Application of New Chain-Growth Algorithms for Lattice Polymers

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Abstract
We apply recently developed enhancements of the Pruned Enriched Rosebluth 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.


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 $W^{(m)}(E)$ in addition to the Rosenbluth and the Boltzmann weights. The partition sum according to the new distribution thus becomes

$$Z_{muca} = \sum_{\phi} W^{(m)}(E)$$

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

$$W^{(m)}(E) = \frac{W^{(m)}(E')}{Z_{muca}} \times \chi(E')$$

where $H_{\phi}(E)$ 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.

Coil-Globule Transition
With the presented algorithms one can study the coil-globule transition of homopolymers up to lengths of order $10^5$. The upper figure shows $\ln(C_{muca}^{(m)})$ (the ‘density of states’) for chains up to length $m=256$, 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.

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.

Crystalization
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 $10^4$ 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.

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

Check with Exact Results
Firstly we compare with exact results from enumeration. An example gives the figure: It shows the heat capacity of an homotetramer 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 $2 \times 10^6$ conformations, $5 \times 10^5$ are from independent growth starts.

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