Parallel Tempering Algorithm in Monte Carlo Simulation

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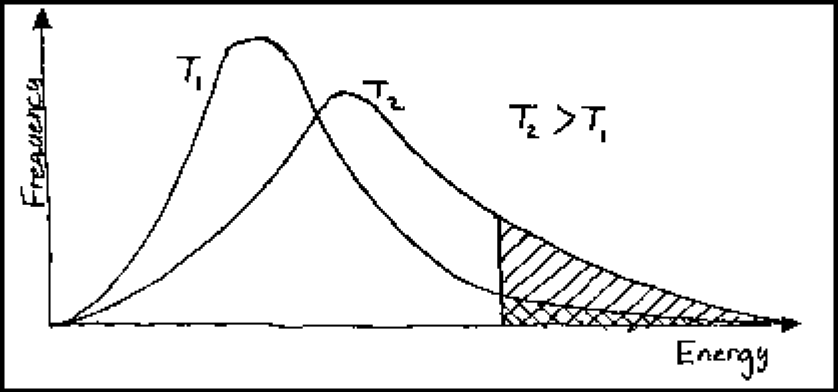
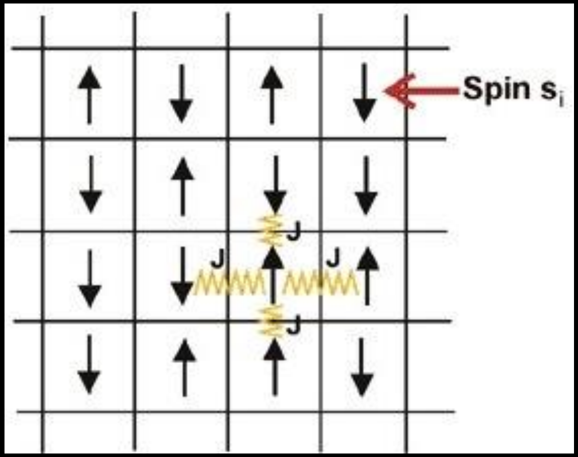
Metropolis Algorithm on Ising Model

- Reason: difficulty of direct sampling
- Objective: compute average physical quantities of interest
- Idea: generate microstates according to Boltzmann distribution (canonical ensemble) after sufficient number of steps
- Boltzmann distribution: $P(s;T) = \frac{\exp(-\beta E_s)}{Z}, \beta = \frac{1}{KT}$
- Underlying principle: detailed balance





Metropolis Algorithm on Ising Model

- Simulation process
  1. Randomly initialize the model
  2. Choose a spin at random & make a trial flip
  3. Accept the flip with probability

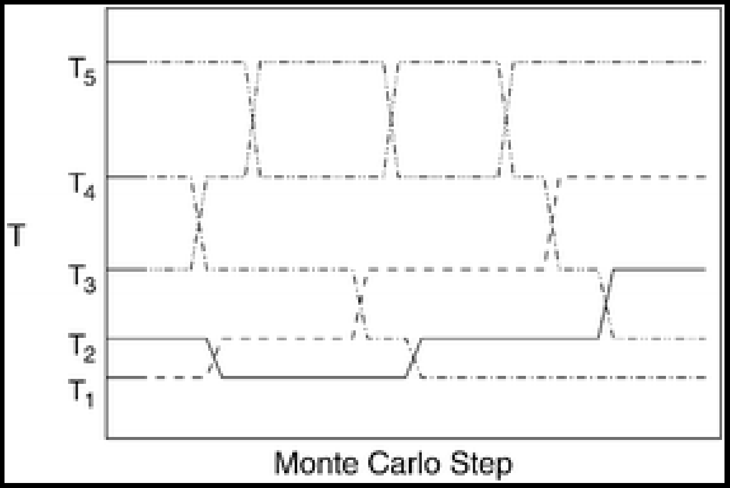
     $$P_{flip} = \min\{1, \exp(-\beta \Delta E)\}, \beta = \frac{1}{KT}$$

  4. If the flip is accepted, determine the desired physical quantities
  5. Repeat steps 2-4 to obtain a sufficient number of microstates
  6. Calculate the ensemble average of quantities

Parallel Tempering

- Recall: $P_{flip} = \min\{1, \exp(-\beta\Delta E)\}, \beta = \frac{1}{KT}$
- Drawback: Low temperature
  - ➔ Unlikely to accept flips with positive energy difference
  - ➔ Trapped in energy local minimum
- Motivation: Run Metropolis algorithm on different temperatures & allow exchange of microstates
  - ➔ High-temperature configuration at low-temperature system
- The probability of accepting an exchange is given by

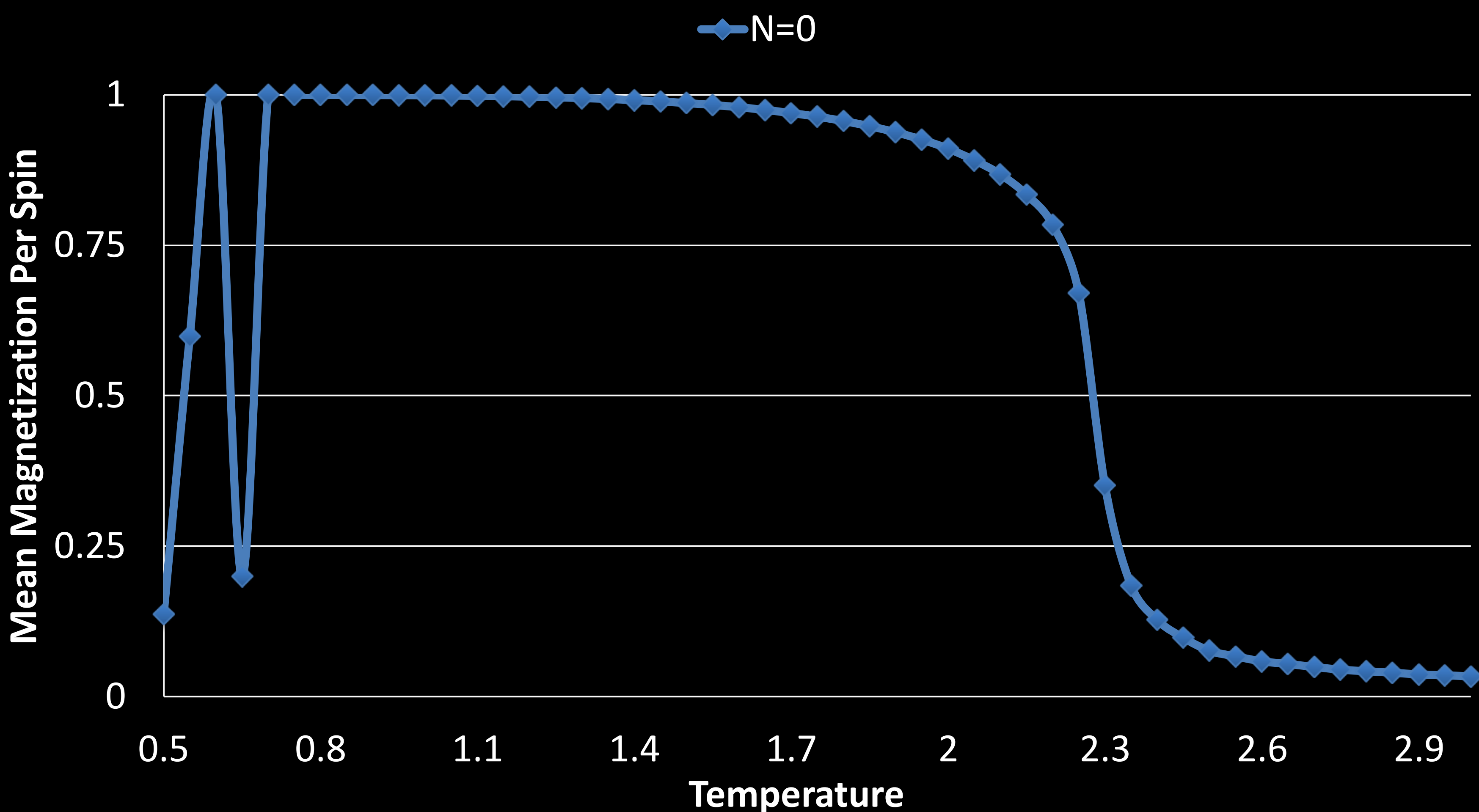
$$P_{exchange} = \min\{1, \exp(\Delta\beta\Delta E)\}$$



Temperature dependence of mean magnetization per spin with various replica exchange frequency

N = # of replica exchange

Total # of MC steps fixed to be 10^9; equilibration time set to 10^9



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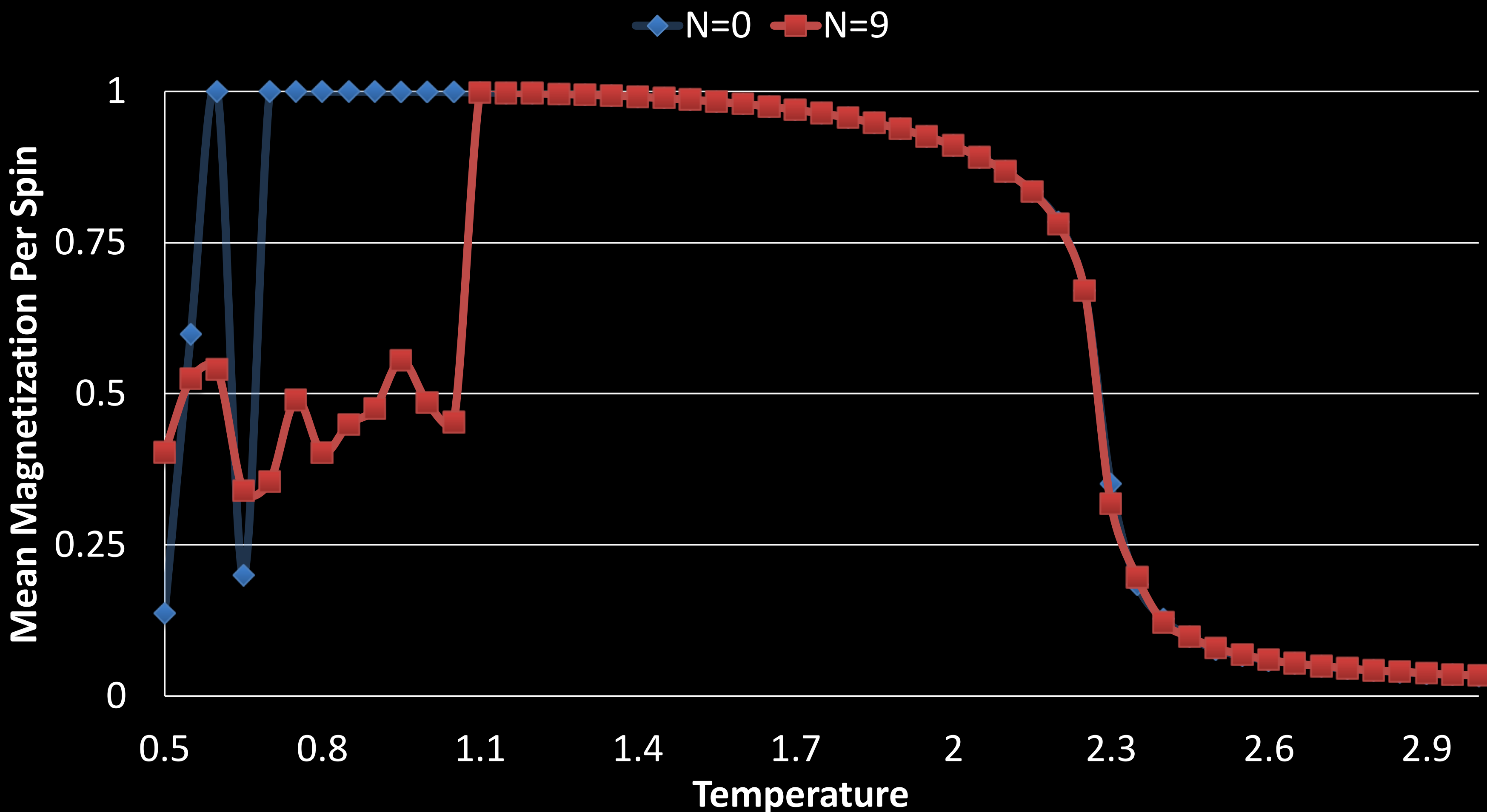

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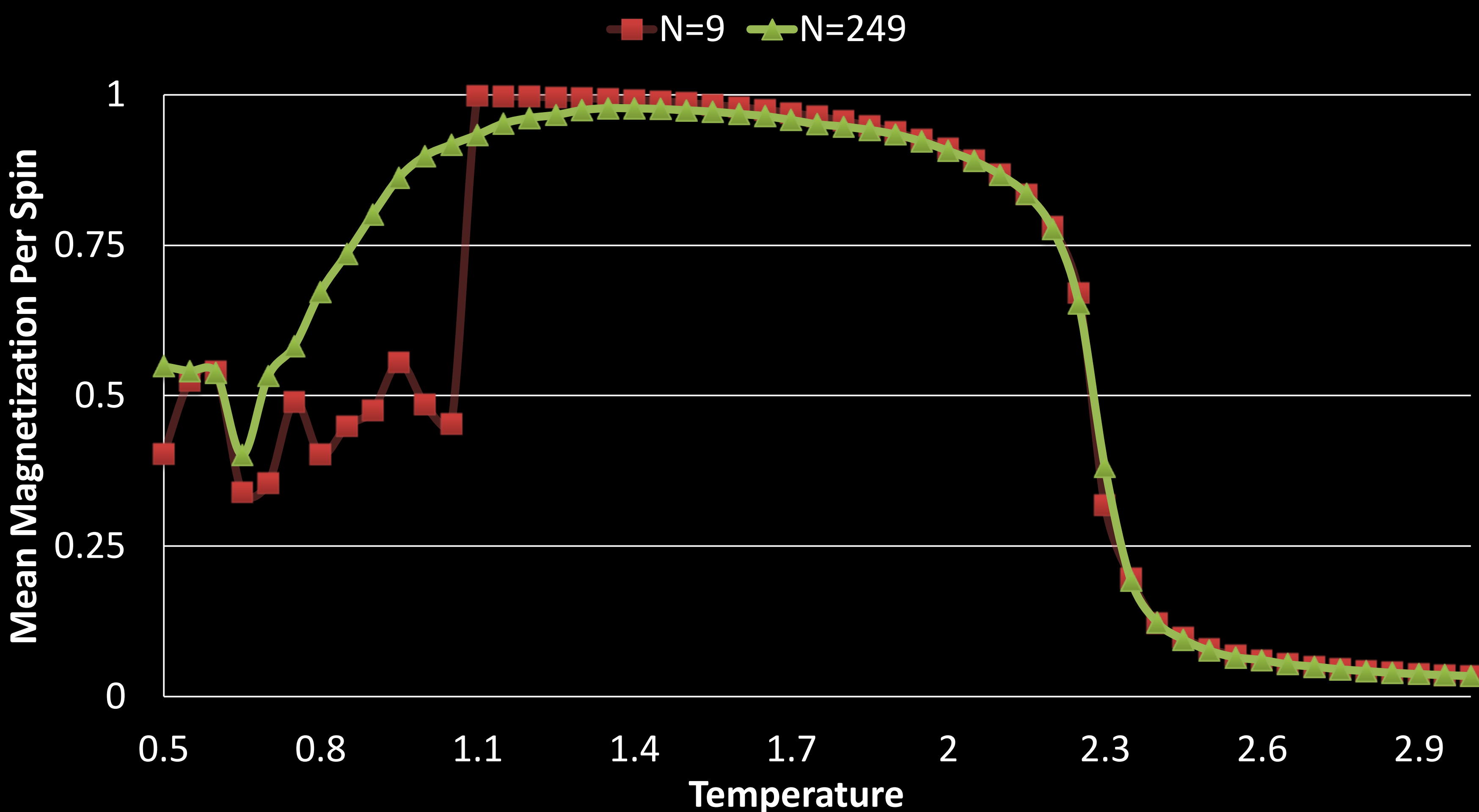

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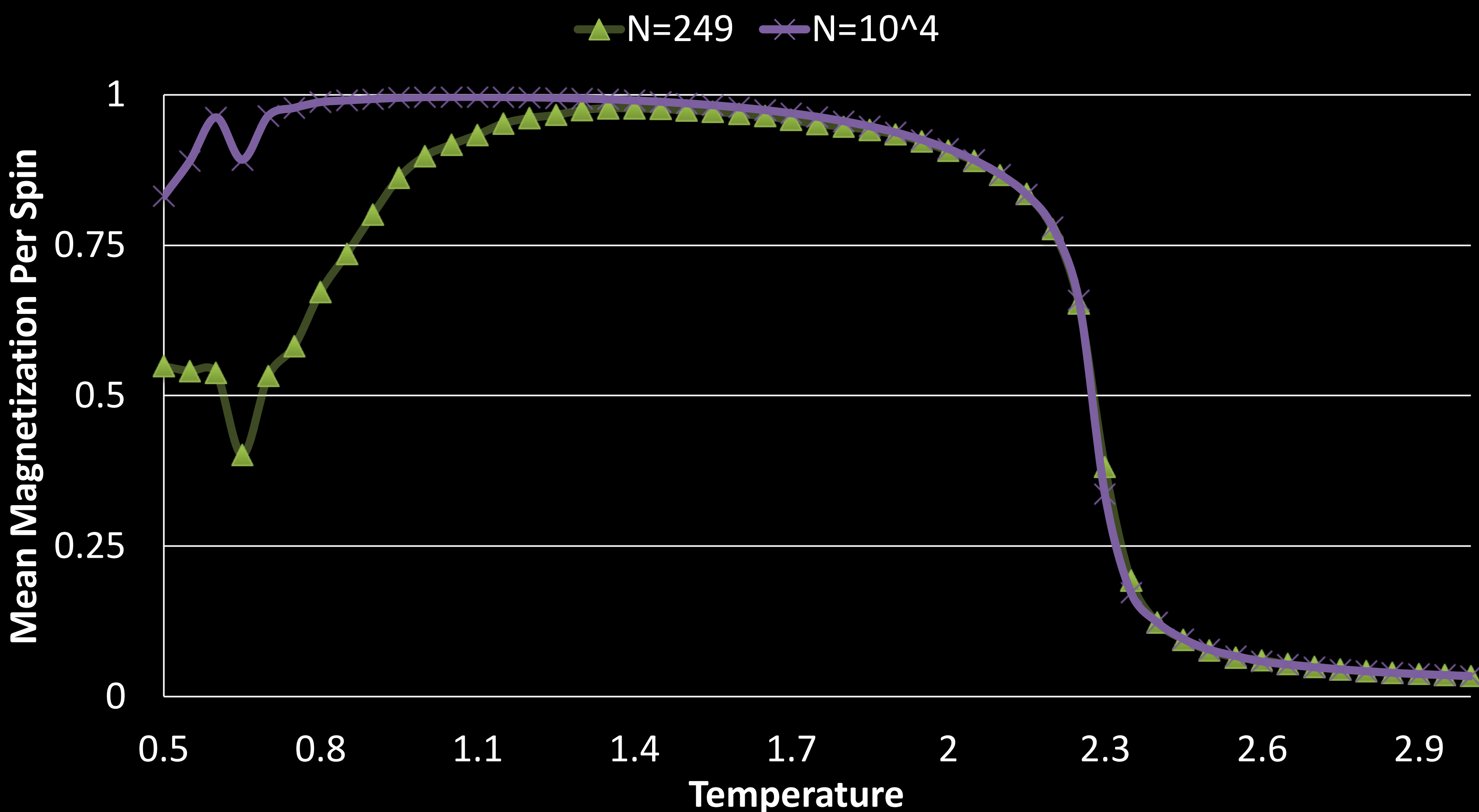

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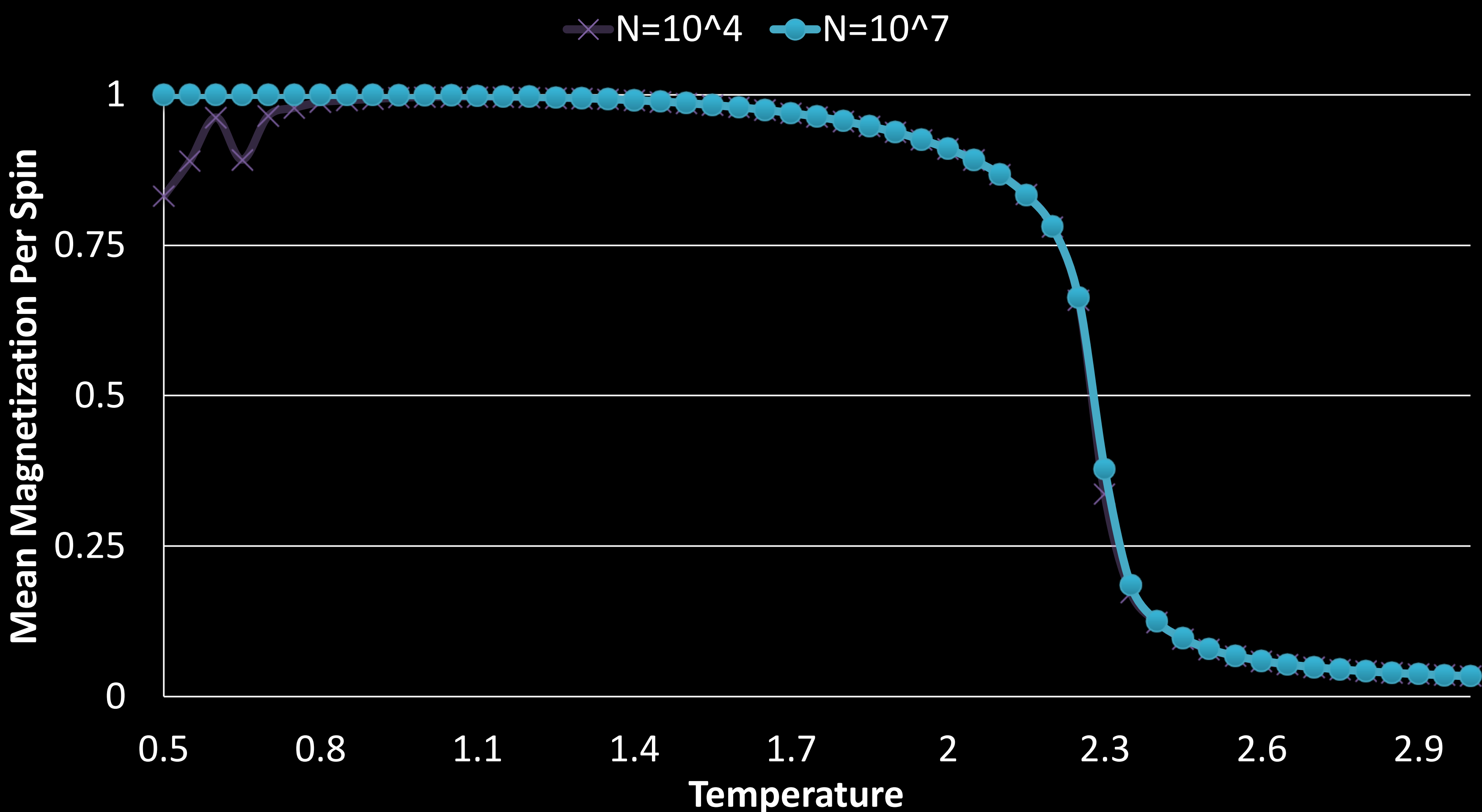

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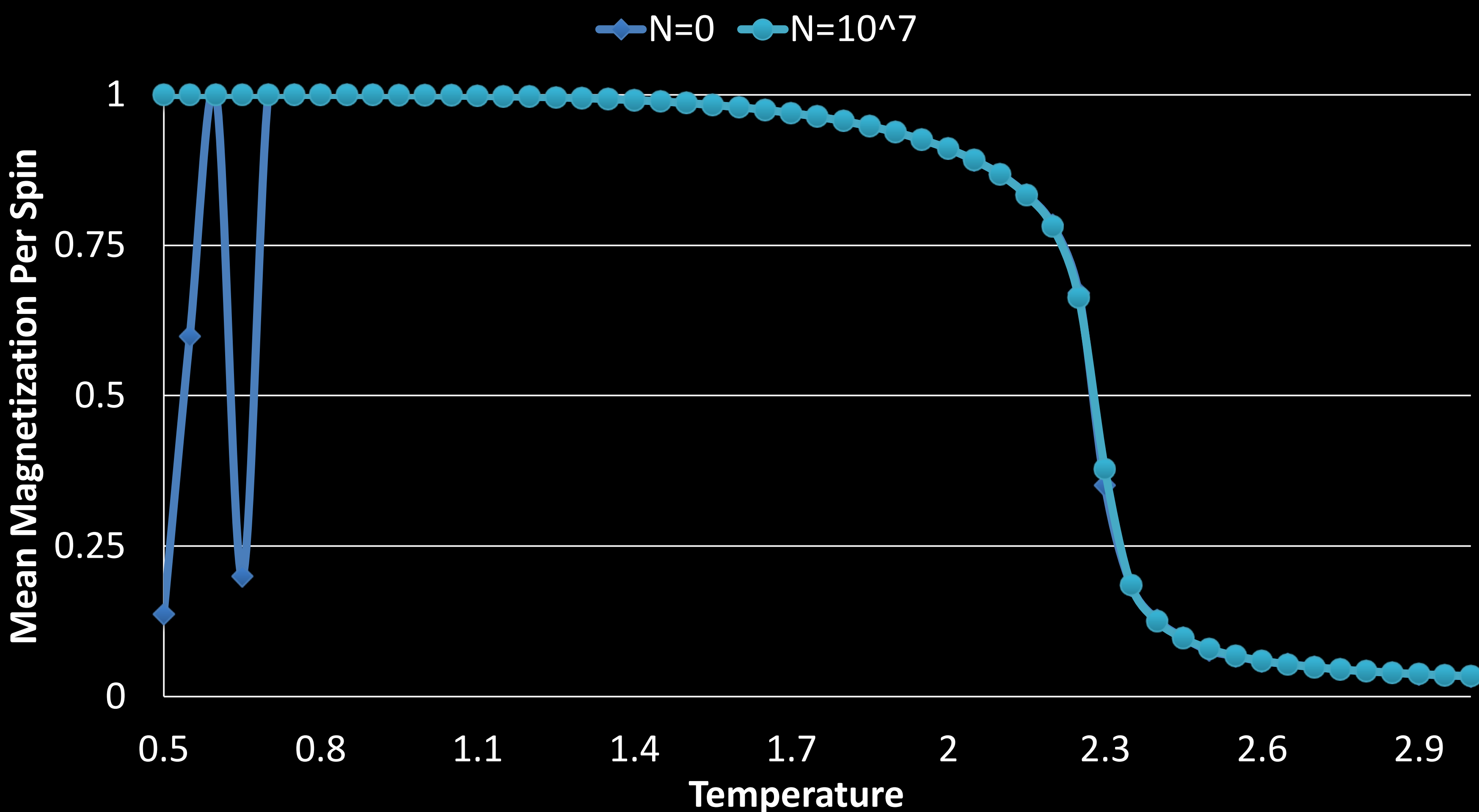

Temperature dependence of energy fluctuation (SD) with various replica exchange frequency

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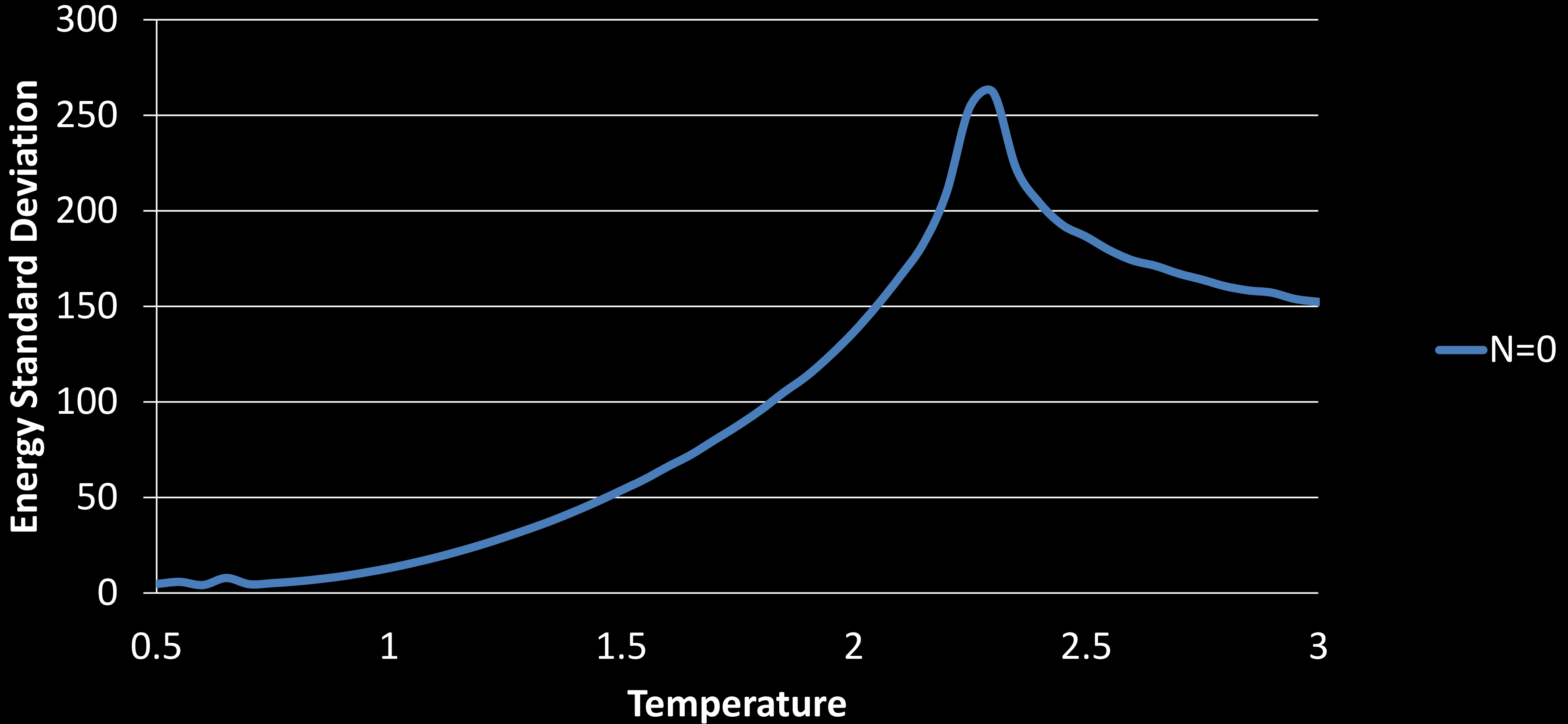

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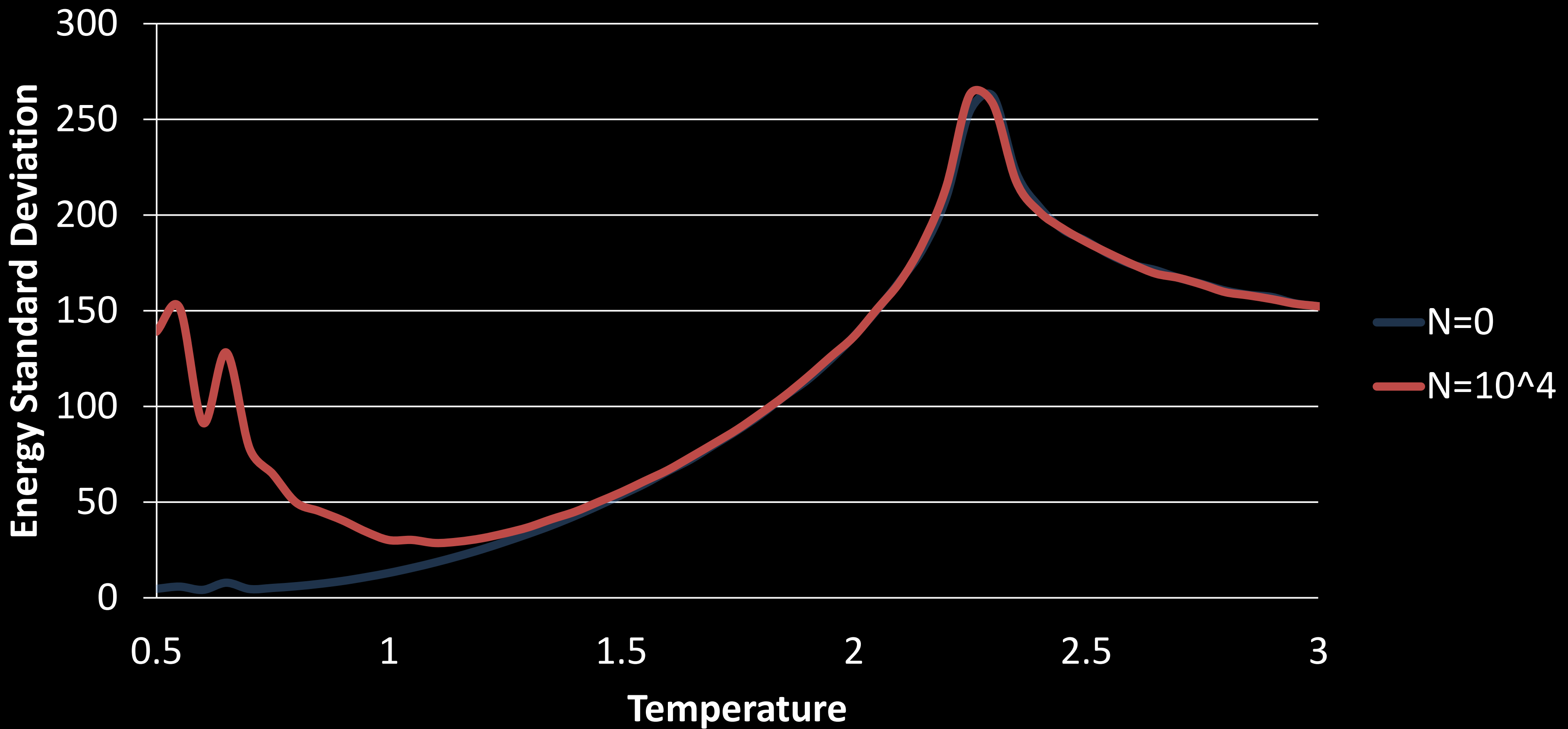

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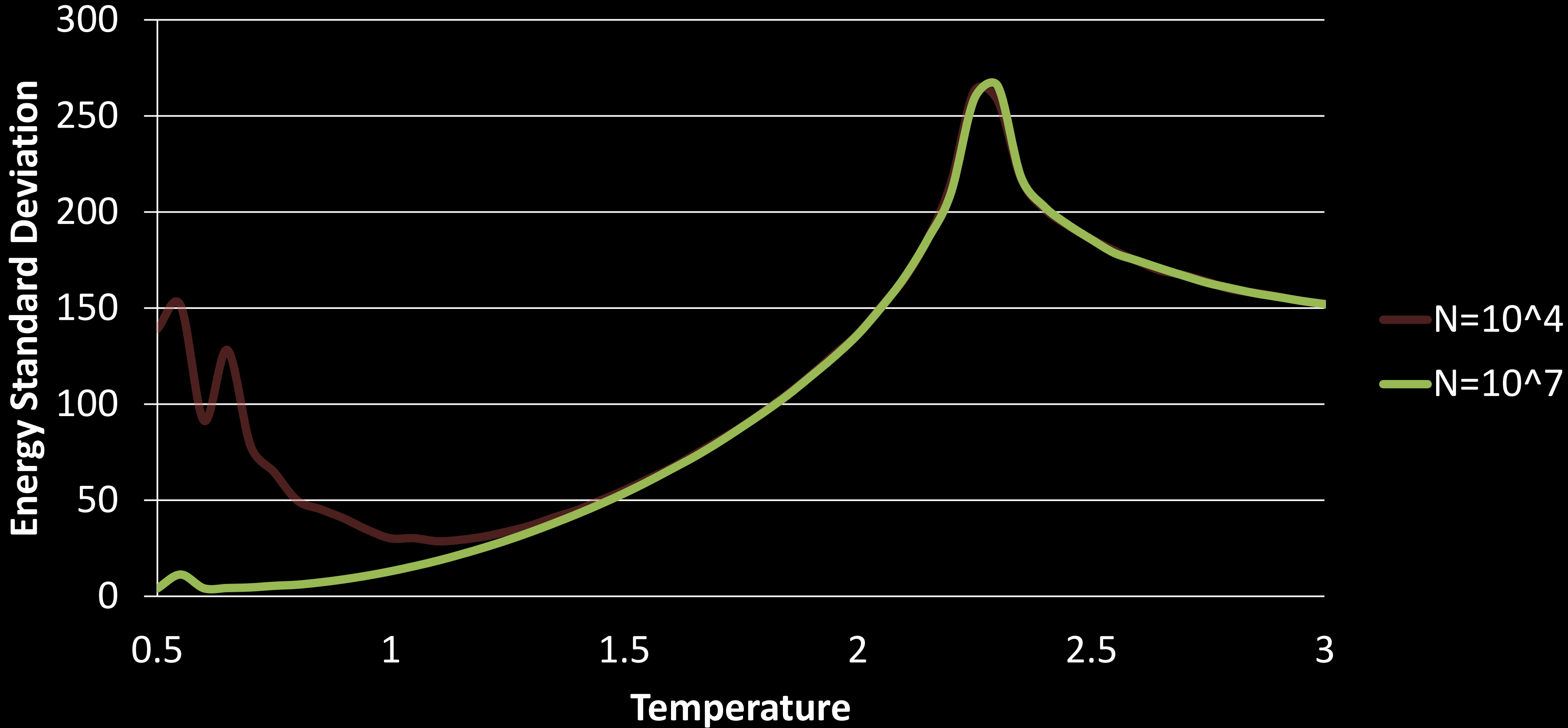
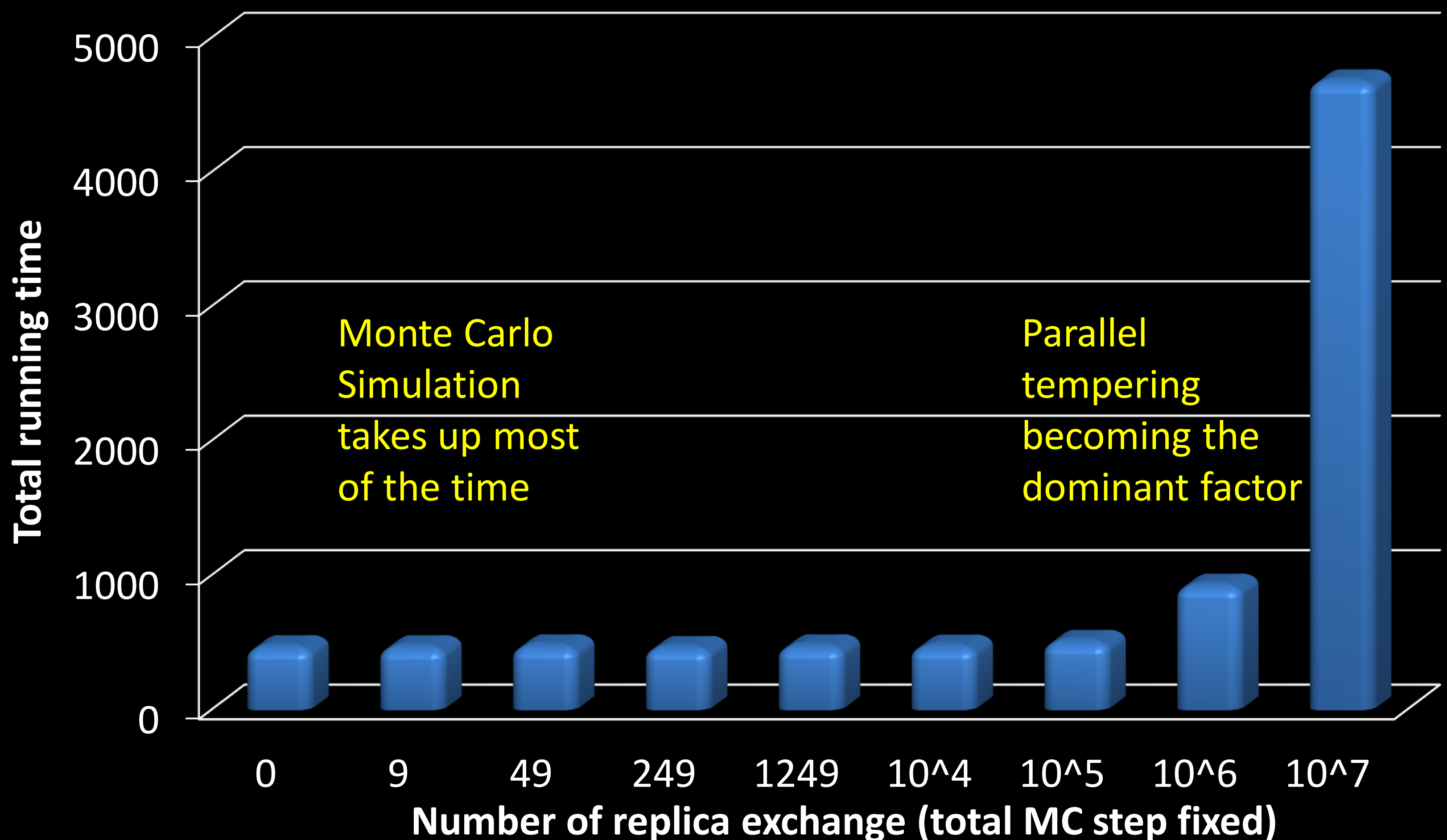


Running Time Dependence on # of Replica Exchanges



Coming soon

- Parallel tempering Metropolis running with:
  - Various temperature spacing (# of processors)
  - Different exchange patterns
  - Geometric temperature sequence
- Implementation on other models
- Goal: optimize the algorithm
  - Better convergence with less time
  - Self adjusting algorithms