The SAPBC Method on local, non-Cluster updates algorithms of Monte Carlo simulation: A study on more convergence of spin correlation at critical temperature.

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Abstract. In this method, we propose computational technique of Screw-Antisymmetric Periodic Boundary Condition (SAPBC Method) on local, non-cluster update algorithms of Isotropic square lattice Ising model of Monte Carlo simulations, as well. The SAPBC Method, actually, is an extended mixed method of Screw (helical) and Antisymmetric periodic boundary conditions beyond connection from of nearest neighbor spin of the main lattice to even far away block of the outer (foreign) neighbor spin arrays. Here, meanwhile of description of geometry exact details of method and way of spin interaction, have applied to critical slowing down in order to achieve more convergence of spin correlation at critical temperature. Actually, in general, at critical temperature algorithms performed by using SAPBC Method have faster correlation and much shorter autocorrelation time than algorithms performed by using PBC Method. We will also see that autocorrelation function for the typewriter Metropolis algorithm was found to be zero at high temperatures. For low temperatures it fell to zero and stayed there. The SAPBC Method also confirms and consists with the law of the spatial correlation length with its dynamical critical exponent. Therefore, it can be used as a trenchant method applied to boundary conditions of Monte Carlo simulation problems extending on a variety of other models such as XY-Pots-Heisenberg model and also cluster algorithms such as Wolf, Swendsen-Wangs, Hoshen-Koppelman as well.

1. Introduction

The dynamics of equilibrium or near equilibrium system is slow, at low temperatures. The Metropolis/Glauber dynamics is very slow when the system is close to a critical state. The Metropolis Monte Carlo method act very well in simulating the properties of the 2-D Ising model. However, close to the Curie temperature, the simulations suffer from critical slowing down. Therefore, algorithms that are more efficient are needed. The Metropolis algorithm is a local algorithm, i.e., one spin is tested and flipped at a time. Near critical temperature, the system develops large domains of correlated spins, which are difficult to break up. So the most likely change in configuration is the movement of a whole domain of spins. But one Metropolis sweep of the lattice can move a domain at most by approximately one lattice spacing in each time step. The advantage of this simple algorithm is its flexibility which allows the application to a great variety of physical systems. The great disadvantage, however, is that this algorithm is plagued by large autocorrelation times, as most other local update algorithms (one exception is the over-relaxation method [1]. Since correlation length diverges at criticality, the Metropolis algorithm thus severely suffers from critical slowing down. Because of that, the autocorrelation times become large near the critical temperature of the infinite system. Near the critical temperature, the relaxation time becomes large. It diverges for an infinite system. The correlation length also diverges at the critical temperature:
Which accounts for long range spin correlations as $T$ approaches $T_c$. Quantity is the relaxation time, which is the time scale over which the system approaches equilibrium. If $A(t)$ is a quantity which relaxes towards its equilibrium value $A$, the relaxation time can be theoretically as:

$$
\tau = \int_0^\infty dt [A(t) - \bar{A}] \\
\int_0^\infty dt [A(t) - \bar{A}]
$$

Near the critical temperature, the relaxation time becomes large. It diverges for an infinite system:

$$
\tau \approx \xi^z \approx \frac{1}{|T - T_c|^z} \quad (3)
$$

here $z$ is the dynamical critical exponent associated with the observable $A$. This phenomenon is called critical slowing down [2-8].

In the 2-D Ising system, the correlation length $\xi$ becomes very large. The correlation time $\tau$, which measures the number of steps between independent Monte Carlo configurations behaves like [9]:

$$
\tau \sim \xi^z \quad (4)
$$

The time autocorrelation function:

$$
c_{AA}(k) = \langle A_n - \langle A_n \rangle \rangle \langle A_{n+k} - \langle A_{n+k} \rangle \rangle = \langle A_n A_{n+k} \rangle - \langle A_n \rangle^2
$$

where $n$ labels the Monte Carlo time step. If Monte Carlo steps separated in time by $k$ intermediate steps are truly uncorrelated then, $c_{AA}(k)$ should be zero.

If the correlation function decays exponentially, we have [9]:

$$
C_{AA}(t) \approx e^{-t/\xi} \quad (6)
$$

Then, the exponential correlation time can be computed as the average:

$$
\tau_{exp} = \left \langle \frac{t}{\log \frac{C_{AA}(t)}{C_{AA}(0)}} \right \rangle \quad (7)
$$
If the decay is exponential then, we have:

\[
\int_0^\infty dt C_{AA}(t) = \int_0^\infty dt C_{AA}(0)e^{-t/\tau} = \frac{1}{\tau} C_{AA}(0) \quad (8)
\]

which is called the integrated correlation time. The formulas above suggest that it is useful to normalize the autocorrelation function by its value at \( t = 0 \):

\[
C_A(K) = \frac{C_{AA}(k)}{C_{AA}(0)} = \frac{\langle A_n A_{n+k} \rangle - \langle A_n \rangle^2}{\langle A^2 \rangle - \langle A \rangle^2} \quad (9)
\]

At the Curie temperature, some observables like the heat capacity per spin and magnetic susceptibility per spin become divergent (infinite) in the thermodynamic limit of an infinite system. These critical divergences are due to long range correlations between spins. Consider two spins, \( S_0 \) at the origin of coordinates and \( S_n \) at some other lattice site labeled by the index \( n \). The correlation between the pair of spins is defined to be \( \langle S_0 S_n \rangle \). If the two spins are uncorrelated then this average will be zero or very small. At \( T = 0 \), the spins are all lined up and so:

\[
\langle S_0 S_n \rangle = 1 \quad (10)
\]

However, this is a somewhat trivial correlation because flipping \( S_0 \) will hardly affect \( S_n \) if it is not a neighbour of \( S_0 \). Near critical temperature, the situation is very different as the spins are constantly changing, but not independently. There are large domains (droplets) of parallel spins, which persist for long periods. Thus, spins far apart from one another are strongly correlated. At high temperatures, the spins fluctuate rapidly but almost independently of other spins.

2. Definition of model and boundary condition

We consider the isotropic Ising model with \( J \) couple interaction [10-14]. They interact with foreign-neighbor of spins. The Hamiltonian reads:

\[
H = -J \sum_i \left( S_{mod(i+1,K\times L)} + S_{mod(i-1+K\times L, K\times L)} + S_{mod(i+K, K\times L)} + S_{mod(i-1+K\times L, K\times L)} \right) (11)
\]

where, \( S_i = \pm 1 \) is the spin at a site (x) and \( K=L \). In most cases, we take all couplings to be Positive, i.e., ferromagnetic. Comparison between different boundary condition has been done completely in ‘figures1-6’.

We perform interaction between spins according to Hamiltonian sentences for Ising model at different boundary conditions.
Figure 1. Application of typical boundary conditions for the two-dimensional Ising model: (left) periodic boundary, (center) screw periodic, (right) free edges [2-5].

\[ \mathcal{H} = -J(\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \ldots + \sigma_{N-1} \sigma_N) \]

Figure 2. A profile of interaction between spins according to Hamiltonian sentences in the free boundary condition (FBC method) [2-5].

\[ \mathcal{H} = -J(\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \ldots + \sigma_{N-1} \sigma_N + \sigma_N \sigma_1) \]

Figure 3. The illustration of interaction between spins according to Hamiltonian sentences in the periodic boundary condition (PBC method) in a one-dimensional array.

Figure 4. Representation of interaction array between spins with Screw(helical) periodic boundary condition (SPBC Method) for lattice with the size of \( N \times N \) in a one-dimensional array.
Figure 5. The illustration of interaction between spins with different boundary condition in a one-dimensional array with the size of 3*3. (a): The periodic boundary condition (PBC) method in a one-dimensional array with the size of 3*3 (b): Screw(helical) periodic boundary condition (SPBC) method in a one-dimensional array with the size of 3*3. (c): Screw (helical) periodic boundary condition (SPBC) method in a one-dimensional array with the size of 5*5.
Figure 6a. Sketch of the interactions in the anisotropic Ising model with $N=100$ of spins, which perform SAPBC simulation techniques, according to the first sentence of Hamiltonian in ‘equation 11’. Here, the last spin in the first row, instead of link with the first spin in the second row according to SPBC method, which performed in ‘figure1-b’, is connected with the last spin in the ninth row (L-1) with a screw-antisymmetric approach. The first spin in the first row also connects with a penultimate spin in the last row (L) on the main lattice (main block).

Figure 6b. Here, the first spin in the second row, instead of link with the last spin in the first row according to SPBC method, which performed in ‘figure1-b’, will be connected with the first spin in the tenth row (L) with a screw-antisymmetric approach. The second spin in the first row also will connect with the last spin in the last row (L) on the main lattice (the main block).
Figure 6c. The second spin in the second row connects with the second spin in the tenth row (L) with a screw-antisymmetric approach. The third spin in the first row will connect with the first spin of the first row of the foreign neighbor block of the lattice. The connection between spins will be removed from the core lattice (the main block). Then their interaction will easily be done with the first block of foreign neighbors.

Figure 6d. The third spin in the second row connects with the third spin in the tenth row (L) with a screw-antisymmetric approach. The fourth spin in the first row will connect with the second spin of
the first row of the foreign neighbor block of the lattice. Here, the connection between spins will be removed from the core lattice (the main block). Their interaction will then be done with the first block of foreign-neighbors.

3. Simulation and Results

Autocorrelation function has been measured through expected statistical quantities, which are done during the Monte Carlo algorithm process. In the method, we consider the autocorrelation function [5] as a division of statistical quantity at t th moment to its initial value. The trend of fluctuation of function is done with the method of Screw anti-symmetric periodic boundary condition (SAPBC Method). Spins are placed on a two-dimensional lattice. The number of 1000000 loops of Monte Carlo is used in this experiment. In the ‘figure 8’, autocorrelation function versus time has been done for different algorithms by using PBC Method. Clearly, the Metropolis update with typewriter ordering is the fastest of these algorithms (See ‘table 1-2’). The autocorrelation function for the Metropolis algorithm using SAPBC method is shown in the ‘figure 8’.

According to the ‘equation 9’, we describe the autocorrelation function as the quantity of \( \frac{A_t}{A_0} \) (as \( A_t \) is actually the value of the susceptibility in the t th of Markov point) for 500 consecutive Markov points with sizes of \( L = 10, 50, 60, 90 \). As the size of lattice increases, correlation function increased proportionally. Autocorrelation time become loner, too. This is due to the fact that autocorrelation time grows proportional to the spatial correlation length. Critical exponent is approximately \( z \approx 2 \) [9].

![Figure 7](image.png)

**Figure 7.** The comparison of autocorrelation function versus time for different algorithm by using PBC Method.
Figure 8. The autocorrelation function for Metropolis algorithm at critical temperature $T = 2.28KT$ for various lattice $L = 10, 50, 60, 90$ by using SAPBC Method on 500 Markov Points.

In general, algorithms performed by using SAPBC Method have faster correlation than algorithms performed by using PBC Method, ‘figures 7-8’. The SAPBC Method also confirms the law of the spatial correlation length with its dynamical critical exponent (See ‘figures 7-10’ and ‘table 2’). In ‘figures 7-10’, there has been done a relatively good comparison between autocorrelation function variations based on Markov Points in three different temperature category: ($T=0.5KT$, $T=2.28KT$, $T=10KT$) by SAPBC Method.

By looking at the figures, we completely realize that in the critical temperature ($T=2.28KT$) the correlation has decreased exponentially, that is expected by ‘equation 5’ and ‘equation 6’ by SAPBC Method. In the temperatures phase $T=0.5KT$ (low temperature) and $T=10KT$ (high temperature), the trend of correlation is completely different (See ‘figures 9-10’).

In ‘figure 9’, the autocorrelation function for the Metropolis algorithm at low temperature ($T=0.5$) performed by SAPBC Method satisfying ‘equation 9’ is done as well. Here, we also can see a similar situation in the correlation between spins, as there is a sudden fall in the correlation of data because of reducing the distance between points and then with the increase in time remained uncorrelated. For high temperature ($T=10$) only the first few data points were correlated and the rest were uncorrelated with their autocorrelation function fluctuating randomly about zero what has been done in PBC Method too (see ‘figure 9’ and ‘figure 10’).

In ‘figure 10’, there is a comparison of fluctuation of autocorrelation function at different temperature (high temperature, critical temperature and low temperature). We can easily see that autocorrelation function has the correlation at critical temperature with slow down trend between points. Both methods (PBC and SAPBC) have similar results on the issue that autocorrelation function for the Metropolis algorithm was found to be zero at high temperatures. For low temperatures, it fell to zero and stayed there.
Figure 9. The graph of autocorrelation function variations based on 600 Markov Points in different temperatures $T = 0.5KT$ (Low Temperature), $T=10KT$ (High Temperature) by SAPBC method.

Figure 10. The autocorrelation function for the Metropolis algorithm at different temperature phase by SAPBC method.

In ‘table1’, there are the measurement of integrated correlation time ($\tau_{int}$) between different algorithms such as Metropolis and heat bath algorithm with typewriter ordering and random ordering on 600 of Markov Points. It is done for $L=64$ with PBC Method. One can see from ‘table1’, the time autocorrelation of Metro-typew is shorter than other algorithms.
Table 1. There is the measurement of integrated correlation time ($\tau_{\text{int}}$) between different algorithms such as Metropolis and heat bath algorithm with typewriter ordering and random ordering on 500 of Markov Points for $L=64$ with PBC Method. As it is seen, the time autocorrelation of Metro, typew is shorter than other algorithms, specifically.

| For 500 of Markov Points with PBC $L=64$ | Different Algorithms | Metro, typew | HB, typew | Metro, random | HB, random |
|----------------------------------------|---------------------|-------------|-----------|--------------|------------|
| $\tau_{\text{int}}$                   | 54                  | 157         | 271       | 316           |            |

In ‘table 2’, we have calculated integrated correlation time for several Markov Points and the different size of lattice on Importance Sampling Metropolis algorithm with typewriter ordering by SAPBC Method [5], according to equation below:

$$\tau_{\text{int}} = \frac{1}{2} \sum_{i=1}^{M} C(t) \quad (12) [5].$$

As the length of lattice increase, the integrated correlation time will be longer for all of Markov Points. We perform the method on the Importance Sampling local, Non-cluster Metropolis algorithm of a square lattice with typewriter method. We measure autocorrelation time for several Markov points according to data on the ‘table2’. By comparison between ‘tables1-2’, we will see that SAPBC Method has a much shorter time than the PBC Method.

Table 2. Calculation of integrated correlation time for several Markov Points and various sizes on Importance Sampling Metropolis algorithm with typewriter ordering by SAPBC method is performed. By comparison between ‘tables1-2’, we will see the SAPBC Method has a much shorter time than the PBC method.

| L=10         | L=50         | L=60         | L=90         |
|-------------|--------------|--------------|--------------|
| Integrated correlation time ($\tau_{\text{int}}$) for 200 of Markov Points with SAPBC method | 20.01252581  | 32.21603988  | 35.68318808  | 38.46125807 |
| Integrated correlation time ($\tau_{\text{int}}$) for 300 of Markov Points with SAPBC method | 20.72135409  | 31.4260469   | 35.69518504  | 41.94682875 |
| Integrated correlation time ($\tau_{\text{int}}$) for 400 of Markov Points with SAPBC method | 19.58417429  | 29.5525833   | 34.67845486  | 44.11686418 |
Integrated correlation time (\(\tau_{int}\)) for 500 of Markov Points with SAPBC method

|                | 16.13552043 | 26.72262622 | 35.07733829 | 45.15720244 |
|----------------|-------------|-------------|-------------|-------------|

Integrated correlation time (\(\tau_{int}\)) for 600 of Markov Points with SAPBC method

|                | 16.01292042 | 22.14786839 | 35.33316382 | 45.2833748  |

4. Conclusions

Here, for overcome to critical slowing down and reach to the shorter autocorrelation time and a faster correlation between spins, the SAPBC Method (computational technique of Screw-Antisymmetric Periodic Boundary condition on local, non-cluster update algorithms of Isotropic square lattice Ising model of Monte Carlo Simulations is applied. We realized that algorithms performed by using the SAPBC Method have faster correlation and shorter autocorrelation time than algorithms performed by the PBC Method. More convergence of spin correlation at critical temperature obtained by the new method. The SAPBC Method also confirmed the law of the spatial correlation length with its dynamical critical exponent [10]. It can be used as a method applied to boundary conditions of Monte Carlo simulation problems extending on a variety of other models such as XY model, Heisenberg model and also cluster algorithms such as Wolf and Swendsen-Wang [15,16].

5. References

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