Overcoming critical slowing down

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Projects

Many of the original applications of Monte Carlo methods were done for systems of approxi- mately one hundred particles and lattices of order 322 spins. It would be instructive to redo many of these applications with much better statistics and with larger system sizes. In the fol- lowing, we discuss some additional recent developments, but we have omitted other important topics such as Brownian dynamics and umbrella sampling. More ideas for projects can be found in the references.

Critical slowing down

The large size of the correlated regions and the corresponding divergent behavior of the correlation lengthξ near T_c implies that the time τ required for a region to lose its coherence becomes very long if a local dynamics is used. At $T = T_c$, $\tau \approx L^z$ for $L \gg 1$. For single spin flip algorithms, $z \approx 2$ and τ becomes very large for $L \gg 1$. On a serial computer, the CPU time needed to obtain n configurations increases as L^2, the time needed to visit L^2 spins. However, the time needed to obtain n approximately independent configurations is of order $\tau L^2 \approx L^{2+z} \approx L^4$ for the Metropolis algorithm. We conclude that an increase of L by a factor of 10 requires 10^4 more computing time.

两种构型方式

1. 局域更新 (local update)，一次只随机翻转一个自旋，即

$$Q(\sigma \to \sigma') = \frac{1}{N} \sum_i \delta_{\sigma_i, -\sigma'_i}$$

2. 集团更新 (cluster update)，一次随机翻转一片区域的自旋，可以克服局域更新自相关 (autocorrelation) 时间在相变附近过长的问题。

Bond probability

We will argue in the following that these (and other) critical exponents are identical if we define the bond probability as

$$p = 1 - e^{-2J/KT} \tag{1}$$

Because we want the probability that a cluster is flipped to be unity, we need to have the probability of the two configurations and their corresponding clusters be the same. Hence, we must have

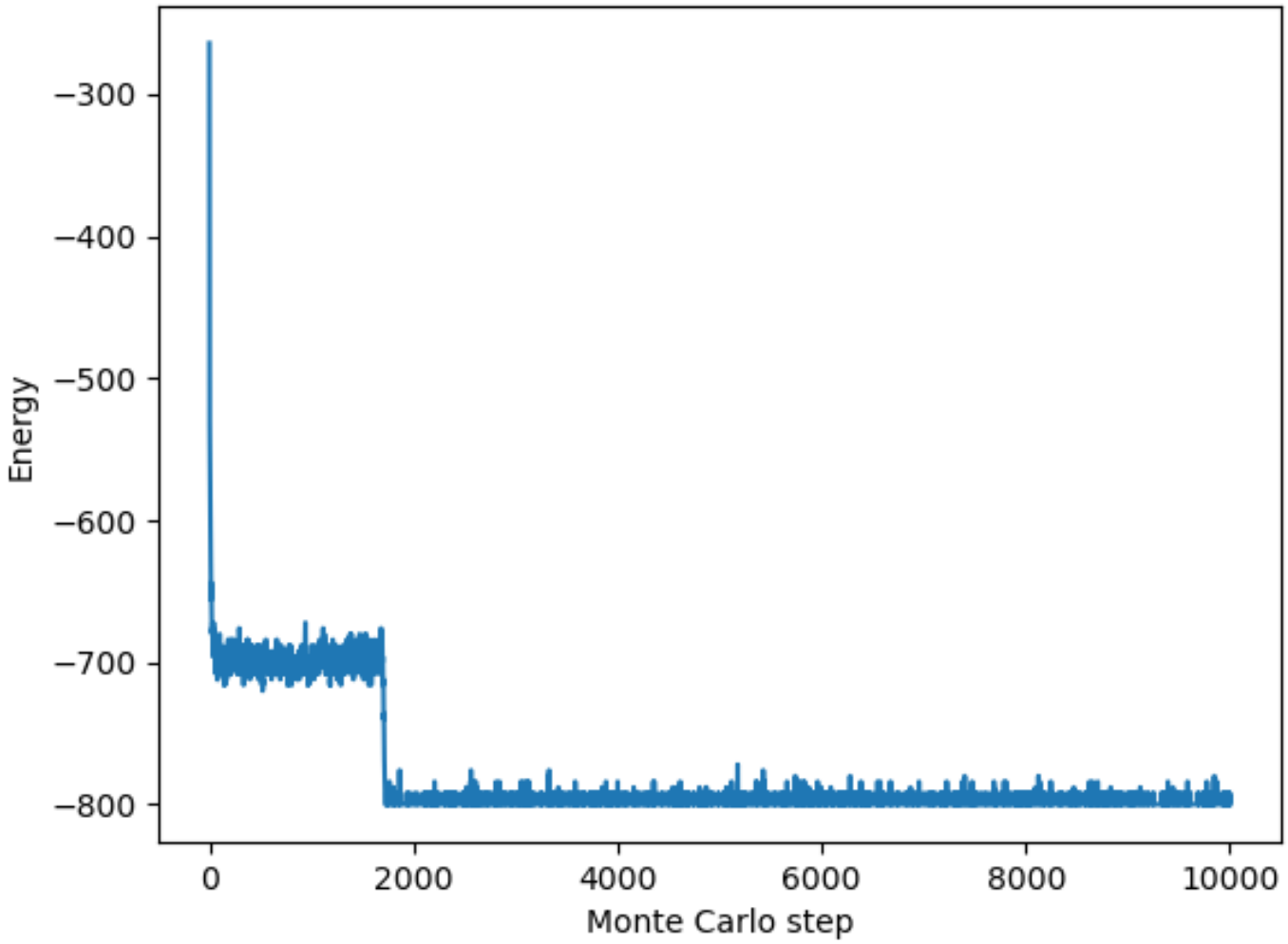
$$pe^{\beta J}e^{-6\beta J} = p\left(1-p\right)^{6} e^{\beta J}e^{6\beta J} \tag{2}$$

Steps

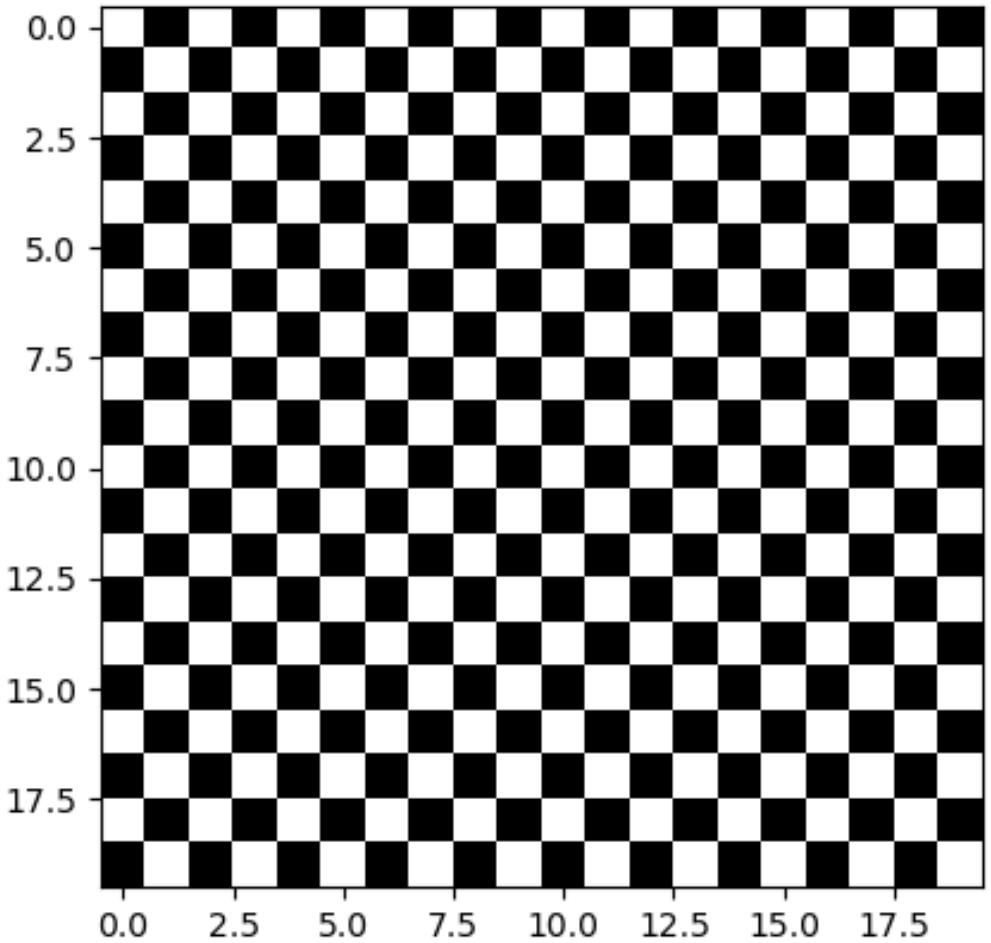
The algorithm can be im-plemented by the following steps:

1. Choose a seed spin at random. Its four nearest neighbor sites (on the square lattice) are the perimeter sites. Form an ordered array corresponding to the perimeter spins that are parallel to the seed spin and define a counter for the total number of perimeter spins.
2. Choose the first spin in the ordered perimeter array. Remove it from the array and replace it by the last spin in the array. Generate a random number r. If $r \leq p$, the bond exists between the two spins, and the perimeter spin is added to the cluster.
3. f the spin is added to the cluster, inspect its parallel perimeter spins. If any of these spins are not already a part of the cluster, add them to the end of the array of perimeter spins.
4. Repeat steps (2) and (3) until no perimeter spins remain.
5. Flip all the spins in the single cluster.

运行结果: Energy-Monte Carlo Step



运行结果: The Spin Configuration



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