# Simulating Polymer Systems on GPU

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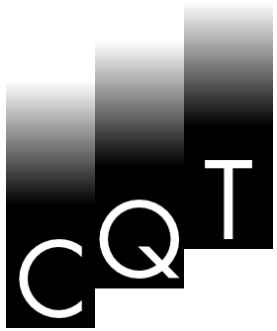


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# Parallel Tempering Method

Parallel tempering (or replica exchange) Monte Carlo with $n_r$ replicas:
Exchange conformations of neighboring replicas $i$ and $i+1$ with probability

$$p = \min\left(1, \exp\left[(E_i - E_{i+1})(\beta_i - \beta_{i+1})\right]\right)$$

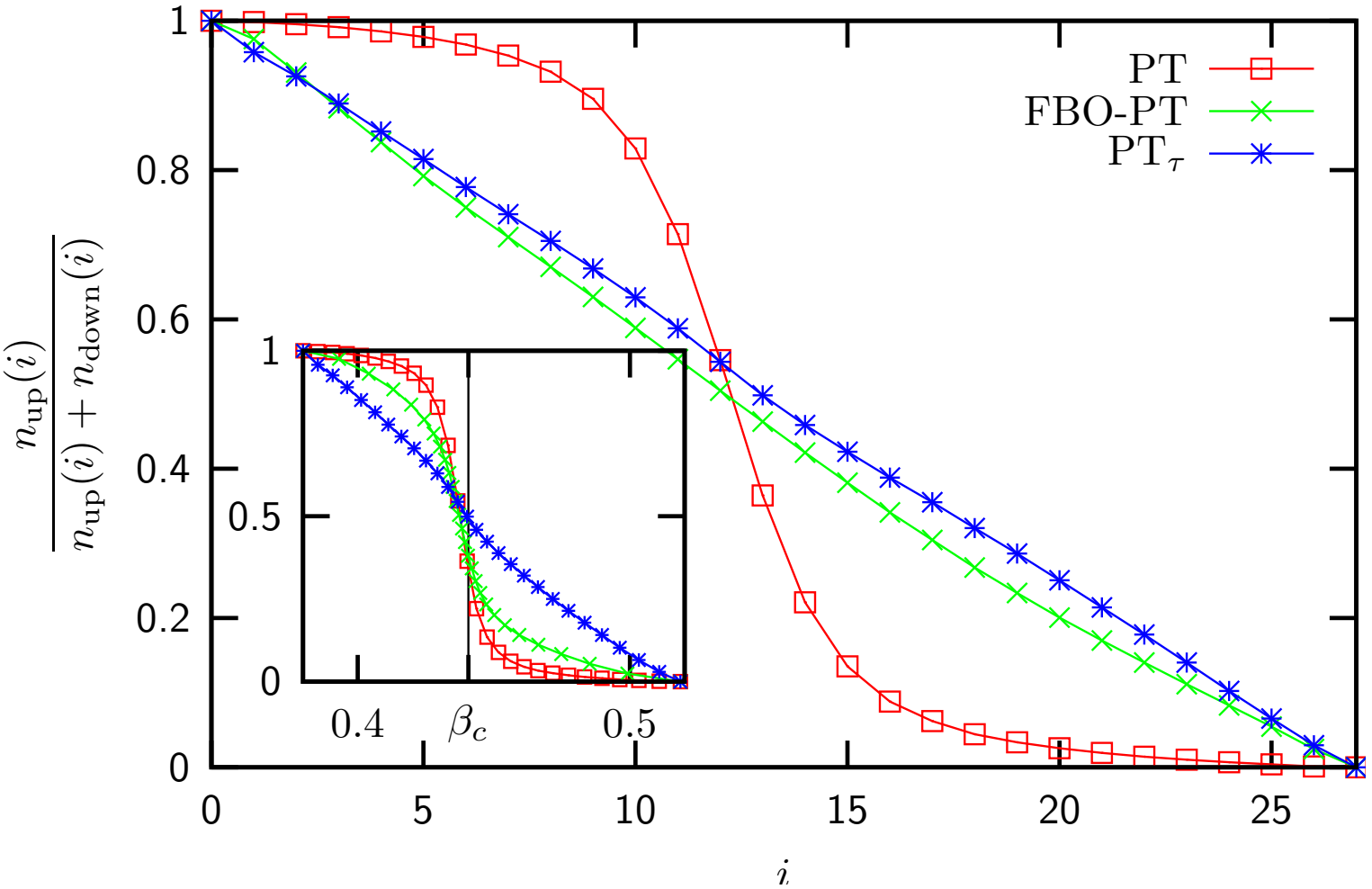
Problem: Appropriate spacing of $\beta_i$ and/or number of sweeps per replica

Here: Focus on autocorrelation times and hence number of sweeps per replica

E. Bittner, A. Nußbaumer, WJ, Phys. Rev. Lett. **101** (2008) 130603; PoS (LAT2009) (2009) 027.

# Flow of Replicas

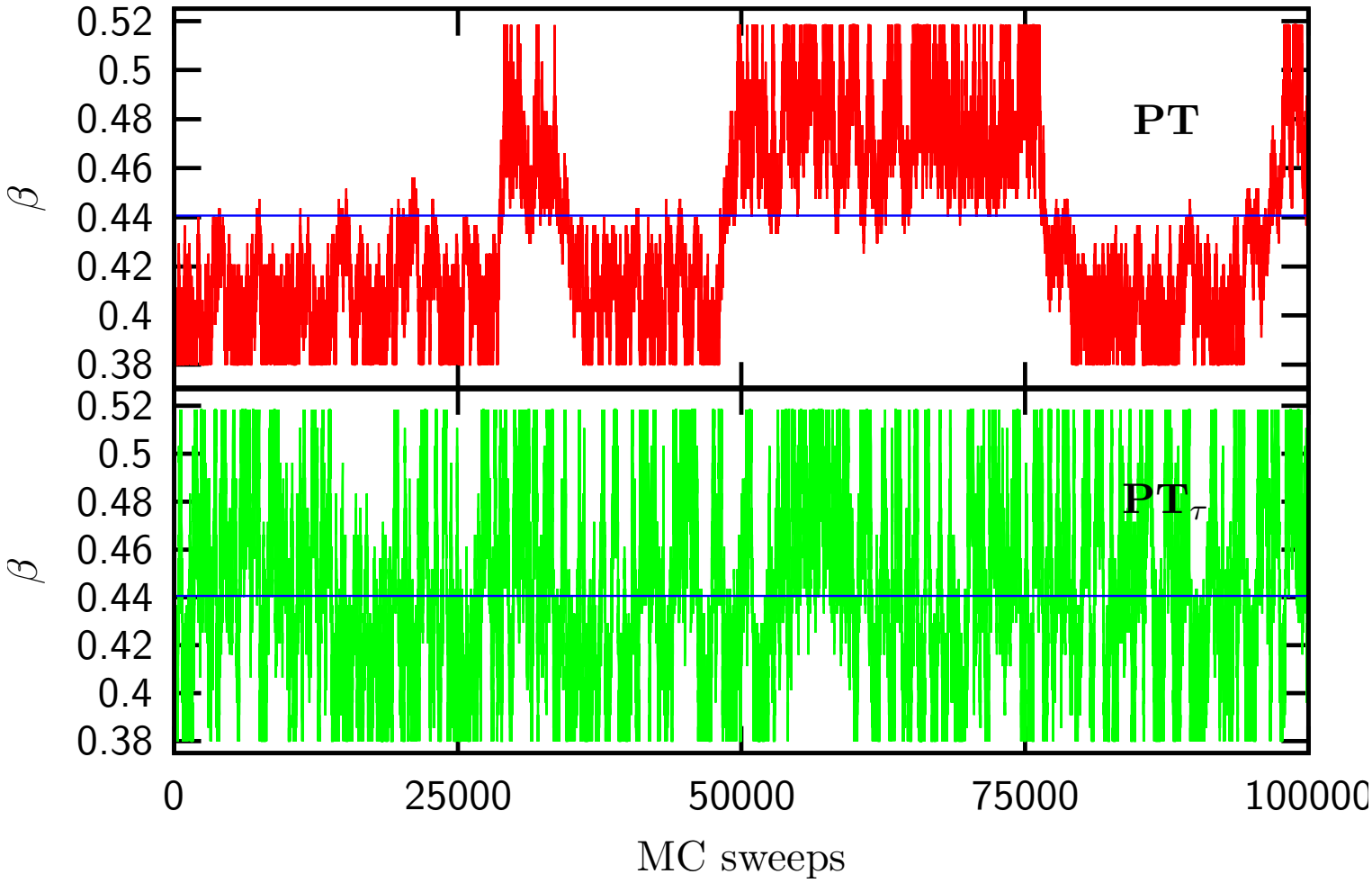
Standard PT exhibits sharp decline close to $\beta_c$




2D Ising model ($L = 80$)

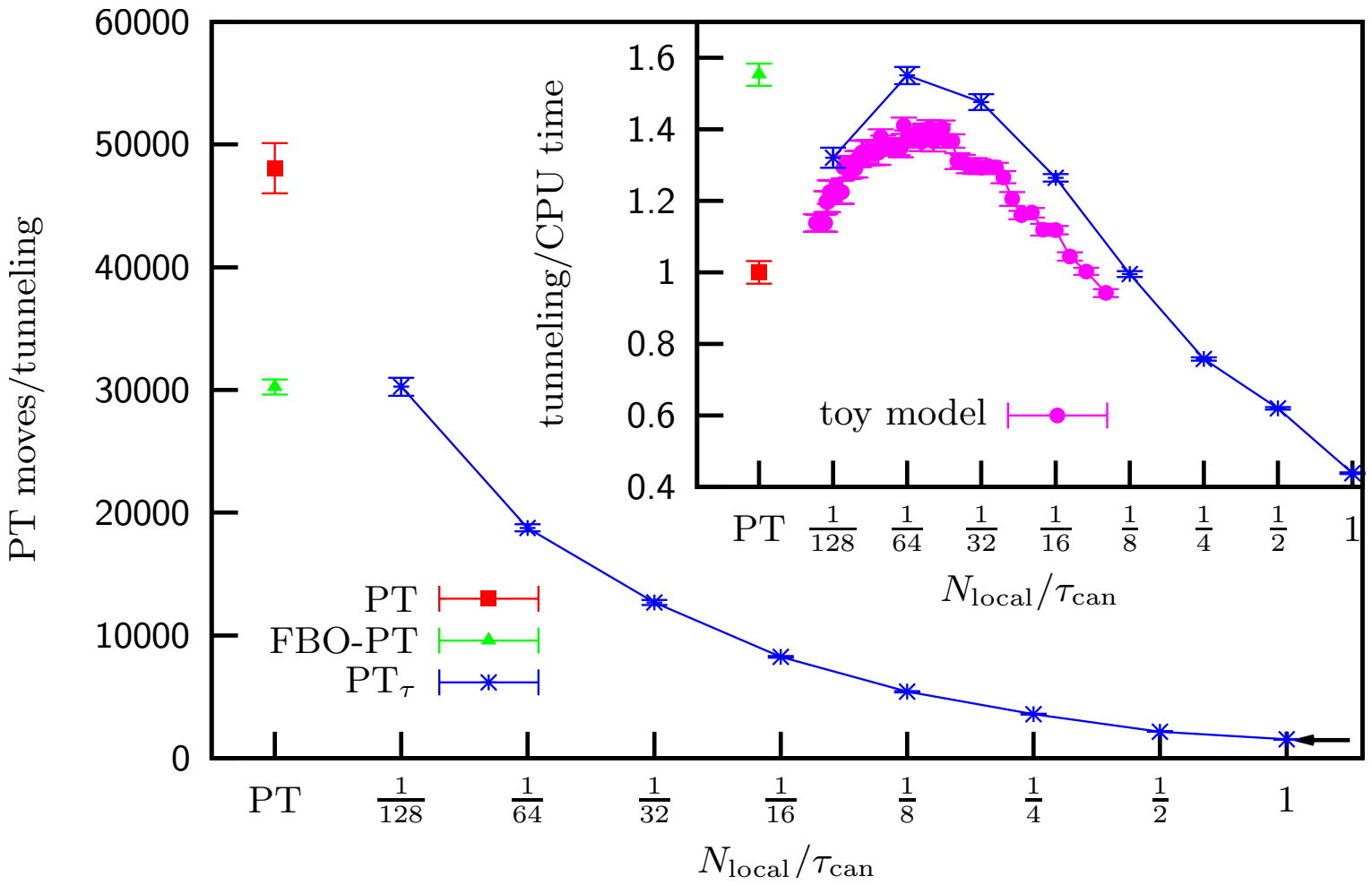
# Time-Series of Arbitrary Replica

Standard PT exhibits “reflections” at $\beta_c$ (similar to time-series for a first-order transition!)



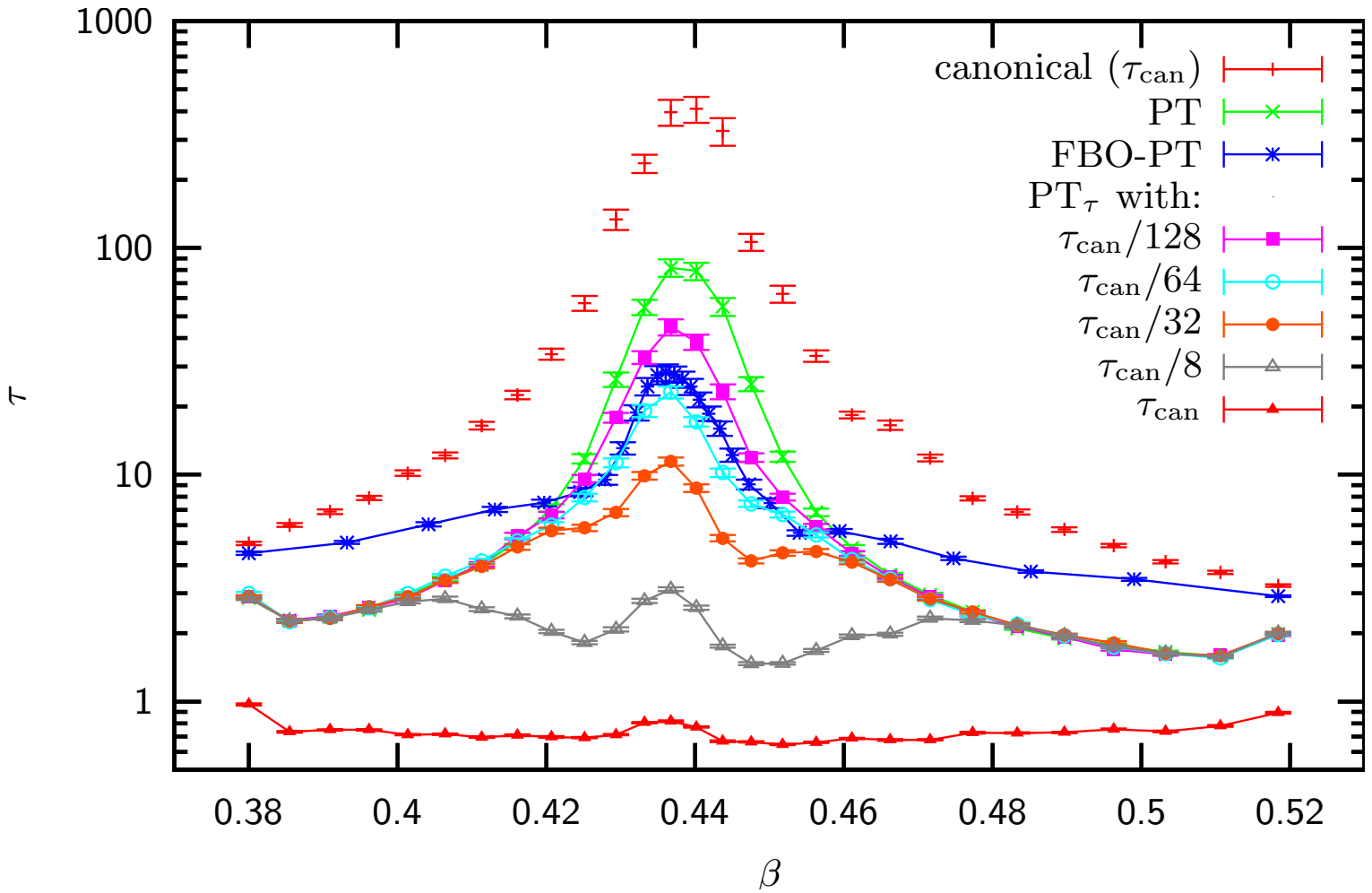

2D Ising model ($L = 80$)

# PT Moves per Tunneling



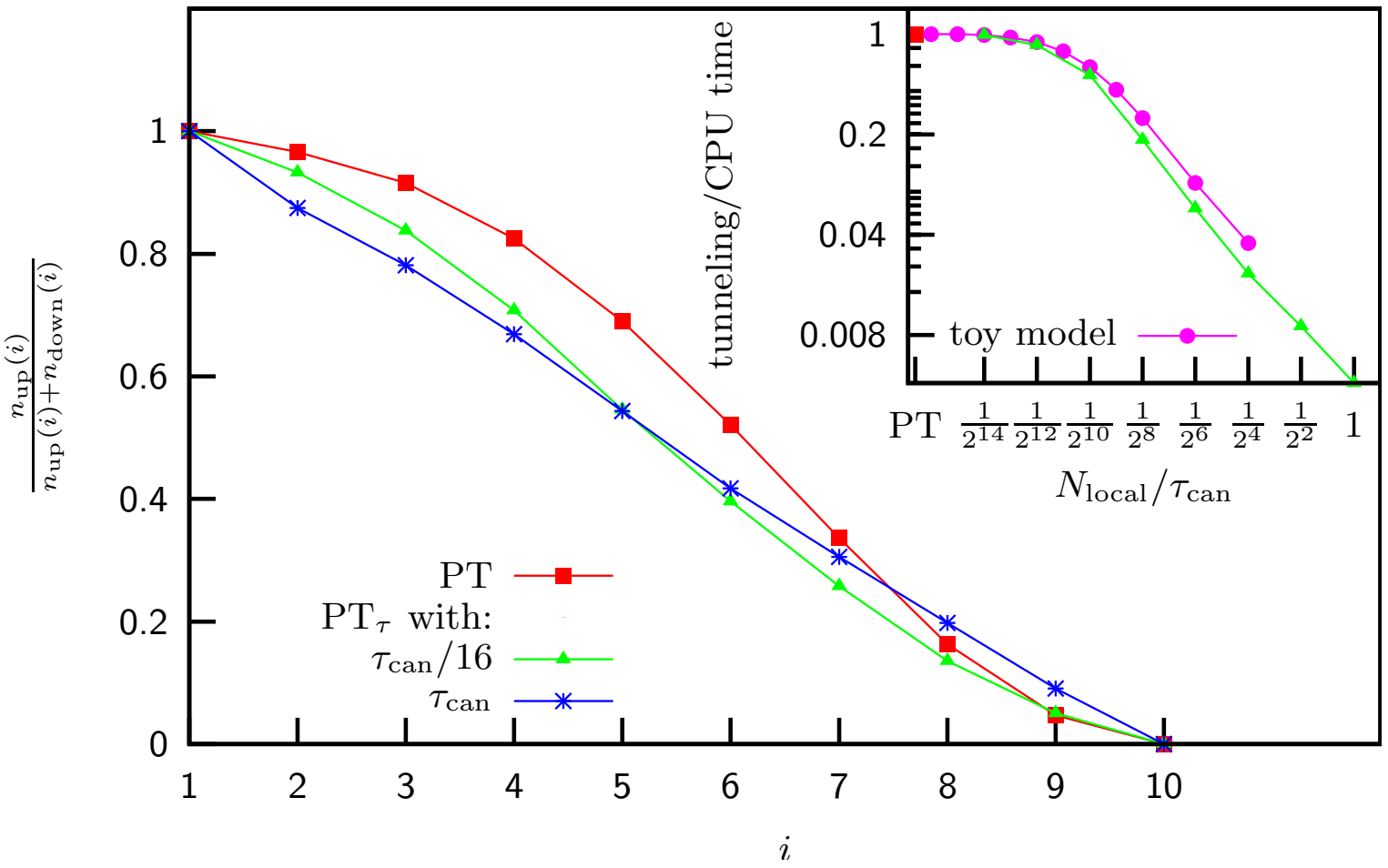

2D Ising model ($L = 80$)

# Autocorrelation Times




2D Ising model ($L = 80$)

# Flow of Replicas for Edwards-Anderson Spin Glass




3D EA Ising spin glass ($L = 6$, 20 disorder realizations)

# Summary and Outlook

Some conclusions

# Acknowledgements

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# Advertisement

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