Local, Cluster, and Transitional Monte Carlo Dynamics*

Jian-Sheng Wang

Department of Computational Science, National University of Singapore, Singapore 119260

(15 July 1998)

We review the local Monte Carlo dynamics and Swendsen-Wang cluster algorithm. We introduce and analyze a new Monte Carlo dynamics known as transitional Monte Carlo. The transitional Monte Carlo algorithm samples energy probability distribution \( P(E) \) with a transition matrix obtained from single-spin-flip dynamics. We analyze the relaxation dynamics master equation,

\[
\frac{dP(E,t)}{dt} = \sum_{E'} T(E,E')P(E',t),
\]

associated with Ising model in \( d \) dimensions. In one dimension, we obtain an exact solution. We show in all dimensions in the continuum limit the dynamics is governed by the partial differential equation

\[
\frac{\partial P}{\partial t'} = \frac{\partial^2 P}{\partial x^2} + x \frac{\partial P}{\partial x} + P.
\]

where \( x \) and \( t' \) are rescaled energy deviation from the equilibrium value and rescaled time, respectively. This equation is readily solved. Thus, we have a complete understanding of the dynamics.

I. MONTE CARLO METHOD

Monte Carlo method \cite{1} in the most basic application is to perform numerical integration of very high dimensional integrals or to compute averages of a given probability distribution. In this respect, the method generates a sequence of states \( X_0, X_1, X_2, \ldots \), by a transition probability \( T(X \rightarrow X') = P(X'|X) \). This is also known as Markov chain Monte Carlo in the statistics community. The state \( X \) can be the set of all the coordinates of the particles in a fluid systems, or the values of spins at lattice points for a classical spin system. The new state \( X' \) is generated according to probability \( P(X'|X) \) given that the previous state is \( X \). \( P(X'|X) \) is usually a simple distribution which can be sampled directly.

We have a lot of freedom in choosing the transition probability \( T(X \rightarrow X') \). If we want that the distribution of \( X \) of the generated sequence follows \( P_{eq}(X) \), it is sufficient to require that

\[
P_{eq}(X) T(X \rightarrow X') = P_{eq}(X') T(X' \rightarrow X).
\]

This is known as detailed balance condition. Subject to some general constraints of ergodicity which can be satisfied easily, the state \( X \) has the unique equilibrium distribution in the large step limit.

Well-known application of Monte Carlo method is to generate Boltzmann distribution \( e^{-H/k_B T}/Z \) in statistical mechanics by Metropolis algorithm, where the transition probability is chosen as

---

*Talk presented at the “98 Workshop on Computational Material Science and Biology”, 8-12, June 1998, Beijing.
\[ T(X \to X') = W(X \to X') \min \left( 1, \frac{P_{eq}(X')}{P_{eq}(X)} \right), \quad X \neq X', \quad (2) \]

where \( W(X \to X') = W(X' \to X) \) is the probability of proposing \( X' \) as the next state given that the current state is \( X \). The next factor \( \min(\cdots) \) is the probability that such a move is accepted.

Averages of thermodynamic variables are computed according to

\[ \langle A \rangle = \sum_X A(X) P_{eq}(X) \approx \frac{1}{M} \sum_{i=1}^{M} A(X_i). \quad (3) \]

The weighted sum (or integral) is replaced by an arithmetic average.

Monte Carlo method is intrinsically an approximate method. Error in Monte Carlo evaluation can be estimated from

\[ \delta A \approx \frac{\sigma_A}{\sqrt{M/\tau}}, \quad (4) \]

where \( \sigma_A^2 \) is the variance of distribution of \( A \), and \( \tau \) is called correlation time. The value \( \tau \geq 1 \) is more precisely defined by so-called integrated correlation time. But in many cases it is equivalent to the exponential correlation time defined by the equation:

\[ \langle A(t_0) A(t_0 + t) \rangle - \langle A(t_0) \rangle^2 \propto e^{-t/\tau}. \quad (5) \]

The exponential correlation time \( \tau \) also characterizes the speed at which arbitrary initial probability distribution \( P(X) \) converges to \( P_{eq}(X) \):

\[ P(X, t) \approx P_{eq}(X) + P_1(X) e^{-t/\tau} + \cdots. \quad (6) \]

II. SOME MONTE CARLO DYNAMICS

The above theory is quite general. We give some more concrete examples and points out some interesting Monte Carlo dynamics.

A. Single-spin-flip Glauber dynamics

We consider a simple classical spin model, the Ising model, as an example of local Monte Carlo dynamics. The model is defined by the energy function

\[ H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad \sigma_i = \pm 1. \quad (7) \]

The spins take only two possible values and live on the sites of a lattice, for example on a square lattice. The total energy is a sum of interactions between nearest-neighbor sites. A Monte Carlo move consists of picking a site at random, and flipping the spin with probability

\[ w = \frac{1}{2} \left[ 1 - \sigma_0 \tanh \left( \frac{J}{k_B T} \sum_i \sigma_i \right) \right], \quad (8) \]
where $\sigma_0$ is the spin value before the flip, and $\sum_i \sigma_i$ is the sum of spins of the nearest neighbors. Another popular choice is the Metropolis rate $\min\{1, \exp(-\Delta H/k_B T)\}$ where $\Delta H$ is the energy increase due to flip. In a computer implementation, the value $w$ is compared with a uniformly distributed random number $r$ between 0 and 1. If $r < w$ the flip is performed; otherwise, the old configuration is retained and is also counted as one Monte Carlo move. One Monte Carlo step is a unit (Monte Carlo) time, and is usually defined as $N$ Monte Carlo moves, where $N$ is the number of spins of the system.

The local Monte Carlo dynamics has some common features: (1) the algorithm is extremely general. It can be applied to any classical model. (2) Each move involves $O(1)$ operation and $O(1)$ degrees of freedom. (3) At the second-order phase transition critical point, the dynamics becomes very slow. This is known as dynamical critical slowing down, characterized by the fact that

$$\tau \propto \xi^z, \quad z \approx 2.$$  \hspace{1cm} (9)

where $\xi \propto |T - T_c|^{-\nu}$ is called correlation length which will diverge at the critical point. On finite system, $\xi$ is replaced by the system linear size $L$. The value $z$ is the dynamical critical exponent. Its value is slightly greater than 2 for a large class of models with order-parameter nonconserving dynamics, such as the single-spin-flip dynamics discussed above [4].

This last feature hampers the effective use of local Monte Carlo algorithms. It is the nonlocal algorithms that come to rescue.

**B. Nonlocal dynamics — cluster algorithms**

Swendsen-Wang algorithm [5,6] is one of the first nonlocal Monte Carlo algorithms which have very different dynamical characteristics. The algorithm uses a mapping from Ising model to a type of percolation model. Each Monte Carlo step consists of putting a bond with probability

$$p(\sigma_i, \sigma_j) = 1 - \exp(-J(\sigma_i \sigma_j + 1)/k_B T)$$ \hspace{1cm} (10)

between each pair of the nearest neighbors. By ignoring the spins and looking only at the bonds, we obtain a percolation configuration of bonds [8]. A new spin configuration is obtained by assigning to each cluster, including isolated sites, a random sign $+1$ or $-1$ with equal probability.

In the Swendsen-Wang algorithm, we generated many clusters and then flipped these clusters. Wolff algorithm [7] is a variation on the way clusters are flipped. One picks a site at random, and then generates one single cluster by growing a cluster from the seed. The neighbors of the seed site will also belong to the cluster if the spins are in parallel and a random number is less than $p = 1 - e^{-2J/k_B T}$. That is, the neighboring site will be in the same cluster as the seed site with probability $p$ if the spins have the same sign. If the spins are different, neighboring site will never belong to the cluster. Neighbors of each new site in the cluster are tested for membership. This testing of membership is performed on pair of sites (forming a nearest neighbor bond) not more than once. The recursive process will eventually terminate. The spins in the cluster are turned over with probability $1$.

The following is a fairly elegant way of implementing the Wolff algorithm in C. The function is the core part which performs a Wolff single cluster flip. This function is recursive. The array for spins $s[]$, percolation probability $P$, and coordination number $Z$ (the number of neighbors) are passed globally. The first argument $i$ of the flip function is the site to be flipped, the second argument $s0$ is the spin of the cluster before flipping. The function neighbor returns an array of neighbors of the current site. The function drand48() returns a random number uniformly distributed between 0 and 1.
void flip(int i, int s0)
{
    int j, nn[Z];
    s[i] = - s0;  // flip the spin immediately
    neighbor(i, nn);  // find nearest neighbor of i
    for(j = 0; j < Z; ++j)
        if(s0 == s[nn[j]] && drand48() < P)  // spins are equal and
            random number is smaller than p
            flip(nn[j], s0);
}

Some of the salient features of cluster algorithms: (1) algorithm is applicable to models containing Ising symmetry. (2) Computational complexity is still of $O(1)$ per spin per Monte Carlo step. (3) Much reduced critical slowing down, i.e., $\tau \propto \xi^{z_{sw}}$. The dynamical critical exponent $z_{sw}$ is 0, 0.3, 0.5, 1, in dimensions 1, 2, 3, and greater or equal to 4, respectively. In addition, Li and Sokal [9] showed that $\tau \geq ac$ for some constant $a$, and $c$ is the specific heat. For some of the latest developments on nonlocal algorithms, see [10–13].

III. TRANSITIONAL MONTE CARLO DYNAMICS

The transitional Monte Carlo dynamics [14] is a new dynamics with the following interesting features: (1) It is a constrained random walk in energy space. (2) The transitional rates are derived from single-spin-flip dynamics. (3) It has a fast dynamics, $\tau \propto c$, and (4) it suggests a different histogram reweighting method.

A. What is transitional Monte Carlo

The transitional Monte Carlo is related to the single-spin-flip dynamics in the following sense but it has a totally different dynamics. A single-spin-flip Glauber dynamics of the Ising model is described by

$$\frac{\partial P(\sigma, t)}{\partial t} = \sum_{\sigma'} \Gamma(\sigma, \sigma') P(\sigma', t)$$

$$= \sum_{i=1}^{N} \left[ -w_i(\sigma_i) + w_i(-\sigma_i) F_i \right] P(\sigma, t), \quad (11)$$

where $N$ is the total number of spins, and $w$ is given by Eq. (8), and $F_i$ is a flip operator such that $F_i P(\ldots, \sigma_i, \ldots) = P(\ldots, -\sigma_i, \ldots)$. Transitional Monte Carlo dynamics is defined by

$$\frac{dP(E, t)}{dt} = \sum_{E'} T(E, E') P(E', t), \quad (12)$$

where $P(E, t)$ is the probability of having energy $E$ at time $t$, and

$$T(E, E') = \frac{1}{n(E')} \sum_{H(\sigma)=E} \sum_{H(\sigma')=E'} \Gamma(\sigma, \sigma'), \quad (13)$$

where $n(E)$ is the degeneracy of the states. We can not derive Eq. (12) from Eq. (11) in general, the “derivation” is valid only at equilibrium when $P(E) = \sum_{H(\sigma)=E} P(\sigma) = n(E) \exp(-E/k_B T)$. 

4
The transition matrix $T(E, E')$ has some general properties: (1) The matrix is banded alone the diagonal. (2) The column sum is zero, $\sum_E T(E, E') = 0$, due to the conservation of total probability. (3) $\sum_{E'} T(E, E') P_{eq}(E') = 0$, due to existence of equilibrium distribution. (4) The transition rate satisfies detailed balance condition, $T(E', E) P_{eq}(E) = T(E, E') P_{eq}(E')$.

The eigenvalues of $T(E, E')$ are real and $\lambda_k \leq 0$. The significance of the eigenspectrum $\lambda_k$ is that the general solution of the master equation can be written as $P(E, t) = \sum_k a_k(E) \exp(\lambda_k t)$.

B. Computer realization of transitional Monte Carlo and reweighting techniques

The transitional Monte Carlo dynamics can be implemented on computer in at least two different ways, we’ll call them algorithm A and B.

Algorithm A

1. Do sufficient number of constant energy (microcanonical) Monte Carlo steps, so that the final configuration is totally uncorrelated with the initial configuration. This step is equivalent to pick a state $\sigma$ at random from all states with energy $E$.

2. Do one canonical Monte Carlo move by picking a site at random.

Clearly, this algorithm is not very efficient computationally, due to step 1. However, it will be helpful in understanding the dynamics.

Algorithm B

- A direct implementation of the master Eq. (12), i.e., a random walk in energy with a transition rate $T(E, E')$.

Other possibility is to solve the equation on computer. Then in this method and algorithm B, we need to know $T(E, E')$ explicitly, this can be done numerically by Monte Carlo sampling, from

$$T(E + \Delta E, E) = w(\Delta E) \langle N(\sigma, \Delta E) \rangle_{H(\sigma)=E}$$

and $w(\Delta E) = \frac{1}{2} (1 - \tanh(\Delta E/(2k_B T)))$. $N(\sigma, \Delta E)$ is the number of cases that energy is changed by $\Delta E$ from $E$ for the $N$ possible single-spin flips.

Note that computation of $\langle N(\sigma, \Delta E) \rangle_{H(\sigma)=E}$ can be done with any sampling technique which ensures equal probability for equal energy. It is a kind of “combinatorial” number independent of the spin flip rates and in particular, independent of the temperature. Thus the transition matrix can be formed with any temperature. The equilibrium distribution and thus the density of states $n(E) = P_{eq}(E) \exp(E/k_B T)$ is obtained by solving

$$\sum_{E'} T(E, E') P_{eq}(E') = 0.$$  

The above scheme is similar in spirit to the histogram method of Ferrenberg and Swendsen [15], and the method has a close connection with, but different from the broad histogram of Oliveira et al [16].
C. Exact results in transitional Monte Carlo dynamics

We have more or less a complete understanding of the transitional Monte Carlo dynamics through exact results in limiting cases. The transition matrix $T(E, E')$ can be computed exactly in one-dimensional chain of length $L$ (with periodic boundary condition), by some combinatorial consideration, as

$$T_{k,k+1} = \frac{(k+1)(2k+1)}{L-1}(1+\gamma), \quad (16)$$

$$T_{k+1,k} = \frac{(L-2k)(L-2k-1)}{2(L-1)}(1-\gamma), \quad (17)$$

where $\gamma = \tanh(2J/k_BT)$. The diagonal term is computed from the relation

$$T_{k-1,k} + T_{k,k} + T_{k+1,k} = 0, \quad (18)$$

and the rest of the elements $T_{k,k'} = 0$ if $|k-k'| > 1$. The integer $k = 0, 1, 2, \ldots, \lfloor L/2 \rfloor$ is related to energy by $E = -LJ + 4k$. While the eigen spectrum at temperature $T = 0$ can be computed exactly as $\lambda_k = -2(k+1)(2k+1)/(L-1)$, the eigenvalues at $T > 0$ is obtained only numerically. The most important feature is that $\tau \propto L^z$, given an unusual dynamical critical exponent of $z = 1$.

The dynamics in any dimensions in the large size limit obeys a linear Fokker-Planck equation:

$$\frac{\partial P(x, t')}{\partial t'} = \frac{\partial}{\partial x} \left( \frac{\partial P(x, t')}{\partial x} + xP(x, t') \right), \quad (19)$$

where $t'$ and $x$ are properly scaled time and energy.

$$x = \frac{E - u_0 N}{(Nc')^{1/2}}, \quad u_0 N = \bar{E}, \quad (20)$$

and $t' = bt$ with

$$b = \lim_{N \to \infty} \frac{1}{2c'N} \sum_{E'} T(\bar{E}, E')(E'-\bar{E})^2, \quad (21)$$

where $u_0$ is the average energy per spin and $c' = k_BT^2c$ is the reduced specific heat per spin. The major consequence of this result is that the relaxation times are $\tau_n = ac'/n$, $n = 1, 2, 3, \ldots$, with some constant $a$.

We can cast the equation in the form of a continuity equation,

$$\frac{\partial P}{\partial t} + \frac{\partial j}{\partial x} = 0, \quad \text{with} \quad j = -\frac{\partial P}{\partial x} - xP. \quad (22)$$

There are two competing effects in the current; $-\partial P/\partial x$ is the usual diffusion, while $-xP$ is a counter drift. $j = 0$ produces the equilibrium distribution $P_{eq}(x) \propto \exp(-x^2/2)$.

With a change of variable $P(x, t') = \exp(-x^2/4)\Phi(x, t')$, the Eq. (19) is transformed into a one-dimensional quantum harmonic oscillator equation, with a general solution of the form

$$\sum_{n=0}^{\infty} c_n \exp(-nbt - x^2/2)H_n(x/\sqrt{2}), \quad (23)$$
where \( H_n \) is Hermite polynomials.

We sketch the derivation of the continuum limit equation, which is known as Ω expansion [17]. Starting from the master equation, Eq. (12), we introduce the new variable \( x \) which describes the scaled deviations from equilibrium,

\[
E = \bar{E} + \delta E = u_0 N + x (Nc')^{1/2}. \tag{24}
\]

The function \( P(E, t) \) is written in terms of \( x \), and \( P(E', t) \to P(x + \delta x, t) = P(x, t) + \frac{\partial P}{\partial x} \delta x + \frac{1}{2} \frac{\partial^2 P}{\partial x^2} \delta x^2 + \cdots \). For the matrix \( T(E, E') \), we assume that the changes along the diagonal are smooth and can be expanded, but across diagonals the changes are still discrete. For \( T(E, E') \) we also expand around \( x = 0 \); we can show that such an expansion is also an expansion in power of \( N^{-1/2} \). Expanding all the relevant terms in powers of \( N^{-1/2} \), the leading terms of order \( N^0 \) give the desired equation. The rest of the correction terms go to zero in the large size limit \( N \to \infty \). We used some of the general properties of \( T(E, E') \) to simplify the equation.

D. Simple pictures of the dynamics

The exact results can be interpreted with intuitive pictures. First, we consider the result of \( \tau \propto L \) in one dimension as \( T \to 0 \). At sufficiently low temperatures with a correlation length \( \xi \) comparable with the system size \( L \), only the ground state (all spins up or down) and the first excited states (with a kink pair) are important. Let’s consider the time scale for \( E_0 \to E_1 \), a spin with opposite sign is created with probability \( \exp(-4K) \) from Boltzmann weight, where \( K = J/(k_B T) \), in each of the canonical move. Thus

\[
\tau \propto \exp(4K) \frac{1}{L} \propto \frac{\xi^2}{L} \propto L. \tag{25}
\]

where \( K \) is chosen such that there is about one kink pair, so that \( \xi \sim \exp(2K) \sim L \).

The reverse process, \( E_1 \to E_0 \) has also the same time scale. In this case, it is advantageous to use the equivalence of Algorithm A and B. Given that the system is in the state of kink pair (a string of up spins followed by a string of down spins, with periodic boundary condition), the first step of Algorithm A randomizes the locations of the kinks. The probability that two kinks are the nearest neighbors is \( 1/L \); the probability that this pair is chosen and destroyed by a spin flip is \( 1/L \). Thus, the transitional Monte Carlo moves needed to destroy a kink pair are \( 1/((1/L)(1/L)) = L^2 \). The time in terms of Monte Carlo step is then \( \tau \propto L^2/L = L \).

Similarly, the result of \( \tau \propto c \) can be obtained by the following argument. The transitional Monte Carlo is a random walk constrained in the range \( \delta E \), due to the gaussian distribution nature of the equilibrium distribution \( P_{eq}(E) \). The width of this distribution is related to the specific heat by \( \delta E^2 = cN k_B T^2 \). Each walk changes \( E \) by \( O(1) \). To change \( E \) by \( \delta E \), we need \( \delta E^2 \) moves, invoking the theory on random walks. In units of transitional Monte Carlo steps,

\[
\tau \approx a \frac{\delta E^2}{N} \propto c. \tag{26}
\]

ACKNOWLEDGEMENTS

Part of the work presented in this talk is in collaboration with Tay Tien Kiat and Robert H. Swendsen. This work is supported in part by a NUS Faculty Research Grant PR950601.
[1] M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods*, (John Wiley & Sons, New York, 1986).
[2] K. Binder, (ed), *Monte Carlo Methods in Statistical Physics*, Topics Curr Phys. Vol 7, 2nd ed, (Springer, Berlin, 1986); *Applications of the Monte Carlo Method in Statistical Physics*, Topics Curr Phys. Vol 36, 2nd ed. (Springer, Berlin, 1987).
[3] R. J. Glauber, J. Math. Phys. 4, 294 (1963).
[4] J.-S. Wang and C. K. Gan, Phys. Rev. E. 57, 6548 (1998).
[5] R. H. Swendsen and J.-S. Wang, Phys. Rev. Lett. 58, 86 (1987).
[6] R. H. Swendsen, J.-S. Wang, and A. M. Ferrenberg, in *The Monte Carlo Method in Condensed Matter Physics*, ed. K. Binder, (Springer, Berlin), Topics in Applied Physics Vol 71 p. 75, (1992).
[7] U. Wolff, Phys. Rev. Lett. 62, 361 (1989).
[8] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, (Taylor & Francis, London, 1992).
[9] X.-J. Li and A. D. Sokal, Phys. Rev. Lett. 63 827 (1989); Phys. Rev. Lett. 67, 1482 (1991).
[10] H. G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett., 70, 875 (1993).
[11] C. Dress and W. Krauth, J. Phys. A. Math. Gen. 28 L597 (1995).
[12] J. Machta, Y. S. Choi, A. Lucke, T. Schweizer, and L. V. Chayes, Phys. Rev. Lett. 75, 2792 (1995).
[13] B. B. Beard and U. J. Wiese, Phys. Rev. Lett. 77, 5130 (1996).
[14] J.-S. Wang, T. K. Tay, and R. H. Swendsen, in preparation (1998).
[15] A. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. 61 2635 (1988); 63, 1195 (1989).
[16] P. M. C. de Oliveira, T. J. P. Penna, and H. J. Herrmann, Eur. Phys. J., B1, 205 (1998); Braz. J. Phys. 26, 677 (1996).
[17] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, (Horth-Holland, Amsterdam), (1981).