Application of New Chain-Growth Algorithms for Lattice Polymers

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Abstract

We apply recently developed enhancements of the Pruned Enriched Rosenbluth Method (PERM) [1], namely the Multicanonical Chain-Growth Algorithm [2] and the Flat Histogram Method [3], to polymers and peptides on lattices.

Both methods are based on the idea to sample independently of temperature the complete energy space of polymer conformations. They thus enable, for example, the determination of the density of states within one simulation run for lattice polymers.

We apply both algorithms to interacting self-avoiding walks to compare the behaviour of the two versions and, of course, to get new results for statistical properties of polymers and peptides.

[1] P. Grassberger, Phys. Rev. E 56 (1997) 3682.

[2] M. Bachmann and W. Janke, Phys. Rev. Lett. 91 (2003) 208105.

[3] T. Prellberg and J. Krawczyk, Phys. Rev. Lett. 92 (2004) 120602.

flatPERM

The flat histogram version follows a strategy from a microcanonical view of the problem. The basic ideas are:

Use growth steps as in the normal PERM chain growth algorithm.

Consider then a microcanonical estimator for the total number of configurations of size n with energy m

$$C^{est}_{n,m} = \langle W \rangle_{n,m} = \frac{1}{S} \sum_i W^{(i)}_{n,m}$$

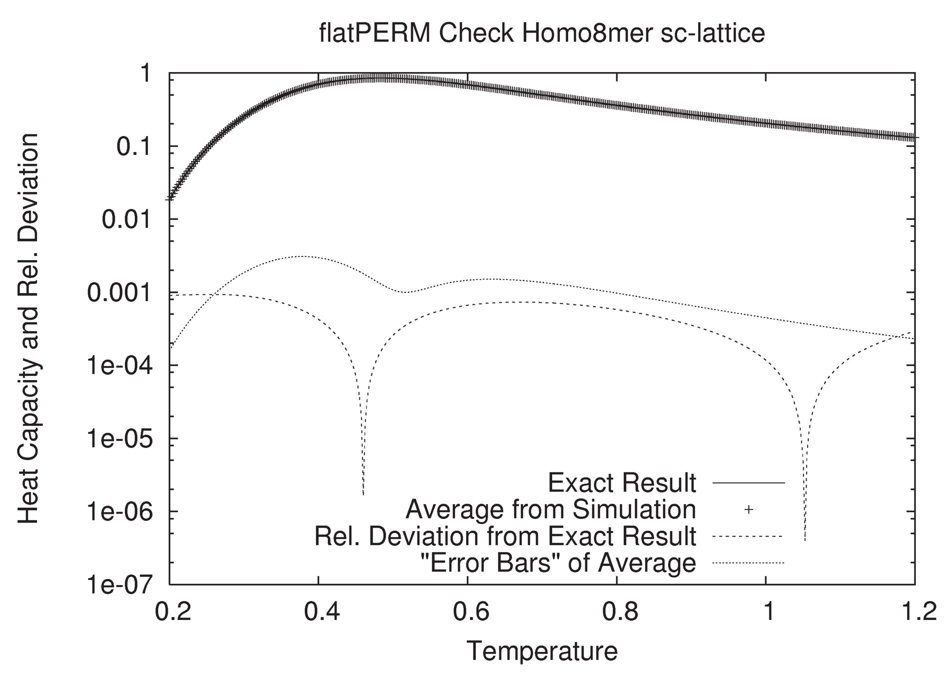
where $W^{(i)}_{n,m}$ is the Rosenbluth weight of the ith configuration. Now define r as the ratio of actual Rosenbluth weight and $C^{est}_{n,m}$:

$$r = \frac{W^{(i)}_{n,m}}{C^{est}_{n,m}}$$

Apply population control by pruning, when $r<1$ and enrichment, when $r>1$.

Check with Exact Results

Firstly we compare with exact results from enumeration. An example gives the figure: It shows the heat capacity of an homo8mer on the sc lattice, as well as the relative deviation from the exact value. The deviation is at all temperatures lower than 10^{-3}, the statistics includes 2×10^6 conformations, 5×10^5 arose from independent growth starts.



mucaPERM

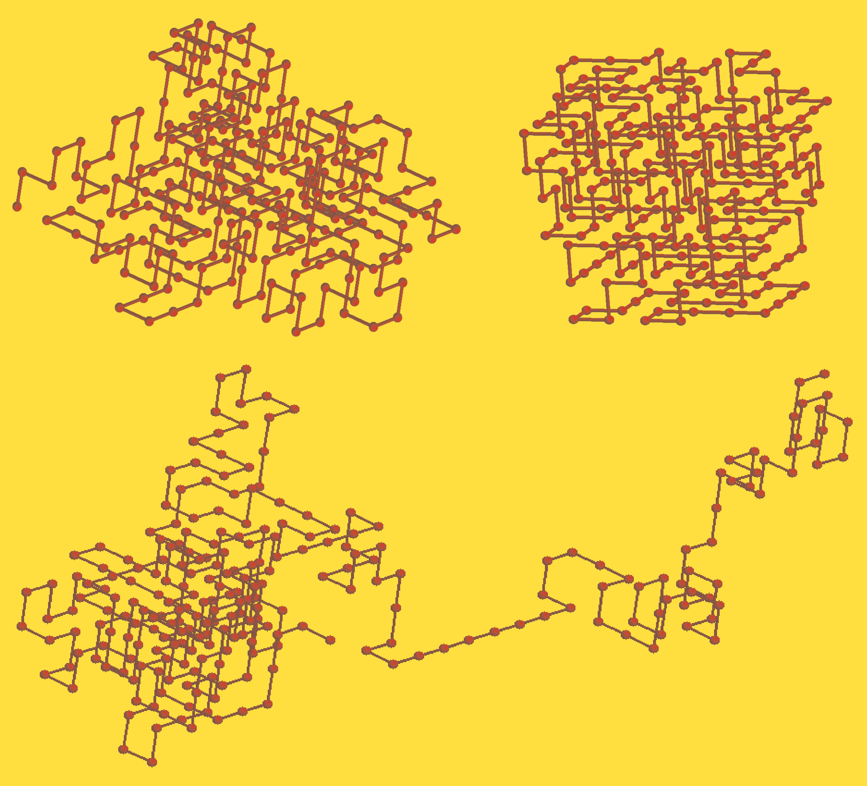
As in all multicanonical simulations, the idea of mucaPERM is to sample a flat energy distribution instead of the canonical one. Therefore we apply a weight $W^{flat}_n(E)$ in addition to the Rosenbluth and the Boltzmann weights. The partition sum according to the new distribution thus becomes

$$Z^{flat}_n = \sum_i W^{(i)}_n e^{-\beta E^{(i)}} W^{flat}_n(E^{(i)})$$

The weights $W^{flat}_n(E)$ have to be determined iteratively:

$$W^{flat,(iter)}_n(E) = \frac{W^{flat,(iter-1)}_n(E)}{H^{(iter-1)}_n(E)}, \quad \forall\, n, E$$

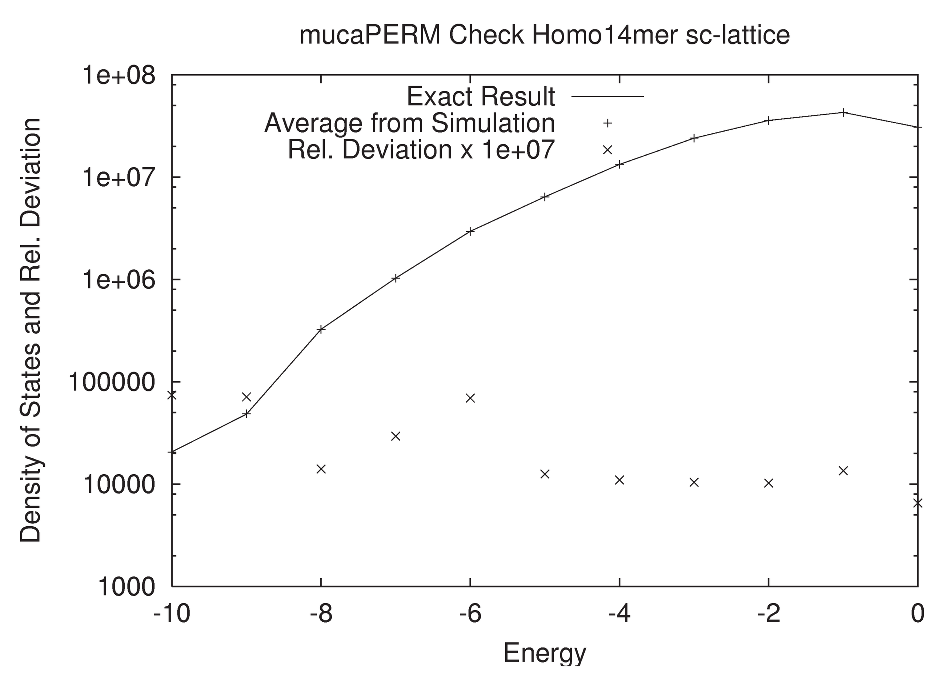
where $H_n(E)$ is the histogram of the accumulated weights, which is reset to 0 after each iteration. One applies population control by comparing the weight with some threshold values.

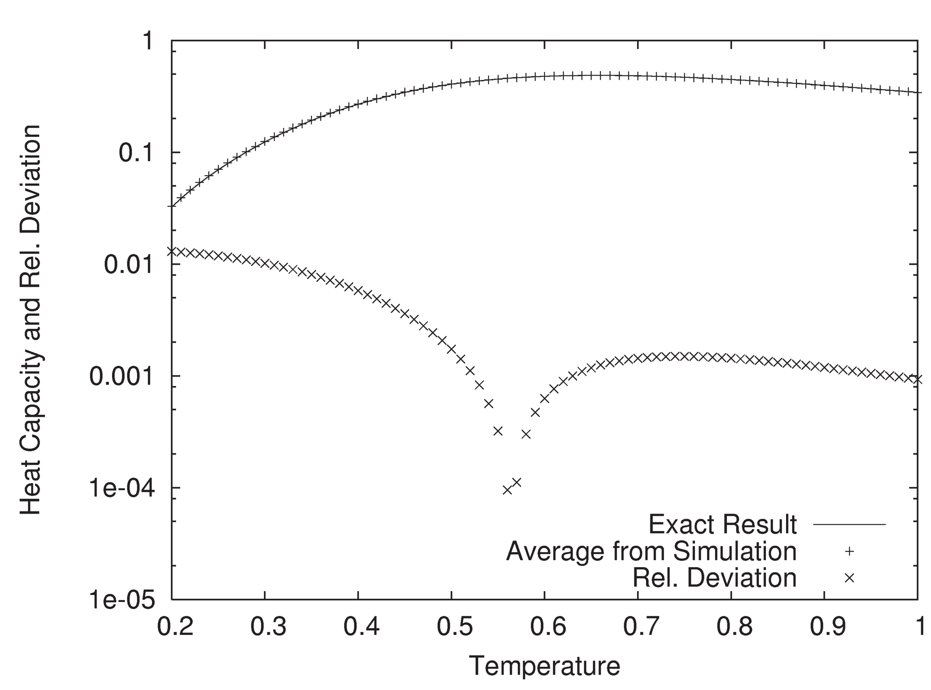


Three typical conformations of an homo256mer on the sc lattice at different temperatures.

Check with Exact Results

The figures show the density of states as well as the heat capacity of an homopolymer on the sc lattice, here with 14 monomers. With very little computing time, the relative deviations from the exact values are already lower than 1 percent.

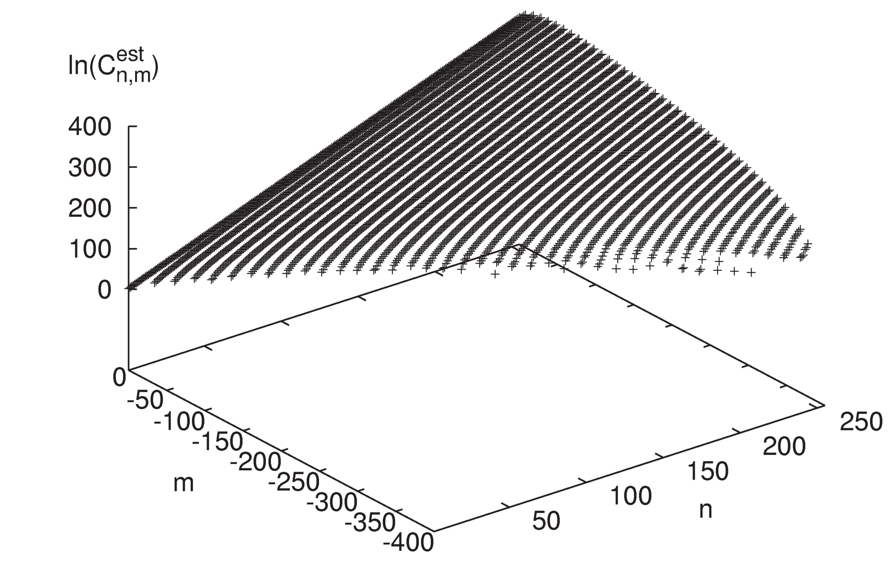


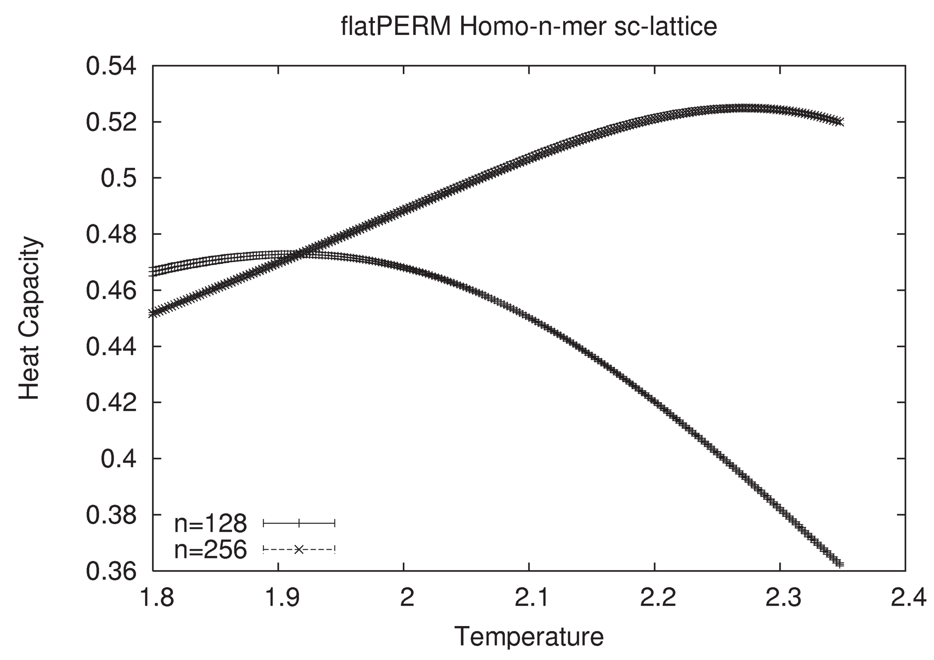


This project is partly supported by the Deutsche Forschungsgemeinschaft (DFG) under contract No. JA 483/24-1.

Coil-Globule Transition

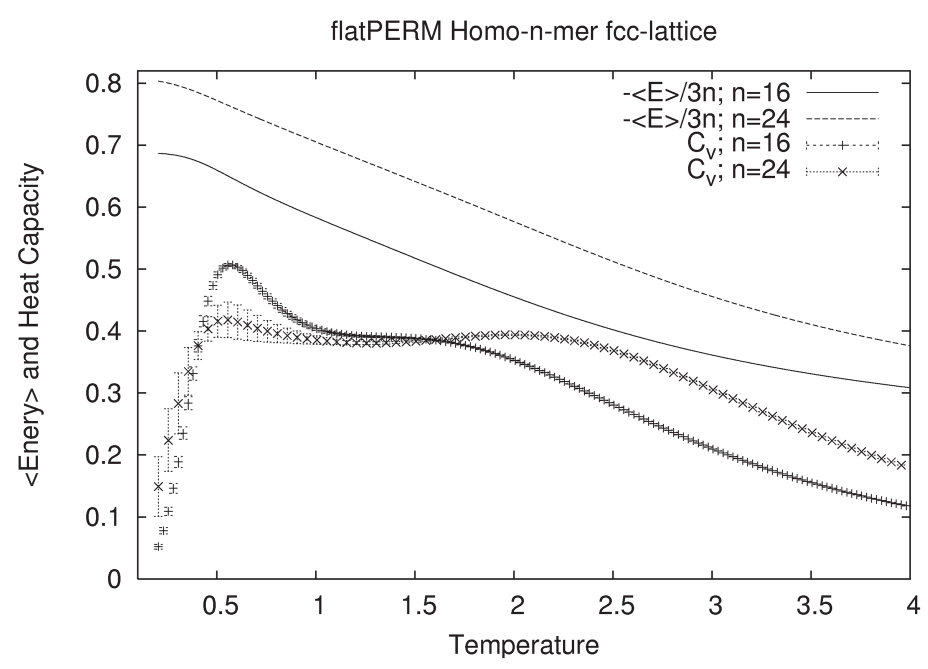
With the presented algorithms one can study the coil-globule transition of homopolymers up to lengths of order 10^3. The upper figure shows $\ln(C^{est}_{n,m})$ (the "density of states") for chains up to length n=256, where m is the energy. The lower figure shows the heat capacity for the homopolymers with lengths n=128 and n=256 near the coil-globule transition temperature. Both figures are for polymers on the sc lattice.





Crystallization

At much lower temperatures as considered above, we find a second peak in the heat capacity that can be interpreted as a liquid-solid transition (crystallization) point [4]. But low-energy conformations (i.e., conformations at very low temperatures) are that rare (by a factor of over hundred orders of magnitudes for considered lengths) that even with the presented powerful methods, chain lengths only up to order 10^2 can reliably be studied at these temperatures. The figure shows the average energies and the respective heat capacities for two shorter chains on a fcc lattice.



[4] F. Rampf, W. Paul, and K. Binder, Europhys. Lett. 70 (2005) 628.

Outlook

Further work will include:
- Application of both methods to other models
- Systematic comparison of excellence of both methods in different fields
- Study of finite-size scaling of both transitions
- Improvement of efficiency

Gedruckt im Universitätsrechenzentrum Leipzig