Application of the exchange Monte Carlo method to ordering dynamics

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Abstract. We have applied the exchange Monte Carlo method to the ordering dynamics of the three-state Potts model with conserved order parameter. Even for the deeply quenched case to low temperatures, we have observed a rapid domain growth; we have proved the efficiency of the exchange Monte Carlo method for the ordering process. The late-stage growth law has been found to be \( R(t) \sim t^{1/3} \) for the case of the conserved order parameter of a three-component system.

The ordering dynamics in spinodal decomposition has attracted a lot of attention [1]. It is considered that the domain-size growth in the late stage is governed by an algebraic law, \( R(t) \sim t^n \). The classical Lifshitz–Slyozov theory [2] gives the growth exponent \( n = 1/3 \) in the case of the spinodal decomposition of the conserved order parameter. On the other hand, the late-stage ordering process of the nonconserved order parameter is described by the classical Lifshitz–Allen–Chan law, \( n = 1/2 \) [3,4]. Although there has been controversy about the value of the growth exponent \( n \), especially for the conserved order parameter case, recent studies [5,6] have revealed that those growth exponents are universal, that is, they do not depend on the space dimensionality or the number of the components of the order parameter.

In simulative studies of the ordering process of phase separation we often encounter the problem of slow dynamics, which is found in a wide range of problems in computer simulation. Other examples are the critical slowing down near the critical point and slow dynamics due to randomness or frustration. There have been several attempts to overcome slow dynamics in the Monte Carlo (MC) simulation. We may classify these attempts into two categories. The first is the cluster algorithm, such as that of Swendsen–Wang [7] and of Wolff [8]. The other is the extended ensemble method. The multi-canonical method [9], simulated tempering [10] and the exchange MC method [11] are examples of the second category. The exchange MC method has been successfully applied to the problem of spin glasses [11,12].

Usually it is considered that the extended ensemble method can be used only for static problems because the extended ensemble affects the dynamics. Is this always so? In this paper, we apply the exchange MC method [11], which treats the exchange of replicas with different
temperatures, to the ordering problem, and test if we can describe the ordering dynamics by 
using the exchange MC method. We pay attention to the fact that the ordering phenomena after 
quenching are controlled by a zero-temperature fixed point, in the language of the renormalization 
group, irrespective of quenched temperature below the critical temperature, $T_c$. We also note 
that, in the case of algebraic growth, the composite of the growth law of different temperatures 
may become an algebraic one again in the leading order, which will be discussed later.

As a model system, we pick up the three-component system of the conserved order 
parameter. The reason is as follows. The ordering dynamics of the three-component system 
(three-state Potts model) is slower compared to the two-component system (Ising model) and, 
moreover, the temporal growth of the conserved order parameter is slower than that of the 
nonconserved order parameter [5, 6]. Since it is a difficult job to determine the late-stage growth 
law of the conserved order parameter due to the slow dynamics, the three-component system of 
the conserved order parameter is suitable for testing the efficiency of the exchange MC method. 

We perform the MC simulation of the three-state ferromagnetic Potts model [13, 14] on the 
square lattice, whose Hamiltonian is given by

$$
H = -J \sum_{<i,j>} \delta(S_i, S_j),
$$

(1)

where $S_j$ takes one of the three states, say, $a, b$ and $c$. For the spin-update of the MC simulation, 
we employ the Kawasaki dynamics of nearest-neighbour pair exchange because we are treating 
the conserved order parameter.

Here, we briefly review the exchange MC method [11]. We treat a compound system which 
consists of $M$ replicas of the system. The $m$th replica is associated with the inverse temperature 
$\beta_m$. We consider the extended ensemble, which is denoted by $\{X\} = \{X_1, X_2, \ldots X_M\}$. Then, 
the partition function of the compound system is given by

$$
Z = \text{Tr}(X) \exp \left( -\sum_{m=1}^{M} \beta_m H(X_m) \right).
$$

(2)

To obtain an equilibrium distribution of all the replicas, a replica exchange update process 
is introduced. By considering the detailed balance condition, the transition probability of 
exchanging the $i$th replica and the $j$th replica may be chosen as

$$
W(\{X_i, \beta_i; X_j, \beta_j\} \rightarrow \{X_i, \beta_j; X_j, \beta_i\}) = \begin{cases} 
1 & (\Delta \leq 0) \\
e^{-\Delta} & (\Delta > 0)
\end{cases}
$$

(3)

where

$$
\Delta = -(\beta_i - \beta_j)(H_i - H_j).
$$

(4)

It should be noted that there is freedom of choice in inverse temperatures of replicas, $\beta_m$. We 
should take account of conditions such that the replica exchange happens with a non-negligible 
probability for all adjacent pairs of replicas, and each replica moves around the whole temperature 
range in suitable Monte Carlo steps (MCS) per spin.

We make a few comments on the coding of the MC simulation. We use the technique of 
the multispin coding [15, 16, 17, 18], where each bit within one word is assigned to the spin of 
different systems. When using a 32-bit machine, one is able to treat 32 systems simultaneously. 
For the case of the three-state Potts model, two words are needed to represent one set of spin 
states. This is different from the case of the Ising model, where spin states can be represented by 
one word. The multispin coding algorithm for the three-state Potts model obeying the Glauber
Figure 1. Schematic illustration of the sublattice decomposition for the MC simulation of Kawasaki dynamics.

dynamics has already been presented [18]. Here we extend this algorithm to the case of the Kawasaki dynamics of nearest-neighbour pair exchange. As far as we know, the multispin coding algorithm for the Kawasaki dynamics has not been publicized so far even for the Ising model.

It is well known that vectorization is possible if one decomposes the lattice into interpenetrating sublattices. This technique is effective for fast computation when using a vector computer. In the case of the MC simulation of the Kawasaki dynamics, sublattice decomposition into eight sublattices is useful, as illustrated in figure 1. If a single spin represented by a black closed circle is picked up, we can choose either a red circle or a blue circle as a pair spin. For calculation of the local energy, we need information on the states of spins connected by dotted lines. All the spins concerned are independent of other black spins. Thus, all the calculations become vectorized, and this choice of sublattice decomposition is useful for calculation of the fast Fourier transform (FFT).

We have made simulations for the three-state ferromagnetic Potts model with linear sizes \( L = 64, 128 \) and 256. We quench the system to the desired temperatures, starting from the disordered state \((T = \infty)\). Actually, we assign 16 systems of 32 multispin-coding systems to the replica exchange MC calculation of 16 temperatures. The other 16 systems are used for the standard MC calculation. For example, we consider 16 temperatures starting from 0.3 in units of \( J \) with a separation of 0.04; that is, the highest temperature is 0.9. The transition temperature of the three-state ferromagnetic Potts model on the square lattice is exactly known as \( T_c = \left[ \ln(1 + \sqrt{3}) \right]^{-1} = 0.99497 \) [14]. Since we are dealing with the ordering phenomena, we have chosen all the temperatures to be lower than \( T_c \). The number of the spins which take each of three states are fixed to be the same. We make a trial for the replica exchange after one MCS for a single spin flip. Typical MCS are \( 8.0 \times 10^5 \).

There are several ways to estimate the characteristic length scale of the domain size. Binder and Stauffer [19] pointed out that the temporal change of the total energy from the equilibrium energy is appropriate for estimating the domain size; that is,

\[
R_E(t) = N[(\langle H(t) \rangle) - \langle H \rangle_T]^{-1}
\]

(5)

where \( \langle H \rangle_T \) is an equilibrium energy, and \( \langle \ldots \rangle \) represents a sample average. There are other
Figure 2. Time evolution of the excess energy, equation (6), for the three-state Potts model of size $128 \times 128$ quenched to $T = 0.3$ and 0.42. The results for the exchange MC and the standard MC are compared.

Quantities to estimate the domain size. For example, we may use the moment of the time-dependent structure factor $S(k)$. We have calculated $S(k)$ by performing the FFT. However, since the results are essentially the same, we only plot the time evolution of the excess energy

$$E = \frac{\langle H(t) \rangle - \langle H \rangle_T}{N}$$

in figure 2. The MCS is used for time $t$. We compare the data of the exchange MC method and those of the standard MC method. The system size is $128 \times 128$, and quenched temperatures are $T = 0.3$ and 0.42. The average has been taken over 16 samples for each data set.

Comparing the purple and green curve in figure 2, we see that the domain growth becomes very slow at low temperatures for the standard MC. It is because the thermal diffusion is not so frequent at low enough temperatures. In contrast, from the red and blue curves in figure 2, we find that the growth rate is faster for lower temperature in the case of the exchange MC because of the replica exchange process.

Examples of real-space snapshots and the corresponding structure factor $S(k)$ are given in figure 3, where the system size is $256 \times 256$ and the quenched temperature is $T = 0.3$. The time is $8.0 \times 10^5$ MCS and the data for the exchange MC and for the standard MC are compared in (a) and (b), respectively. The three colours, red, green and blue, are used for representing three states in the real-space snapshots. The vertical and horizontal axes for the structure factor span $-\pi$ to $\pi$ in units of the inverse lattice spacing. We can see from figure 3 that even for the deeply quenched case to low temperatures, we have observed a rapid domain growth with the use of the exchange MC method. In the case of $T = 0.3$, to attain the same domain size, the calculation with the exchange MC method is about 200 times faster than that with the standard MC method at the cost of 16 simultaneous calculations with different temperatures. We can use the data for all the temperatures, and the efficiency becomes more prominent for much lower temperatures.

In order to estimate the growth exponent, it is convenient to consider the effective exponent
defined by

\[ n_{\text{eff}} = \frac{d \ln R(t)}{d \ln t}. \]  

We can estimate the growth exponent \( n \) by extrapolating \( n_{\text{eff}} \) in the limit of \( t \to \infty \). Following Huse [20], we plot the effective exponent \( n_{\text{eff}} \) as a function of \( 1/R_E \) in figure 4. We calculate \( n_{\text{eff}} \) from the data shown in figure 2. We compare the data of the exchange MC method and those of the standard MC method. From the data of the exchange MC method shown in figure 4, we may reliably estimate \( n \) as 1/3, which is consistent with the conclusion of [5]. In the study of the standard MC simulation [5], the growth exponent has been estimated as 1/3 from a long extrapolation process; the value of the effective exponent for the largest domain size was 0.23. In contrast, our value of \( n_{\text{eff}} \) by the use of the exchange MC simulation is 0.32. Thus, the estimate of the exponent \( n \) is more reliable.

Although the replica exchange dynamics is not considered to be related to a real one, we have found that a domain growth is controlled by a simple algebraic growth law, \( R(t) \sim t^{1/3} \). The value is consistent with a direct simulation [5] for the same model. In the standard MC the domain growth becomes very slow at low temperatures because of the lack of the thermal diffusion. In order to study the late-stage dynamics in the standard MC, we often choose a relatively high temperature, for example, \( T = 0.5T_c \). Then interfacial fluctuations become large. The advantage of using the exchange MC method is that we can have rapid growth of order together with small interfacial fluctuations. The problem is whether the exchange process of replica modifies the dynamics or not. The answer is generally yes. However, for the problem of ordering phenomena,
it works well even for the estimate of the growth exponent. Why can the exchange MC method simulate the dynamics of ordering phenomena? The ordering phenomena are controlled by a zero-temperature fixed point, in the language of the renormalization group, irrespective of quenched temperature; thus the replicas associated with different (inverse) temperatures obey the same growth law. Even if the growth process is described by the composite of the growth law of different temperatures, the resulting growth behaviour again becomes an algebraic one,

\[ C_1 t^n + C_2 t^n + C_3 t^n + \cdots \propto t^n. \]  

(8)

One comment should be made here on the choice of temperatures of replicas. Although we have shown only the data for the 16 temperatures from 0.3 to 0.9 with the temperature separation of 0.04, other choices of temperatures give essentially the same results.

In summary, we have tested the efficiency of the exchange MC method in the case of the ordering process by quenching. Even for the deeply quenched case at low temperatures, we have observed a rapid domain growth. Although the dynamics including the exchange process is not a simple one, a domain growth has been found to be controlled by a simple algebraic growth law, \( \tilde{R}(t) \sim t^{1/3} \), for the case of the conserved order parameter of a three-component system. It is interesting to apply this method to more complicated problems. The effect of surfactants in the phase separation dynamics is now studied by using this method [21].

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Figure 4. The effective exponent \( n_{\text{eff}} \) as a function of \( 1/R_E \).
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