PARALLEL TEMPERING CLUSTER ALGORITHM FOR COMPUTER SIMULATIONS OF CRITICAL PHENOMENA

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Parallel Tempering

- provides an efficient method to investigate systems with rugged free-energy landscapes, particularly at low temperatures

- used in many disciplines:
    - biomolecules
    - bioinformatics
    - classical and quantum frustrated spin system
    - QCD
    - spin glasses
    - zeolite structure solution

Parallel Tempering

- How it works?

- different replica are simulated at different temperatures
- regular intervals an attempt is made to exchange the replica
- replica are exchanged via a Monte Carlo process the attempt is accepted with a probability

$$P_{\mathrm{PT}}(E_1, \beta_1 \rightarrow E_2, \beta_2) = \min[1, \exp(\Delta\beta\Delta E)]$$

with $\Delta\beta = \beta_2 - \beta_1$ and $\Delta E = E_2 - E_1$

Parallel Tempering

- How it works?

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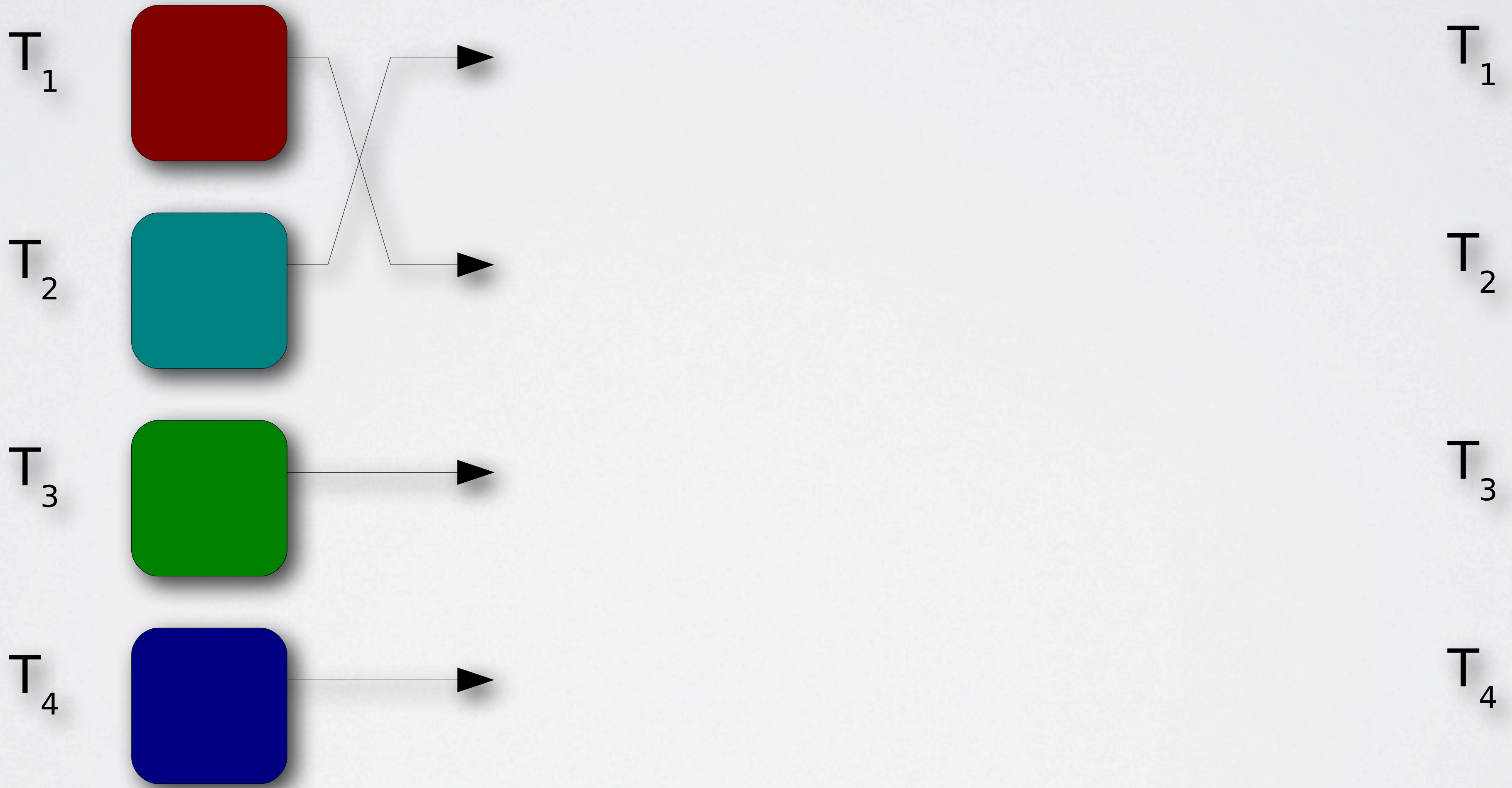
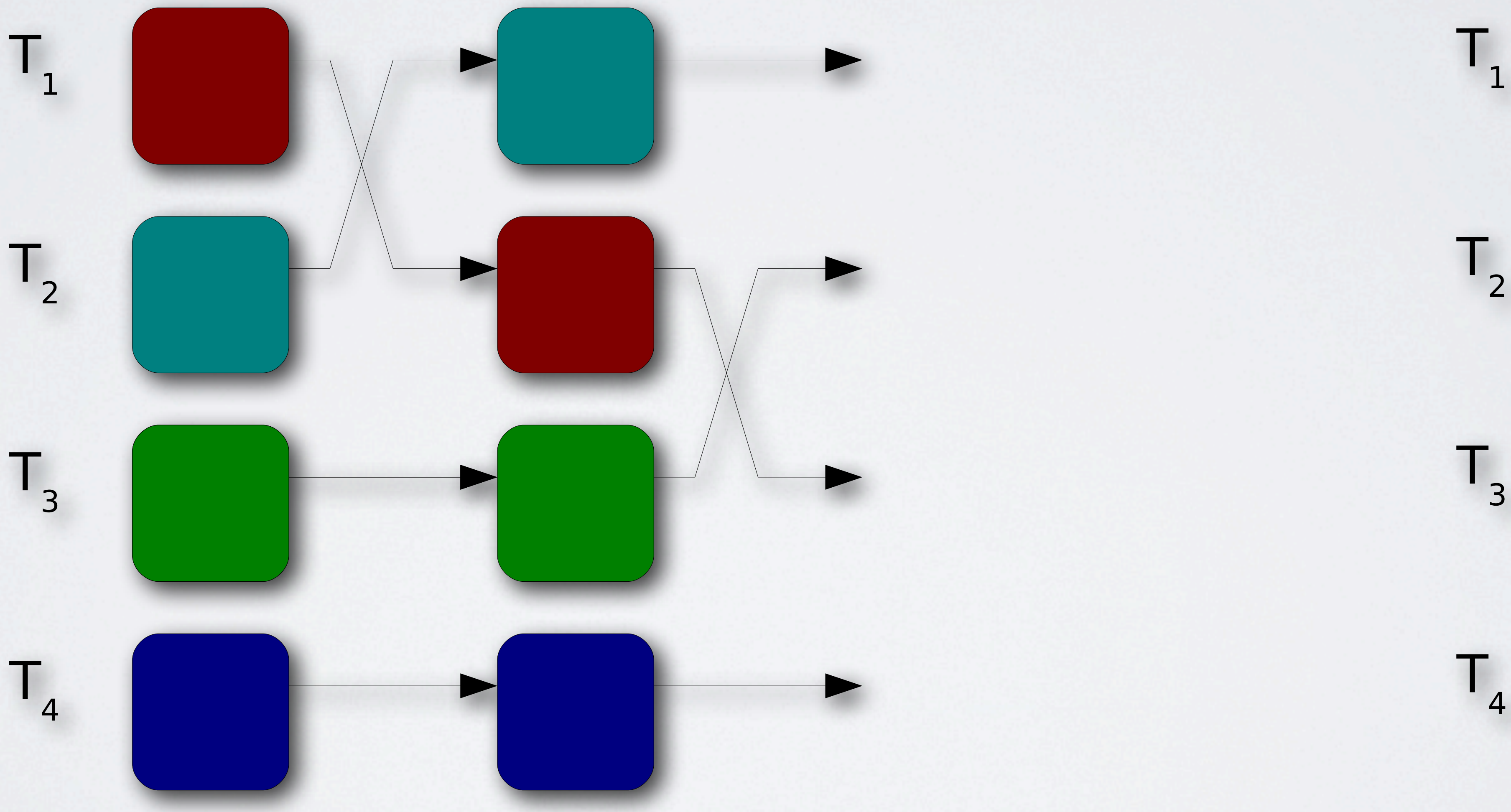


Parallel Tempering

- How it works?



Parallel Tempering

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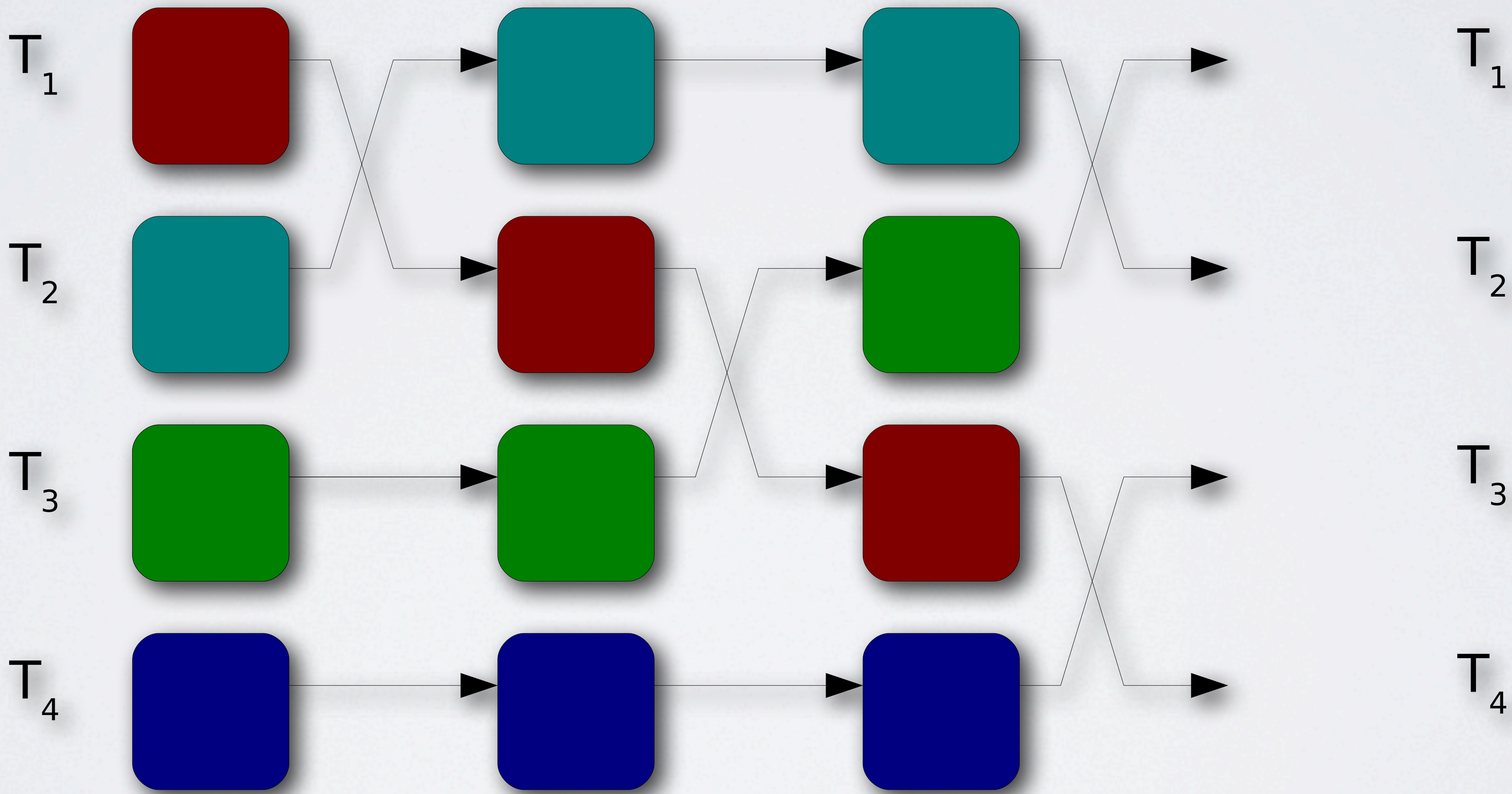

Parallel Tempering

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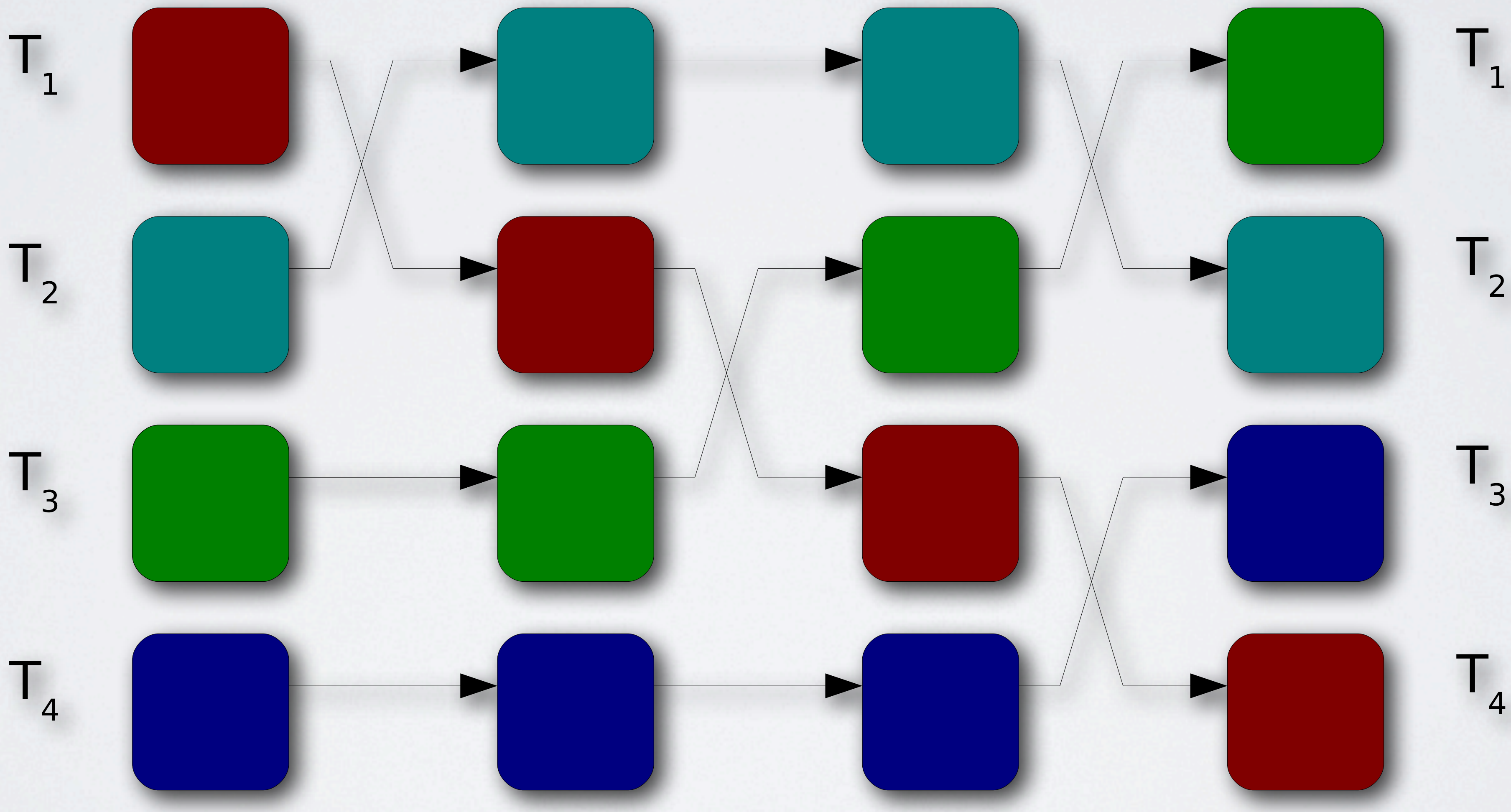
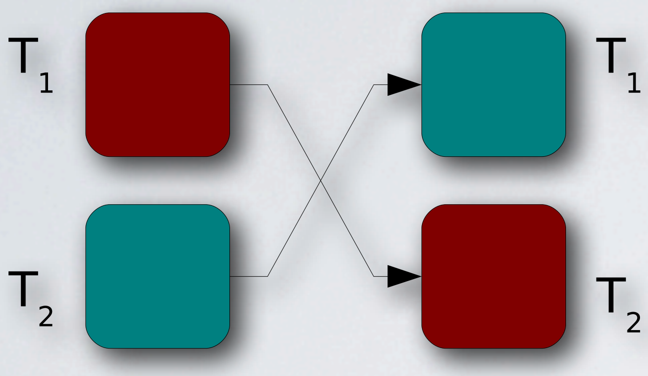


Parallel Tempering



$$P_{\mathrm{PT}}(E_1, \beta_1 \rightarrow E_2, \beta_2) = \min[1, \exp(\Delta\beta\Delta E)]$$

An efficient selection of the temperature intervals for PT simulations is still an open problem.

Several strategies have been proposed:

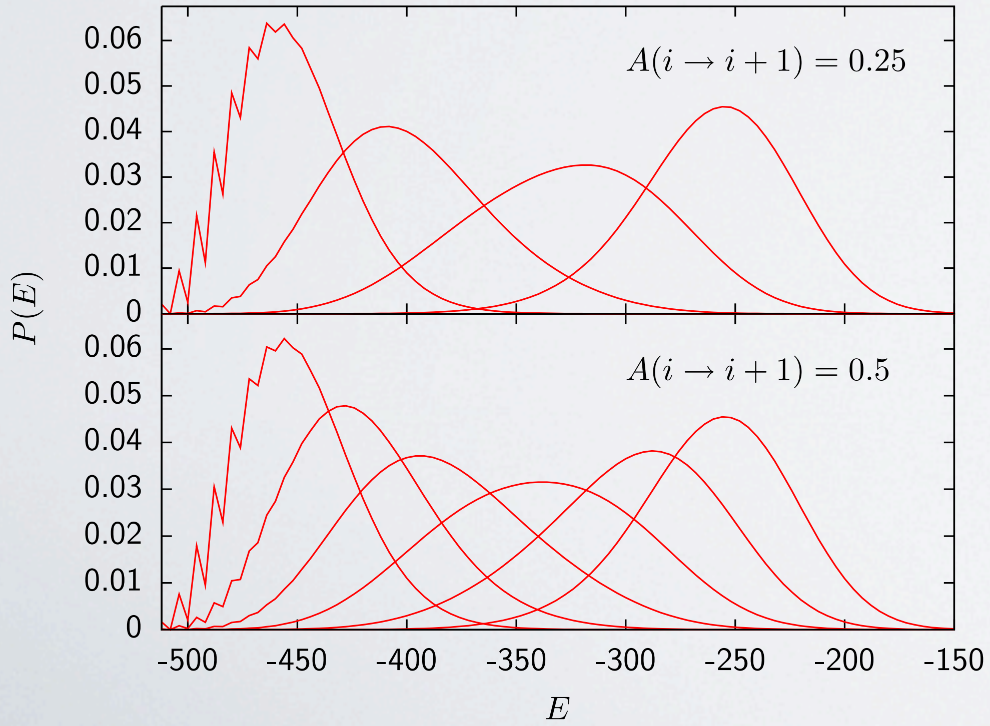
- based on the assumption of constant overlap between the replica
- based on the maximum flow in the temperature space

Parallel Tempering

Following the concept of constant acceptance rate between replica:

$$A(1 \to 2) = \sum_{E_1, E_2} P_{\beta_1}(E_1) P_{\beta_2}(E_2) P_{\mathrm{PT}}(E_1, \beta_1 \to E_2, \beta_2),$$

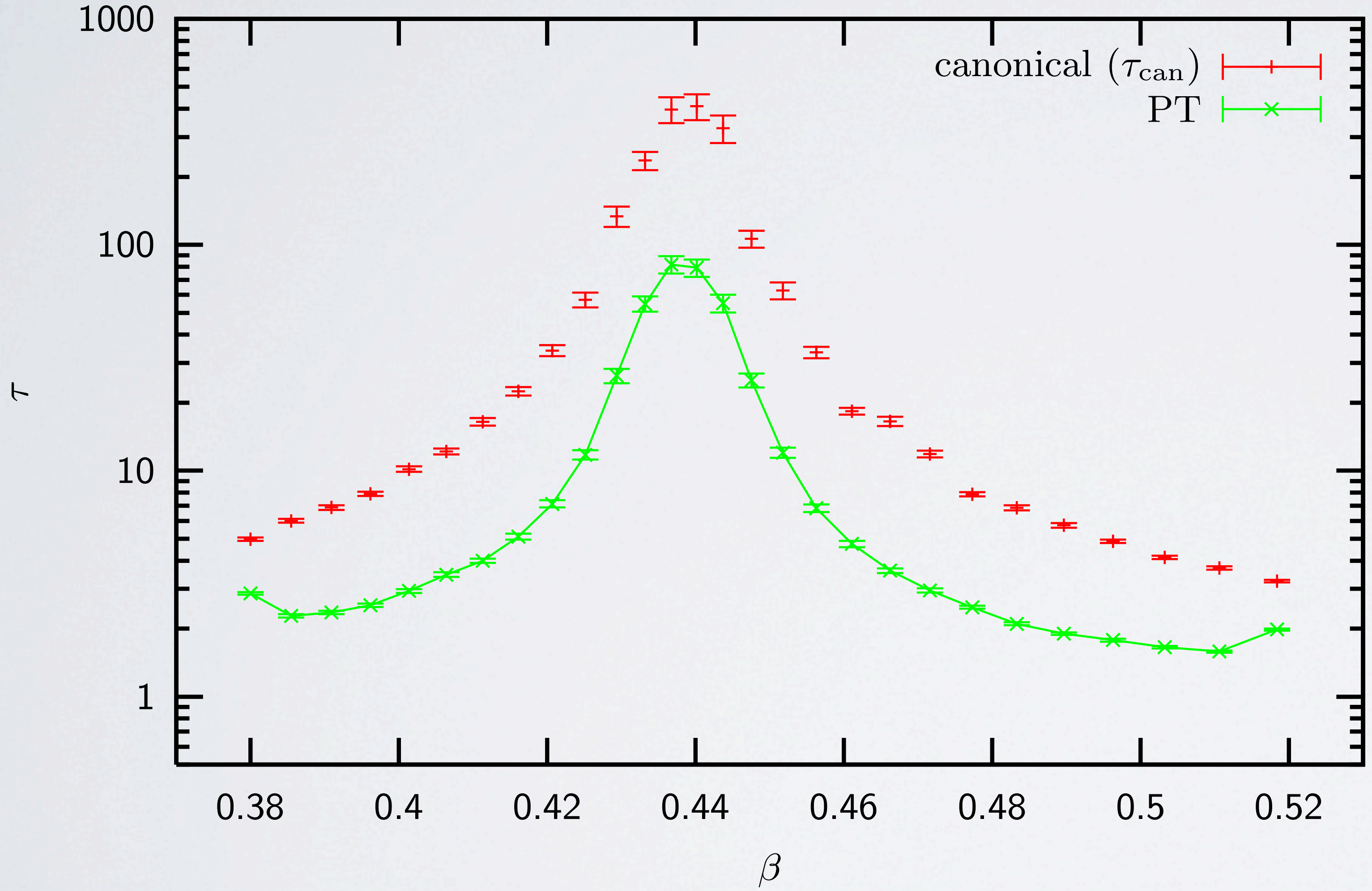
where $P_{\beta_i}(E_i)$ is the probability for replica i with β_i to have the energy E_i.



Energy distributions of the 2D Ising model with $L = 16$ for a set of inverse temperatures starting $\beta_i = 0.38$ and $A(i \to i+1) = 0.25$ and 0.5.

[P. Beale, Phys. Rev. Lett. 76, 78 (1996)]

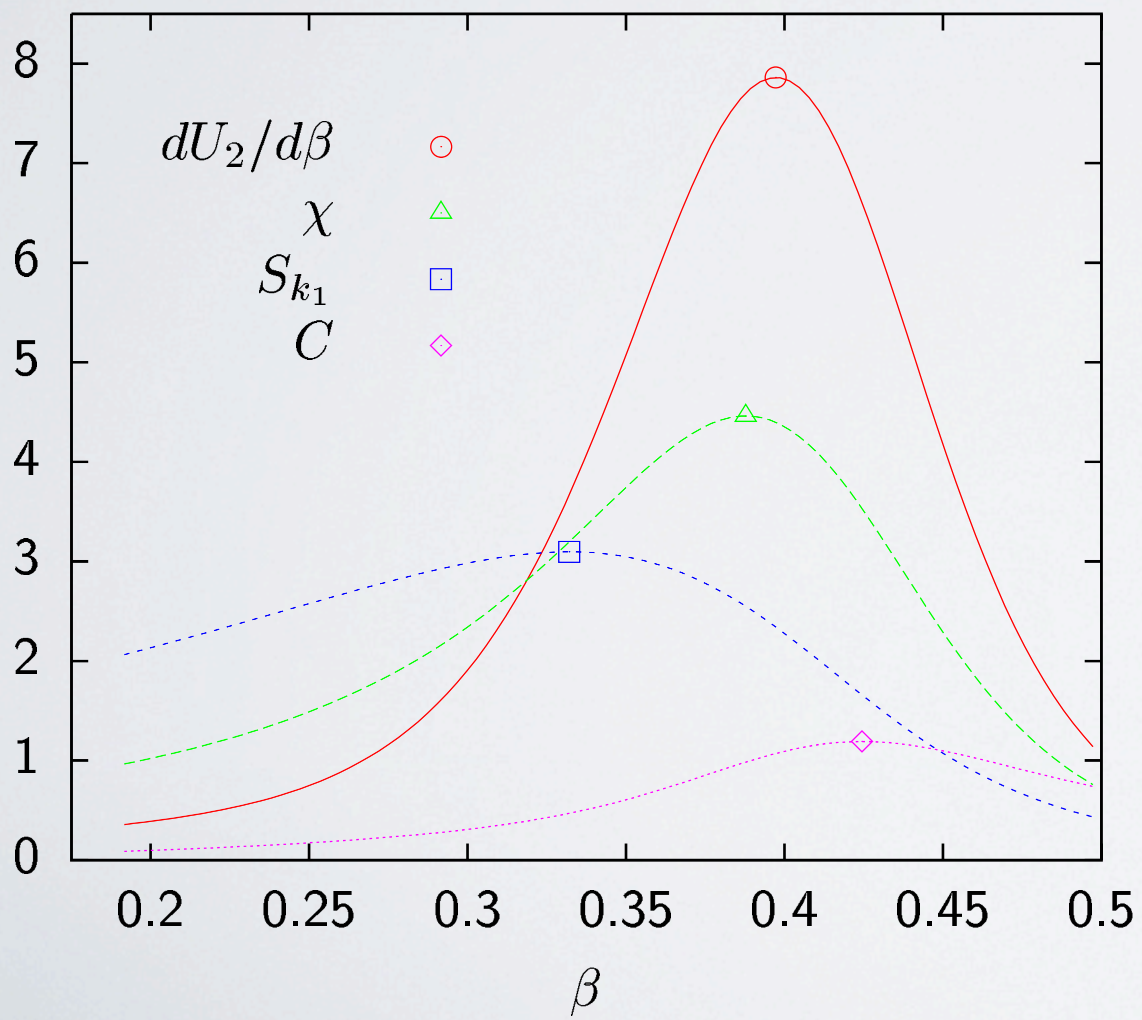
Autocorrelation times



Autocorrelation times τ as a function β of for the independent simulations and the parallel tempering update scheme for the 2D Ising model $(L = 80)$.

Temperature Interval

✤cover the complete desired "critical" temperature range



$$C(\beta) = \beta^2 V(\langle e^2 \rangle - \langle e \rangle^2)$$

$$\chi(\beta) = \beta V(\langle m^2 \rangle - \langle |m| \rangle^2)$$

$$U_{2k}(\beta) = 1 - \langle m^{2k} \rangle / 3 \langle |m|^k \rangle^2$$

$$\ldots$$

Temperature Interval

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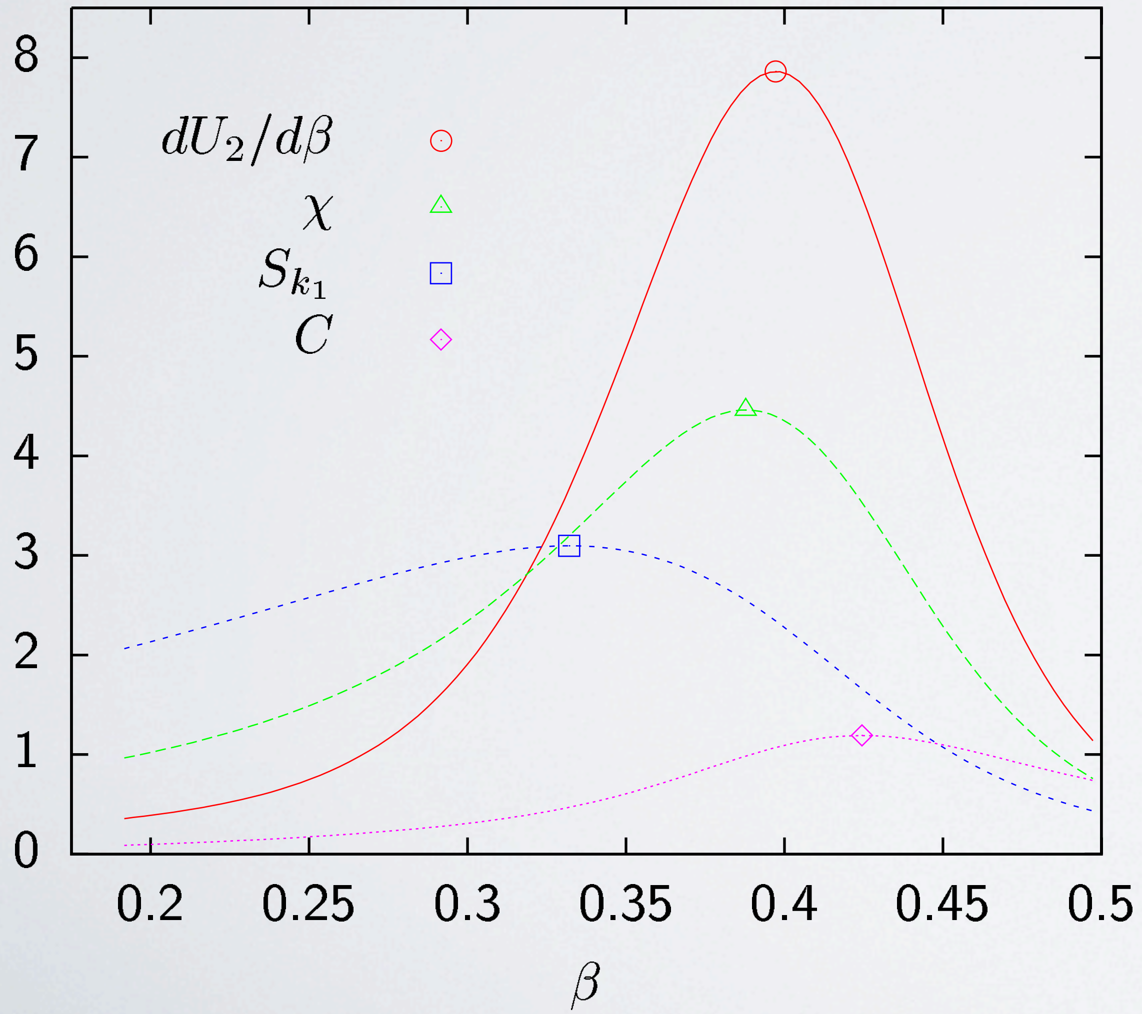

$$S = \{C, \chi, \ldots\}$$

$$S^{\max} = S(\beta_S^{\max})$$

$$S(\beta_S^{+/-}) = rS^{\max}$$

$$\beta_S^+ > \beta_S^{\max} \text{ and } \beta_S^- < \beta_S^{\max}$$

"desired" range: $[\beta^-_{S_{k_1}}, \beta^+_C]$

Temperature Interval

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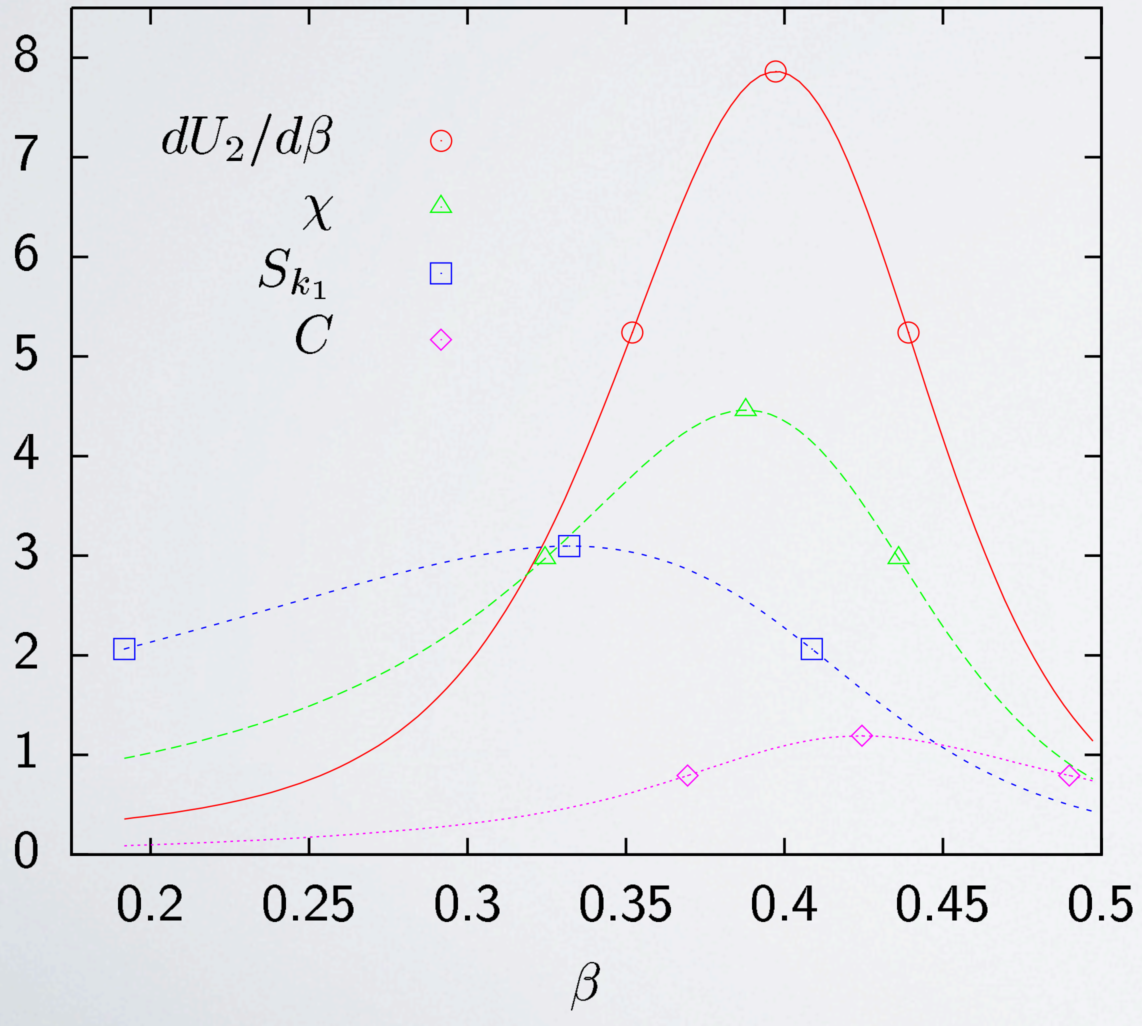


$$S = \{C, \chi, \dots\}$$

$$r = \frac{2}{3}$$

$$S^{\max} = S(\beta_S^{\max})$$

$$S(\beta_S^{+/-}) = r S^{\max}$$

$\beta_S^+ > \beta_S^{\max}$ and $\beta_S^- < \beta_S^{\max}$

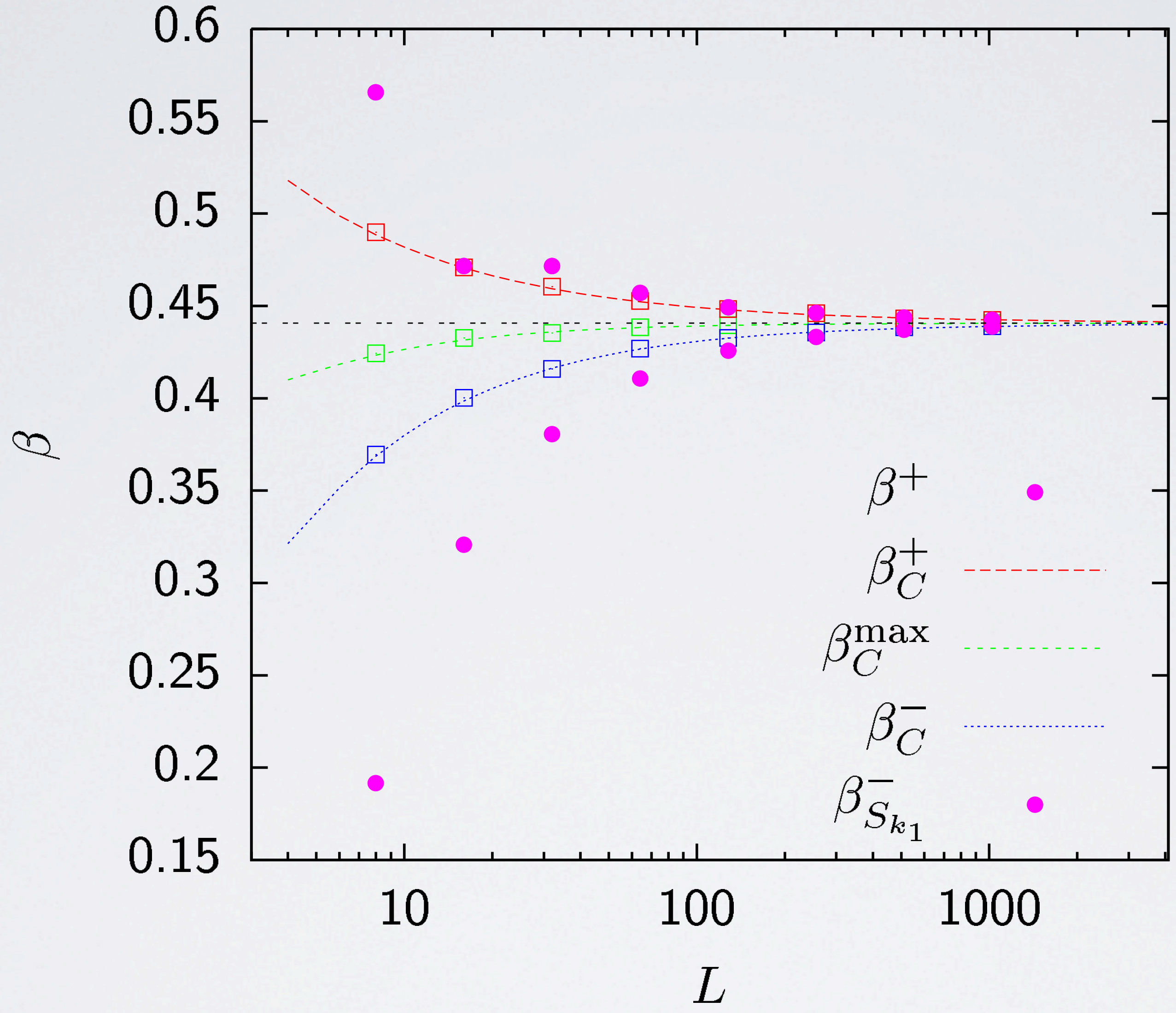
"desired" range: $[\beta_{S_{k_1}}^-, \beta_C^+]$

Temperature Interval

general recipe:

1. compute the simulation temperatures of the replica equidistant in β,
2. perform several hundred thermalization sweeps and a short measurement run,
3. check the histogram overlap between adjacent replica: if the overlap is too small, add on or two replica and goto step 1, else go on,
4. use multi-histogram reweighting to determine β_S^- and β_S^+ for all observables S,
5. leading to the temperature interval $[\beta_{\min}^-, \beta_{\max}^+] = [\min_S\{\beta_S^-\}, \max_S\{\beta_S^+\}]$,
6. start with $\beta^- = \beta_{\min}^-$ and compute a sequence of temperatures β_i with fixed acceptance rate $A(1 \to 2)$ until $\beta_i = \beta^+ \geq \beta_{\max}^+$,
7. perform several hundred thermalization sweeps and a long measurement run.

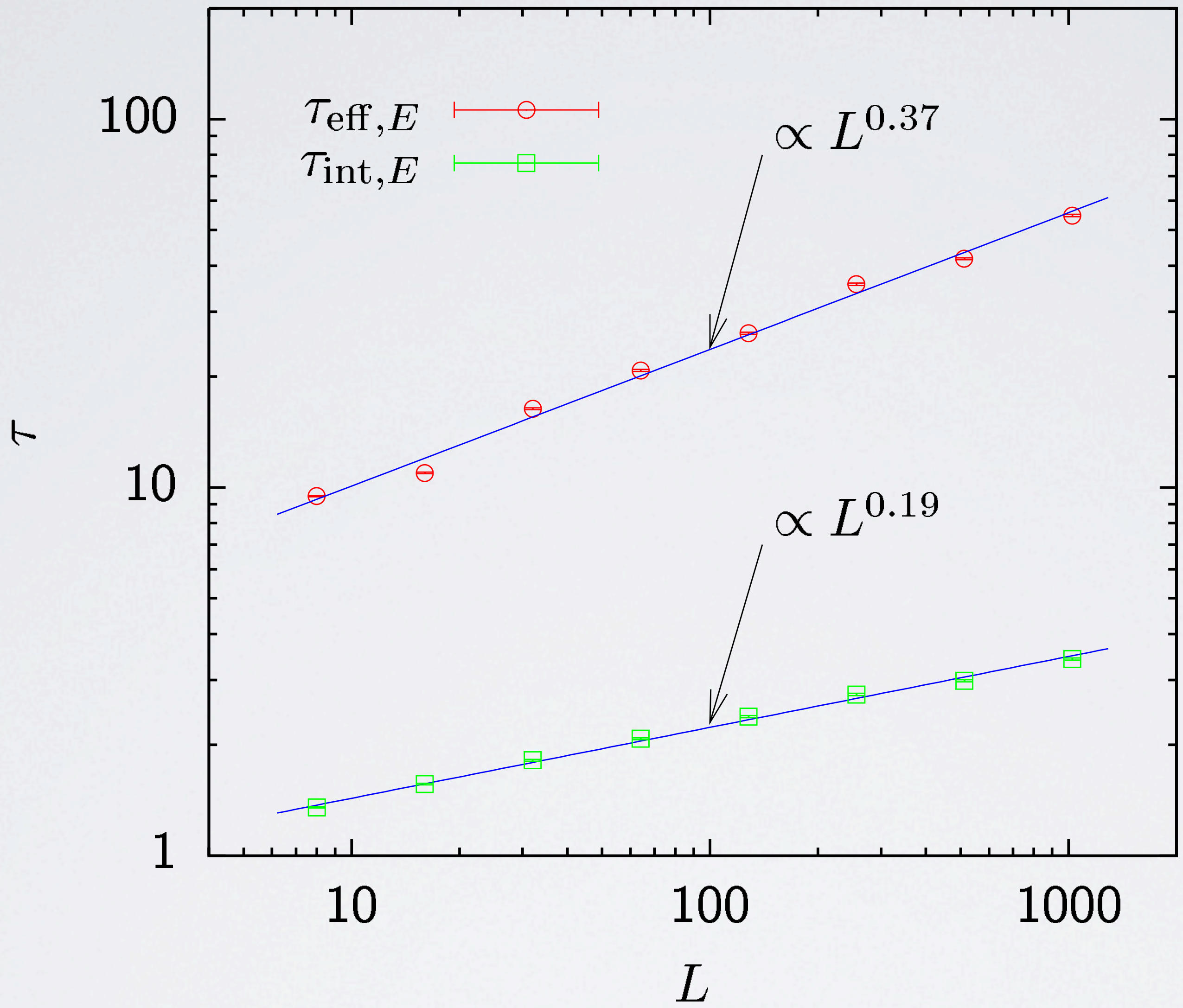
Temperature intervall



$$r = \frac{2}{3}$$

The “desired” temperature interval for r = 2/3 as a function of the system size.

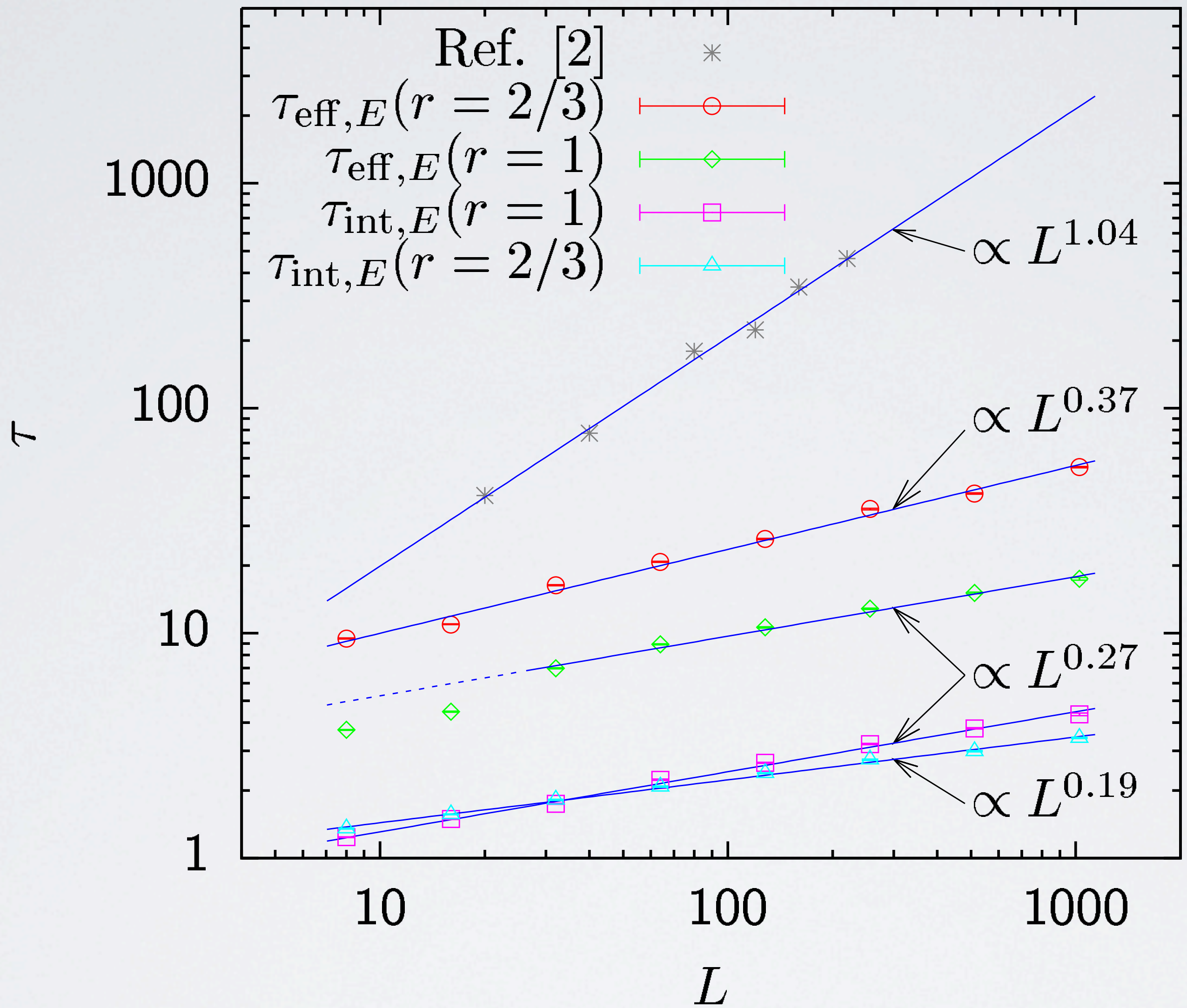
Autocorrelation times



$$r = \frac{2}{3}$$

Autocorrelation times τ_{int} and τ_{eff} for the energy of the 2D Ising model, where $\tau_{\mathrm{eff}} = N_{\mathrm{rep}}\tau_{\mathrm{int}}$ and N_{rep} is the number of replica.

Autocorrelation times



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Temperature intervall

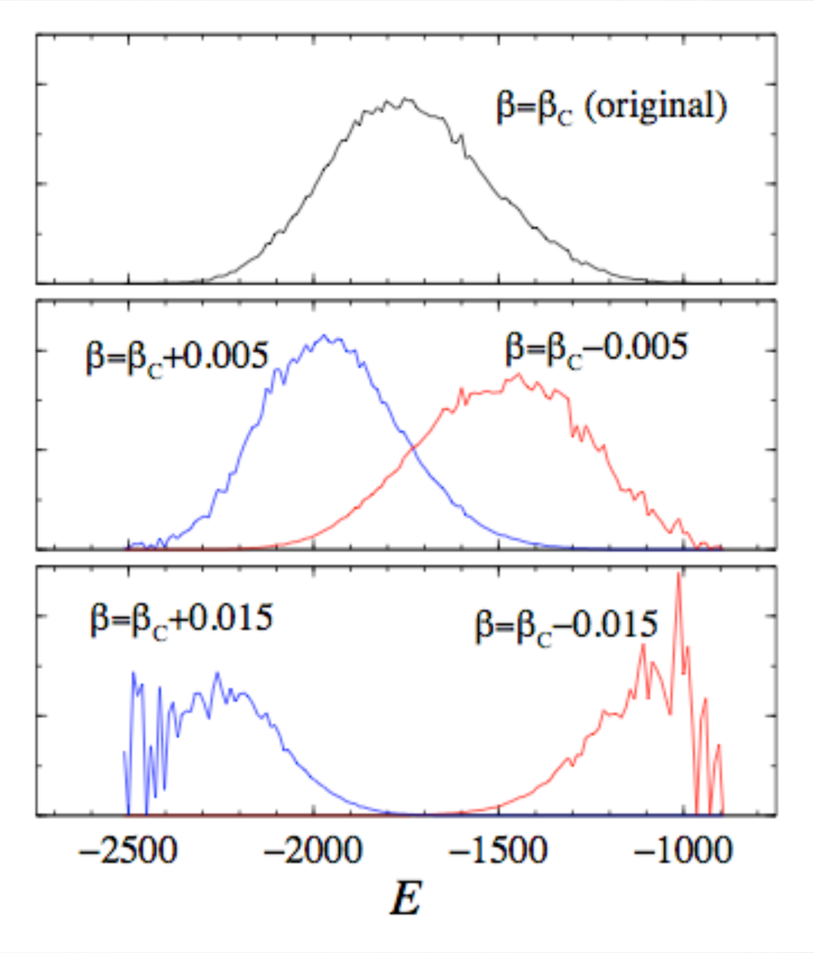
understand the FSS of τ_{eff} in 2D Ising

$$\Delta\beta_{\text{rew}} \propto L^{-1/\nu}/\sqrt{\ln L}$$

$$\beta^+ - \beta^- \approx \beta^+_C - \beta^-_{S_{k_1}} = aL^{-1/\nu} + bL^{-r/\nu}$$

$$N_{\text{rep}} = (\beta^+ - \beta^-)/\Delta\beta_{\text{rew}} \rightarrow L^{(1-r)/\nu}\sqrt{\ln L}$$

$$\beta^+ - \beta^- \propto L^{-\kappa'}$$



64x64

Temperature intervall

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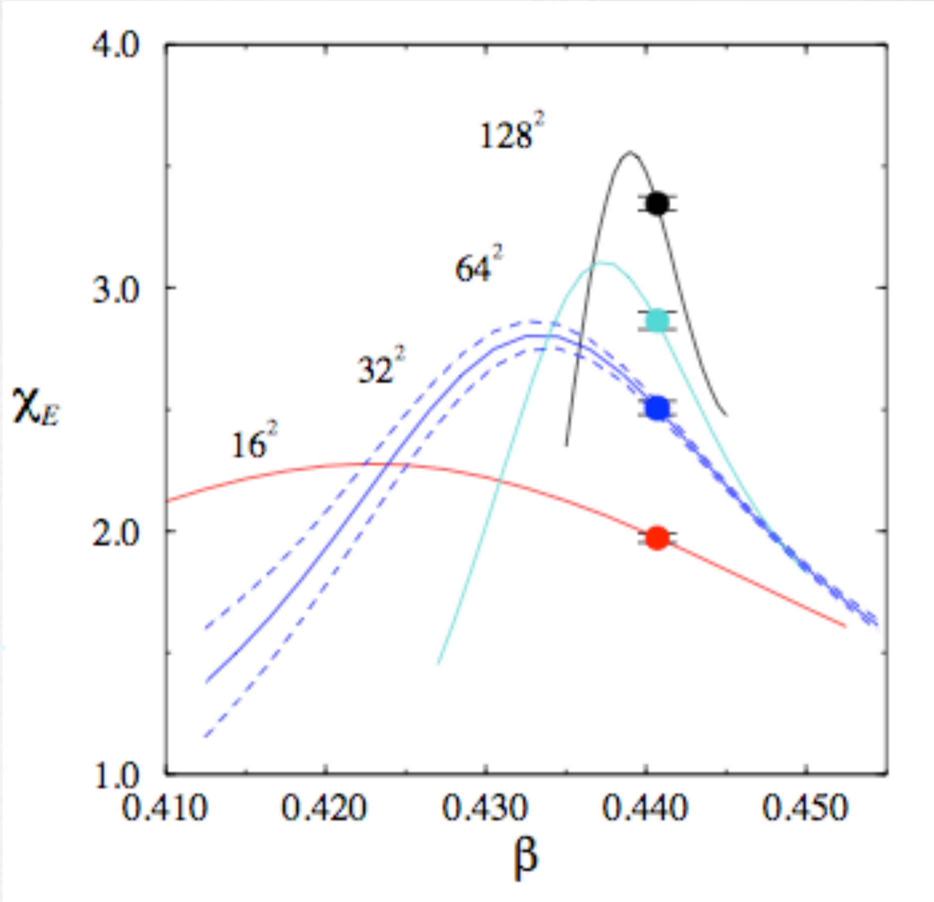
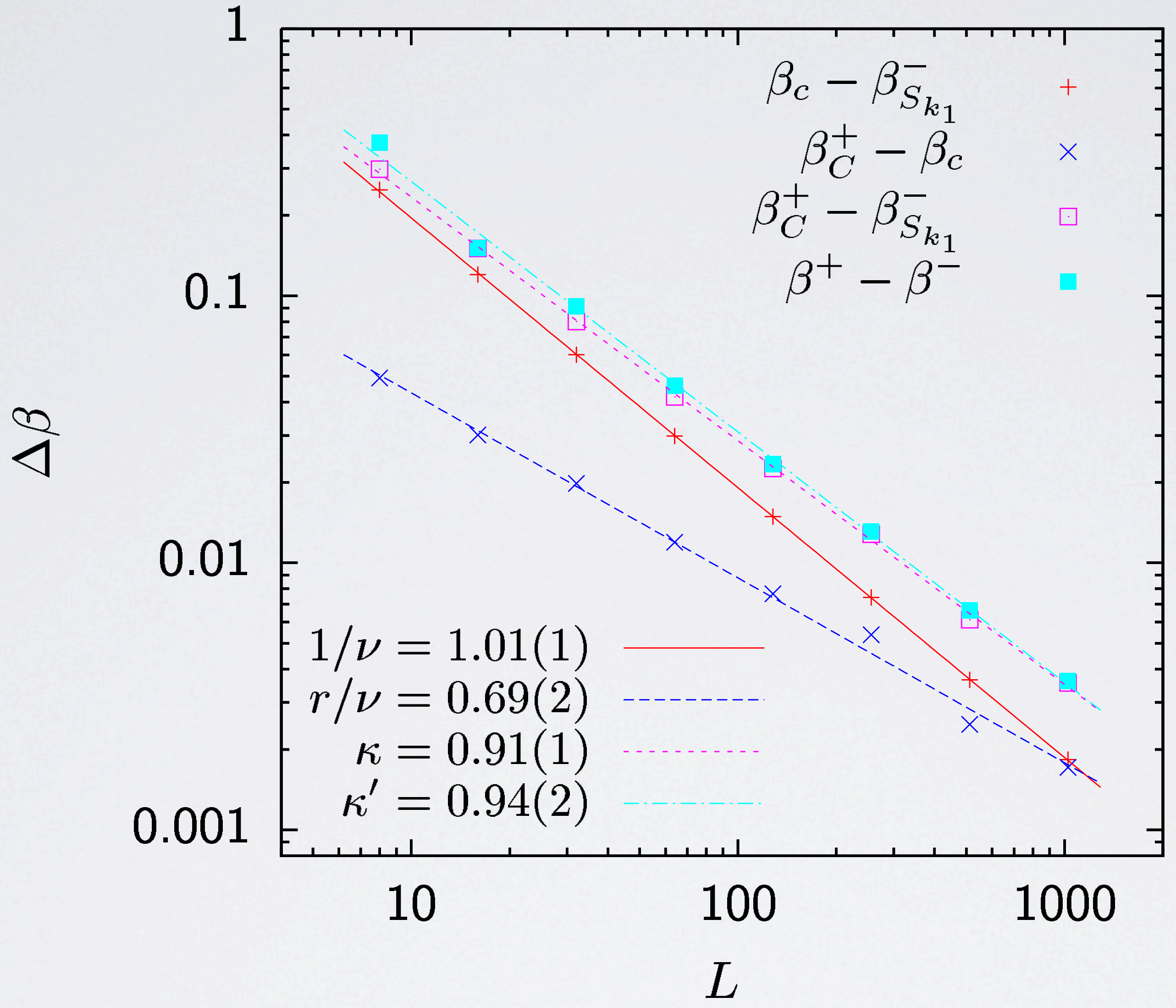
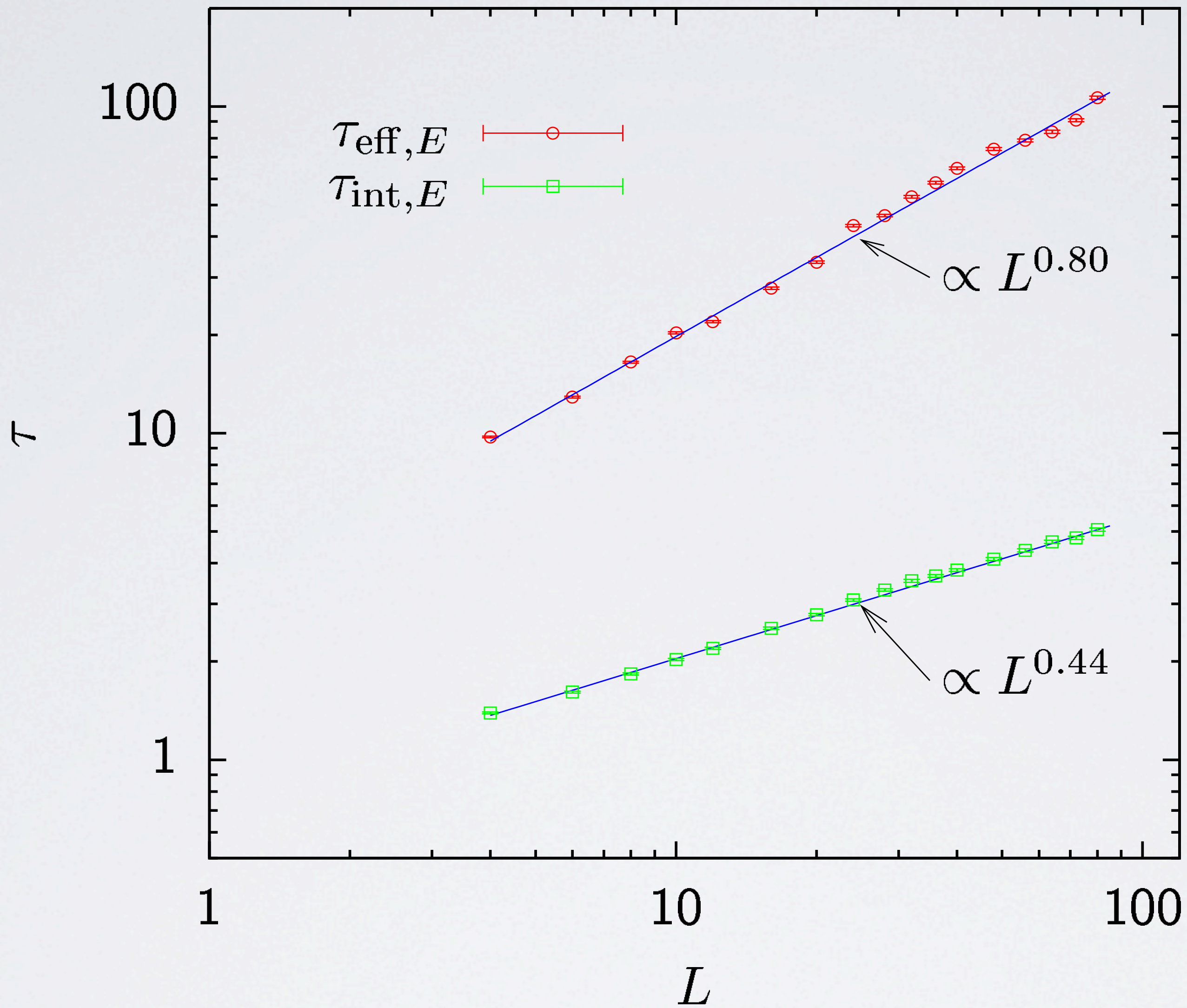


Temperature intervall



FSS of the "desired" simulation window for the 2D Ising model with r = 2/3.

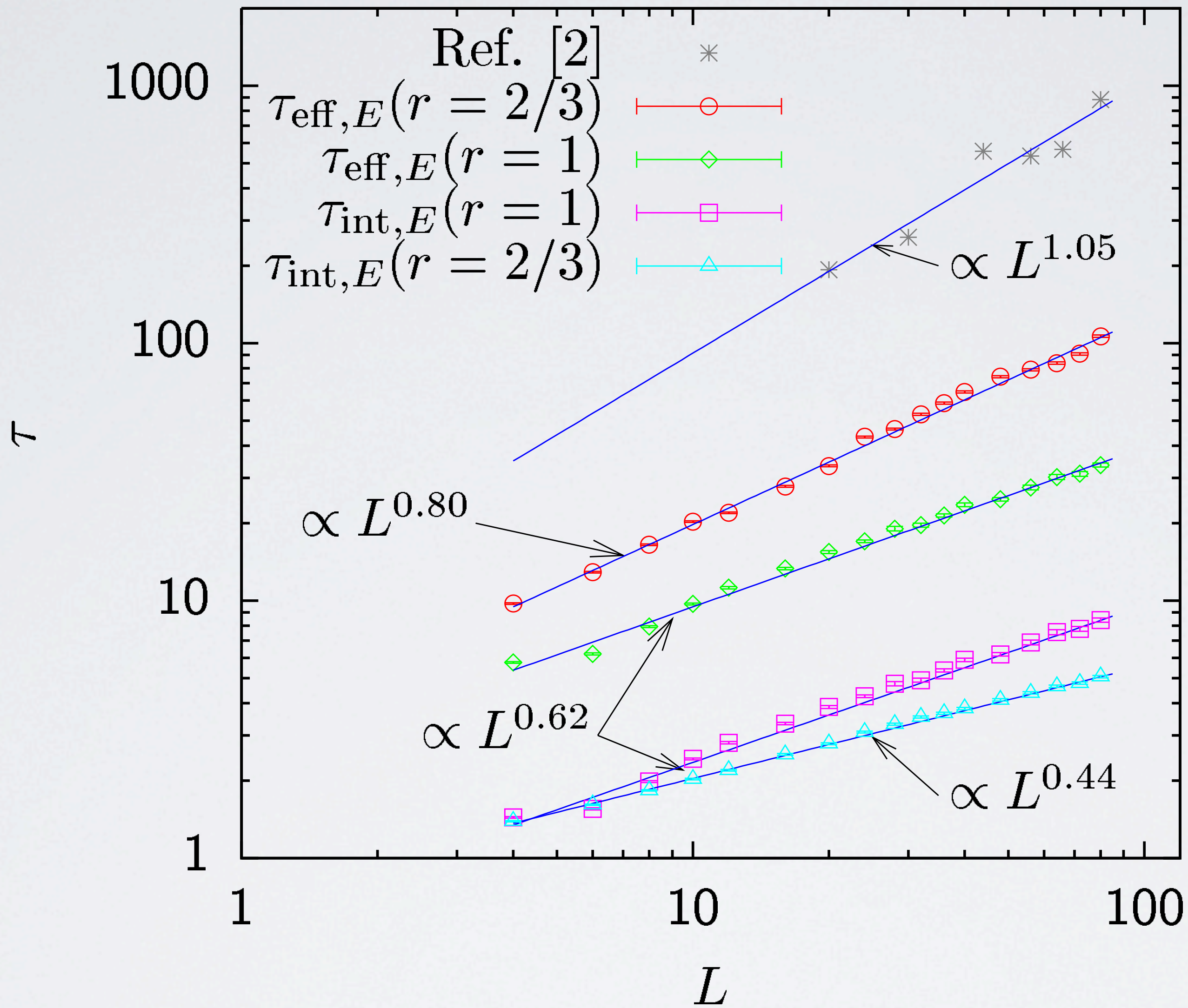
Autocorrelation times



$$r = \frac{2}{3}$$

Autocorrelation times τ_{int} and τ_{eff} for the energy of the 3D Ising model, where $\tau_{\text{eff}} = N_{\text{rep}}\tau_{\text{int}}$ and N_{rep} is the number of replica.

Autocorrelation times



Autocorrelation times τ_{int} and τ_{eff} for the energy of the 3D Ising model, where $\tau_{\mathrm{eff}} = N_{\mathrm{rep}} \tau_{\mathrm{int}}$ and N_{rep} is the number of replica.

Summary

What can we do to improve the parallel tempering algorithm?

- use the replica-exchange cluster algorithm

or

- use a constant acceptance rate between the replica
- keep the temperatures fixed
- take the temperature dependence of autocorrelation times into account

EB, A. Nußbaumer, and W. Janke, Phys. Rev. Lett. 101 (2008) 130603
EB and W. Janke, Phys. Rev. E 84 (2011) 036701

Acknowledgements

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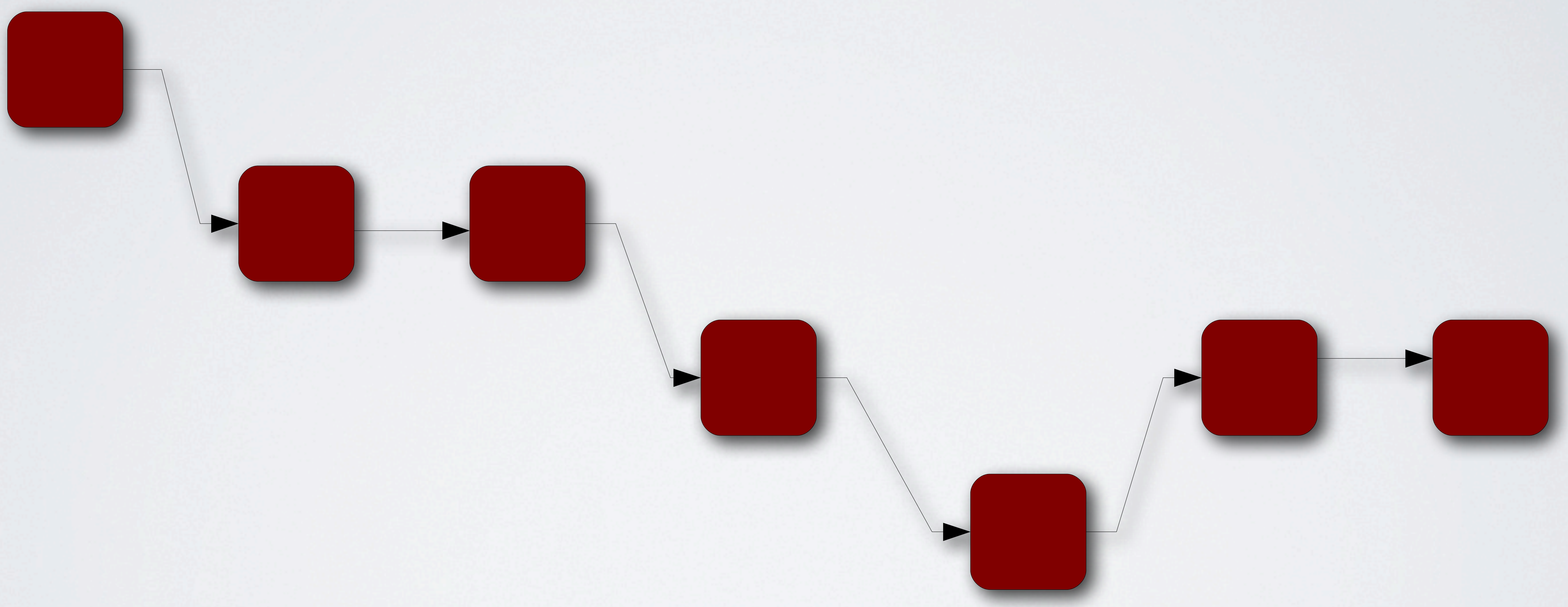
- Deutsche Forschungsgemeinschaft (DFG)
- EU-RTN Network "ENRAGE"

THANK YOU!

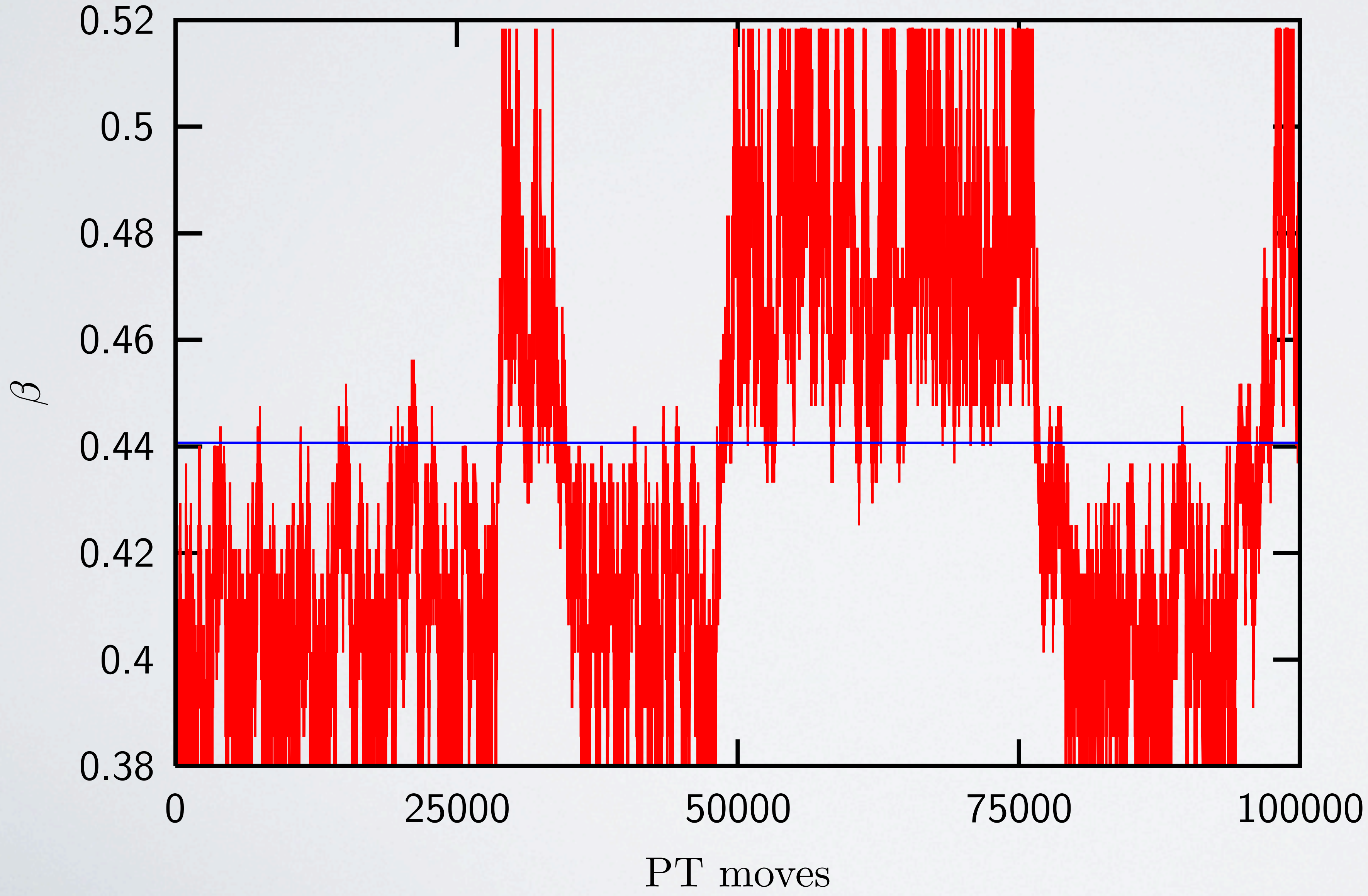
Flow

The way through inverse temperature space of an arbitrarily chosen replica:



Flow

The way through inverse temperature space of an arbitrarily chosen replica:

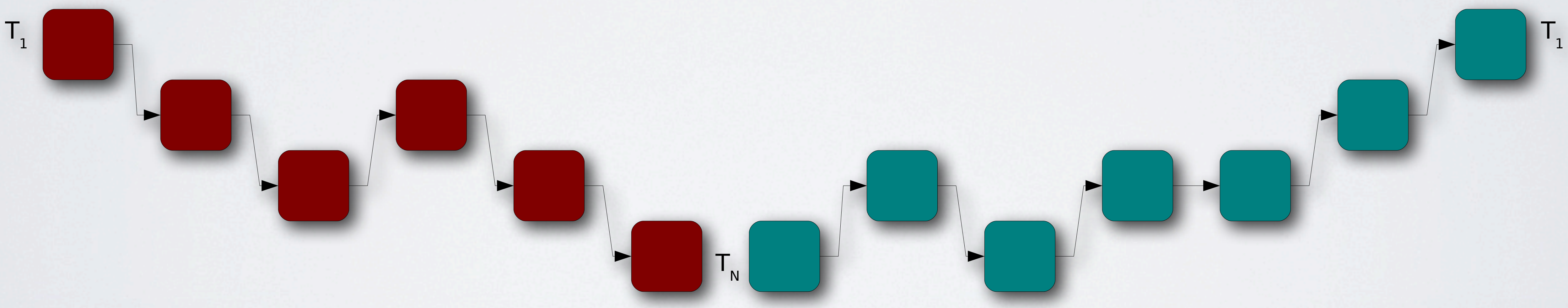


2D Ising model
$(L = 80)$

Flow

The flow η is the fraction of replica which wander from the largest β to the smallest as a function of the replica index i.

$$\eta = \frac{n_{\mathrm{up}}(i)}{n_{\mathrm{up}}(i) + n_{\mathrm{down}}(i)}$$



[H.G. Katzgraber, S. Trebst, D.A. Huse, and M. Troyer, J. Stat. Mech. P03018 (2006)]

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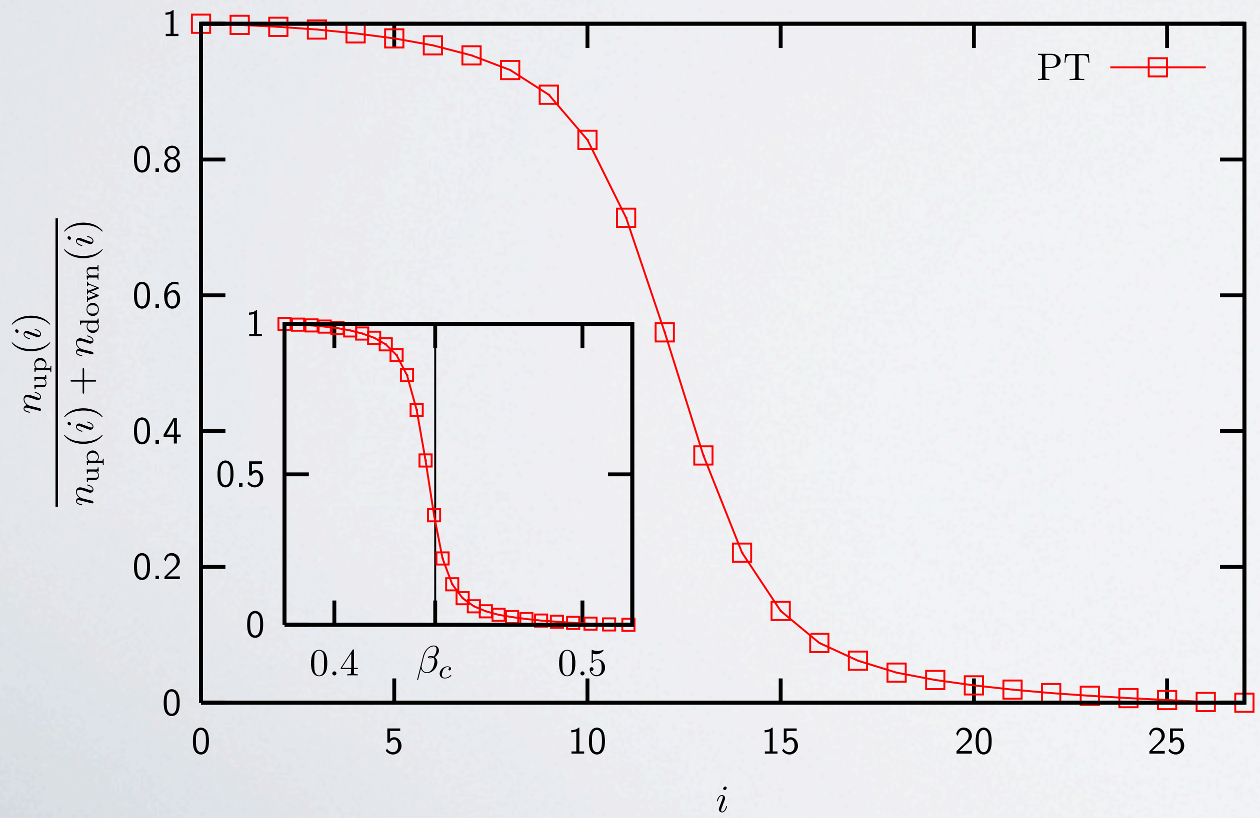

flow for the 2D Ising model ($L = 80$)

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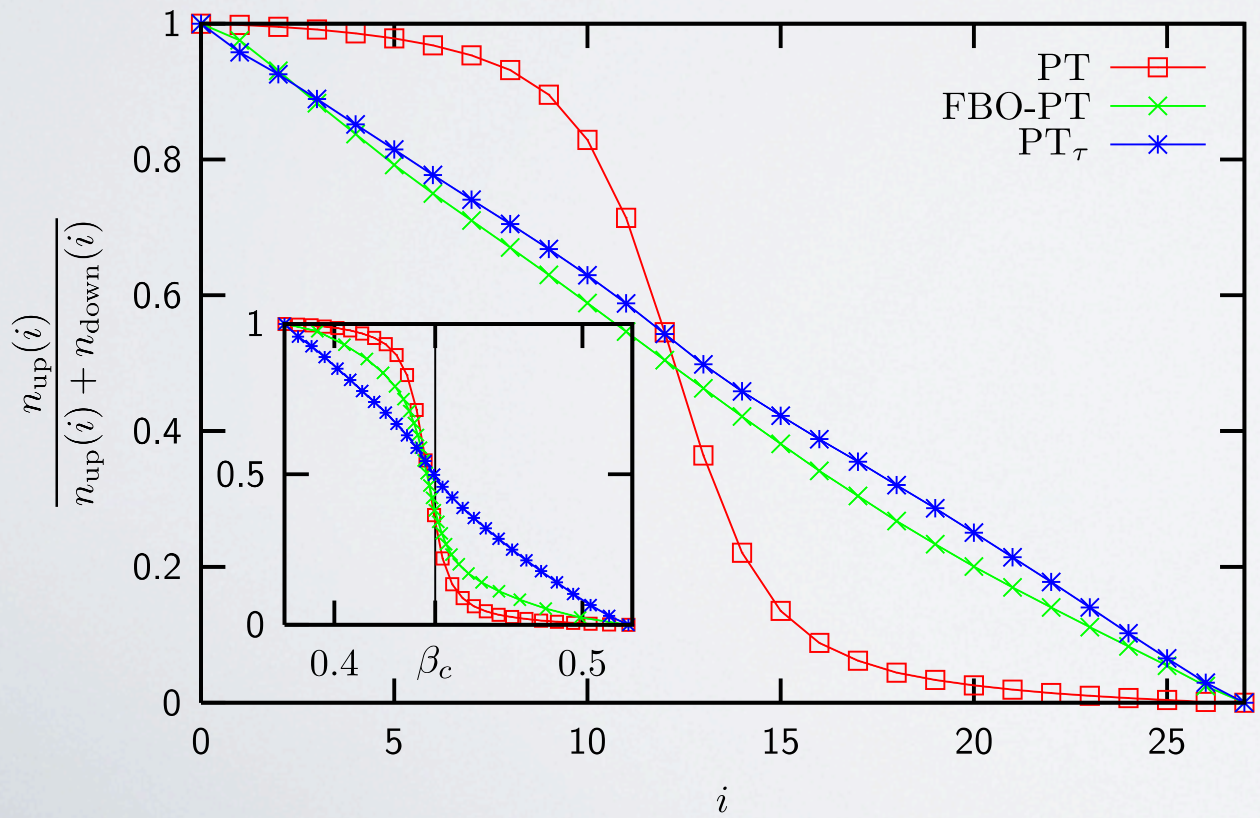
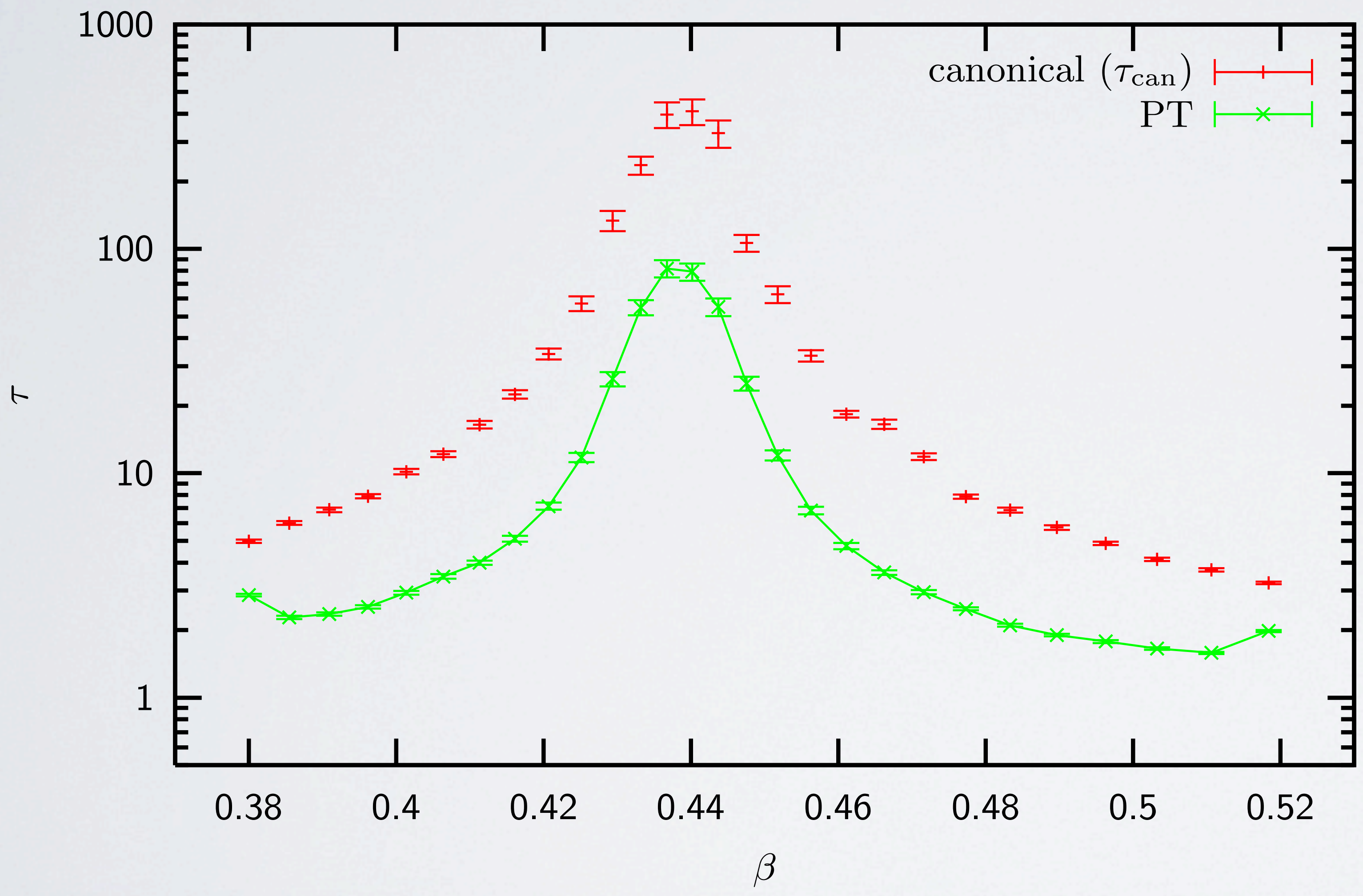


flow for the 2D Ising model ($L = 80$)

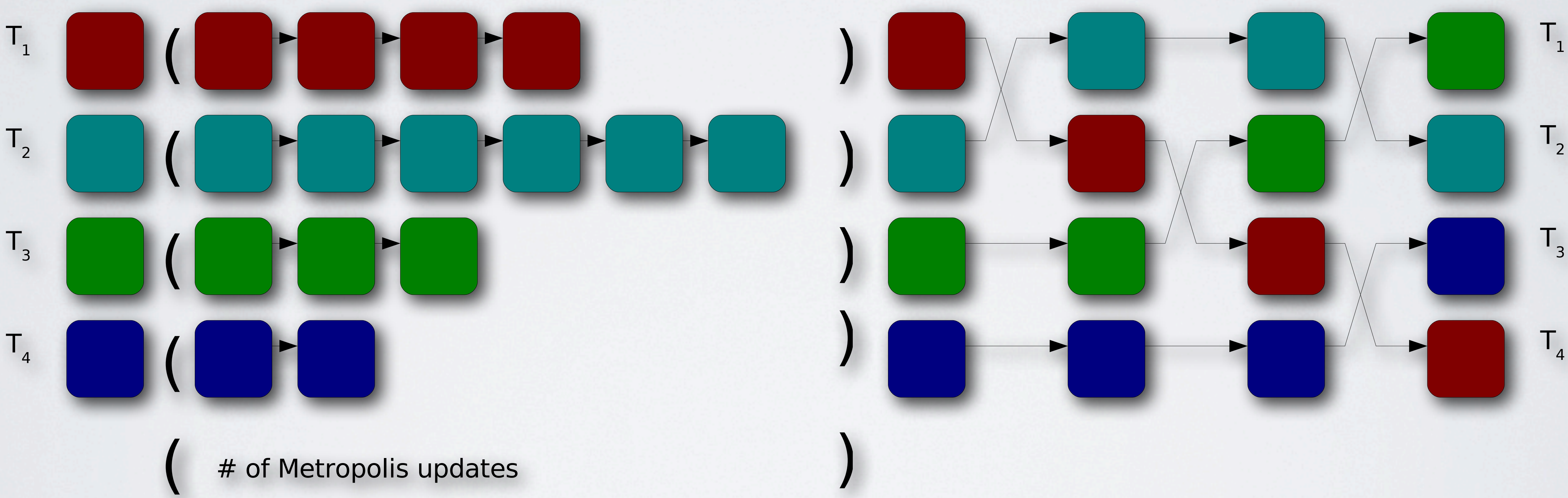
Autocorrelation times



Autocorrelation times τ as a function β of for the independent simulations and the parallel tempering update scheme for the 2D Ising model ($L = 80$).

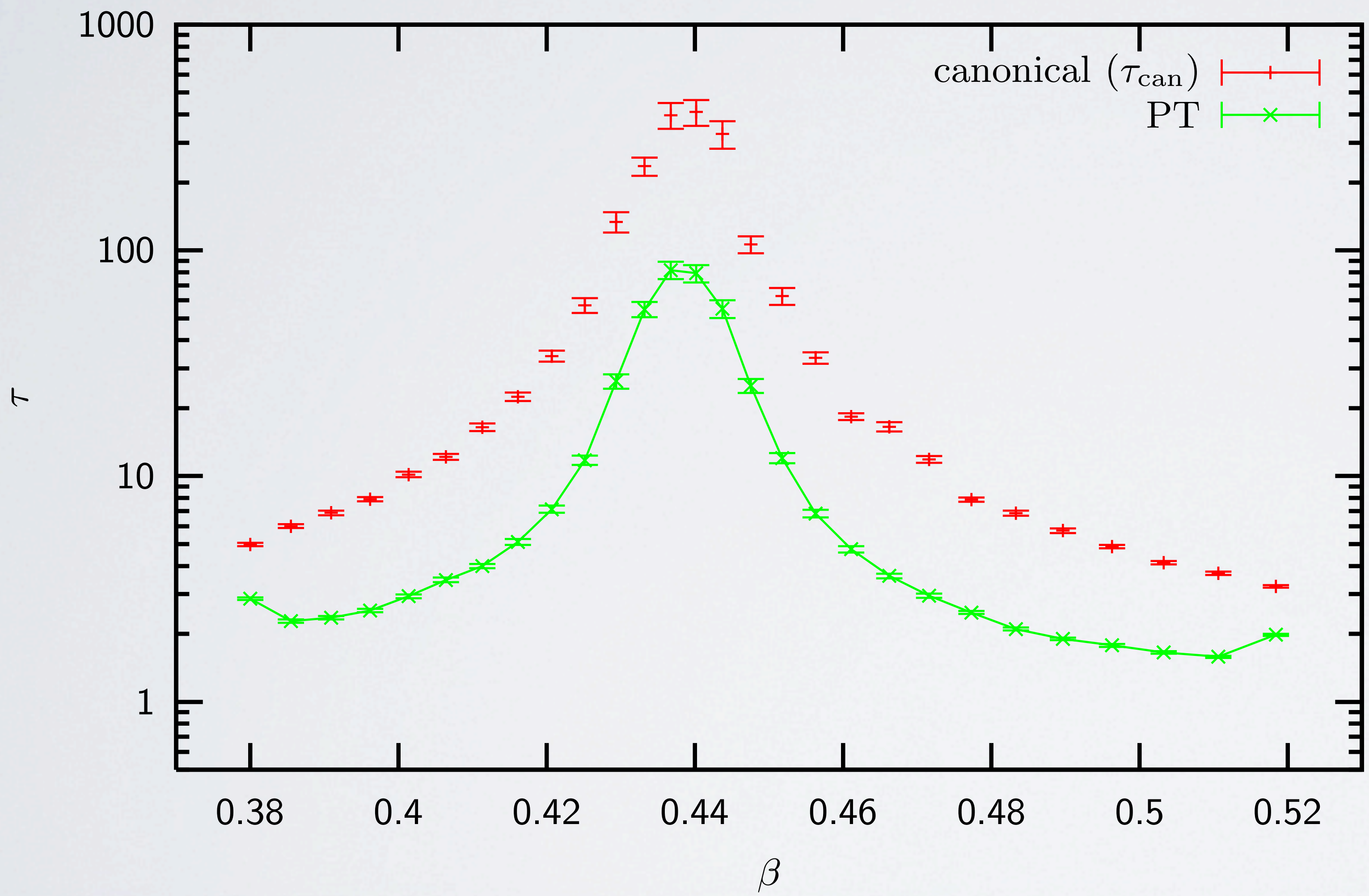
Improved parallel tempering update scheme

✤How it works?



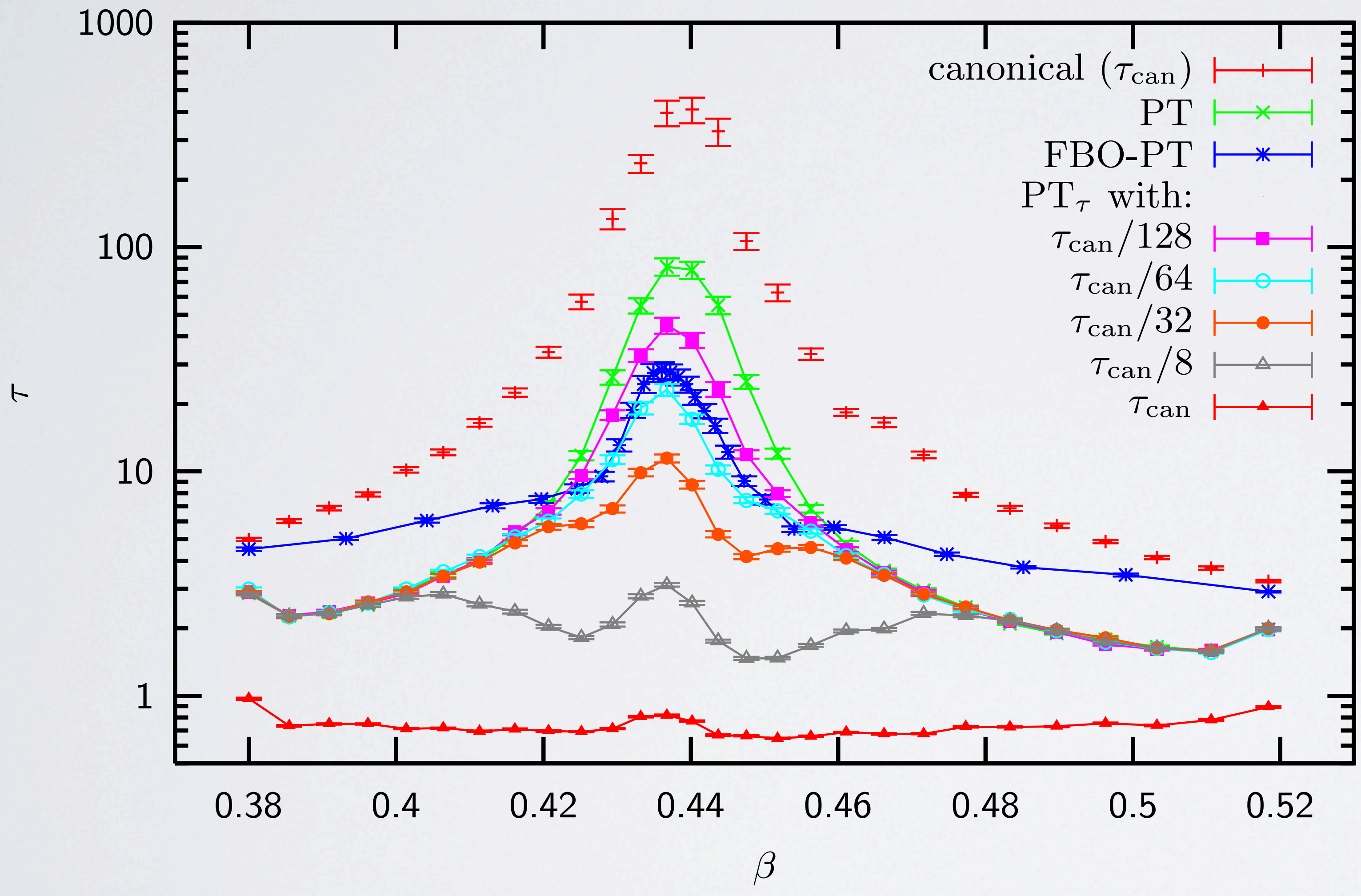
$$N_{\mathrm{local}}(\beta) \propto \tau_{\mathrm{can}}(\beta)$$

Autocorrelation times



Autocorrelation times τ as a function β of for the independent simulations and the parallel tempering update scheme for the 2D Ising model $(L = 80)$.

Autocorrelation times



Autocorrelation times τ as a function β of for the independent simulations, the parallel tempering update scheme, the feedback-optimized parallel tempering method, and the improved parallel tempering update scheme for the 2D Ising model $(L = 80)$.

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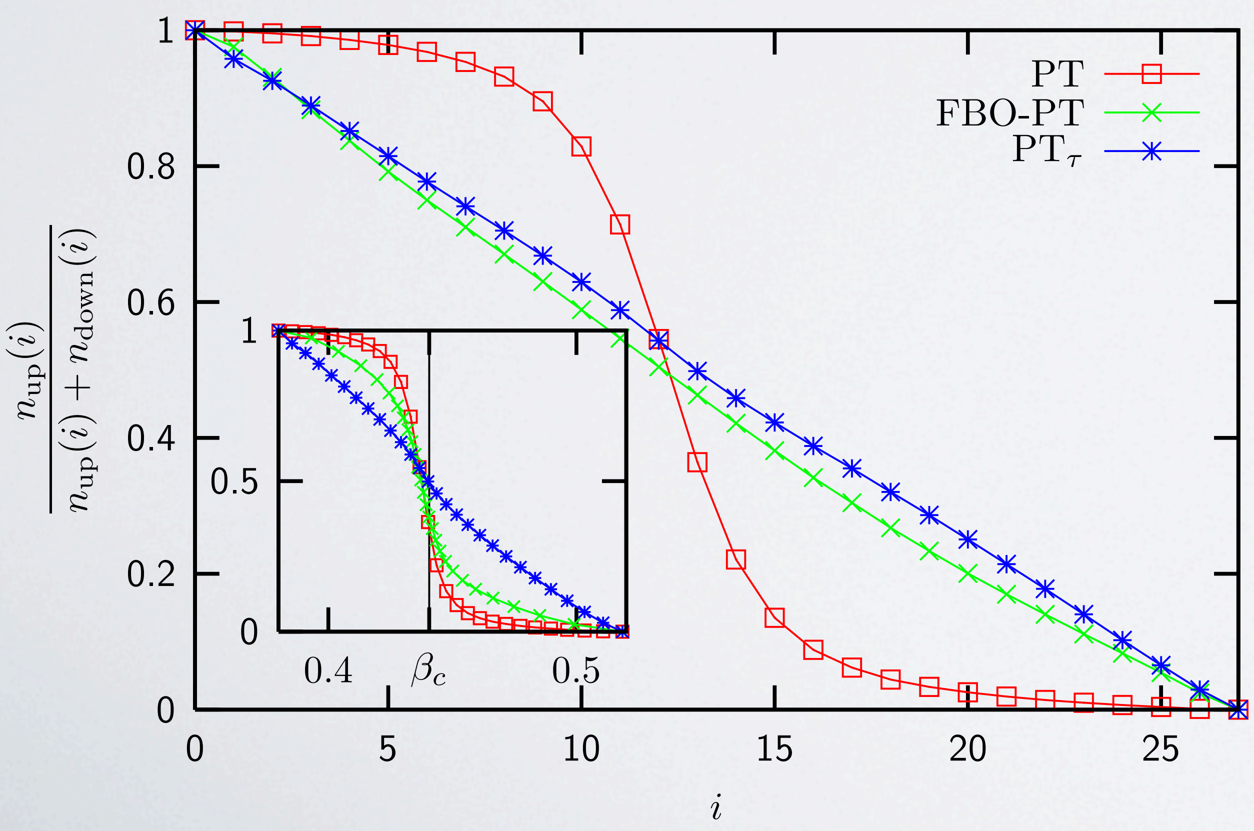
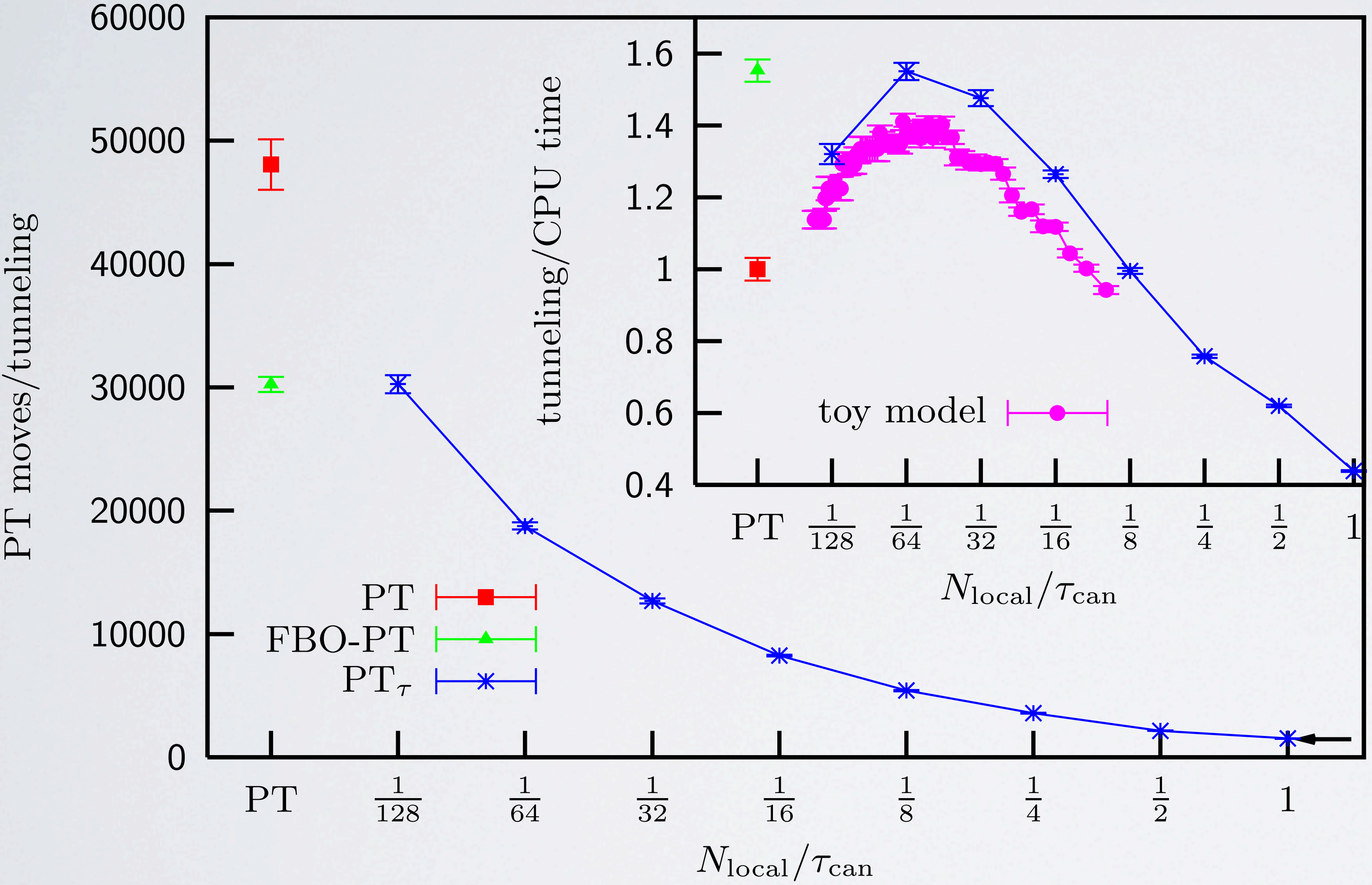


flow for the 2D Ising model ($L = 80$)

Sweeps per tunneling



Sweeps per tunneling as a function of N_{local} for the 2D Ising model $(L = 80)$.