Non-Flat Histogram Techniques for Spin Glasses

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Abstract

We take into consideration the 3D Edwards-Anderson model with bimodal bond distribution. Since the model is characterized by spin-glass behavior, finding ground states is an NP-hard problem. Employing different simulation techniques the round trip time distribution is investigated and the performance of the different methods is compared. The methods taken into consideration are the most established broad energy ensemble methods including the parallel tempering method and, in addition, a specially designed non-flat histogram technique which is shown to outperform the currently existing methods.

Introduction

- bimodal Edwards-Anderson-model:

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

  - sum over all next neighbors in simple cubic lattice
- spin glass model
- properties:
  - frustration
  - disorder
  - finding ground states is NP-hard [1]
- optimization problem
- formulation of many optimization problems in Ising-type Hamiltonians available [2]

The flat MUCA method

- aims at producing flat histograms in energy
- generalized metropolis criterion employing inverse density of states

$$P_{\text{acc}} = \min\left(1, \frac{W(E_{\text{new}})}{W(E_{\text{old}})}\right), \qquad W(E) \propto \Omega^{-1}(E)$$

- estimator for density of states $\Omega(E)$ determined iteratively before actual simulation

Parallel Tempering

- run several replicas at fixed temperatures $\{\beta_i\}$
- allow for exchange of replicas between temperatures with probability

$$P_{EX} = \min\left(1, e^{\Delta\beta\Delta E}\right),$$

- constant acceptance rates protocol employed with next neighbor exchanges [3]

The non-flat MUCA method

- histogram shaped to P_{SH} with weights

$$W(E) \propto \Omega^{-1}(E) P_{\text{SH}}(E).$$

- PT concentrates effort towards low energy region
- idea: imitate PT by power law shaped histograms

$$P_{\text{SH}}(E, E_0, \alpha) \propto (E - E_0)^{\alpha}$$

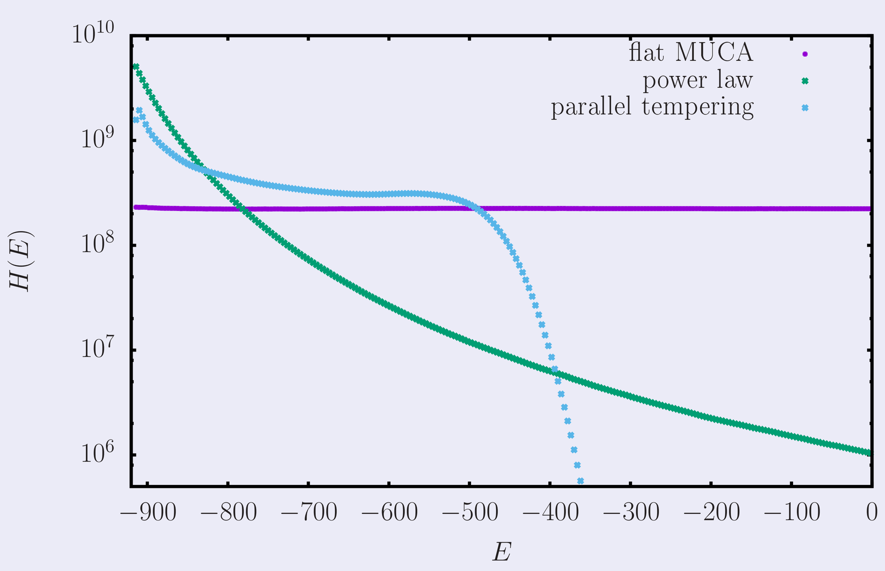
- expressing relatively to the ground state

$$P_{\text{SH}}(E, \Delta E, \alpha) \propto (E - (E_g - \Delta E))^{\alpha}$$

- best size-independent parameter set found: $\{\Delta E = 96, \alpha = -3.6\}$
- error in estimator for $\Omega(E)$

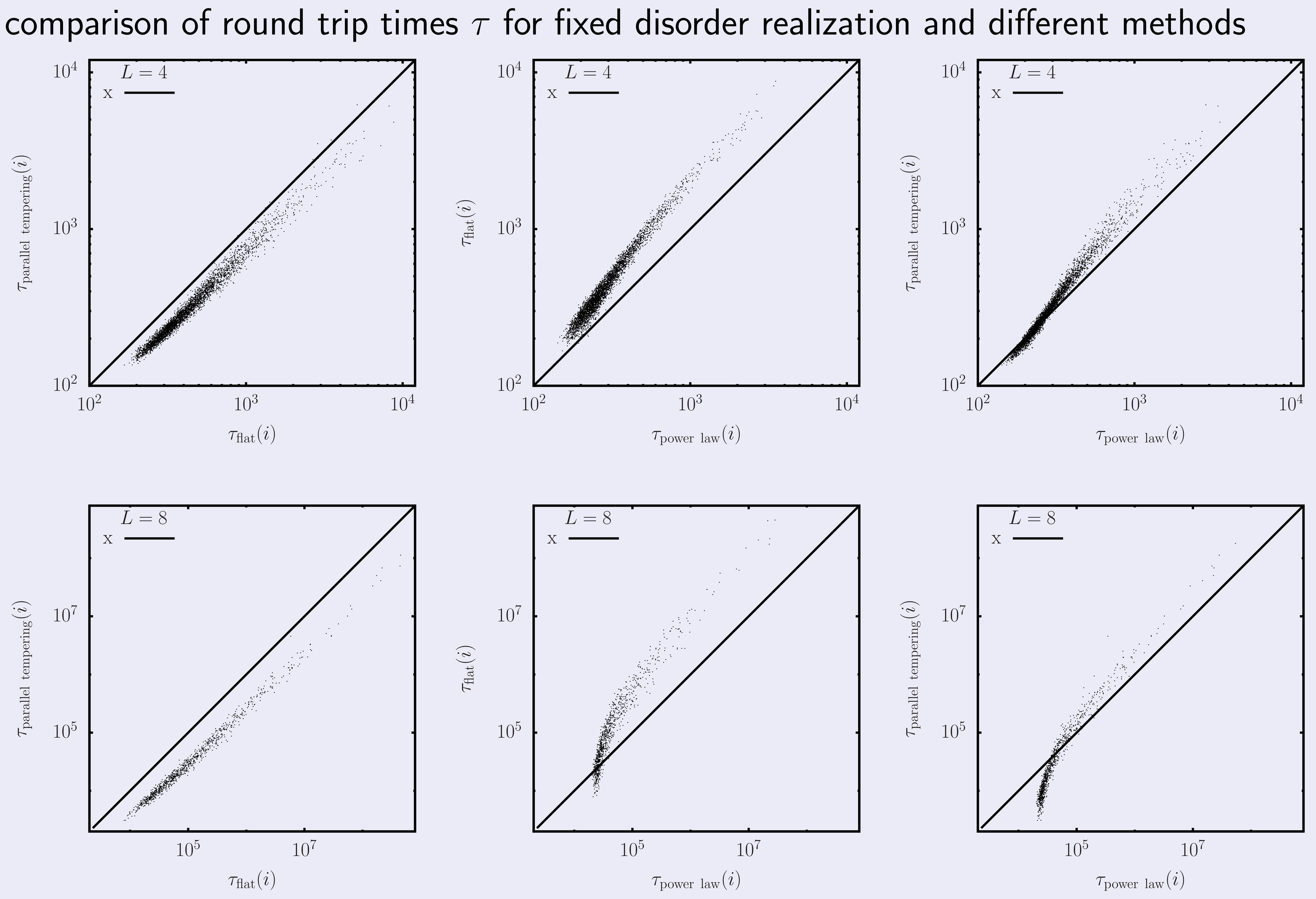
$$\Delta\Omega(E) \propto 1/\sqrt{N_{\text{round trips}}}$$

- $\rightarrow$ faster estimation of $\Omega(E)$ with non-flat histograms
- also applicable to Wang-Landau method



Scattering Plots

- comparison of round trip times τ for fixed disorder realization and different methods



- power law MUCA performs better for hard disorder realization with performance loss for the easy disorder realizations

Benchmarks and Extreme Value Statistics

- visiting ground state represents extreme event
- $\Rightarrow$ extreme value statistics are needed
- all round trip times distributions of Fréchet type
- Fréchet cumulative distribution function

$$\text{CDF}(\tau) = \exp\left(-\left(1 + \xi\frac{\tau - \mu}{\beta}\right)^{-1/\xi}\right)$$

- ξ shape, β scale, μ position
- Mean $\begin{cases} \mu + \beta/\xi\,(\Gamma(1-\xi) - 1) & \text{for } \xi < 1 \\ \infty & \text{otherwise} \end{cases}$
- Quantile Function

$$Q(p) = \mu + \frac{\beta}{\xi} \cdot \left[(-\log(p))^{-\xi}\right], \quad p \in (0, 1)$$

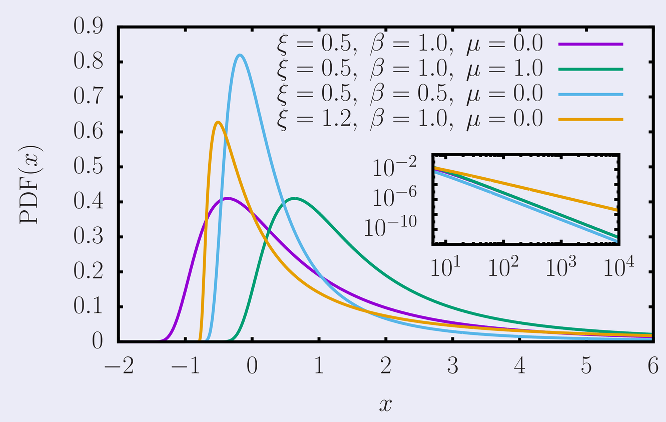
$\rightarrow$ distribution mean not always defined

$\rightarrow$ consider integral up to the $(1 - \epsilon)$ - quantile:

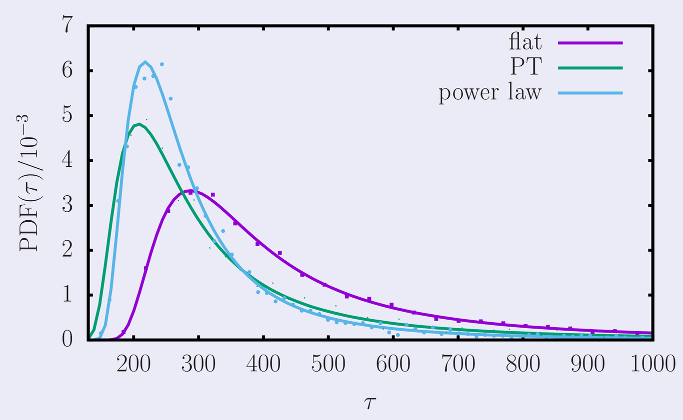
$$\overline{\tau}_{\epsilon} = \int_{\beta/\xi - \mu}^{Q(1-\epsilon)} \frac{\tau}{\beta}\left(1 + \xi\frac{\tau - \mu}{\beta}\right)^{-1/\xi - 1} \exp\left[-\left(1 + \xi\frac{\tau - \mu}{\beta}\right)^{-1/\xi}\right] d\tau.$$

- takes account for the properties of the distribution
- allows for an extrapolation to higher round trip times

Fréchet distribution for different parameter sets

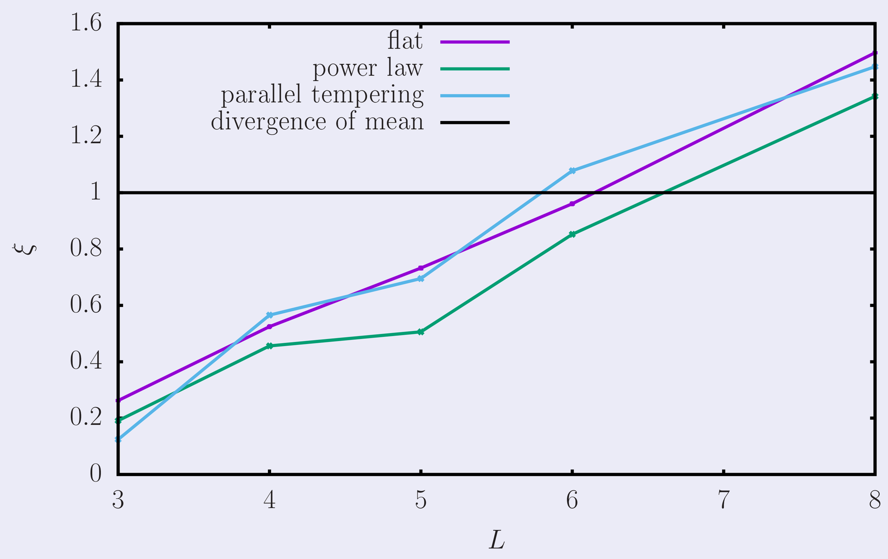


Fréchet distributions for $L = 4$

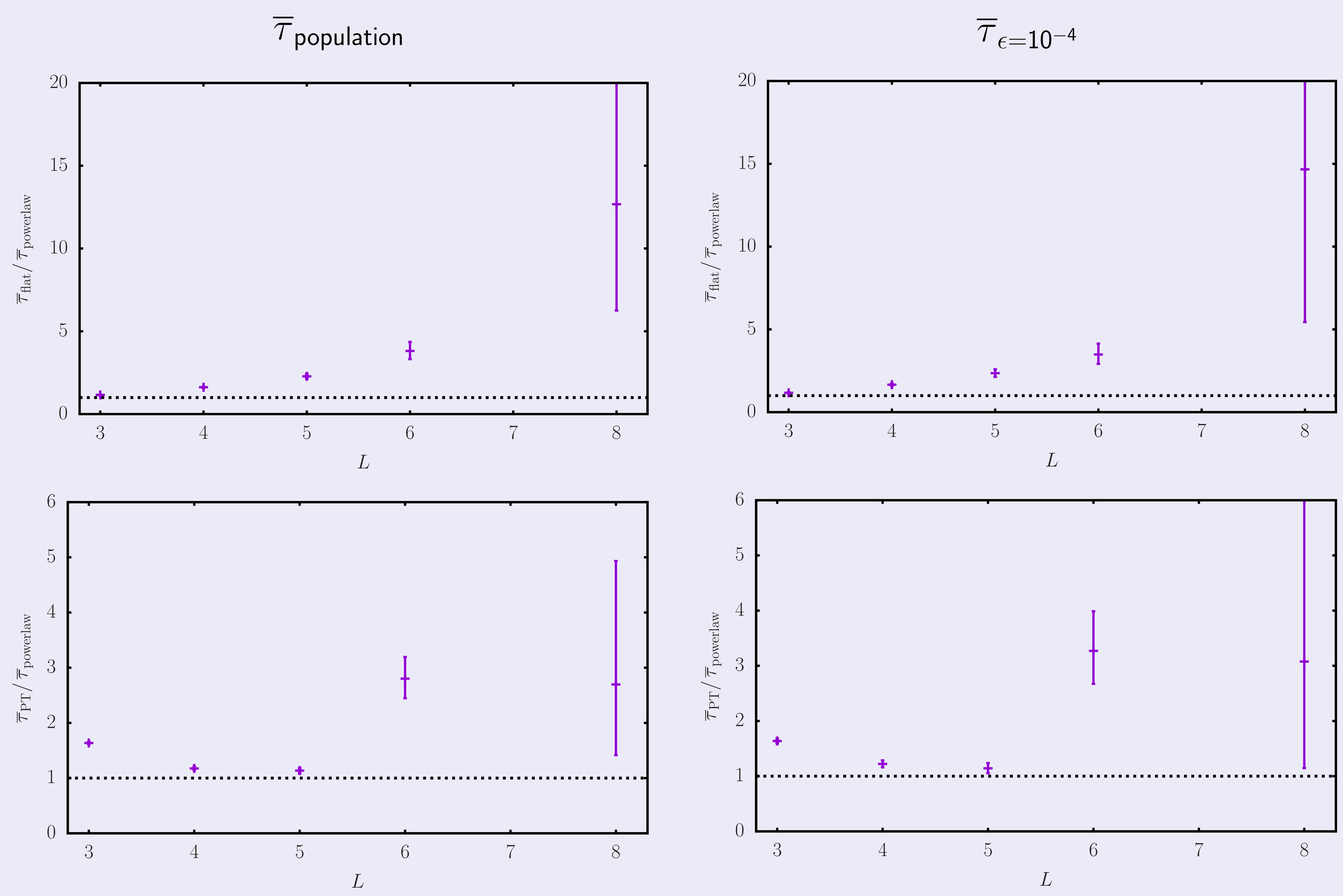


Finite-Size Scaling of the Shape Parameter

- shape parameter as indicator of performance for hard disorder realization
- similar scaling for all different methods
- non-flat MUCA systematically smallest ξ
- distribution means for all methods undefined for $L = 8$



Results



- compared to flat MUCA improvement growing with lattice size
- more then ten times smaller mean round trip time for $L = 8$
- compared to parallel tempering up to roughly 3 times lower mean round trip time

References

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Conclusion

The non-flat histogram method has proven to yield lower mean round trip times for the 3D bimodal Edwards-Anderson spin glass for all considered lattice sizes. We were able to find one universal histogram shape yielding an overall better performance than the existing methods. The shape is particularly well-suited for the hard instances of the problem, which due to the nature of the underlying distribution and the scaling of its shape parameter are likely to play an increasing role with growing lattice size. The gain in performance is therefor expected to increase when even larger system sizes are taken into consideration. The general idea of sampling non-flat histograms can easily be generalized to the Wang-Landau algorithm and may also be successfully applied to other models which are characterized by rugged free energy landscapes.

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