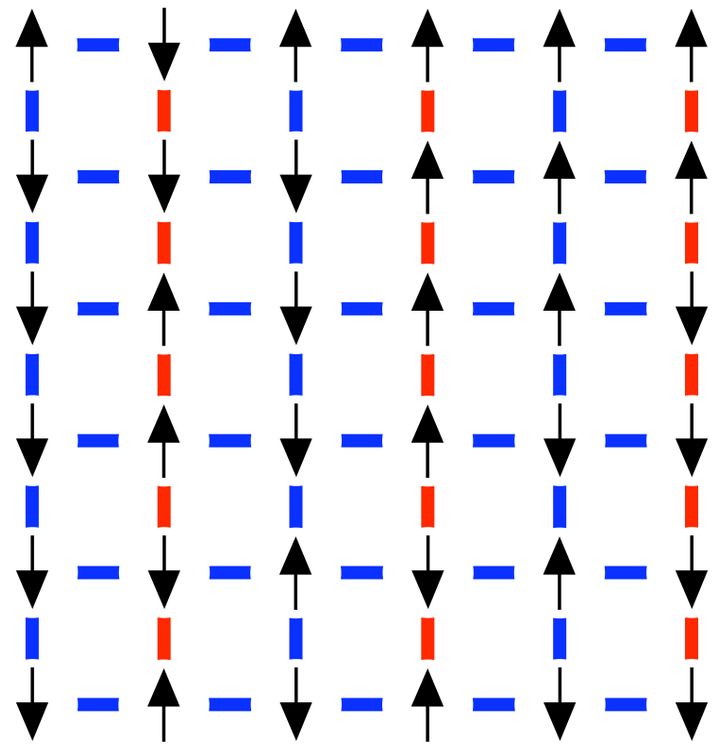

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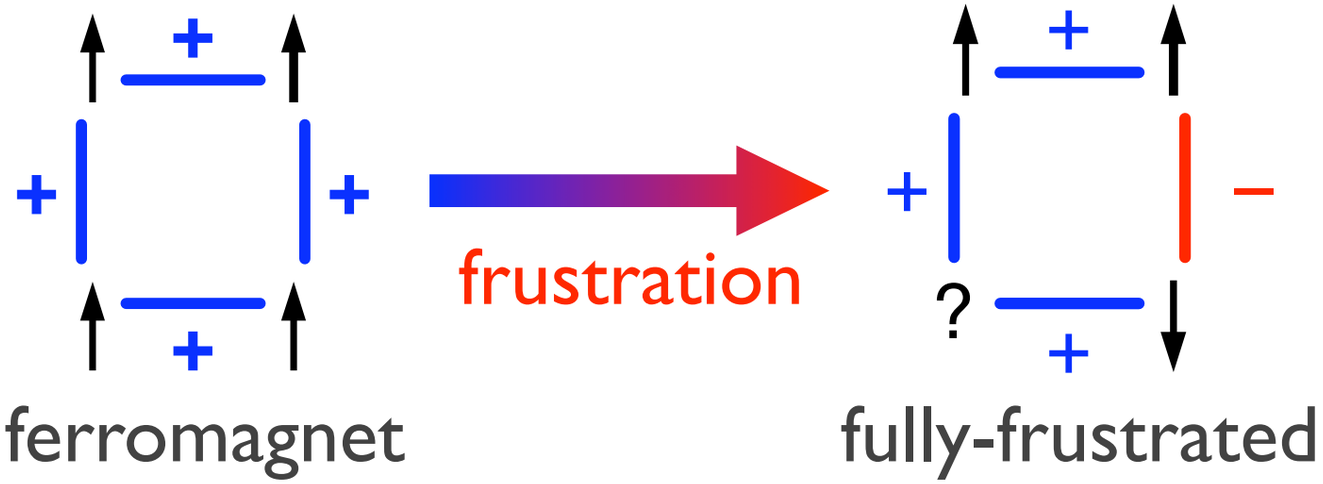


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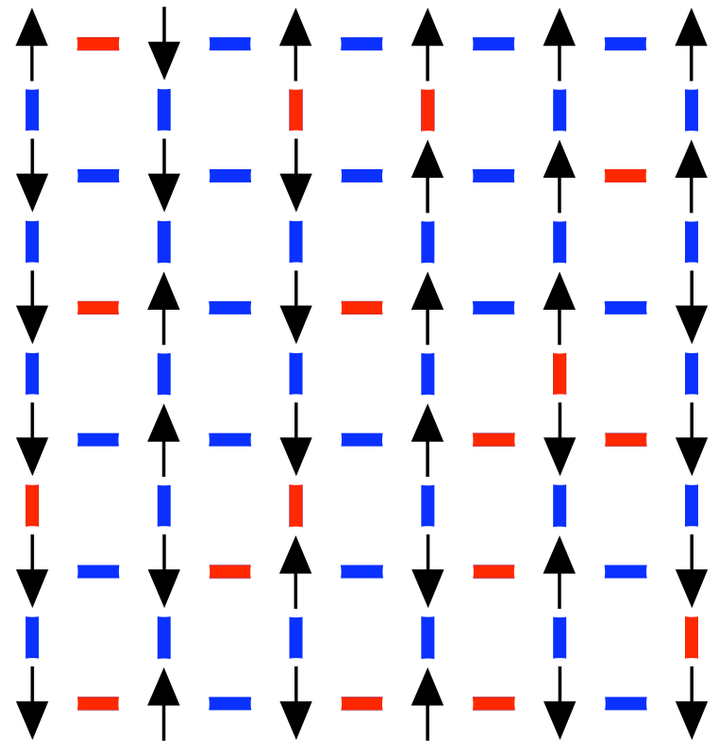

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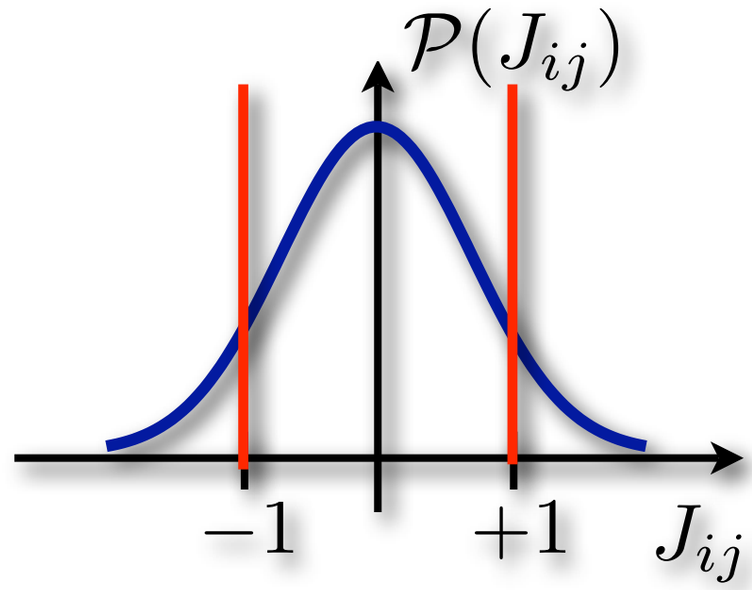
# Adding frustration and disorder: spin glass

- Spin-glass Hamiltonian:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j \qquad S_i \in \{\pm 1\}$$




- Details about the model:
  - Unconventional "order."
  - Only mean-field solution.
  - Bimodal random bonds: high degeneracy.
  - Gaussian random bonds: unique ground state.
  - 2D $T_c = 0$
    3D $T_c = 0.951(2)$
    4D $T_c = 1.805(10)$

- Will be discussed in detail tomorrow and not discussed here further.

# Reminder: Simple Monte Carlo

# The original Metropolis paper (1953)…

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

## Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
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(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

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### II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number $N$ may be as high as several hundred. Our system consists of a square† con-

- They knew this was important… and they were right!

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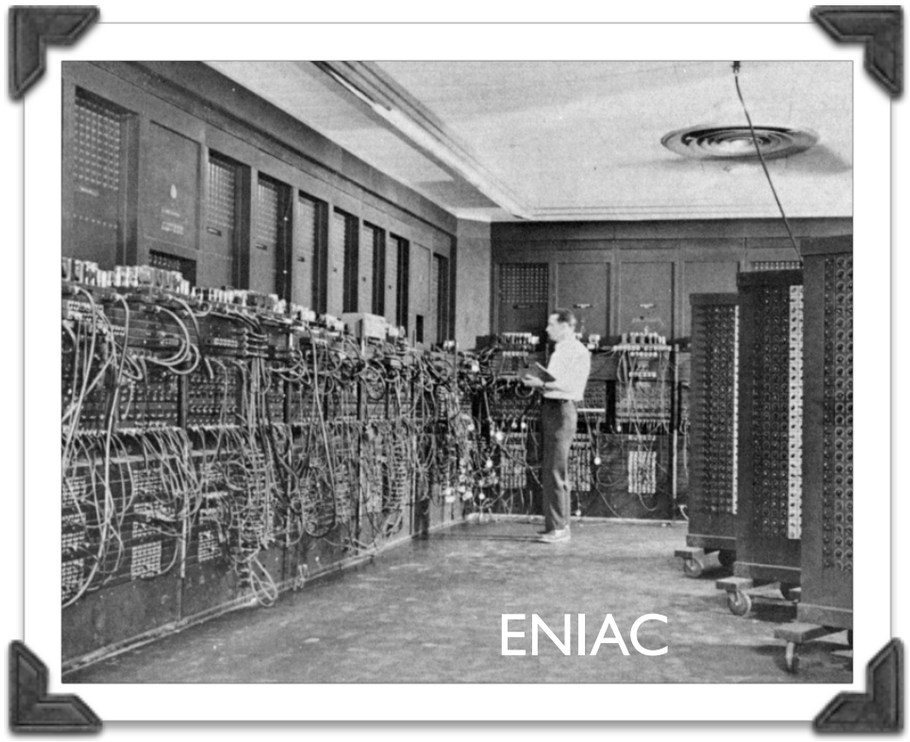
# The original Metropolis paper: some facts

Phys. Plasmas 12, 057303 (05)

- 50 years later at a Los Alamos meeting:
  - Only M. Rosenbluth attended, although with terminal cancer.
  - Metropolis mainly contributed CPU time on MANIAC.
  - von Neumann and Ulam invented the Monte Carlo method in 1946 and pointed out that it could be used for simulations.
  - Teller: Statistical averages can be made as ensemble averages.
  - Interesting author list: two couples. How often does this happen?


ENIAC

- Why Los Alamos?
  - The US was bulding the atomic bomb.
    At least one good thing came out.

# Reminder: simple Monte Carlo

- In statistical mechanics we want to compute the average of an observable *O*:

$$\langle O \rangle = \sum_n P_n^{\mathrm{eq}} O_n \qquad P_n^{\mathrm{eq}} = \frac{e^{\beta E_n}}{\sum_n e^{-\beta E_n}}$$

- Problem: The number of states is exponentially large.
- Solution: Statistically sample a few (smartly chosen) states to obtain an estimate of *O* but with a statistical error.
  - If we chose the states according to $P_n^{\mathrm{eq}}$ and ensure detailed balance we obtain a Markov chain for $\langle O \rangle_{\mathrm{est}}$

$$\langle O \rangle_{\mathrm{est}} = \frac{1}{M} \sum_i^M O_i$$

  where *M* is the number of states sampled.
- Metropolis algorithm: accept a new configuration if $(e^{-\Delta E/T} > \mathrm{rand}())$

$$P_{\mathrm{accept}} = \min(1, e^{-\Delta E/T})$$

# Why does simple Monte Carlo fail here?

- The systems we are interested in have rugged energy landscapes.
- At low temperature, when $\Delta E$ is large

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is "never" accepted.

- How can we resolve the problem?
  - Tunnel trough barrier.
  - Heat up the system to overcome the barrier.

- Note:
  - Simulated annealing has similar problems (stuck in valleys).

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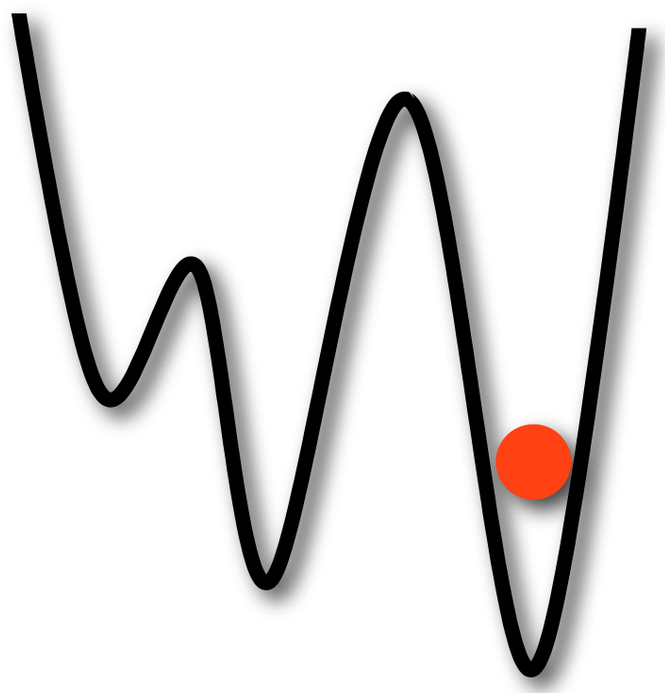

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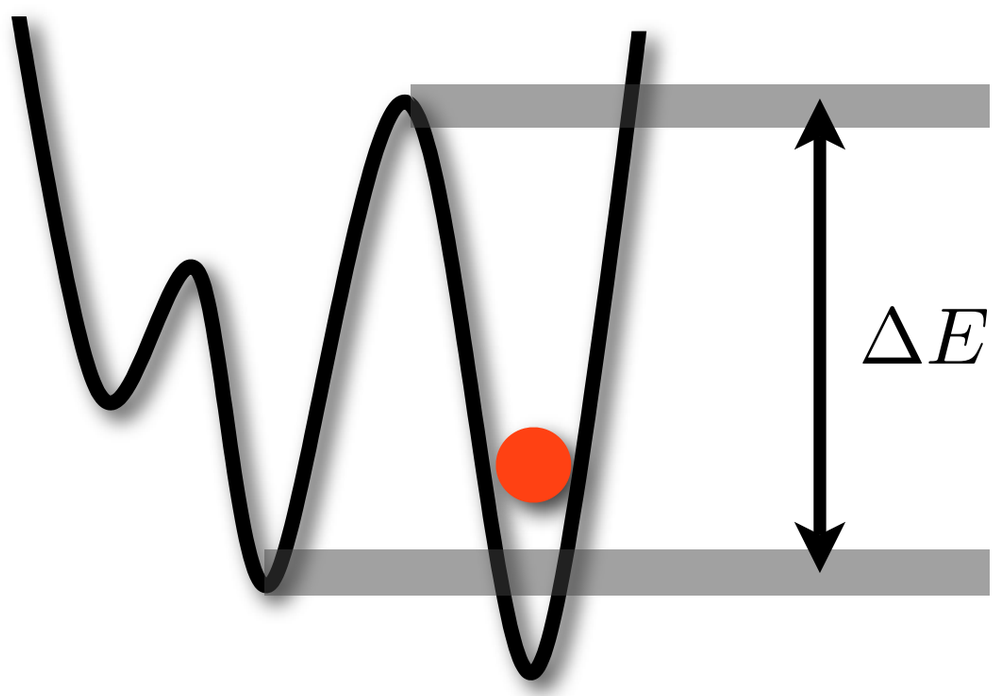


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# Exchange (parallel tempering) Monte Carlo

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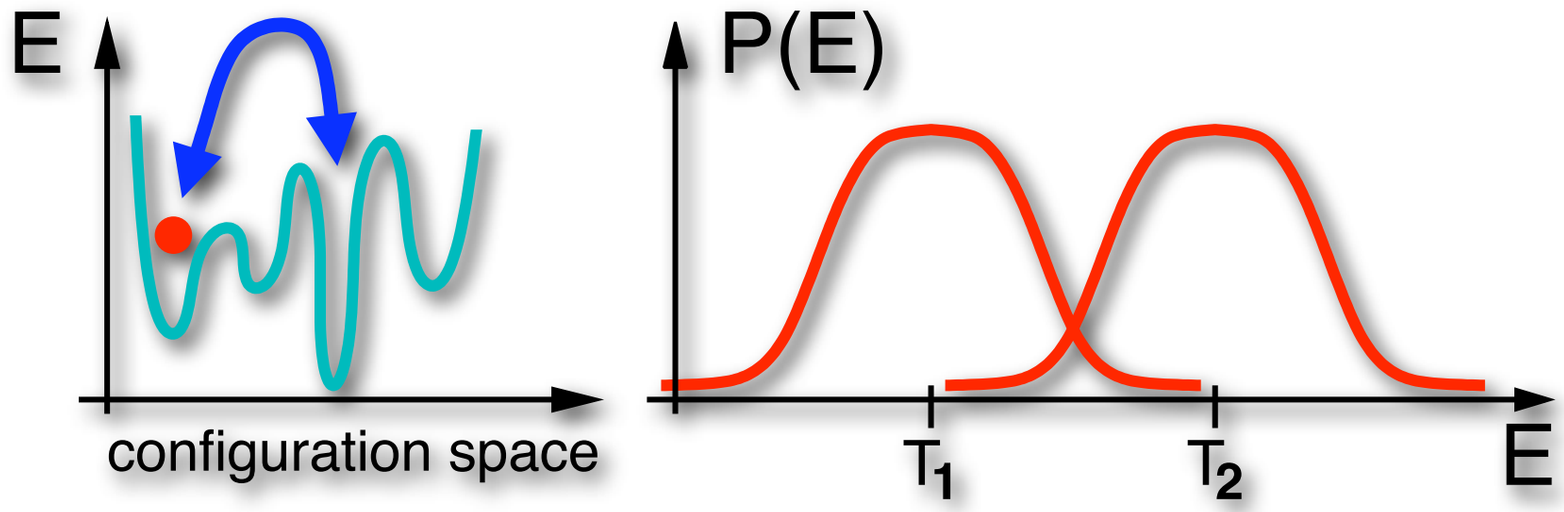
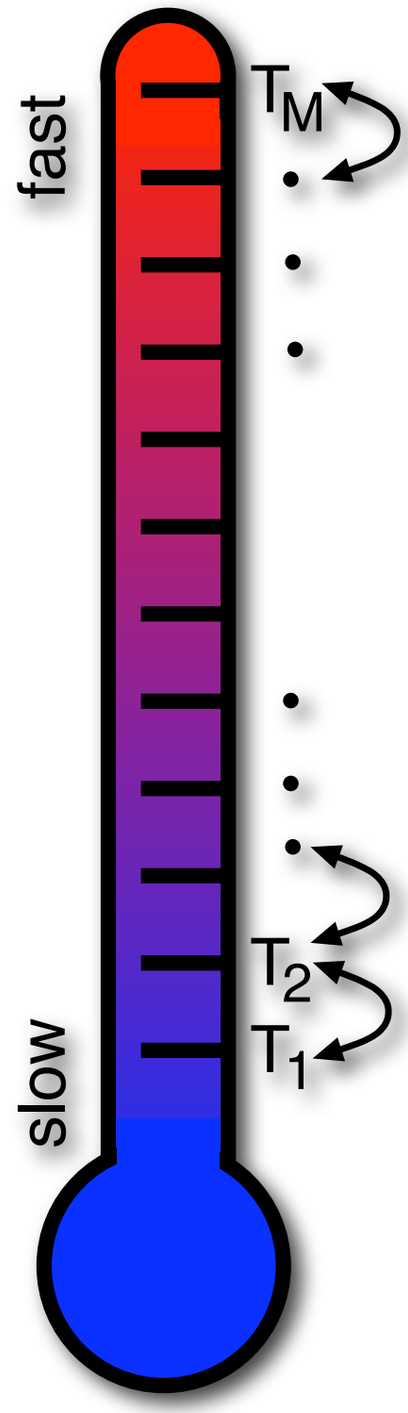
10. I told you so...

# Exchange (parallel tempering) Monte Carlo

Hukushima & Nemoto (96)

- Idea:
  - Simulate *M* copies of the system at different temperatures with $T_{max} > T_c$ (typically $T_{max} \sim 2T_c^{MF}$).
  - Allow swapping of neighboring temperatures: easy crossing of barriers.




- What has to be tuned?
  - Number of temperatures.
  - Position of temperatures.

# Parallel tempering: algorithm and details

- Brief outline of the algorithm:
  - Perform a Monte Carlo update between *neighboring* replicas.
  - Best to keep temperatures and change pointers to configurations.

$$P(S_{m+1} \leftrightarrow S_m, \beta_{m+1} \leftrightarrow \beta_m) = e^{-\Delta} \quad : \quad \Delta > 0$$
$$P(S_{m+1} \leftrightarrow S_m, \beta_{m+1} \leftrightarrow \beta_m) = 1 \quad : \quad \Delta \leq 0$$

$$\Delta = (\beta_{m+1} - \beta_m)(E_m - E_{m+1})$$
$$\beta = 1/T$$

[obeys detailed balance]

- How often do we call the swap routine?
  - Optimal ratio of lattice sweeps (*N* spin updates) and swaps is 1:1, i.e., after each lattice sweep, perform an attempted parallel tempering swap [see Katzgraber *et al*., JSTAT P03018 (2006)].

# How fast is fast? Example: 3D spin glass

- Equilibration times:

$$\tau_{\mathrm{eq}}^{\mathrm{PT}} \approx 300\,\mathrm{MCS}$$

$$\tau_{\mathrm{eq}}^{\mathrm{SM}} \approx 10^6\,\mathrm{MCS}$$

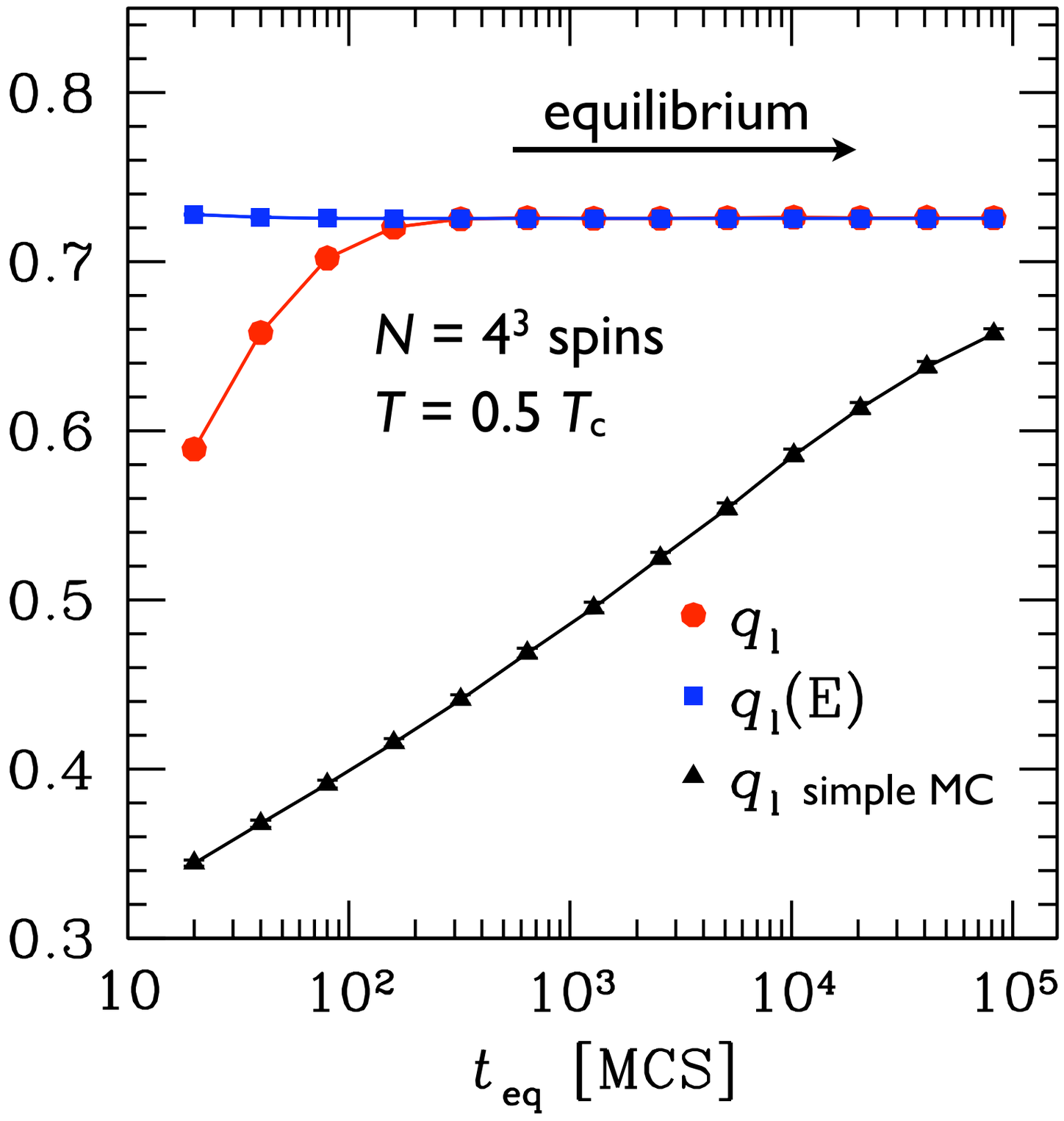
- Equilibration test (later):

$$q_l(E) = \frac{2T|E|}{z} + 1$$

$$z = 2D$$

Once both agree, the system is in equilibrium (only Gaussian disorder).

Katzgraber *et al.* PRB (01)



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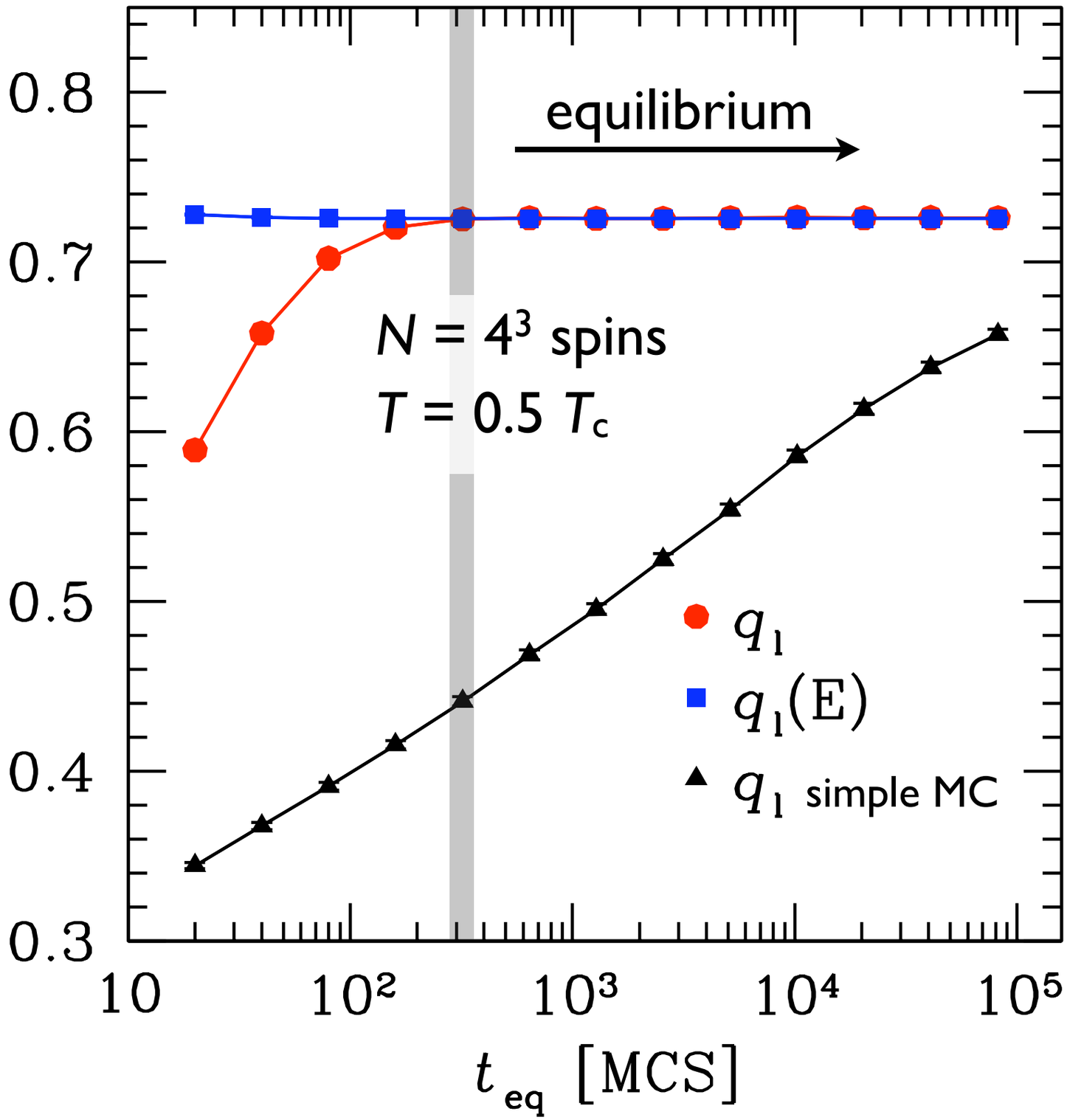

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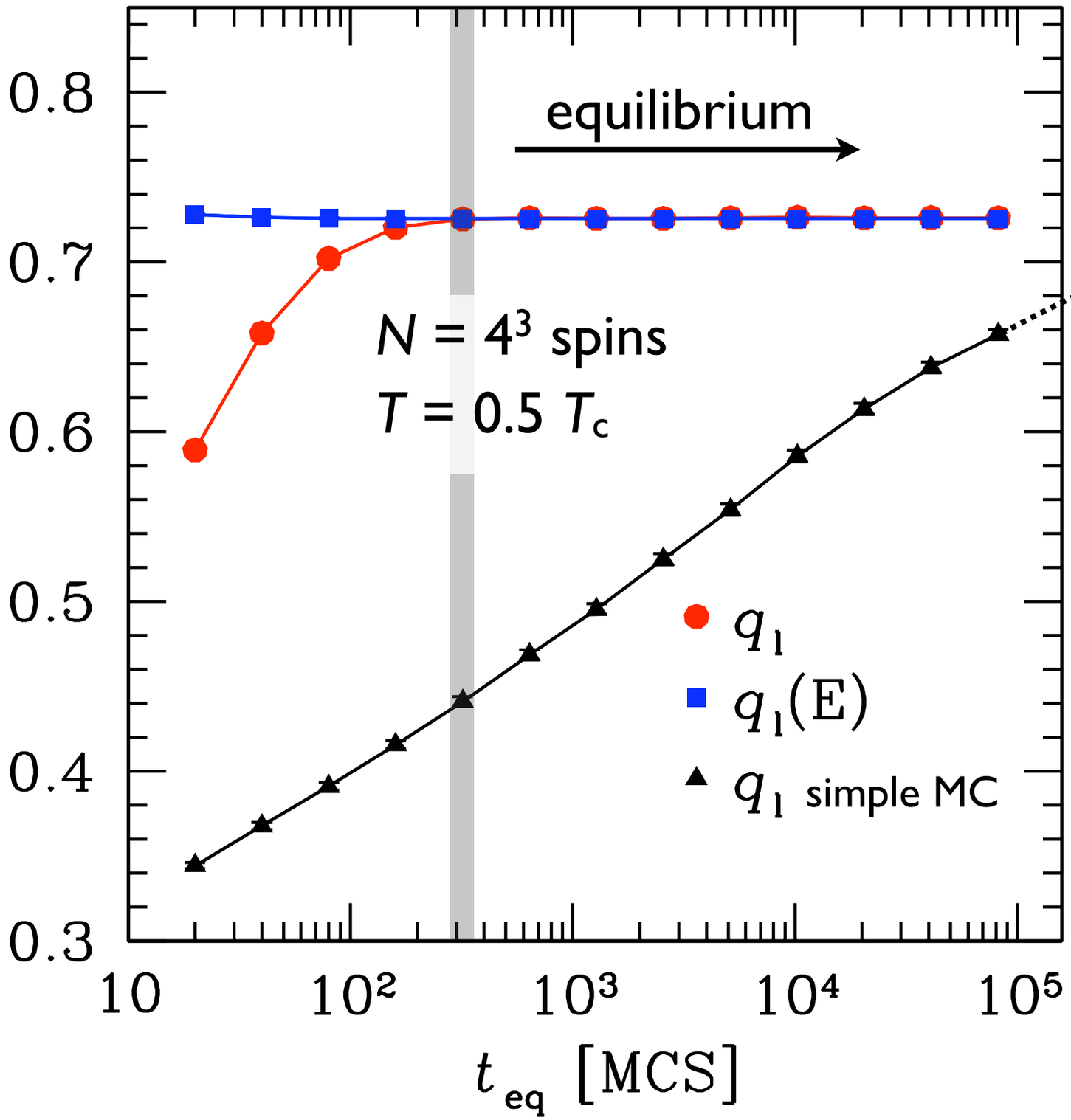
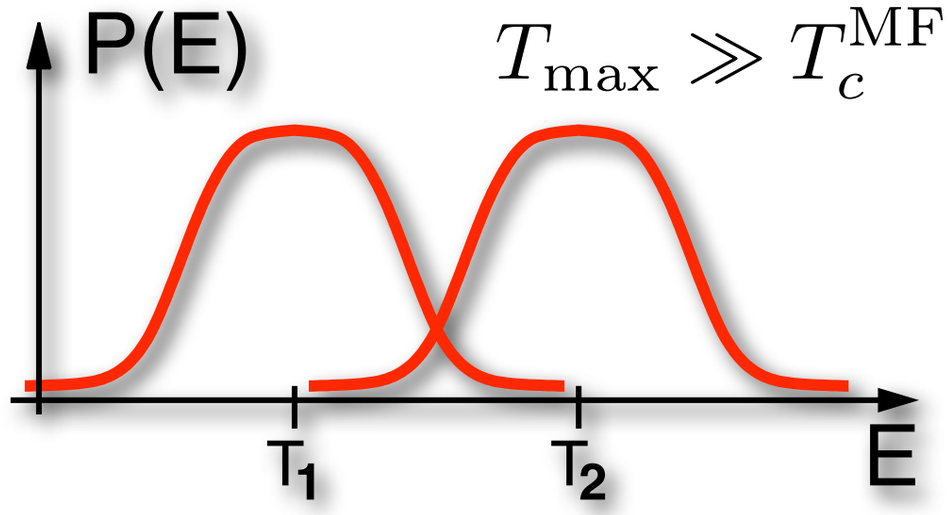


# How do we choose the temperatures?

# How many temperatures do we need?

- Two possible scenarios:
  - Temperatures too far apart: parallel simple Monte Carlo chains.
  - Temperatures too close: overhead.



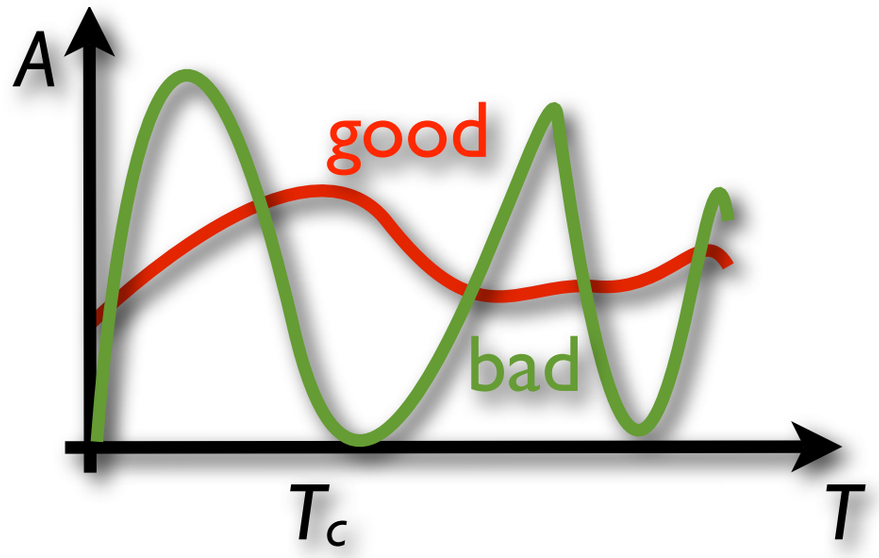

- What determines the number *M* of temperatures?
  - The energy distributions of the system at $T_1$ and $T_2$ have to overlap.
  - Because $\Delta E \sim C_{\mathrm{V}} \longrightarrow M \sim \sqrt{N^{1+\alpha/d\nu}}$
  - Note: Systems for which $C_{\mathrm{V}}|_{T\to 0} \to 0$ require many temperatures.

- In principle, we need as many temperatures such that the method works. Measure? Acceptance rates.

# Measuring acceptance rates

- Definition:

$$A = \frac{N_{\text{accept}}}{N_{\text{trial}}}$$




- Traditional wisdom: Tune the temperature set such that...
  - ... $0.2 \leq A \leq 0.9$.
  - ... $A$ is approximately independent of temperature.

  - Detailed implementation which gives flat acceptance rates: Incomplete beta function law [uses $A = f(C_{\text{V}})$ ].

Predescu *et al.*, JSTAT (03)

- Notes:
  - A quick run (no need to equilibrate) will immediately produce stable acceptance rates (easy tuning by hand).
  - It has been claimed that $A \sim 0.3$ is optimal.

Rathore *et al.*, J. Chem. Phys. (05)

# Practical/traditional approaches

- Geometric progression:
  - Works well when $C_V$ ~ const (like for spin glasses).
  - Iteratively construct a temperature set and tune $M$ with $\lambda$.

$$\frac{1}{T_i} = \lambda R^{i-1} \frac{1}{T_{\min}} \qquad R = \left[\frac{T_{\min}}{T_{\max}}\right]^{1/(M-1)}$$

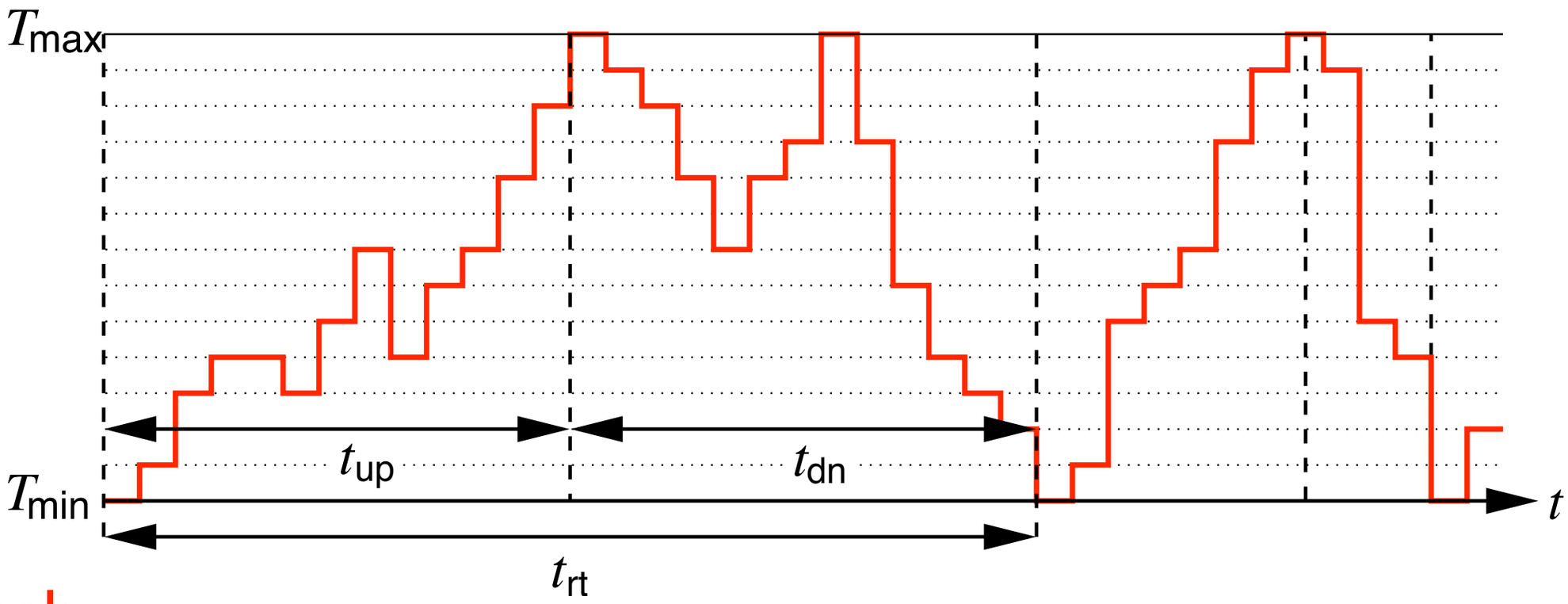
- By hand:
  - If $C_V$ diverges (phase transition) start from a geometric progression.
  - Interlace extra temperatures by hand.
  - Tedious, but after a while you get a feeling for it.

- But... are temperature-independent acceptance rates optimal?
  - Replicas do a random walk in temperature space.

# Optimizing the ensemble $\{T_i\}$

Katzgraber *et al.*, JSTAT (06)

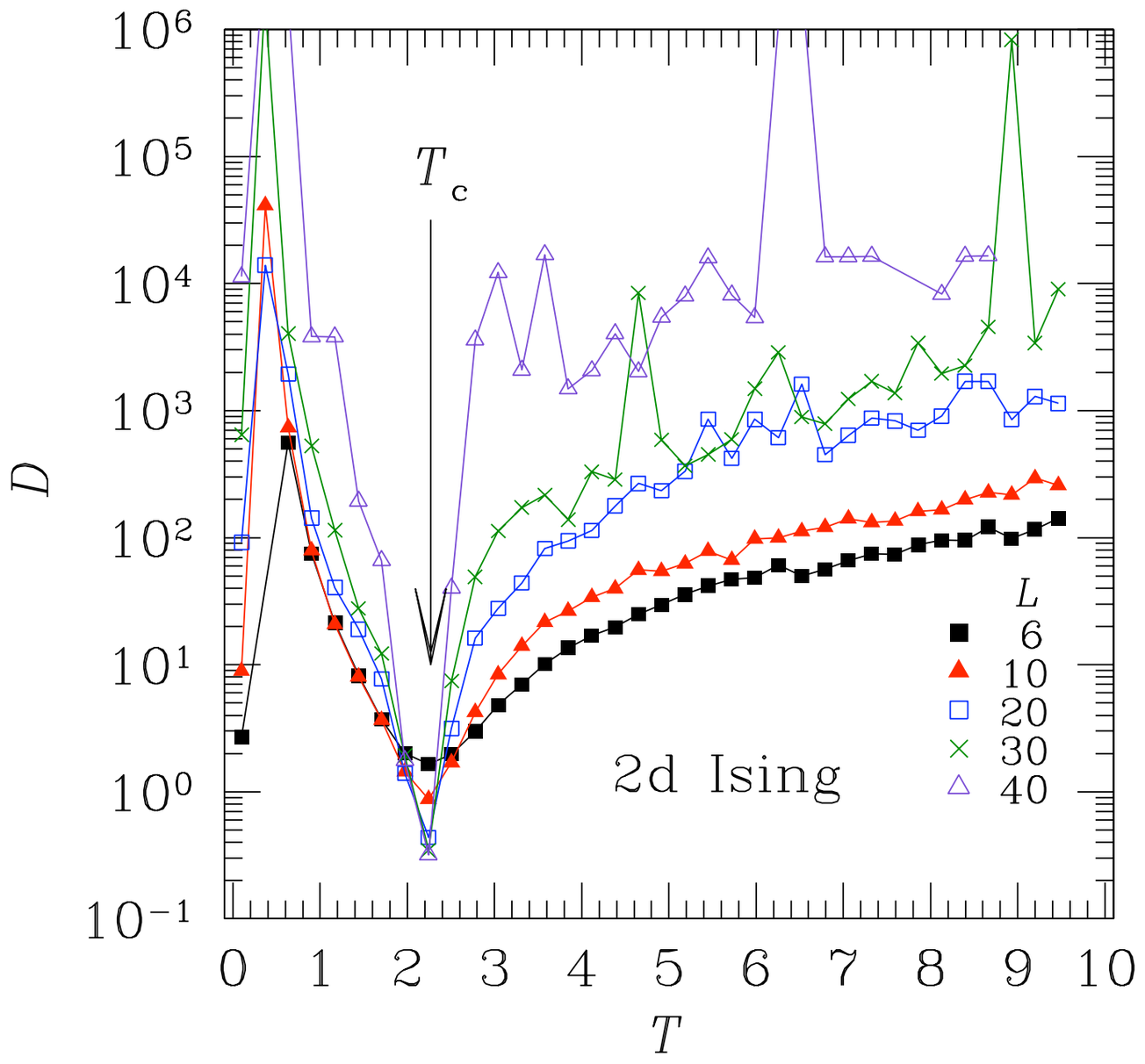
- Track random walk of the replicas in temperature space...




- Goal:
  - Minimize the round-trip time $t_{rt}$ and ensure that $t_{up} \sim t_{dn}$.
  - This shall ensure an efficient sampling of temperature space.
- How?
  - Tune the ensemble $\{T_i\}$ at a fixed number of temperatures $M$.
  - Quick run at the beginning of the simulation.

# Conventional temperature sets...

- Start from a temperature set with $A(T)$ ~ const.
- Track one replica and measure the local diffusivity $D$ in the ensemble $\{T_i\}$.




- Ising model:
  - Bottleneck at $T_c$!
- Fully-frustrated Ising model:
  - Bottleneck at $T = 0$.
- Goal: change $\{T_i\}$ so that $D$ ~ const. for each $\Delta T_i = T_{i+1} - T_i$.

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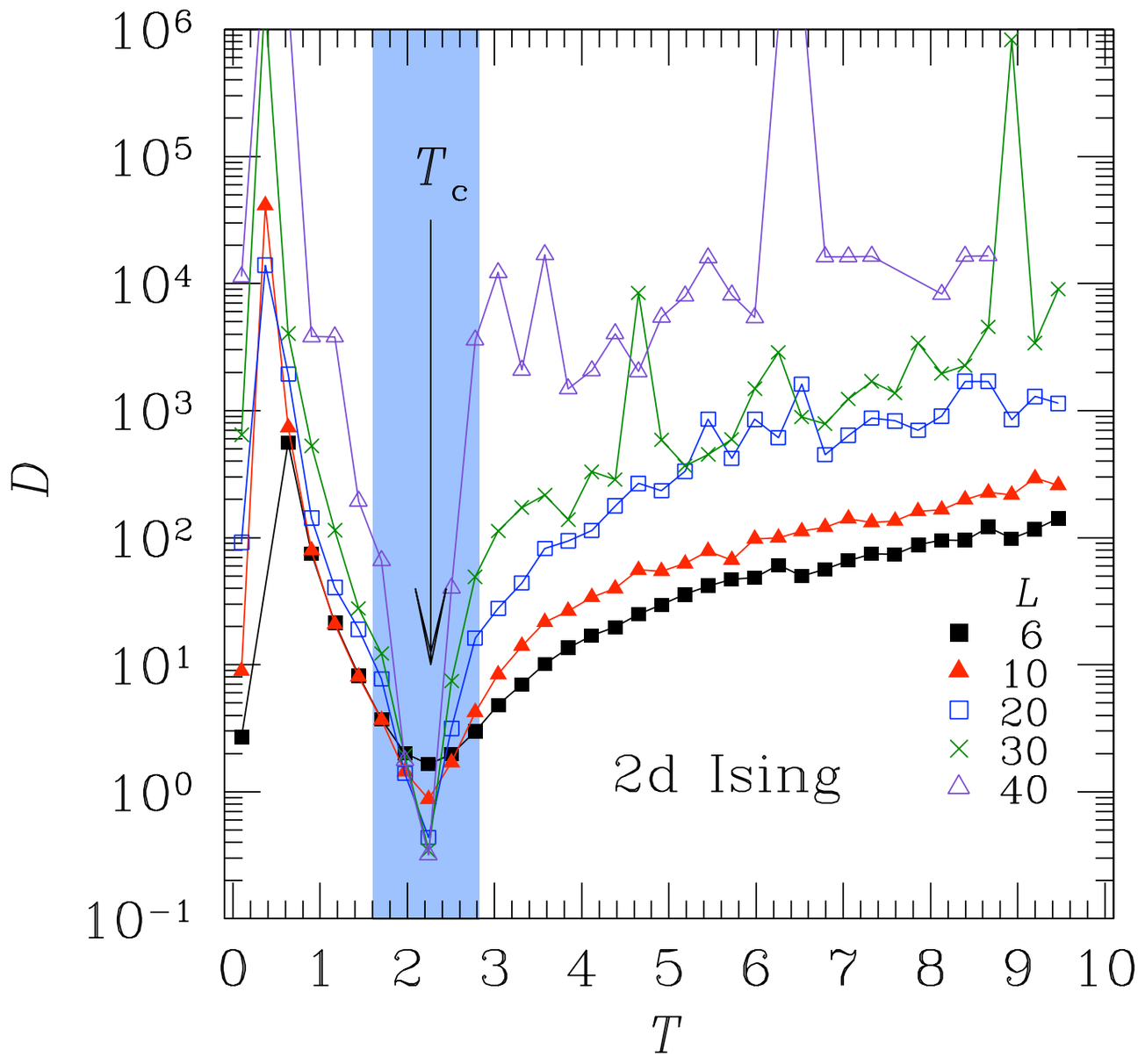


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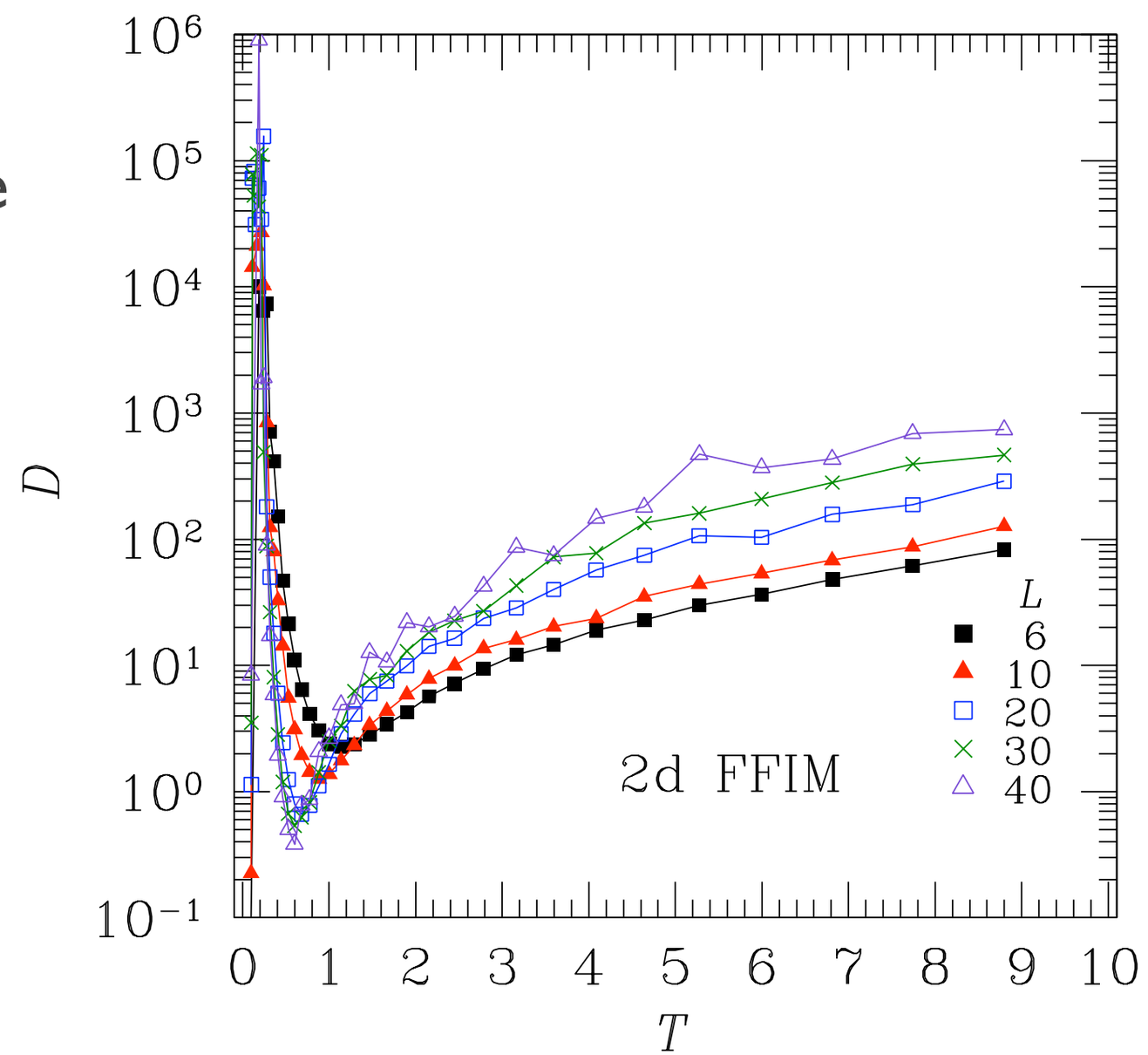


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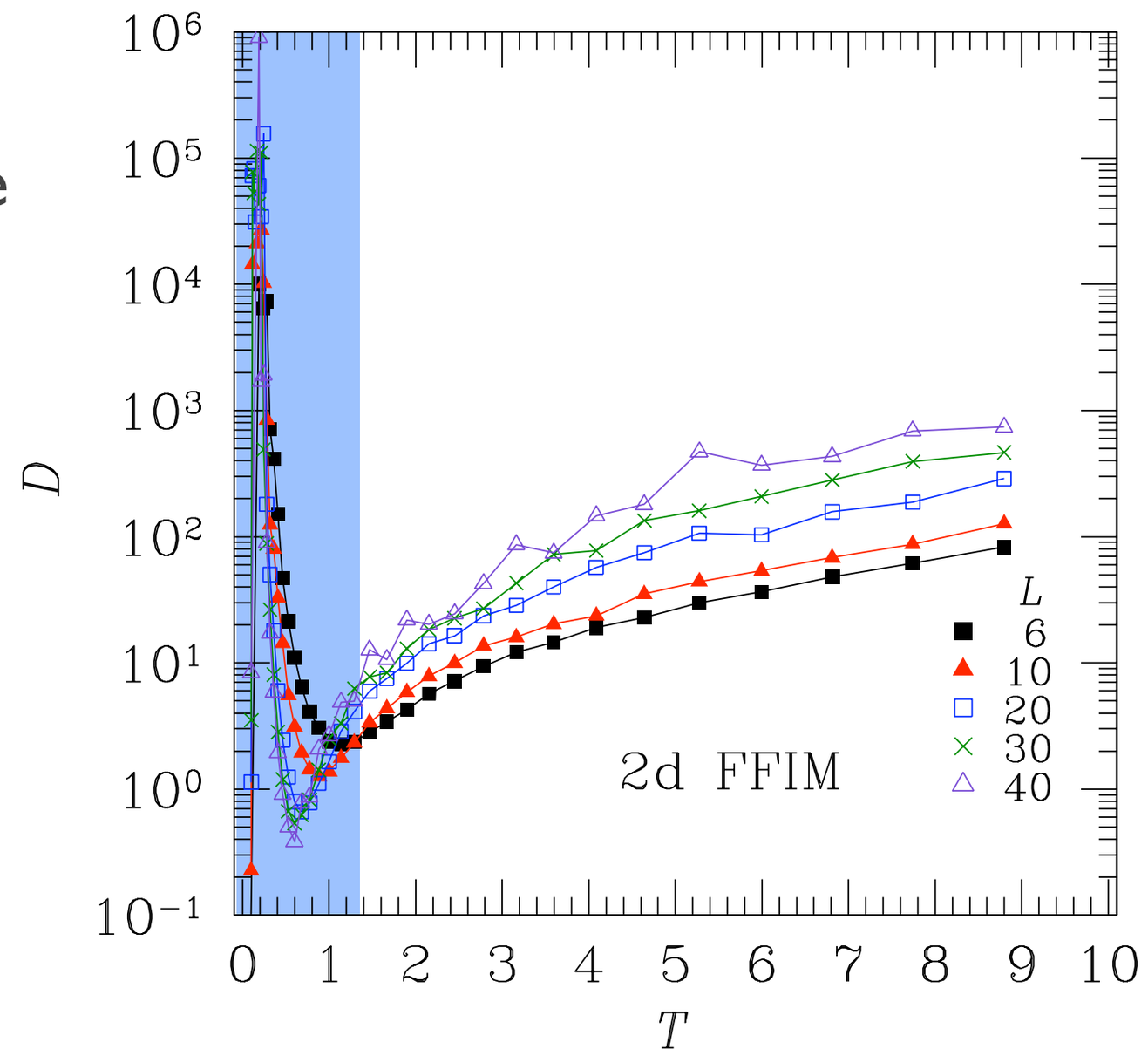


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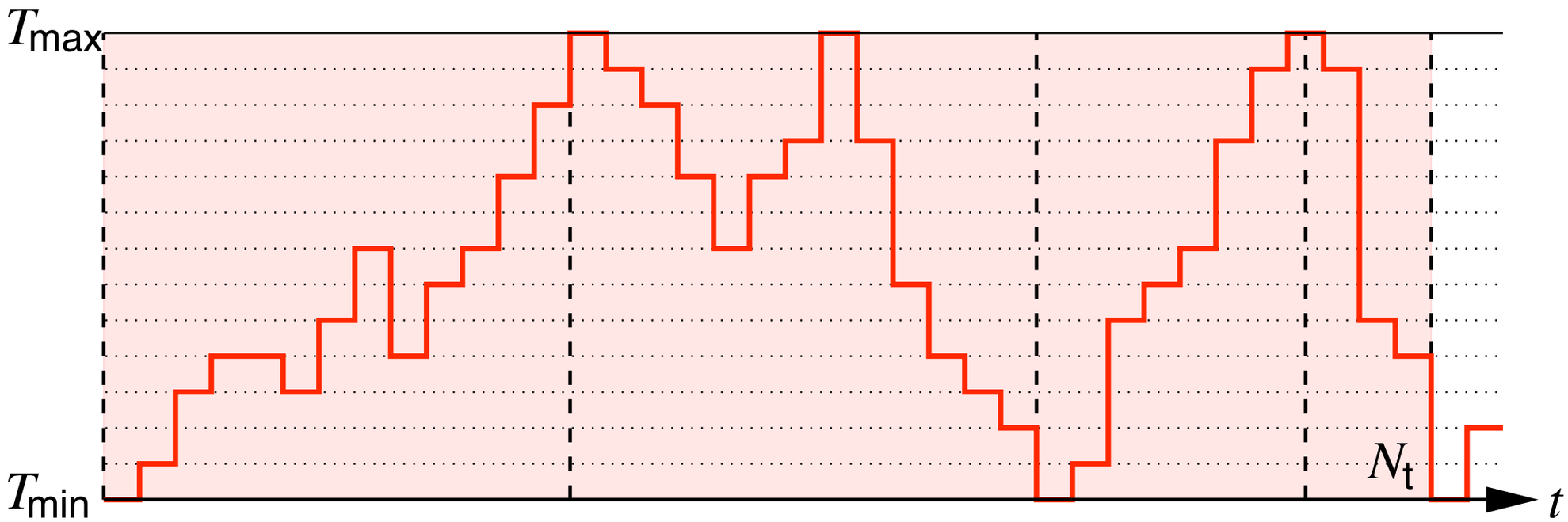
# Feedback method

Katzgraber *et al.*, JSTAT (06)




- Track replicas for $N_t$ MCS and compute a histogram $n(T)$ of the number of times a replica hits a given $T$.
- Compute a histogram of directed walkers $n_{up}(T)$.
- Calculate the fraction $f(T) = n_{up}(T)/n(T)$ $\quad [D(T) = (df/dT)^{-1}]$.
- Calculate $\{T'_i\}$ from $\{T_i\}$:

$$\frac{1}{\Delta T'_i} = C\sqrt{\frac{1}{\Delta T_i}\frac{df}{dT_i}} \sim \frac{1}{\sqrt{\Delta T_i D(T_i)}}$$

- Choose C such that $[T'_{min}, T'_{max}]$ maps back to $[T_{min}, T_{max}]$. Iterate!

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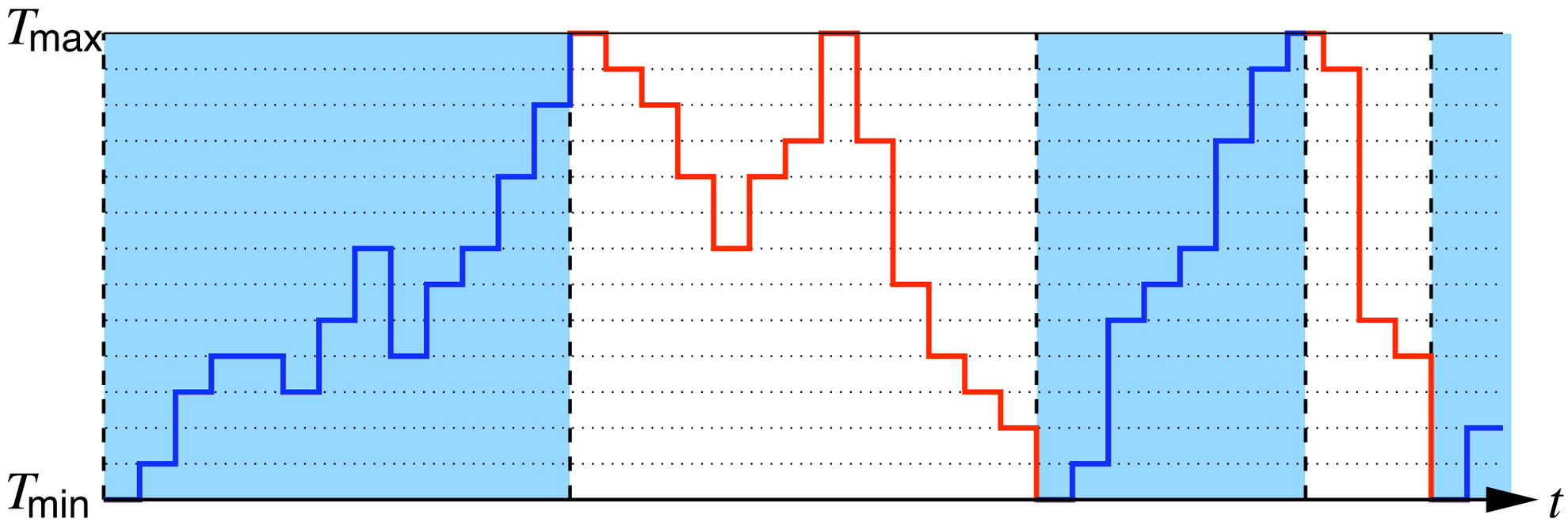
Katzgraber *et al.*, JSTAT (06)

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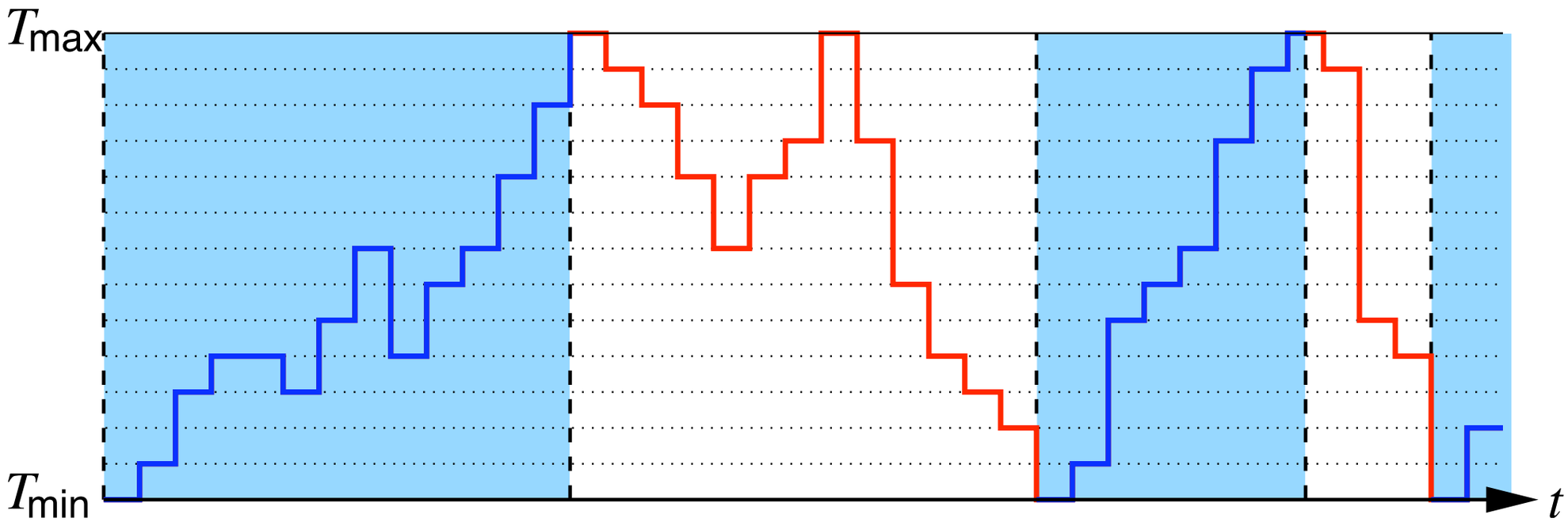


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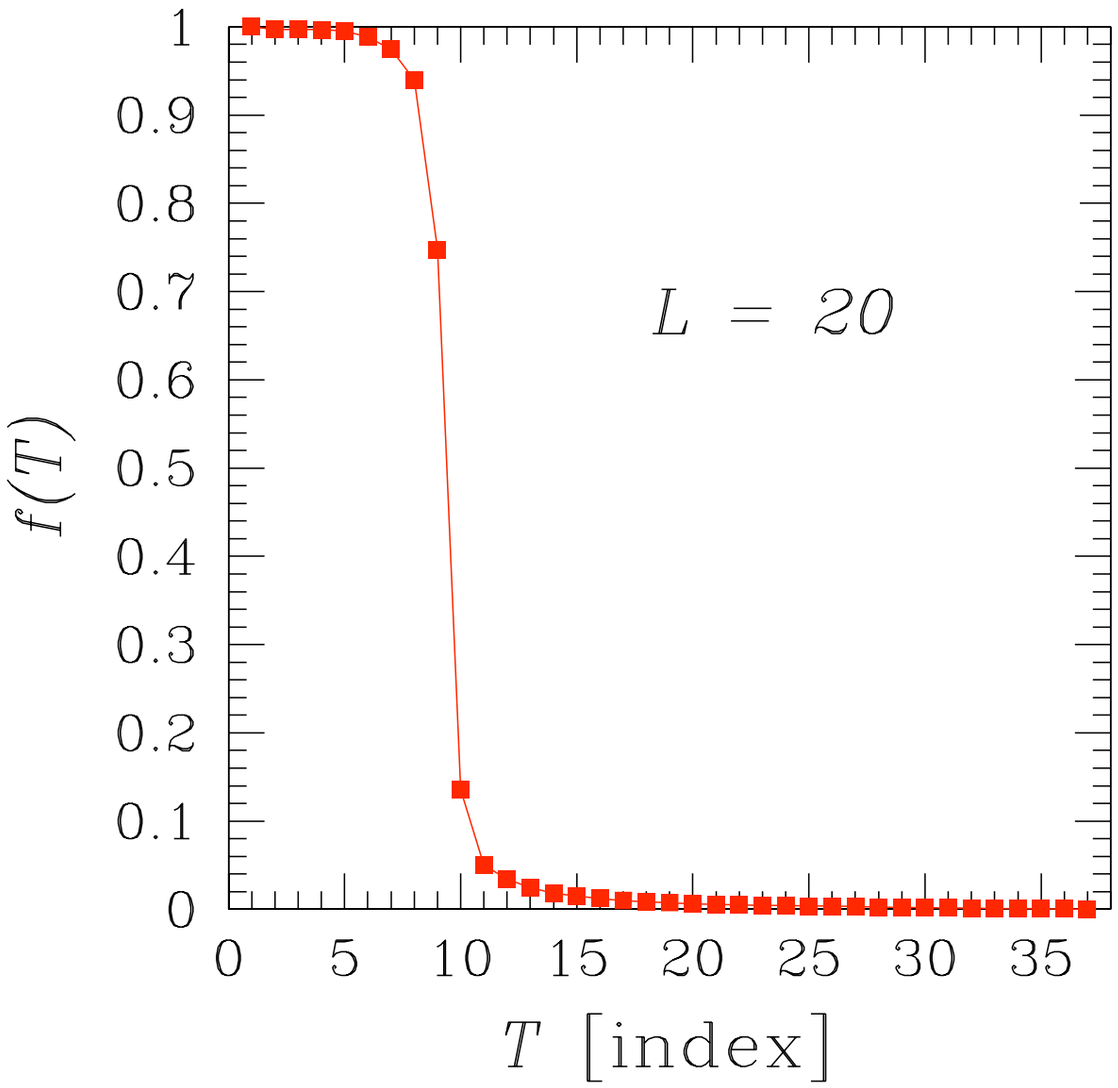


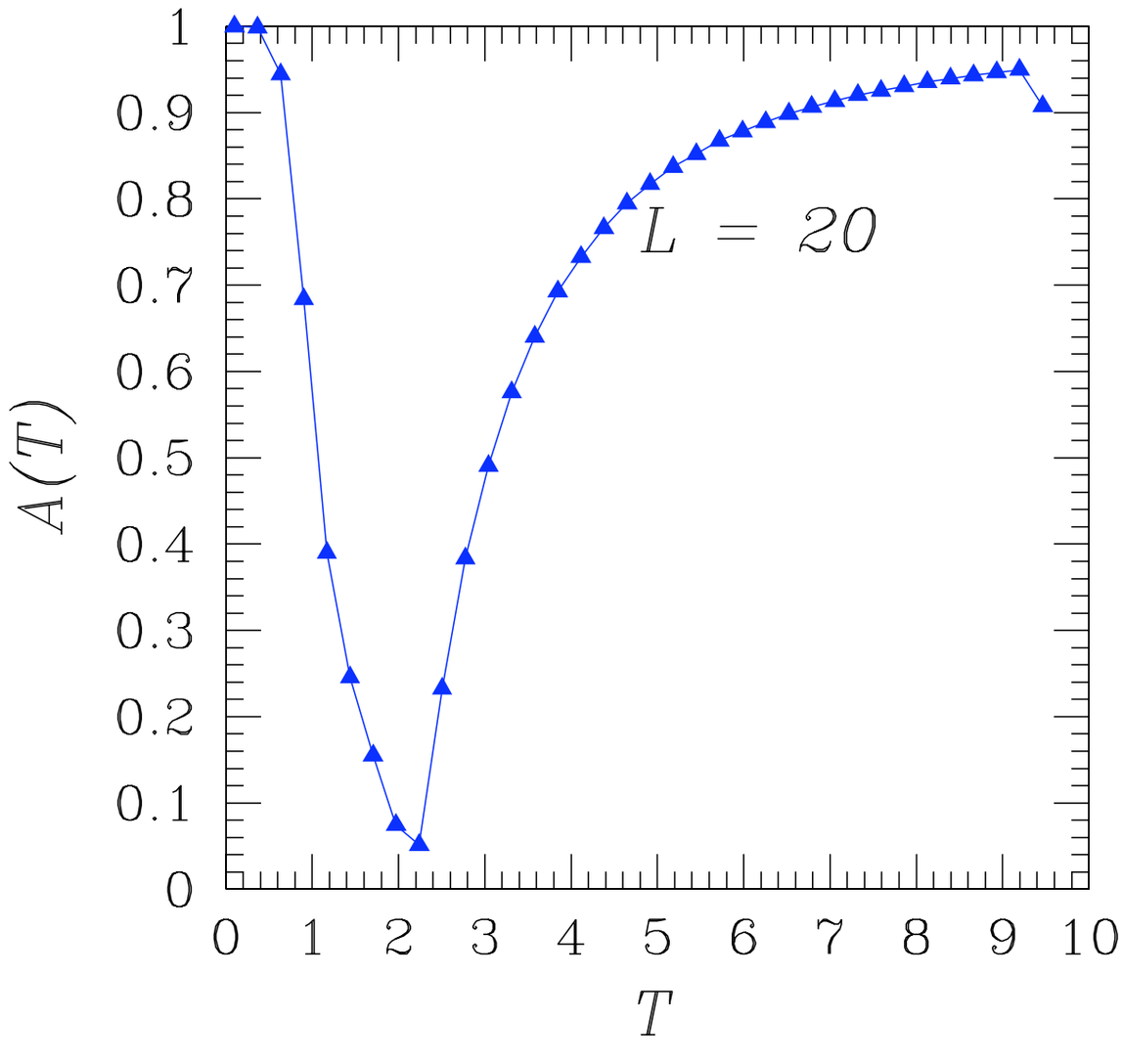


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- Feedback maximizes the rate of round trips.
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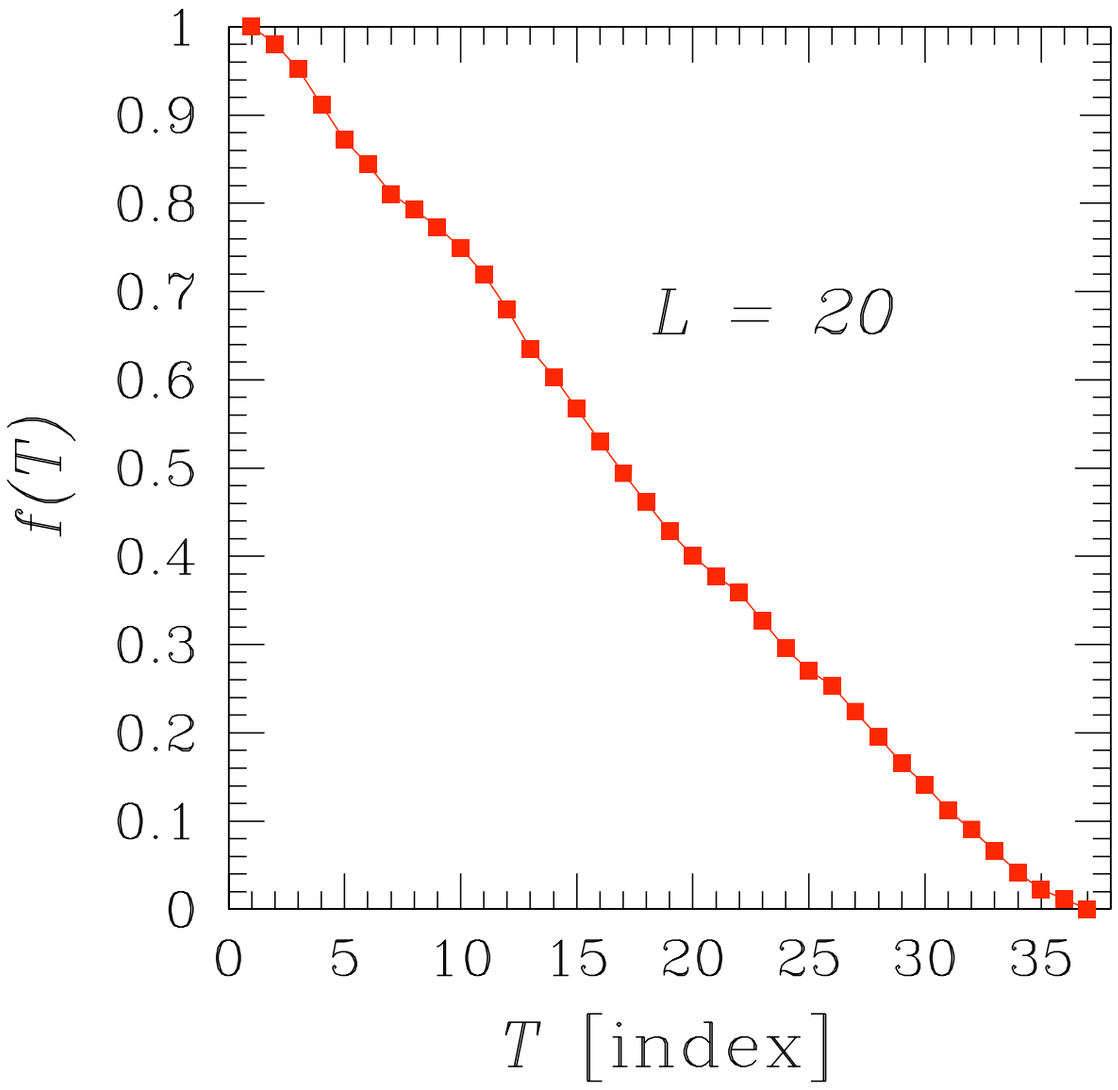


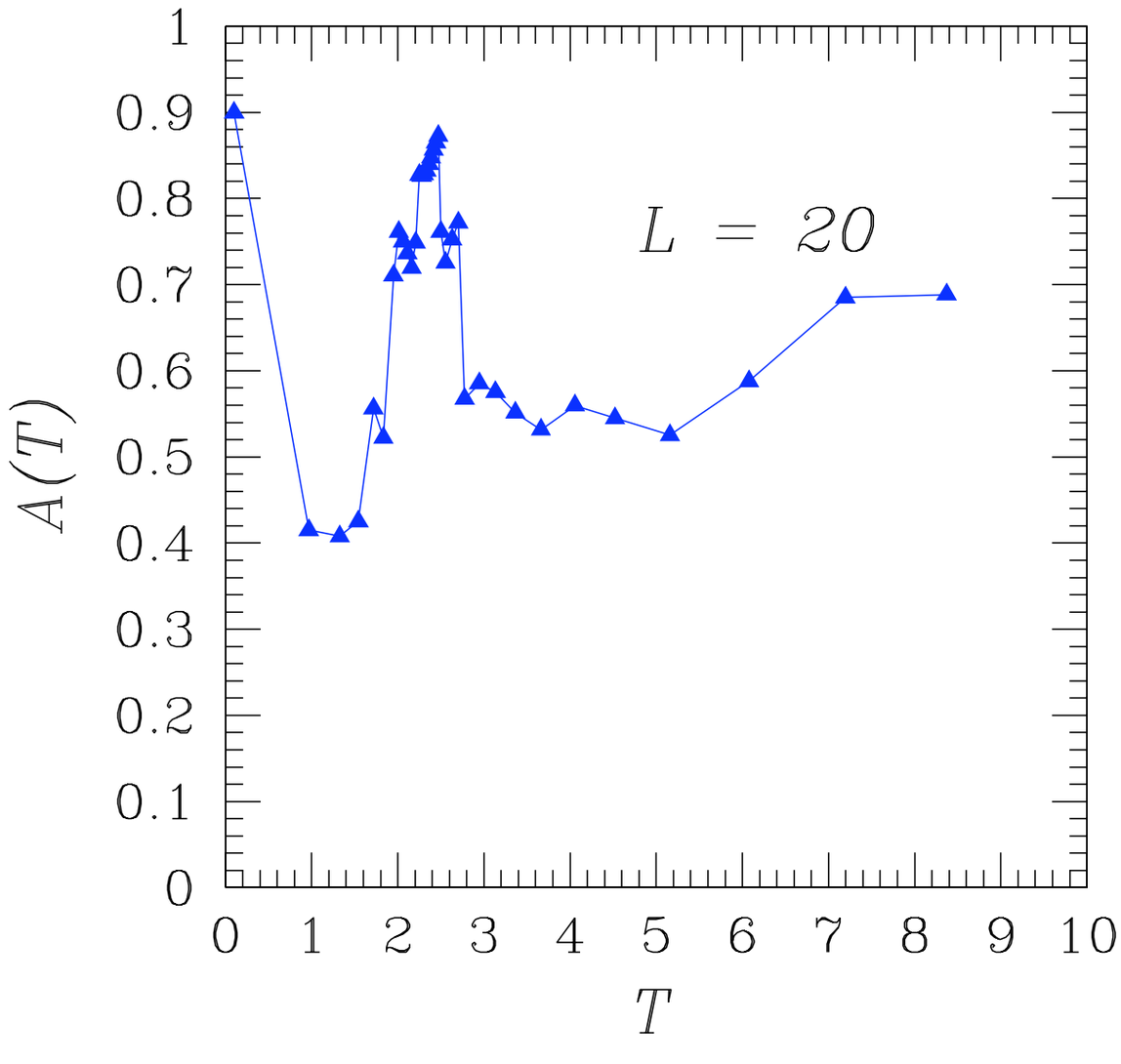


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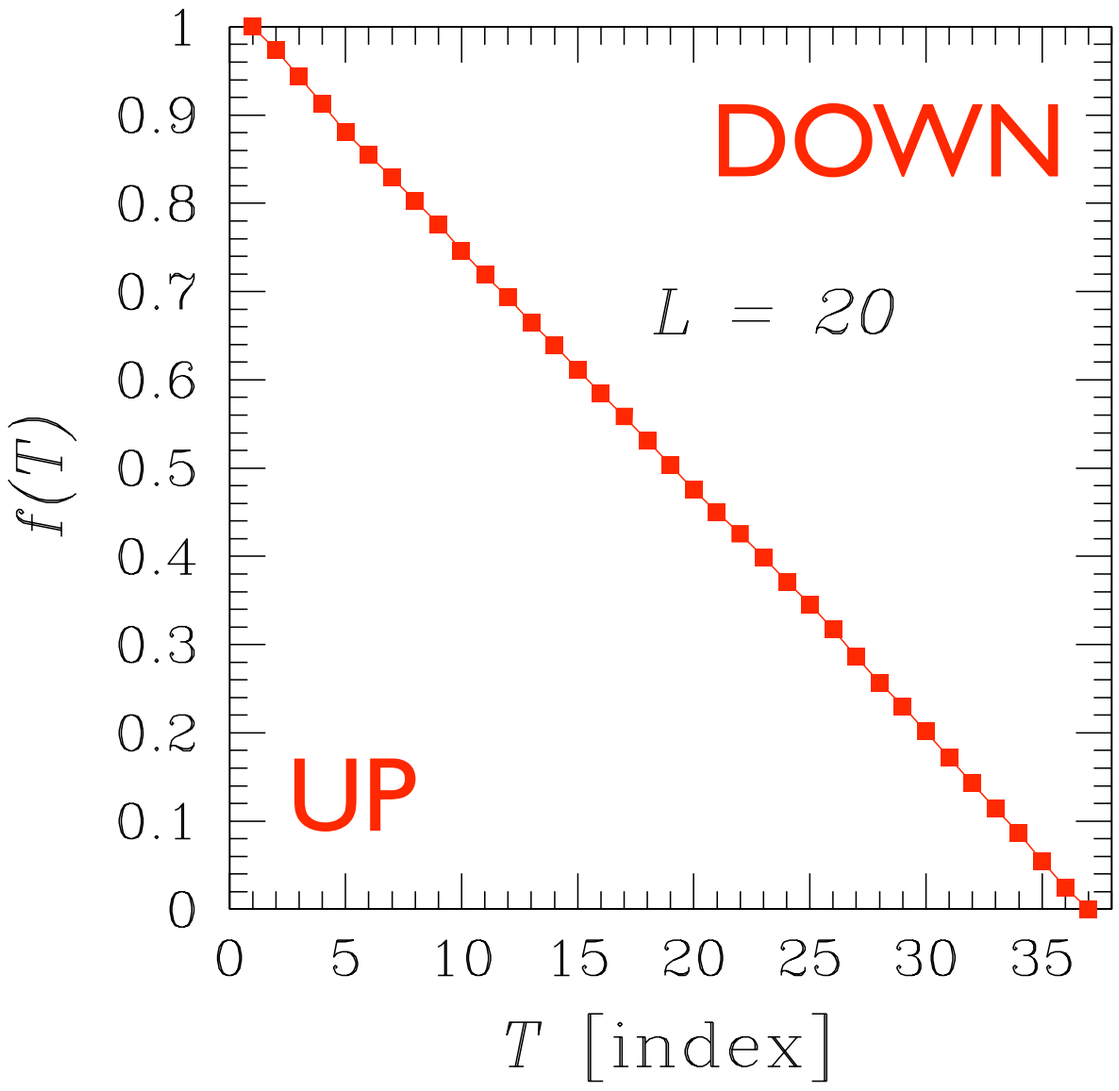


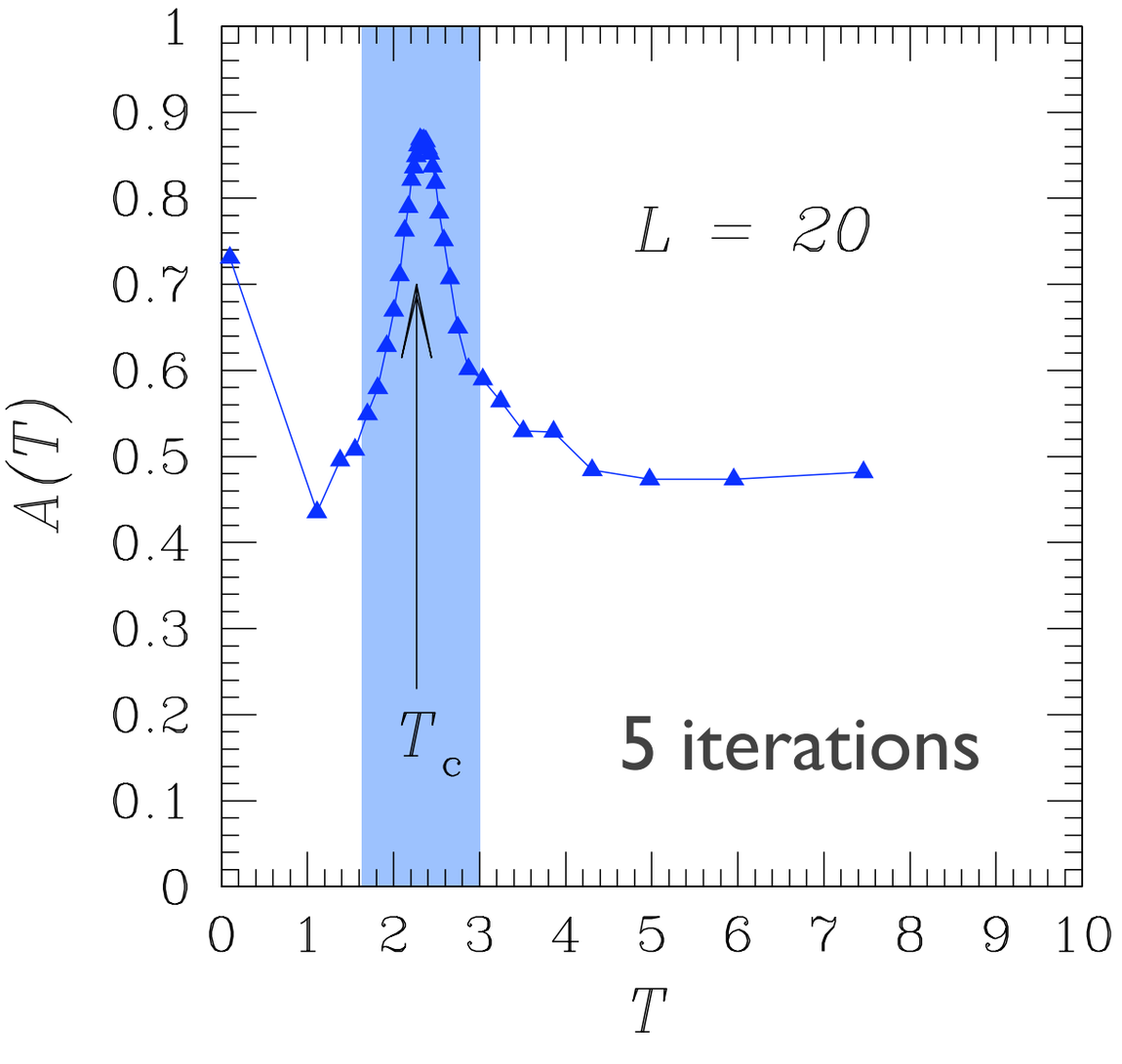


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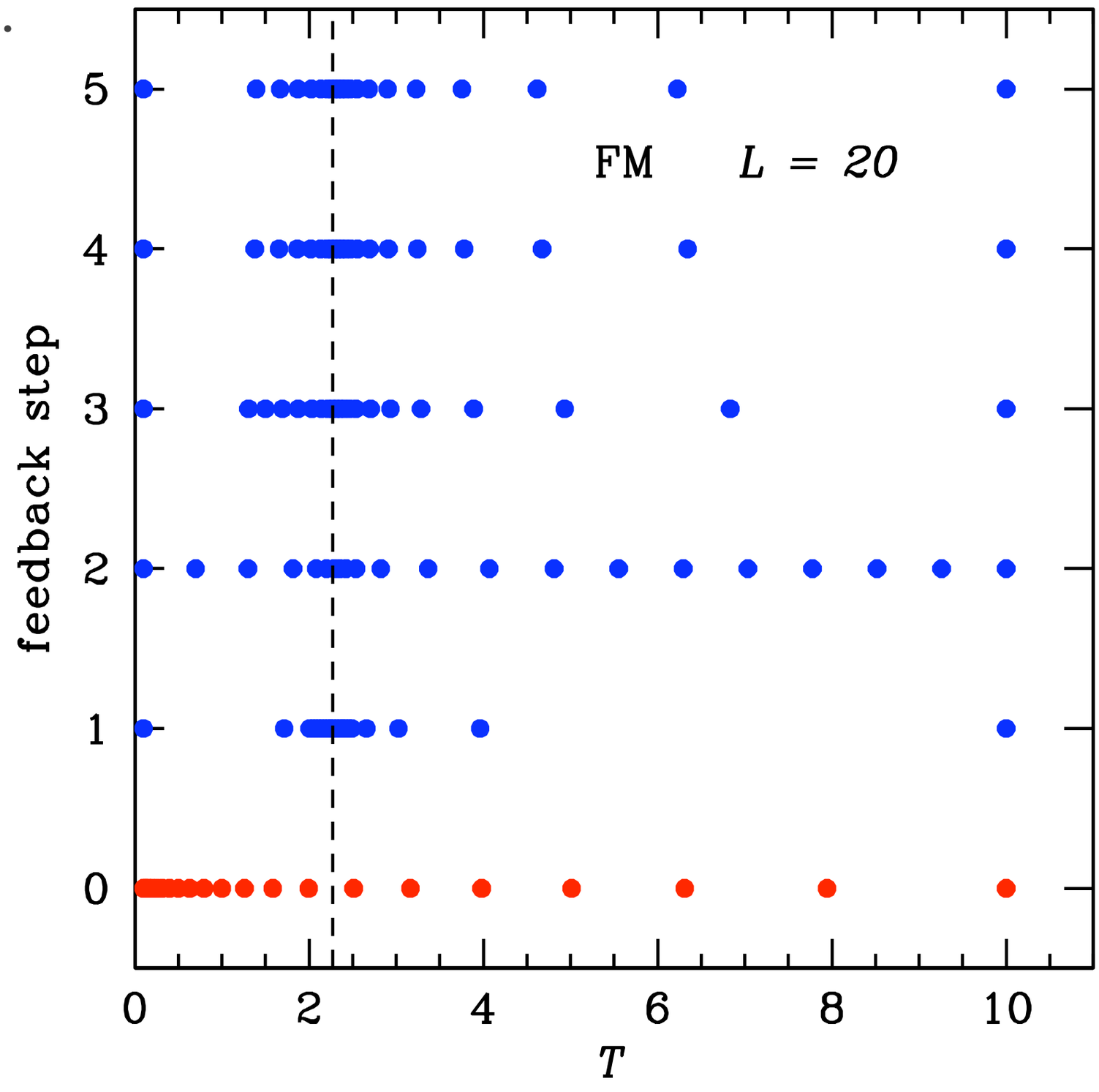
- After few iterations the temperature set converges.
- The method reallocates more temperatures to the bottlenecks.



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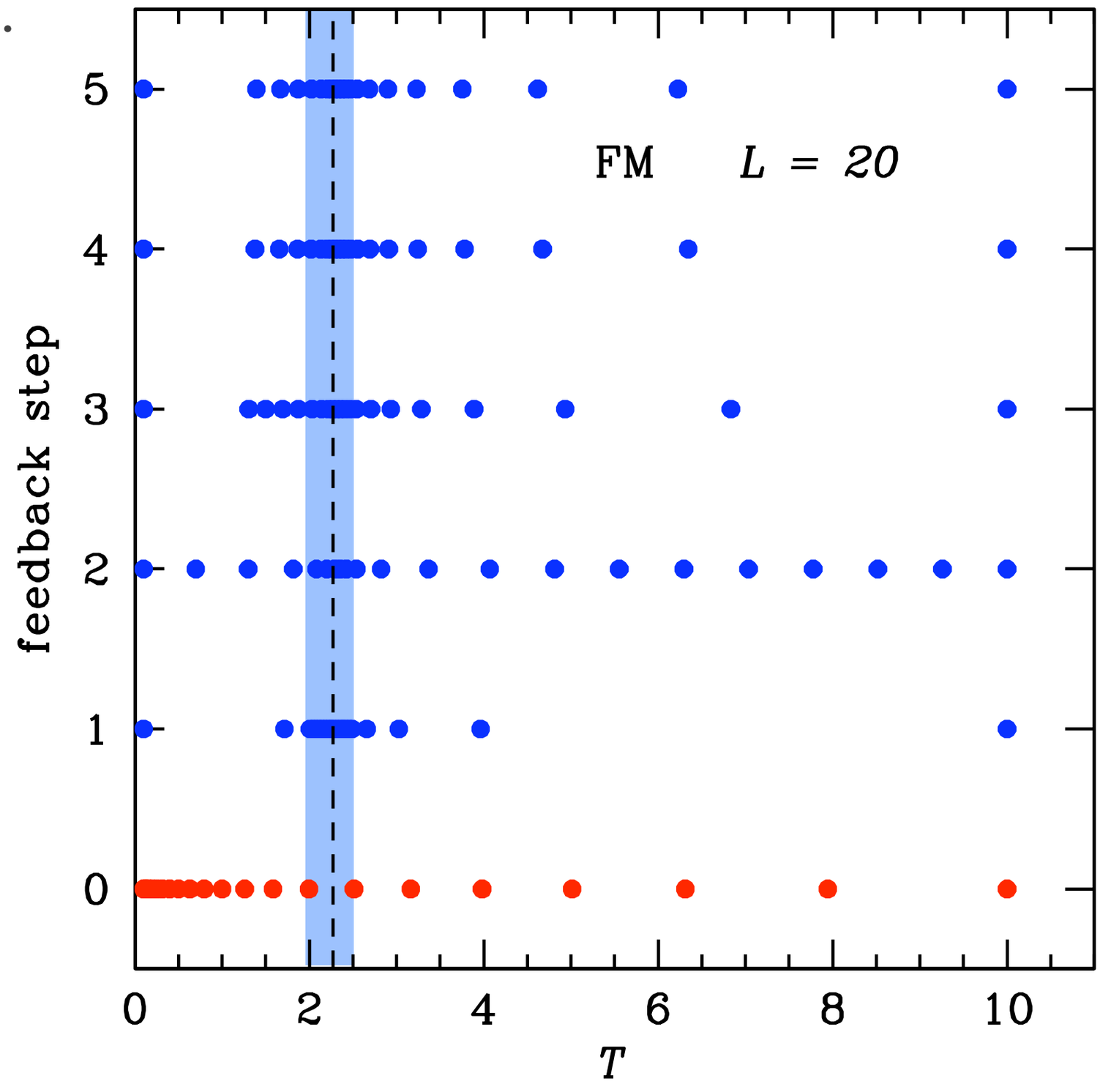

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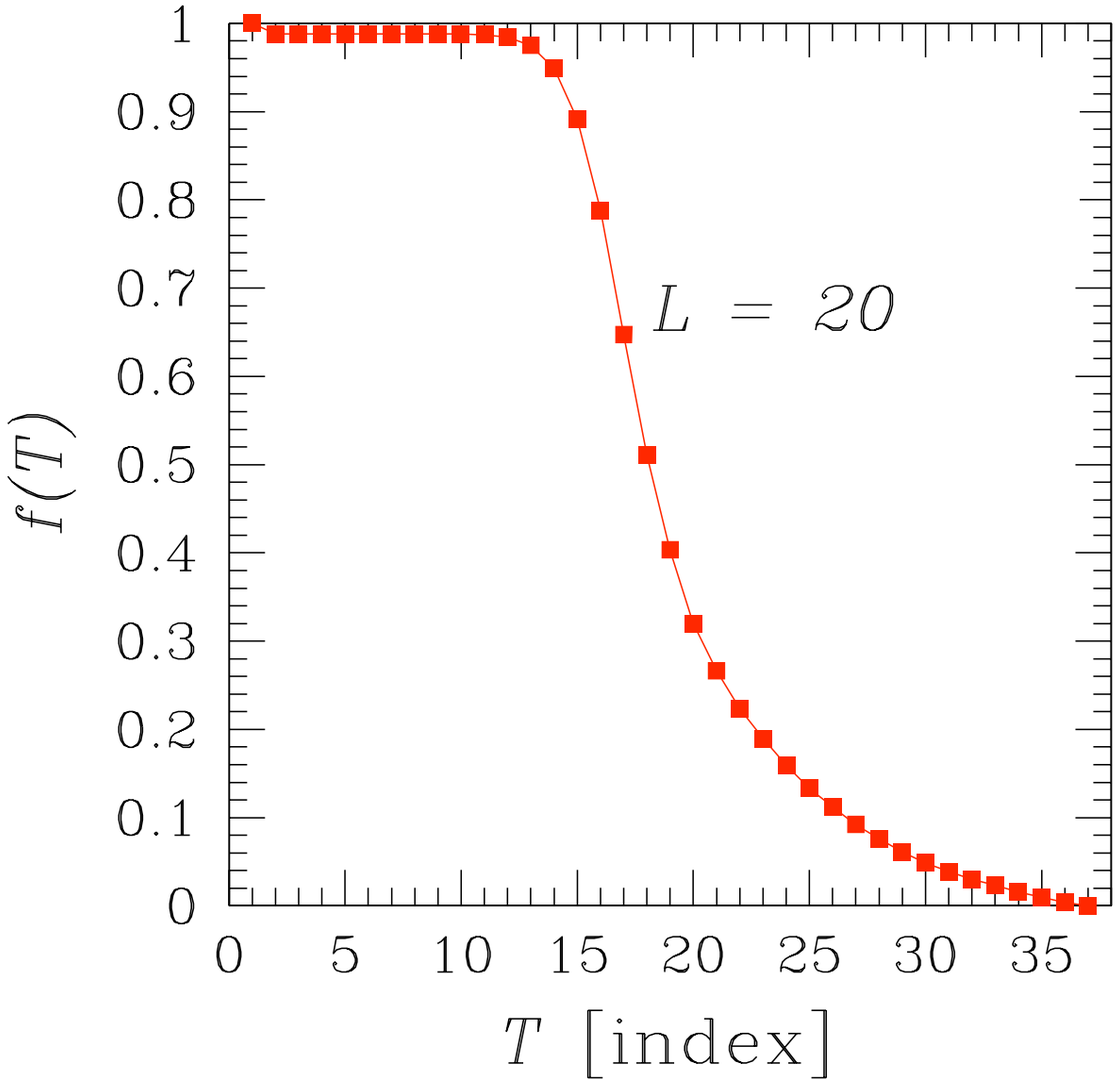


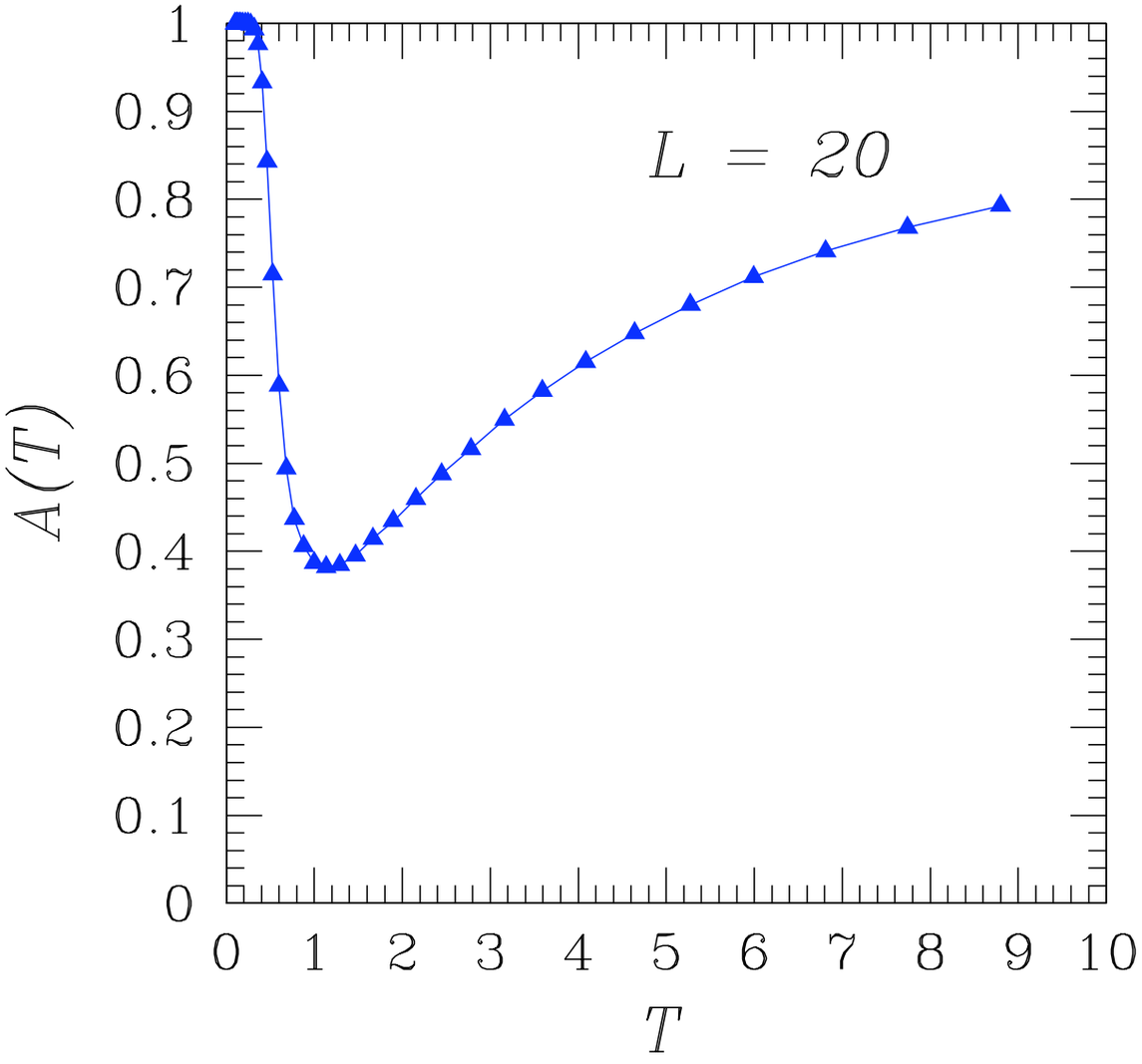


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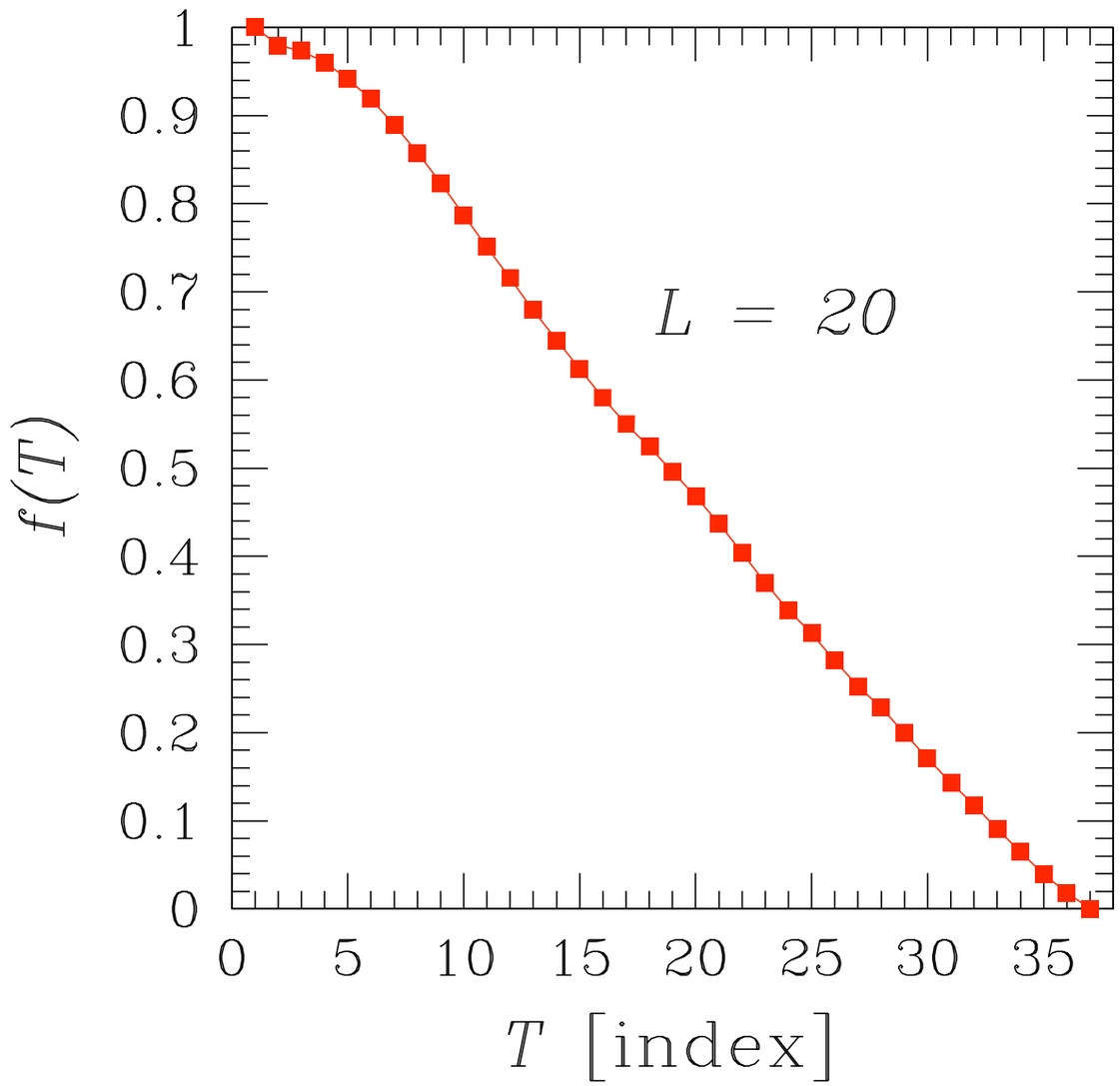


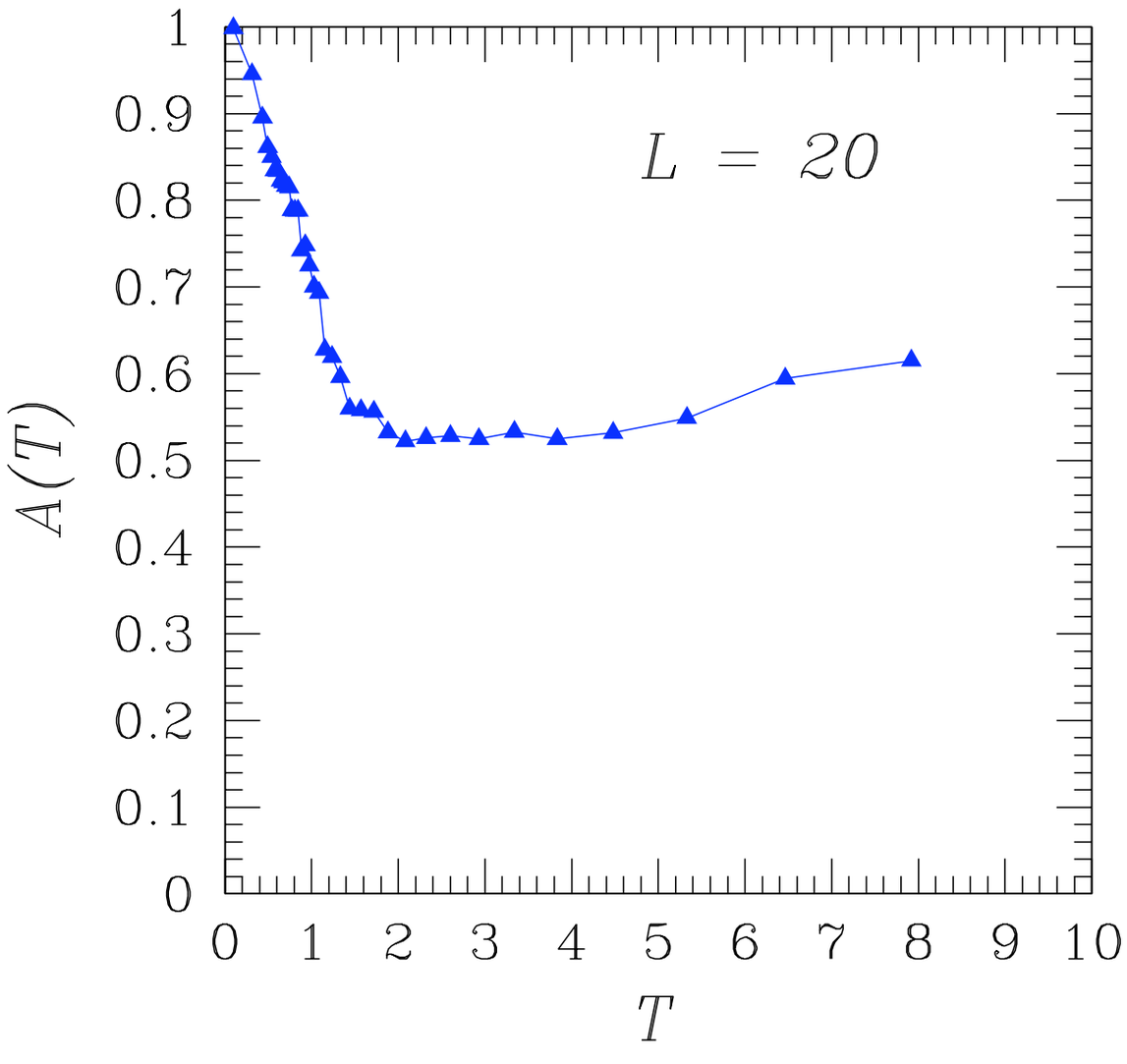


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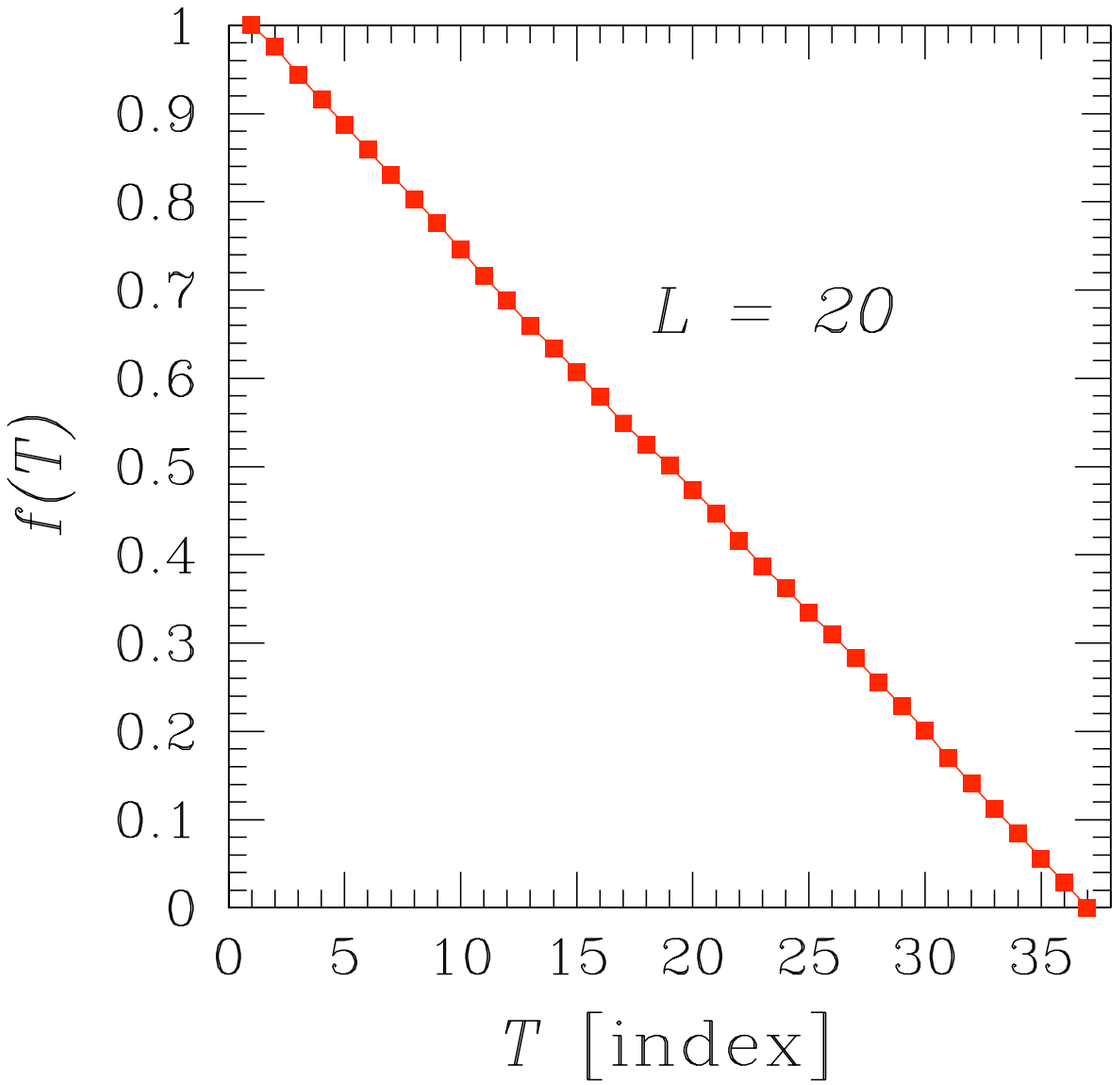


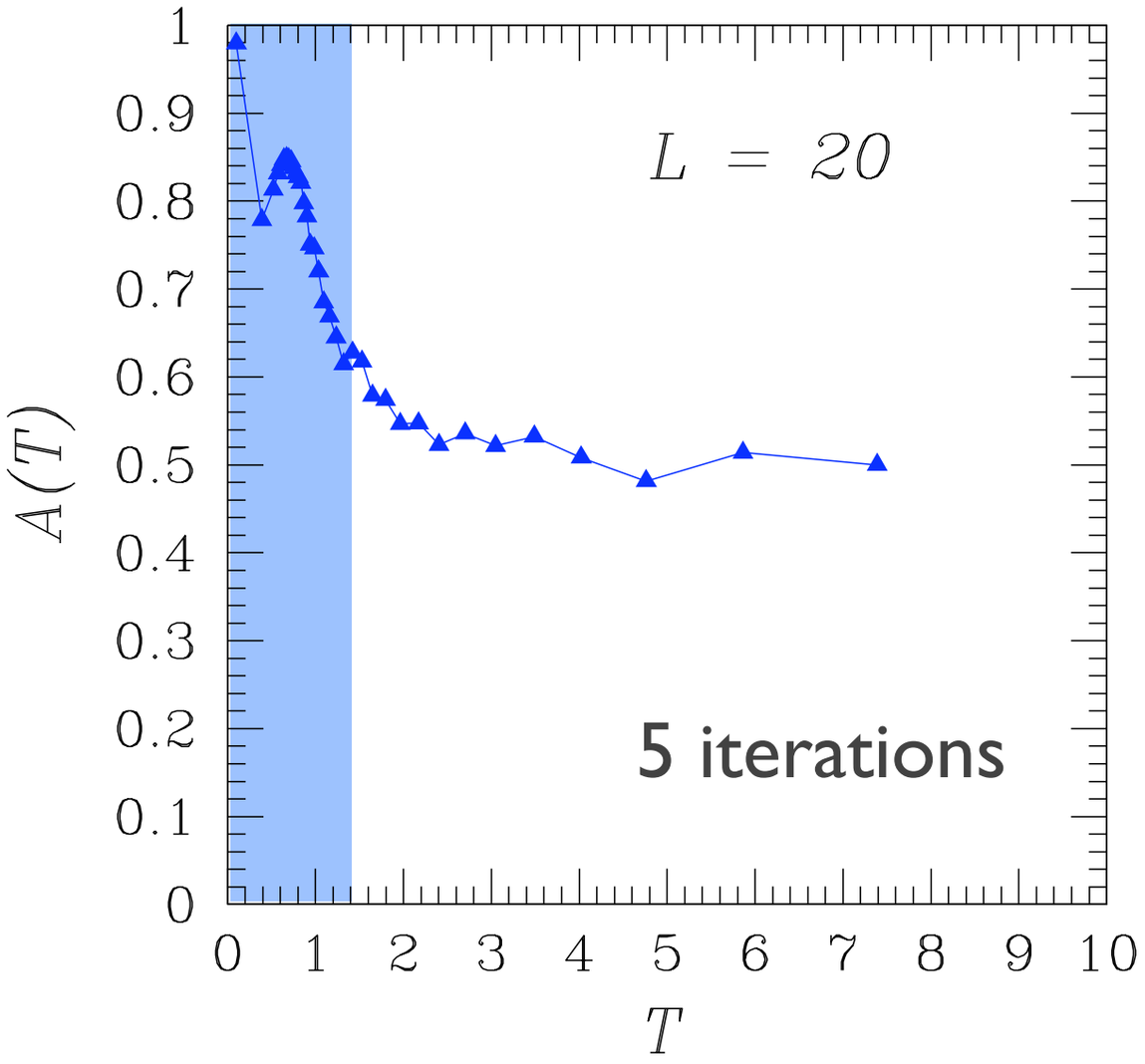


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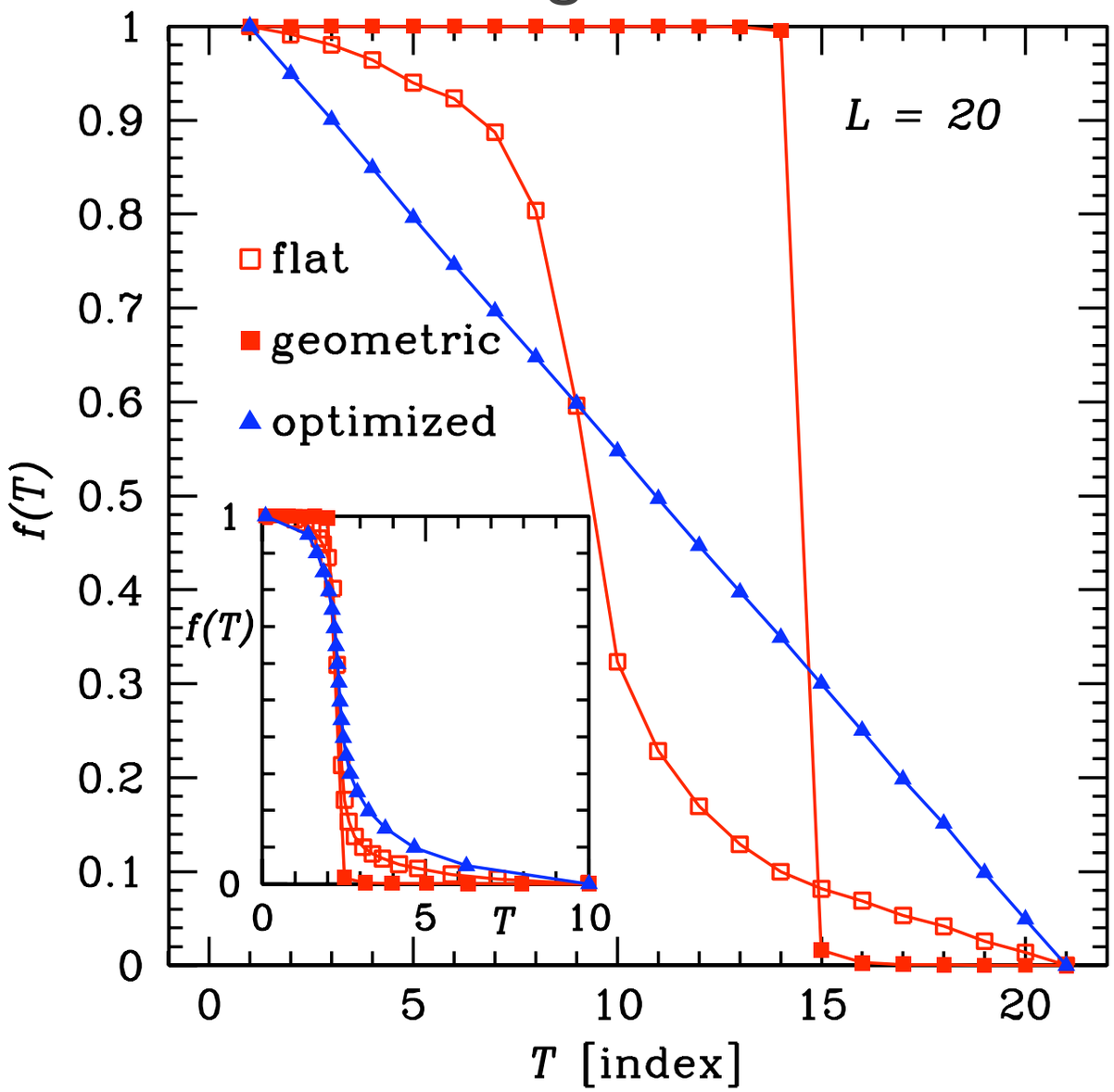
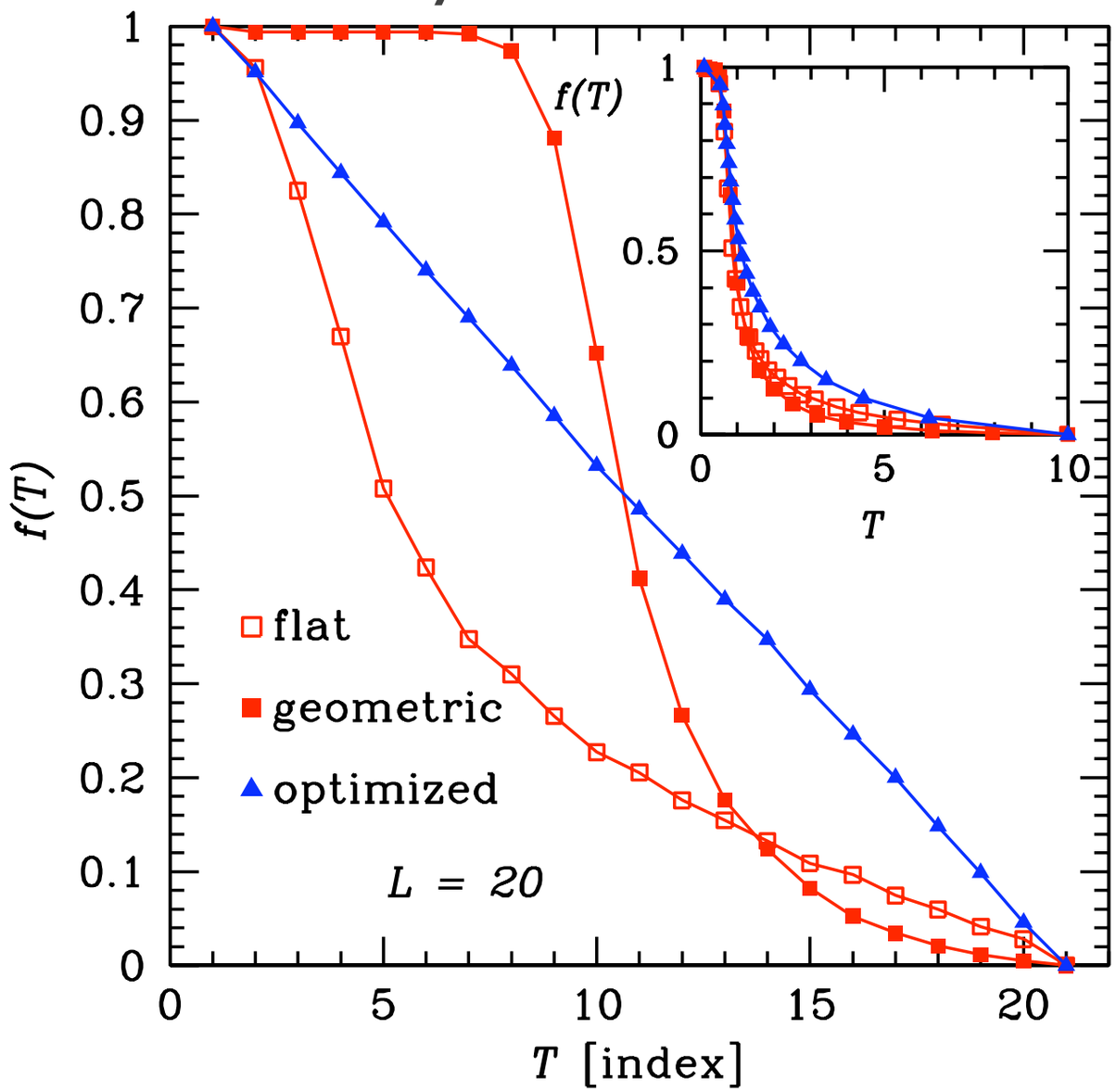
# Comparison of fractions

Ising model



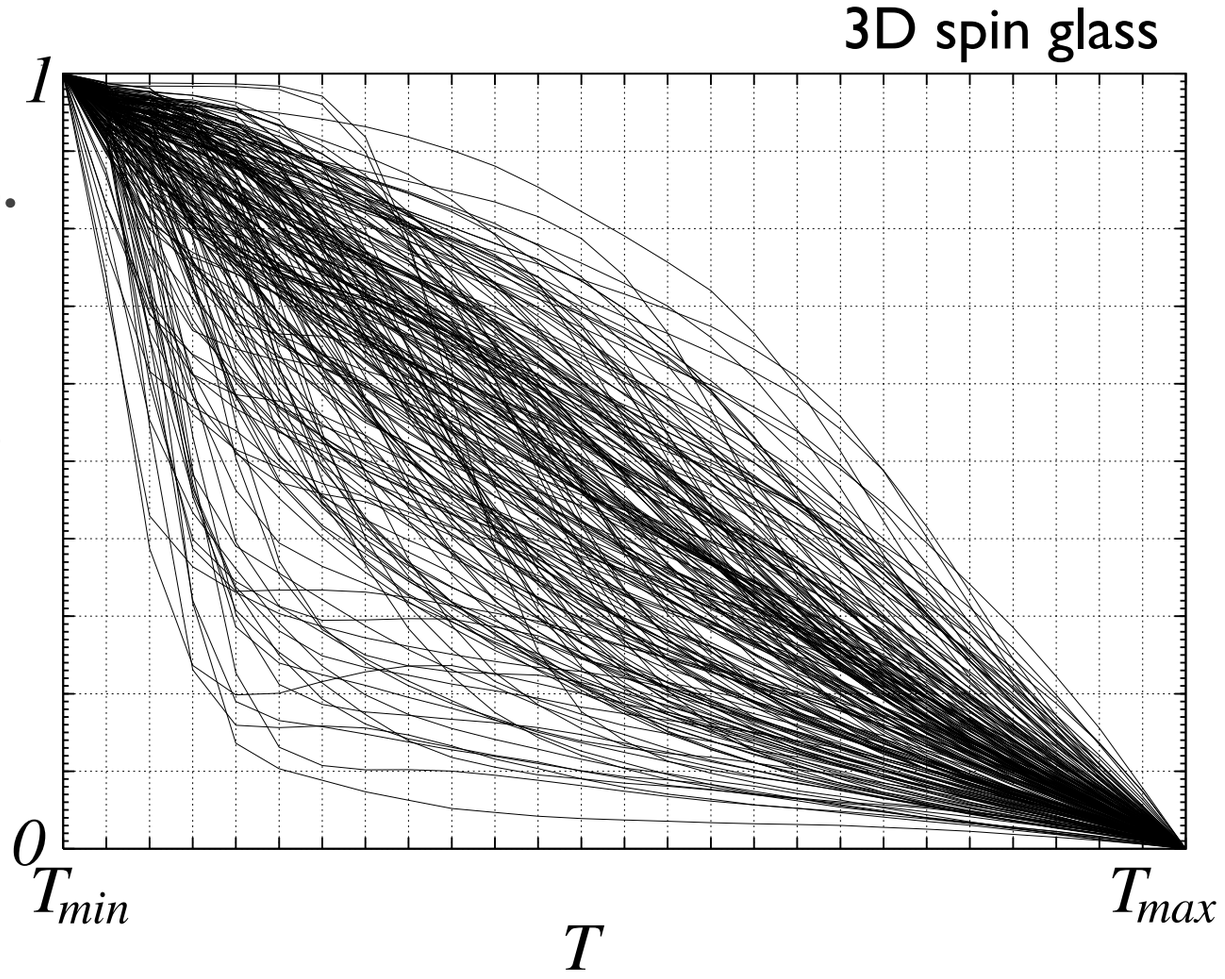

Fully frustrated model




- In general, a "flat" [$A(T)$ ~ const] temperature set is not too bad, but not optimal.
- If $C_v$ diverges, a geometrical progression is bad.

# What happens for systems with disorder?

- Problems:
  - We need to deal with averages.
  - Each fraction depends on the given disorder configuration.
  - Each disorder configurations converges independently...
  - The round-trip times are fat tail distributed.
  - Each disorder realization has its own temperature set.

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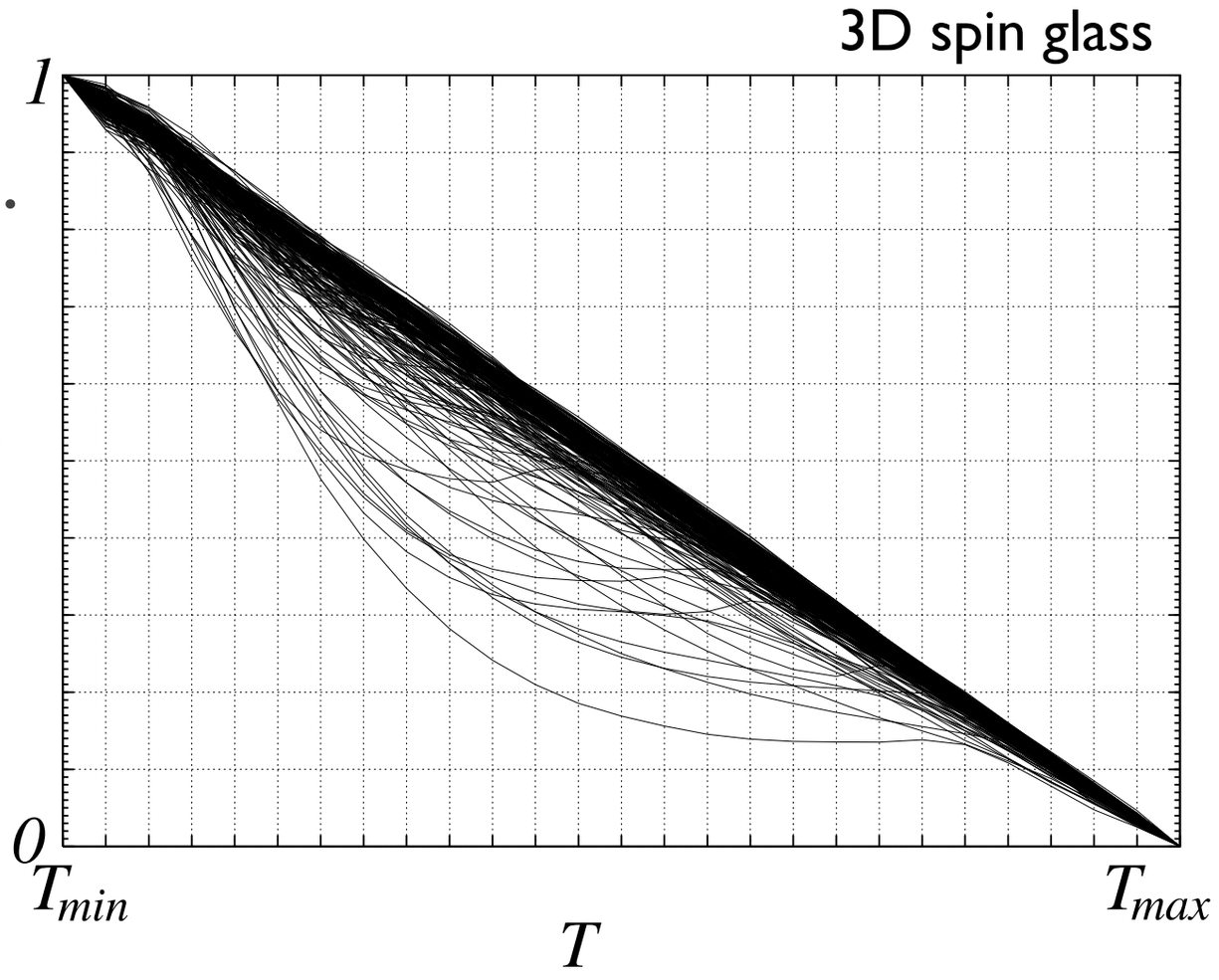


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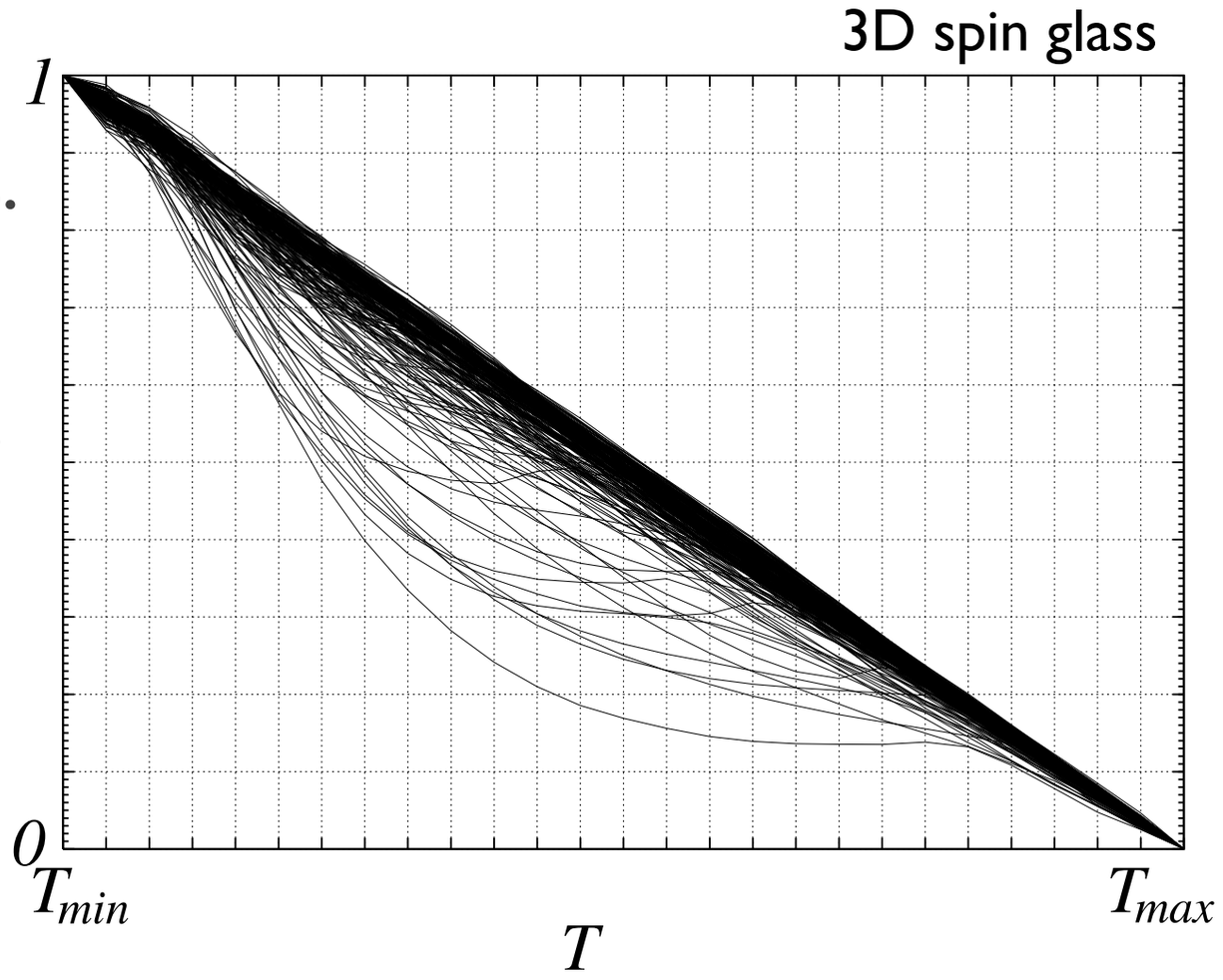


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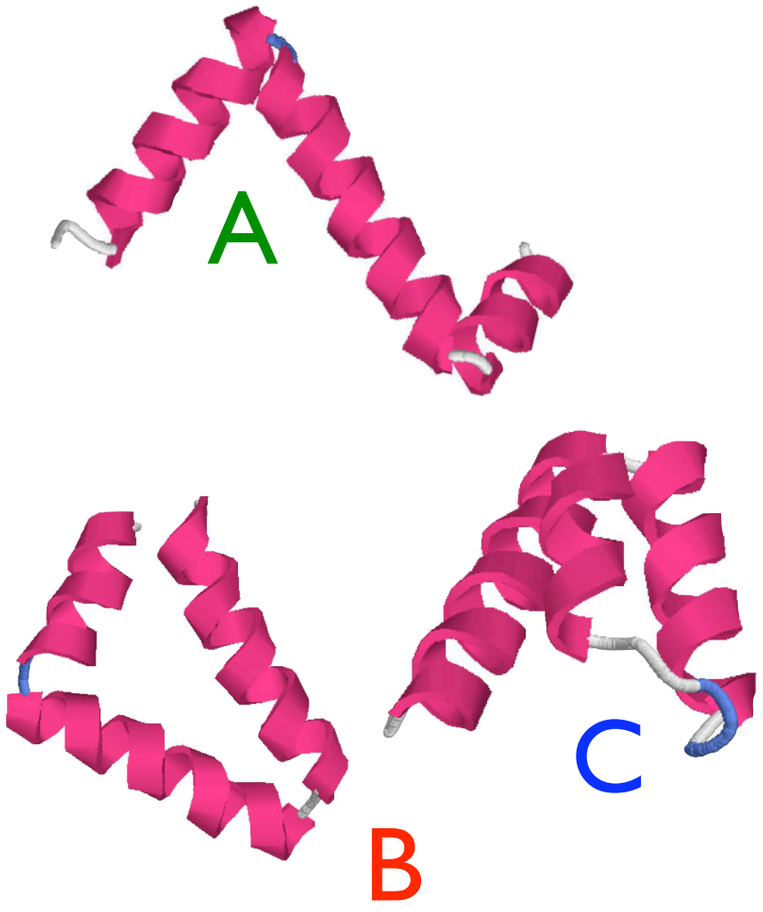
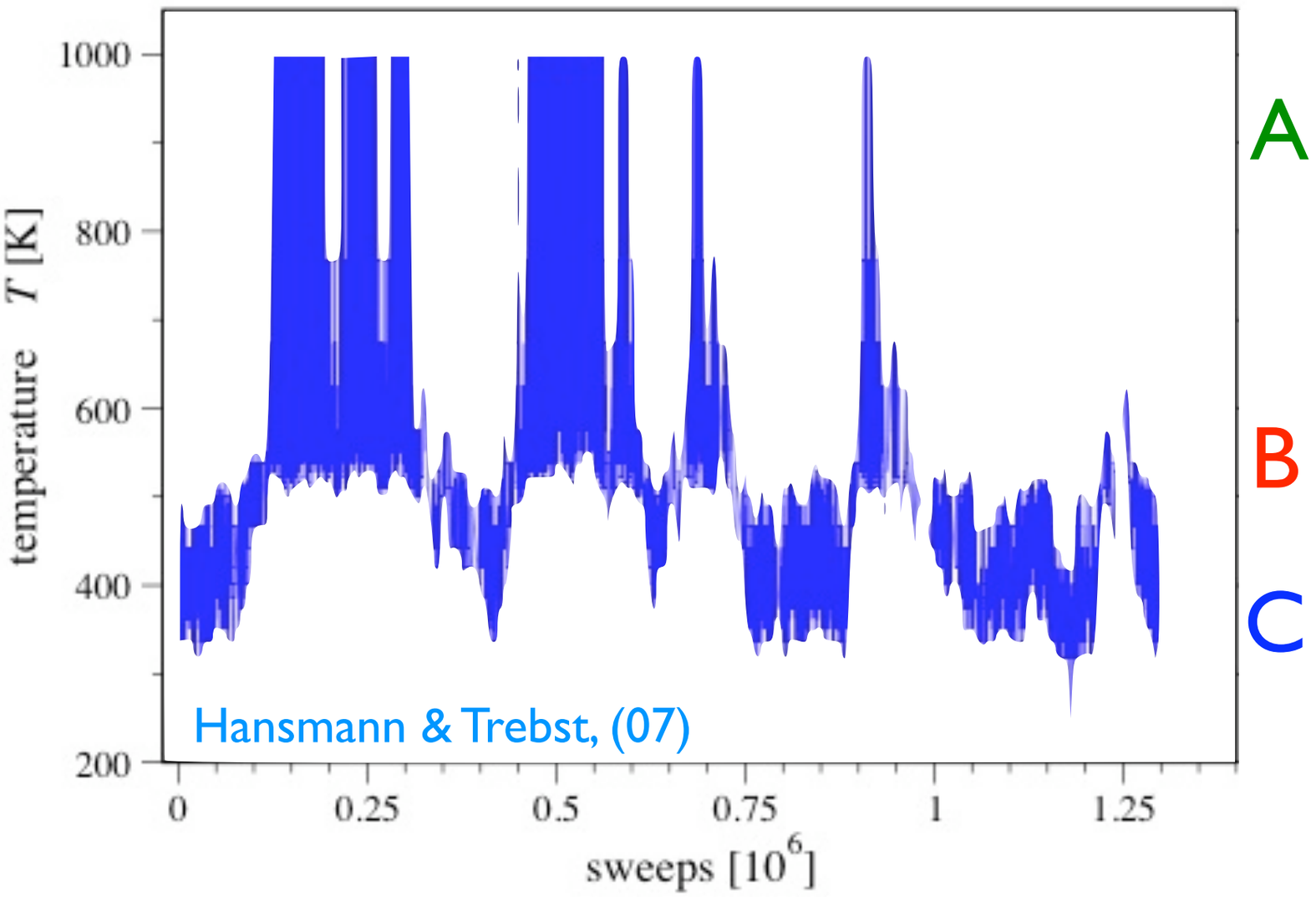
Do not use for glasses...

# Simulations in (bio)chemistry

- Example: Protein A

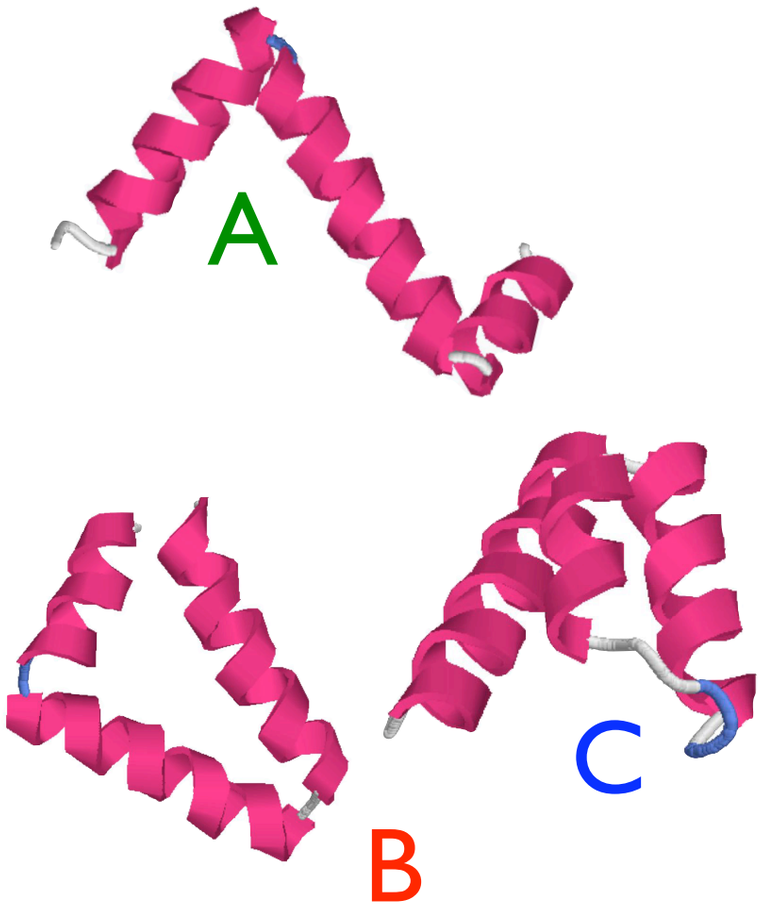


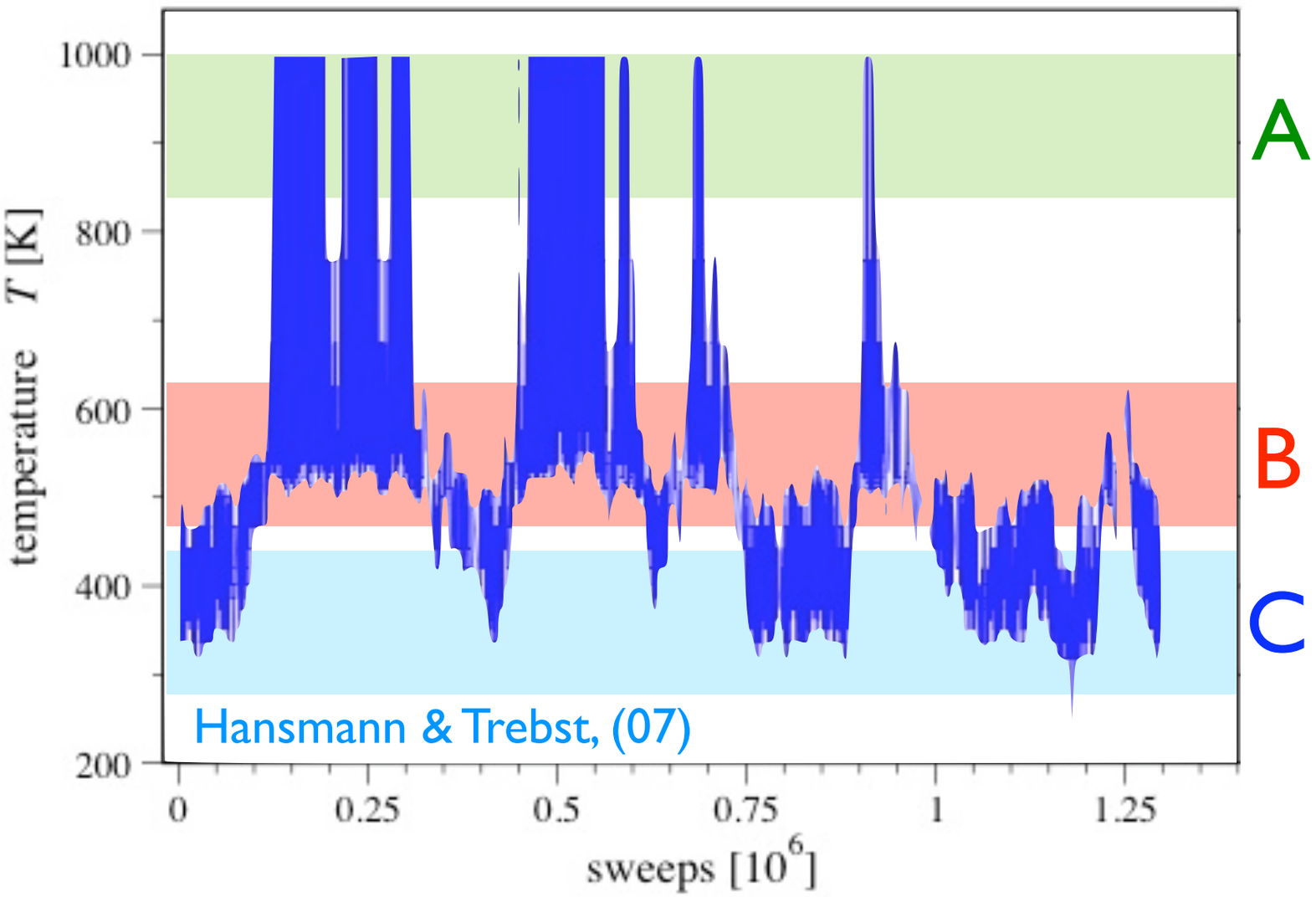




- It can happen that the replicas will only move in subspaces of the phase space (A, B, C).
- Feedback optimization helps overcome these problems easily. Simulations otherwise impossible.

# Simulations in (bio)chemistry

- Example: Protein A

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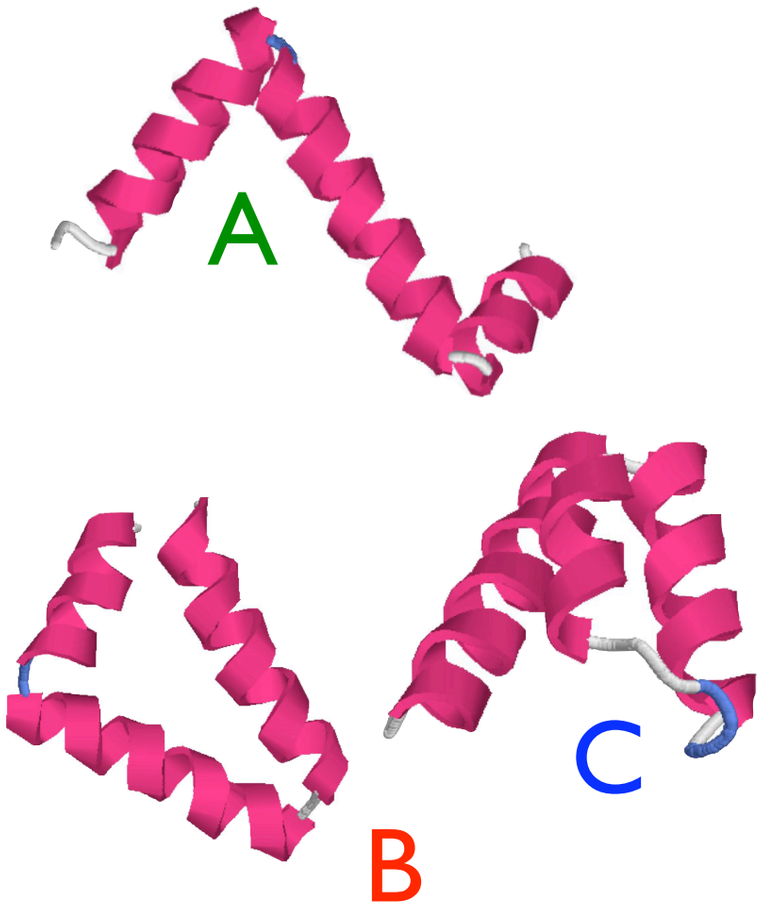
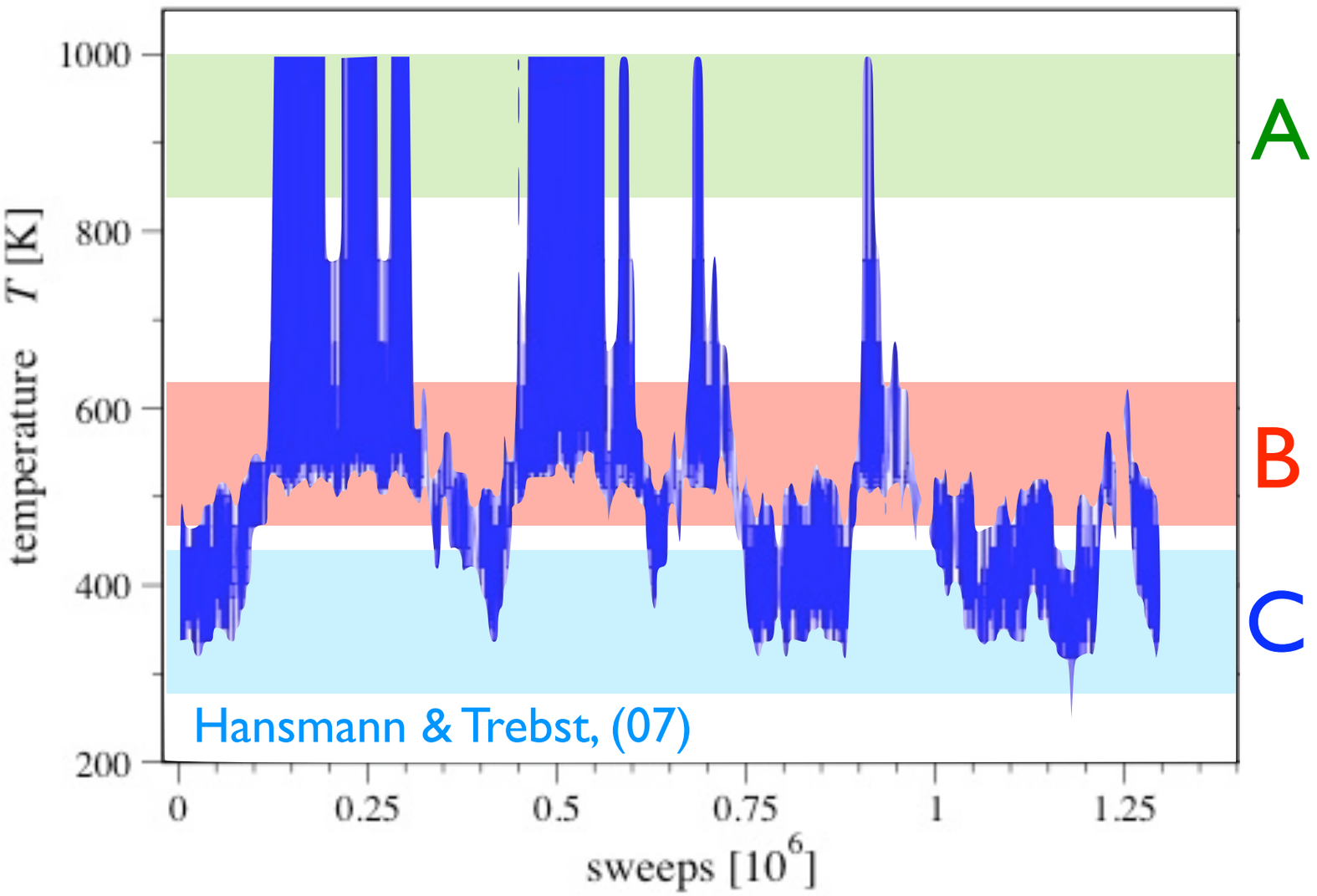
# Simulations in (bio)chemistry

- Example: Protein A

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Use for biology applications...

# Some final thoughts (and extensions)...

# Heuristic ground state search

- Outline of the algorithm:
  - Perform an exchange MC run with $T_{min}$ close to zero.
  - Simulate two copies of the system with different Markov chains.
  - The system is in thermal equilibrium:
    - after each lattice sweep record the spin configuration and energy for the lowest $T$ if these match in both copies.
      - If a lower energy is found, replace the previously recorded energy.
  - Measure for $1/4t_{eq}$.

- For small to intermediate system sizes where other algorithms do not work well the method provides heuristic ground states with high probability (98% up).

# Extensions and combinations

- Any control variable can be used:
  - Field
  - Temperature and field
  - Coupling constants in QCD
  - Frequencies (e.g., in a Holstein model)
  - ...
- Combinations with other algorithms possible:
  - Exchange Monte Carlo molecular dynamics (biomolecules).
  - Exchange quantum Monte Carlo (quantum spin glasses).
  - Bayensian periodigram (planet search in star systems).
  - Iterative search methods (combinatorial problems).
  - Cluster exchange Monte Carlo (diluted spin glasses).
  - ...

Thank you.