Polymer-chains

Ludwig Rasmijn 4106644
Sebastiaan Lokhorst 4005058
Shang-Jen Wang 4215974

Abstract

Polymer-chains are simulated and a number of optimization are used to increase the length

1 Introduction

Rosenbluth algorithm and optimizations are used to simulate polymer-chains.

2 Methods

The polymer model is a self-avoiding walk in 2 dimensions, where each effective monomer is a fixed distance from the nearest neighbour. The interaction between the beads are modelled by the Lennard-Jones potential.

2.1 Rosenbluth algorithm

The Rosenbluth algorithm will avoid high-energy conformations, when adding new beads to the polymer. This will avoid any unprobable conformations. It does this by adding the next bead with a distribution $\exp(-E(\theta)/(k_BT))$, where $E(\theta)$ is the interaction energy of the new bead and θ is the angle between the new bead and the previous two beads. This model uses six evenly spaced $(2\pi/6)$ discrete angles with a random offset in which the new bead can be added to the polymer. The weight for each angle can be calculated by:

$$w_j^{(l)} = \exp(-E(\theta_j)/(k_BT)), \qquad (1)$$

where j is the number of the angle and l is the bead that is being added. The sum of all the weights can be expressed as:

$$W^{(l)} = \sum_j \exp(-E(\theta_j)/(k_BT)). \qquad (2)$$

So angle j is accepted with a probability $w_j^{(l)}/W^{(l)}$.

The polymer weight is given by:

$$\text{PolWeight} = \prod_l W^l. \qquad (3)$$

2.2 Pruned-enriched Rosenbluth method

A method which suppresses the high energy conformations better than the Rosenbluth method is the pruned-enriched Rosenbluth method (PERM) by Grassberger [**?**]. This method removes the configurations with a 'low' weight and replaces them with copies of configurations with a 'high' weight. Two thresholds UpLim and LowLim are used to define 'low' and 'high' weights. If at any polymer length the PolWeight > UpLim, then two members of this polymer are created when adding the next bead and each are given a PolWeight which half the PolWeight of the original polymer. This is called 'enriching'. If at any polymer length the PolWeight < LowLim, then the polymer will be removed with a probability of 1/2. If the polymer is not removed, then the PolWeight is multiplied by 2. This will make sure that the distribution does not change. This is called 'pruning'.
The choice of UpLim and LowLim depends on the average weight 'AvWeight' at step L. The average weight is updated for every polymer that reaches that length. UpLim and LowLim are expressed as a ratio of the average weight and the weight 'Weight3' corresponding to the shortest length (3 beads):

$$\text{UpLim} = \alpha \cdot \text{AvWeight}/\text{Weight3}, \qquad (4)$$

$$\text{LowLim} = \alpha \cdot \text{AvWeight}/\text{Weight3}. \qquad (5)$$

A good value for α for UpLim is 2 and for LowLim 1.2. It is possible that α is dependent on L, but this can be removed by multiplying the weight of the polymer by a constant at each step. This constant should be near $1/(0.75N_\theta)$, where N_θ is the number of angles.

References

[1] P. Grassberger, (1997)
Pruned-enriched Rosenbluth method: Simulation of θ polymers of chain length up to 1 000 000.
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