The correlation between a random sequence and its transformed sequences is studied. In the case of a permutation operation or, in other word, the shuffling operation, it is shown that the correlation can be so small that the sequences can be regarded as independent random sequences. The applications to the Monte Carlo simulations are also given. This method is especially useful in the Ising Monte Carlo simulation.

Keywords: random number; Monte Carlo simulation; Ising model.
1 Introduction

Random numbers are indispensable to the Monte Carlo simulation, which is one of the most important applications of supercomputers. The recent development of vector computers makes more accurate Monte Carlo simulation possible. The Ising Monte Carlo simulation is the most highly developed application and the precision now reaches to the order of $10^{-6}$ and sometimes such simulations consume of the order of $10^{14}$ random numbers.

When a high-precision Monte Carlo simulation is made, two points are important. One is the use of correct pseudo-random number. It is a quite reasonable requirement. And the other is the efficient use of random numbers. For example, the fastest Monte Carlo algorithm using the single-spin updating dynamics of the Ising model uses one random number for updating several spins which are coded in a computer word (independent-system coding technique). The spins in a word belong to physically independent systems and therefore it is expected that such a technique does not make a problem. The validity of this algorithm relies on the physical independence of the simulated systems. When we want to know the expectation values at many different temperatures or fields, this kind of efficient use of random number is very helpful and it has been used in many studies. But if we want to know the expectation value at one temperature, this algorithm was not useful. To overcome this difficulty, the random shuffling of the Boltzmann factor tables (BFT, see Section 6) has been proposed. Although it seemed to work, the validity and/or the limitation of such an operation has not been made clear.

If we transform a given sequence of random numbers, $\{r_n; n = 0, 1, 2, 3, \cdots\}$, using some map $f$ from interval $I = [0, 1]$ to $I$, how does the new sequence $\{f(r_n); n = 0, 1, 2, 3, \cdots\}$ behave? If $f(x) = x^2$ or some other smooth analytic function is used, the sequences $\{r_n\}$ and $\{f(r_n)\}$ will be strongly correlated. Intuitively if we use $f(x)$ which maps any real number in $I$ into $I$ randomly, the sequence $\{r_n\}$ and $\{f(r_n)\}$ may be independent random sequences. On the digital computer, the reliable random real numbers distributed between 0 and 1 are usually generated by normalizing random integers which are generated by a recursion relation. This kind of discrete random number is treated in this paper.

The purpose of the present paper is to study the behavior of random sequences under transformations and to clarify whether there is room for improvement in Monte Carlo simulation in terms of this transformation strategy. And a new algorithm named recycle algorithm is proposed. This algorithm makes the meaning, validity and limitation of the BFT shuffling operation clear.

Some relevant lemmas about the random sequence transformation are given in the next section. The algorithm of random permutation generation which is important in the application of our algorithm is studied in the third section. The general study of the efficiency of our algorithm is made in the fourth section. In the fifth section, a simple application to the static Monte Carlo integration is shown. The application to the dynamic Monte Carlo simulation of the Ising model is given in the sixth section. The final section is for the conclusion and remarks.
2 Some Lemmas

In this section, some useful lemmas are given. Their proofs are not given but they are easily proved.

Notation

$K$ is a field (for example, real field or complex field) and $\Omega$ is any set with $N$ elements, where $N$ is a positive integer. $T_N$ denotes the set of all the maps from $\Omega$ to $\Omega$. There are $N^N$ maps in $T_N$. The subset of $T_N$ made of injections are denoted by $S_N$, which is naturally regarded as the symmetric group of order $N$. $F_M^N$ denotes the set of all the maps from $\Omega^M$ to $K$. $f \circ t$ denotes the composition of $t \in T_N$ and $f \in F_M^N$. In the following lemmas, $N$ is assumed to be larger than $2M$.

Although the lemmas below are proved under above-mentioned general situations, we are interested in the application to the random sequence and Monte Carlo simulations. In these cases, the real field is usually used as $K$. And $\Omega$ corresponds to the possible values of random number, that is,

$$\Omega = \{ \frac{i}{N} : i = 0, 1, 2, \cdots, N-1 \}.$$

(1)

Instead of continuous random numbers, discrete random numbers are considered and it is appropriate because the pseudo-random number generated by a digital computer usually takes such discrete values.

Definition

For any $f \in F_M^N$, the average of $f$, $I_M^N[f]$, is defined by

$$I_M^N[f] = \frac{1}{N^M} \sum_{\omega_1, \omega_2, \omega_3, \cdots, \omega_M \in \Omega} f(\omega_1, \omega_2, \omega_3, \cdots, \omega_M).$$

(2)

Lemma 1.

If $I_1^N[f \circ t] = I_1^N[f]$ for a given $t \in T_N$ and any $f \in F_1^N$, $t$ is an element of $S_N$. Inversely, if $t$ is an element of $S_N$, $I_1^N[f \circ t] = I_1^N[f]$ for any $f$ in $F_1^N$.

This Lemma 1 suggests that the permutation operation is better than other operations in $T_N$ to transform the random sequences into other random sequences. If a permutation is used, the averaged value of $f$ is not biased at all. If we use the permutation, there is no deviation of this kind even for $M$ variable function:

Lemma 2.

For any $s \in S_N$ and any $f \in F_M^N$,

$$I_M^N[f \circ s] = I_M^N[f].$$

(3)

Therefore

$$< \Delta I_M^N[f \circ s]^2 >_{s \in S_N} = 0,$$

(4)
where $\langle \cdot \rangle_{a \in A}$ denotes the average over a set $A$ and

$$
\langle \Delta I^N_M[f \circ s]^2 \rangle_{s \in S_N} = \langle I^N_M[f \circ s]^2 \rangle_{s \in S_N} - \langle I^N_M[f \circ s]^2 \rangle_{s \in S_N}.
$$  \hspace{1cm} (5)

But if another transformation is used, a deviation of the order of $1/\sqrt{N}$ appears as shown in the following Lemma 3:

**Lemma 3.**
For any $f \in F^N_M$,

$$
\langle I^N_M[f \circ t] \rangle_{t \in T_N} = I^N_M[f]
$$  \hspace{1cm} (6)

and

$$
\langle \Delta I^N_M[f \circ t]^2 \rangle_{t \in T_N} = \frac{1}{N} I^N_M[\Delta f^2],
$$  \hspace{1cm} (7)

where

$$
I^N_M[\Delta f^2] = I^N_M[f^2] - I^N_M[f]^2.
$$  \hspace{1cm} (8)

The following Lemma 4 shows that the correlation between a random sequence and the sequences obtained by its permutation becomes small when the resolution of the random number $1/N$ becomes high.

**Lemma 4.**
For any $s \in S_N$ and any $f, g \in F^N_M$,

$$
\langle I^N_M[f \cdot g \circ s] \rangle_{s \in S_N} - I^N_M[f] I^N_M[g] = \frac{C_{f,g}}{N} + O\left(\frac{1}{N^2}\right)
$$  \hspace{1cm} (9)

and

$$
\langle \Delta I^N_M[f \cdot g \circ s]^2 \rangle_{s \in S_N} = \frac{E_{f,g}}{N} + O\left(\frac{1}{N}\right),
$$  \hspace{1cm} (10)

where

$$
C_{f,g} = \sum_{i>j} (I^N_M[f] - D^N_{M,i,j}[f])(I^N_M[g] - D^N_{M,i,j}[g]),
$$  \hspace{1cm} (11)

$$
E_{f,g} = \sum_{i=1}^{M} \sum_{j=1}^{M} (I^N_M[f]^2 - W^N_{M,i,j}[f])(I^N_M[g]^2 - W^N_{M,i,j}[g]),
$$  \hspace{1cm} (12)

$$
D^N_{M,i,j}[f] = \frac{1}{N^{M-1}} \sum_{\omega_1=\omega_j} f(\omega_1, \omega_2, \omega_3, \ldots, \omega_M)
$$  \hspace{1cm} (13)

and

$$
W^N_{M,i,j}[f] = \frac{1}{N^{2M-1}} \sum_{\omega_i=\omega_j} f(\omega_1, \omega_2, \omega_3, \ldots, \omega_M) f(\omega'_1, \omega'_2, \omega'_3, \ldots, \omega'_M).
$$  \hspace{1cm} (14)

The summation in eq. (13) runs over all the elements $(\omega_1, \omega_2, \omega_3, \ldots, \omega_M) \in \Omega^M$ which satisfy the conditions that $\omega_i = \omega_j$. The summation in eq. (14) runs over all
the elements \((\omega_1, \omega_2, \omega_3, \cdots, \omega_M) \in \Omega^M\) and \((\omega'_1, \omega'_2, \omega'_3, \cdots, \omega'_M) \in \Omega^M\) which satisfy the conditions that \(\omega_i = \omega'_j\).

The lemma 1, 2 and 4 suggests a new algorithm of random number generation and usage:

**Algorithm (Recycle Use of Random Number)**
From a sequence of random integers, a new random sequence is generated by applying permutation operations which are selected randomly.

The efficiency analysis and real implementations of this algorithm are given in the rest sections.

Here one remark should be made. When a fixed permutation \(s \in S_N\) is applied to a random number repetitively, the randomness of the obtained sequence is worse than the sequence obtained by the above algorithm as is shown in the Lemma 5:

**Definition**
For any \(f \in F_1^N\), \(s \in S_N\) and \(\omega \in \Omega\), \(J^N\) is defined by

\[
J^N[f; s, \omega] = \lim_{L \to \infty} \frac{1}{L} \sum_{k=0}^{L-1} (f \circ s^k)(\omega) \tag{15}
\]

**Lemma 5.**
For any \(f \in F_M^N\) and \(\omega \in \Omega\),

\[
<J^N[f; s, \omega]>_{s \in S_N} = I_1^N[f] + \frac{\rho_N}{N} (f(\omega) - I_N[f]) + O(\frac{1}{N}), \tag{16}
\]

\[
<J^N[f; s, \omega]>_{s \in S_N, \omega \in \Omega} = I_1^N[f] \tag{17}
\]

and

\[
<\Delta J^N[f; s, \omega]^2>_{s \in S_N, \omega \in \Omega} = \frac{\rho_N}{N} I_1^N[\Delta f^2] + O(\frac{1}{N}), \tag{18}
\]

where

\[
\rho_N = \sum_{k=1}^{N} \frac{1}{k} \tag{19}
\]

Note that the \(\rho_N\) behaves as \(C_E + \log N\) when \(N\) is large, where \(C_E\) is Euler’s constant. Therefore the deviation is the order of \(\sqrt{\log N/N}\).

**3 Permutation Generation**
In the previous section, it is shown that a random sequence and its transformed sequence by permutation are *almost* independent with each other. Now the question is whether this recycle algorithm of a random sequence improves the efficiency of the real simulation or not.
In the real application, the random integers uniformly distributed between 0 to $2^n - 1$ are easily generated and such a random integer is to be transformed by one table-lookup. For example, such random integers are generated by Tausworthe's method\cite{23}--\cite{28}. The table holds a permutation of integers between 0 to $2^n - 1$. When 20 bit random integer is used, that is, $n = 20$, the necessary memory storage for one such table is $4$ byte $\times 2^{20} = 4$ Mbyte. This is not a large table on the modern computers.

The use of discrete random integers instead of real random numbers causes a correlation of the order of $2^{-n/2}$ as it is shown in Lemma 4. Therefore we have to analyze the efficiency carefully. For that purpose, it is necessary to know how to generate a permutation randomly. Random numbers are necessary to prepare a permutation randomly and it might be possible that the total amount of necessary random numbers was larger. Therefore the permutation generation methods are studied in this section to clarify the efficiency of the recycle algorithm.

Consider $N$ objects which are in the boxes, $A_0$, $A_1$, $A_2$, $\cdots$, $A_{N-2}$ and $A_{N-1}$ at the beginning. Now we want to shuffle the objects and generate a new order which is independent of the original order. This is called the **shuffling problem**.

This problem is easily solved by the following algorithm: Firstly, all the objects are put out of the boxes. Then select one object randomly and put it in $A_0$. And then select one object from the remains randomly and put it in $A_1$ and so on. An naive implementation is the following FORTRAN subroutine:

```fortran
SUBROUTINE PERM1(N,ILIST)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION ILIST(0:N-1)
DO 10 I=N-1,0,-1
   J=INT(RANDOM()*DFLOAT(I+1))
   ITMP=ILIST(I)
   ILIST(I)=ILIST(J)
   ILIST(J)=ITMP
10 CONTINUE
RETURN
END
```

The function **RANDOM()** is assumed to generate one random real number uniformly distributed in the interval, $I = \{r; 0 \leq r < 1\}$.

Above program is, however, dangerous. We expect that the $J$ generated by $J=\text{INT(RANDOM()}*\text{DFLOAT(I+1)})$ are distributed uniformly on $\{0, 1, 2, \cdots, I\}$ but it is not always correct, especially when $I$ is large. This is because the random real numbers generated by a random number generation routine take only discrete values. For example, if the random real number takes one of the values in $\{0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9\}$ uniformly and $I=7$, the probabilities that $J=0, 1, 2, 3, 4, 5, 6$ and 7 are $1/5, 1/10, 1/10, 1/10, 1/5, 1/10$ and $1/10$, respectively. Of course, if the random number generation routine generates random real numbers which take all real*8 floating precision between 0 and 1, such non-uniform property might be negligible.

The above mentioned problem is removed in the following routine **PERM2**:
SUBROUTINE PERM2(IB,N,ILIST)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION ILIST(0:N-1)
IF((2**(IB-1).GE.N).OR.(2**IB.LT.N))THEN
   WRITE(*,*)'ERROR! IN PERM2. SPECIFIED IB=',IB,' AND N=',N
   WRITE(*,*)' ARE NOT IN PROPER RANGE.'
   STOP
END IF
DO 10 I=1,IB
   IN=2**(IB-I)
   IS=1-I
   IFIRST=IN*2-1
   IF(I.EQ.1)IFIRST=N-1
   DO 20 J=IFIRST,IN,-1
      K=ISHFT(IRNDTW(),IS)
      IF(K.GT.J)GOTO 30
      ITMP=ILIST(K)
      ILIST(K)=ILIST(J)
      ILIST(J)=ITMP
   20 CONTINUE
10 CONTINUE
RETURN
END

The function IRNDTW() is assumed to generate random integers between 0 to $2^{IB-1}$ (See Appendix A). The values of IB and N must satisfy the relation

$$2^{IB-1} < N \leq 2^I B.$$  \hfill (20)

Two different implementations of shuffling routines are given here. The necessary number of random numbers for shuffling N elements, which is denoted by $n_R(N)$, are estimated here. In the first subroutine PERM1, $n_R(N)$ is N. In the second subroutine PERM2, $n_R(N)$ depends on the values of generated random numbers. About one half of the generated random numbers are not used. In average, $n_R(N)$ is 2N but there is some fluctuation. The following will be an overestimate of it:

$$N + 2\sqrt{N} + \left(\frac{N}{2} + 2\sqrt{\frac{N}{2}}\right) + \left(\frac{N}{4} + 2\sqrt{\frac{N}{4}}\right) + \cdots = 2N + \frac{2\sqrt{2}}{\sqrt{2} - 1}\sqrt{N}. \hfill (21)$$

Therefore $n_R(N) = 3N$ is an overestimated value and it is a safe estimate.

The shuffling algorithm implemented in the PERM2 routine is used in the following analysis. And we can say that the random number cost for the shuffling of N elements is 3N in the worst case and this $n_R(N) = 3N$ is used in the next section for the efficiency analysis of our recycle method.
4 Efficiency

The Monte Carlo estimation of an M-dimensional integration:

$$\hat{I}[F] = \int_{x_1}^{x_1} \int_{x_2}^{x_2} \int_{x_3}^{x_3} \cdots \int_{x_M}^{x_M} F(x_1, x_2, x_3, \cdots, x_M) dx_1 dx_2 dx_3 \cdots dx_M$$

is considered to study the efficiency of our recycle method. The dynamic Monte Carlo simulation will correspond to the very large M case. After rescalings, $y_i = (x_i - x_i^{\min})/(x_i^{\max} - x_i^{\min})$ $(i = 1, 2, 3, \cdots, M)$, this integration reduces to the estimation of

$$I[f] = \int_0^1 \int_0^1 \int_0^1 \cdots \int_0^1 f(y_1, y_2, y_3, \cdots, y_M) dy_1 dy_2 dy_3 \cdots dy_M.$$  \hspace{1cm} (23)

Instead of this integral, the discrete approximant $I_M^N[f]$ is estimated by a Monte Carlo simulation. This $I_M^N[f]$ is expected to converge to $I[f]$ when $N$ goes to infinity.

Before the Monte Carlo sampling is started, $L_{\text{table}}$ permutation tables are prepared and it requires $N f(N) L_{\text{table}}$ random numbers. The permutation operation in the $i$-th table is expressed by $s_i$ $(i = 1, 2, 3, \cdots, L_{\text{table}})$. Then a set of $M$ random numbers $r_1, r_2, r_3, \cdots, r_M$ which is denoted by $\vec{r} \in \Omega^M$ is generated and the value of $f(\vec{r})$ is accumulated. The average of $L_{\text{sample}}$ samples is denoted by $E_0(\{\vec{r}_i; i = 1, 2, 3, \cdots, L_{\text{sample}}\})$. At the same time, the values of $s_i(r_1), s_i(r_2), s_i(r_3), \cdots, s_i(r_M)$ $(i = 1, 2, 3, \cdots, L_{\text{table}})$ which is denoted by $f(s_i(\vec{r}))$ are also accumulated. The averages of $L_{\text{sample}}$ samples are denoted by $E_i(\{\vec{r}_i\})$.

Each of these estimations $E_i(\{\vec{r}_i\})$ $(i = 0, 1, 2, \cdots, L_{\text{table}})$ converges to $I_M^N[f]$ as is shown in lemma 3 and the error defined by

$$\delta_i(\{\vec{r}_j\}) = E_i(\{\vec{r}_j\}) - I_M^N[f]$$

converges as

$$< \delta_i(\{\vec{r}_j\}) >_{\vec{r}_1, \vec{r}_2, \vec{r}_3, \cdots, \vec{r}_{L_{\text{sample}}} \in \Omega^M} = \frac{1}{L_{\text{sample}}} I_M^N[\Delta f^2].$$

Therefore the magnitude of the error is

$$|\delta_i(\{\vec{r}_j\})| \sim \sqrt{\frac{I_M^N[\Delta f]}{L_{\text{sample}}}}.$$ \hspace{1cm} (26)

Now the behavior of the averages of $E_i(\{\vec{r}_j\})$ $(i = 1, 2, 3, \cdots, L_{\text{table}})$, that is,

$$E_{\text{all}}(\{s_i\}, \{\vec{r}_j\}) = \frac{1}{L_{\text{table}}} \sum_{i=1}^{L_{\text{table}}} E_i(\{\vec{r}_j\})$$

is studied. It is obvious that this $E_{\text{all}}$ converges to $I_M^N[f]$ when $L_{\text{sample}} \to \infty$ even if $L_{\text{table}}$ is finite. But is it true when $L_{\text{table}}$ goes to $\infty$ and $L_{\text{sample}}$ is finite? The
question is how this quantity converges towards $I^N_M[f]$. And the answer is: The error of the $E_{\text{all}}$ defined by

$$
\delta_{\text{all}}(\{s_i\}, \{\vec{r}_j\}) = E_{\text{all}}(\{s_i\}, \{\vec{r}_j\}) - I^N_M[f] \quad (28)
$$

behaves as

$$
\left\langle \delta_{\text{all}}(\{s_i\}, \{\vec{r}_j\})^2 \right\rangle_{\{s_i\}, \{\vec{r}_j\} \in \Omega^M, s_1, s_2, \cdots, s_{L_{\text{table}}} \in S_N} = \frac{1}{L_{\text{table}}L_{\text{sample}}} (I^N_M[\Delta f^2] + \frac{C_{f,f}}{N}) + \frac{1}{L_{\text{sample}}} \frac{C_{f,f}}{N} + O\left(\frac{1}{N^2}\right). \quad (29)
$$

It is concluded from this eq. (29) that the error does not converge to zero when $L_{\text{table}} \to 0$ and $L_{\text{sample}}$ is finite. From eq. (29), we can derive the condition under which the Monte Carlo simulation with the recycle algorithm is advantageous to the standard algorithm.

The number of necessary random numbers to achieve a given error $\delta$ is denoted by $\Lambda_S(\delta)$ in the standard algorithm case and $\Lambda_R(\delta)$ in the recycle algorithm case. The $\Lambda_S(\delta)$ is obtained by solving the equation the right-hand side of eq. (26) be $\delta$:

$$
\frac{\sqrt{I^N_M[\Delta f^2]}}{\Lambda_S(\delta)/M} = \delta. \quad (30)
$$

Therefore

$$
\Lambda_S(\delta) = \frac{I^N_M[\Delta f^2]M}{\delta^2}. \quad (31)
$$

To get the $\Lambda_R(\delta)$, we have to optimize the number of tables, $L_{\text{table}}$. When we use $L_{\text{table}}$ tables, the accuracy is obtained from eq. (29) and

$$
\Lambda_R(\delta) = ML_{\text{sample}} + n_R(N)L_{\text{table}}. \quad (32)
$$

When one random permutation table is generated, $n_R(N)$ random numbers are necessary as studied in the previous section. After we minimize the $\Lambda_R(\delta)$ under the condition that the error be $\delta$, we reach the expression

$$
\Lambda_R(\delta) = \frac{2}{\delta} \sqrt{n_R(N)M(I^N_M[\Delta f^2] + \frac{C_{f,f}}{N})} + \frac{MC_{f,f}}{\delta^2N} \quad (33)
$$

when

$$
L_{\text{table}} = \frac{1}{\delta} \sqrt{\frac{M}{n_R(N)}} \left( I^N_M[\Delta f^2] + \frac{C_{f,f}}{N} \right). \quad (34)
$$

Therefore the recycle algorithm is efficient when

$$
\frac{I^N_M[\Delta f^2]M}{\delta^2} > \frac{2}{\delta} \sqrt{Mn_R(N)(I^N_M[\Delta f^2] + \frac{C_{f,f}}{N})} + \frac{MC_{f,f}}{\delta^2N} \quad (35)
$$

in terms of the number of random numbers. Generally speaking, $I^N_M[\Delta f^2]/C_{f,f}$ is usually much larger than one as is observed in the next section as an example and
δ · N should be larger than one. After neglecting irrelevant terms, above condition reduces to
\[ \sqrt{\frac{M I_M^N \Delta f^2}{4 \delta^2 n_R(N)}} > 1, \] (36)
which is usually satisfied in the high accuracy simulation case. Furthermore the optimal number of tables is
\[ L_{\text{table}} = \sqrt{\frac{M I_M^N \Delta f^2}{\delta^2 n_R(N)}}, \] (37)
which is a large number also in the high accuracy simulation case.

These efficiency studies here show that our recycle algorithm in some cases is more efficient than the standard algorithm. It is especially efficient for high accuracy Monte Carlo simulations.

Only the number of random numbers was considered to study the efficiency in this section and there will be many other factors to determine the computational time in the real computer simulation. So we have to study the real efficiency and it is made in the next section and the result proves that the recycle algorithm is really efficient in high accuracy simulations.

5 Simple Application

In this section, an example is given to show that our recycle algorithm really reduces the computational time without introducing any bias to the estimate and the lemma 4 and the recycle algorithm in section 2 works successfully. The Monte Carlo estimation of the volume of an M-dimensional hypersphere is considered in the following.

In this case, the integrand is
\[ f(x_1, x_2, x_3, \ldots, x_M) = \begin{cases} 2^M & \text{if } \sum_{i=1}^M x_i^2 < 1, \\ 0 & \text{otherwise} \end{cases}, \] (38)
where \(0 \leq x_i < 1(i = 1, 2, 3, \ldots, M)\). The answer is
\[ I[f] = V_M = \frac{\pi^{M/2}}{1(M/2 + 1)}, \] (39)
where \(V_M\) denotes the volume of the M-dimensional unit hypersphere. The constants relevant to the efficiency analysis, \(I_M^N[\Delta f^2]\) and \(C_{f,f}\), are estimated to be
\[ I_M^N[\Delta f^2] = (2^M - V_M)V_M \] (40)
and
\[ C_{f,f} = \frac{M(M - 1)}{2}(V_M - \sqrt{2V_{M-1}})^2. \] (41)

Two Monte Carlo programs are prepared for \(M = 5\) case. In this case, \(I_5^N[\Delta f^2] = (2^5 - V_5)V_5 \approx 140.7 \) and \(C_{f,f} = 10(V_5 - \sqrt{2V_4})^2 \approx 29.41\). One does not use the
recycle algorithm and the other one uses it. They are optimized to their algorithms and the FORTRAN codes are given in the appendix A. 64 independent samples are used to estimate the statistical errors and each sample is an average over $10^3 \sim 10^7$ independent trials. In the recycle algorithm case, 63 random permutations are prepared and used.

The results and performance for the 13 bit-wide random integer case, that is, the $N = 2^{13} = 8192$ case are given in Table 1. The exact value of the integral is $8\pi^2/15 = 5.26378901 \cdots$. The $I_{\text{est}}$ converges correctly except for the $N_{\text{trial}} = 10^7$ case. The $N_{\text{trial}} = 10^7$ simulation is more accurate than the accuracy limit determined by the random number bit-width. In this calculation, the accuracy limit is of the order of

$$\delta_{\text{limit}} = \frac{2^M}{2^B} = 2^{5-B},$$

where $B$ is the bit-width of the random numbers. The calculation reaches this accuracy after $N_{\text{limit}}$ trials determined by

$$\sqrt{\frac{I_2^N [\Delta f^2]}{N_{\text{limit}}}} = \delta_{\text{limit}},$$

therefore

$$N_{\text{limit}} = \frac{I_2^N [\Delta f^2]}{\delta_{\text{limit}}^2} = \frac{\pi^2}{15} (1 - \frac{\pi^2}{60}) \cdot 2^{2B-2}.$$  

(44)

When $B = 13$, $\delta_{\text{limit}} = 0.0039$ and $N_{\text{limit}} = 9.2 \times 10^6$. The above calculation with $N_{\text{trial}} = 10^7$ means totally $6.4 \times 10^7$ trials which are much longer than $N_{\text{limit}}$. In the $N_{\text{trial}} = 10^6$ case, the estimated accuracy is of the same order as the accuracy limit and therefore the results of those cases are not reliable, although they seem to be acceptable.

In Table 2, the result and performance with 16 bit-wide random integers are shown. In this case, the accuracy limit is 0.00049 and the maximum number of trials is $5.9 \times 10^8$. The calculations are tried up to $N_{\text{trial}} = 10^6$.

The results in Tables 1 and 2 show two things clearly: (1) our recycle algorithm works correctly and (2) it accelerates the high-precision and long Monte Carlo simulations.

6 Ising Monte Carlo Simulation

An example which uses the recycle algorithm naively was shown in the previous section and an advanced application is given in this section. It is the Ising Monte Carlo simulation with an independent-system coding technique.

The most efficient algorithm of this problem prepares and uses tables named Boltzmann-factor tables which convert the value of a random integer into a few bits variable which is useful to update the spins coded in one computer word. For example, in the case of the ferromagnetic Ising model on a cubic lattice with nearest neighbor interaction without external field, two tables IX1 and IX2 are used. The $l$th bits of these tables express the value of two-bit variables for the system.
Table 1: The results and performance for 13 bit-wide random number case are shown. The column named algorithm shows which program was used. NR means the program with conventional random number usage and R means the recycle use algorithm for random numbers. The \( N_{\text{trial}} \), \( I_{\text{est}} \), and \( T_{\text{ratio}} \) denote the number of trials for one sample, the estimated volume of the five-dimensional unit hypersphere and the CPU time ratio of NR and R cases, respectively. 64 samples are used to estimate the value of \( I_{\text{est}} \) and its error. The SUN Sparc Station 2 was used to measure the CPU time. The \( X \) denotes \(( I_{\text{MC}} - I_{\text{exact}} )/\delta I_{\text{MC}}\), where \( I_{\text{MC}} \), \( I_{\text{exact}} \) and \( \delta I_{\text{MC}} \) denote the estimated volume, exact volume and estimated error, respectively.

| \( N_{\text{trial}} \) | algorithm | \( I_{\text{est}} \) | \( X \) | CPU time | \( T_{\text{ratio}} \) |
|-----------------------|-----------|------------------|-------|----------|----------------|
| \( 10^3 \)            | NR        | 5.296 ± 0.043    | 0.75  | 0.8      |                |
|                       | R         | 5.217 ± 0.040    | -1.17 | 2.8      | 0.3            |
| \( 10^4 \)            | NR        | 5.254 ± 0.015    | -0.65 | 6        |                |
|                       | R         | 5.262 ± 0.015    | -0.12 | 4        | 1.5            |
| \( 10^5 \)            | NR        | 5.2648 ± 0.0057  | 0.18  | 57       |                |
|                       | R         | 5.2674 ± 0.0044  | 0.82  | 20       | 2.9            |
| \( 10^6 \)            | NR        | 5.2652 ± 0.0014  | 1.01  | 570      |                |
|                       | R         | 5.2654 ± 0.0017  | 0.95  | 179      | 3.2            |
| \( 10^7 \)            | NR        | 5.2675 ± 0.00044 | 8.77  | 5694     |                |
|                       | R         | 5.26615 ± 0.00049| 4.82  | 1764     | 3.2            |

Table 2: The results and performance for 16 bit-wide random number case are shown. The notations are the same as those in Table 1.
coded in the $l$th bit. When the spins in one word are updated, one random integer $\text{IR}$ is converted into two values $\text{IX1(\text{IR})}$ and $\text{IX2(\text{IR})}$. Each pair of bits in the same bit-positions of these $\text{IX1(\text{IR})}$ and $\text{IX2(\text{IR})}$ holds sufficient information about the random number to update each Ising spin coded in that bit-position. They are used to update the spins and $\text{IR}$ is not necessary anymore. The recycle algorithm can be implemented by shuffling randomly the bit pairs in $\text{IX1}$ and $\text{IX2}$ before the spin updating operations. The subroutine $\text{BFSHUF}$ for this operation is given in Appendix B and the shuffling operation is described in this FORTRAN subroutine. The algorithm is essentially the same as $\text{PERM2}$ routine given in the third section. The performance of this $\text{BFSHUF}$ routine is measured with the NEC SX3/11 in Köln university and the MONTE4 in Japan Atomic Energy Research Institute, and it is given in Table 3. The MONTE4 has four processors and the performance is measured with one processor of them under single job environment, which is appropriate to compare the performance with the single processor machine, NEC SX3/11. The performance of the MONTE4 is largely influenced by the other jobs on other processors and the performance shown in Table 3 suffers from large fluctuations under multi-job environment. Although the time consuming operation of this routine is not vectorizable, the Boltzmann factor tables are shuffled within reasonable CPU time. This Ising Monte Carlo algorithm with table shuffling is useful because the systems at the same temperature can be simulated with the independent-system coding technique.

Fig. 1 shows two sequences of the magnetization of 64 systems at the critical temperature and no correlation is observed in this figure. The correlation between the magnetization sequences is studied quantitatively here to check the validity of our algorithm. The magnetizations from the $i$th permuted random sequences are denoted by

$$M_i(t), \quad t = 1, 2, 3, \cdots, m,$$

where $t$ denotes the sample number in the temporal order and the magnetization is calculated in every constant Monte Carlo steps. We assume that there are $n$ sequences, that is, $i = 1, 2, 3, \cdots, n$. The correlation coefficient between samples $i$ and $j$ is defined by

$$c_{ij} = \frac{< M_i(t)M_j(t) >_t}{\sqrt{< M_i(t)^2 >_t < M_j(t)^2 >_t}},$$

where $< \cdot >_t$ denotes the temporal average, that is,

$$< f(t) >_t = \frac{1}{m} \sum_{t=1}^{m} f(t).$$

The average of $c_{ij}$ over all different samples $i$ and $j$,

$$c = \frac{\sum_{i \neq j} c_{ij}}{\sum_{i \neq j} 1}$$

is estimated for several simulations with different parameters. The results are given in Table 4 and it is clearly observed that the correlation between the samples using permuted random numbers is negligibly small as is expected from our lemma 4.
Table 3: The shuffling performance of the BFISHUF routine given in the Appendix B is listed. The IRBIT denotes the bit-width of the random integer and the size of the Boltzmann factor tables to be shuffled is $2^{\text{IRBIT}}$. The 8 byte integer is specified for integer variables and arrays with -w option of the NEC FORTRAN77/SX compiler. The CPU time for the shuffling is measured and shown. For small value of IRBIT, the BFISHUF routine is called repeatedly so that the time may be the order of tens of seconds and the averaged CPU time is shown. The IRBIT=23 performance of SX3/11 is not available because of the memory-size limitation.

| IRBIT | SX3/11     | MONTE4    |
|-------|------------|-----------|
| 10    | 0.046 sec. | 0.039 sec.|
| 11    | 0.091      | 0.078     |
| 12    | 0.19       | 0.17      |
| 13    | 0.43       | 0.37      |
| 14    | 1.0        | 0.85      |
| 15    | 2.2        | 2.0       |
| 16    | 4.7        | 4.2       |
| 17    | 9.8        | 8.4       |
| 18    | 20         | 17        |
| 19    | 41         | 37        |
| 20    | 82         | 74        |
| 21    | 165        | 149       |
| 22    | 332        | 284       |
| 23    | 568        |           |

Table 4: The correlation $c$ between the magnetization sequences from the simulation with permuted random numbers is shown. $X$ denotes $c/\delta c$, where $\delta c$ denotes the estimated error of $c$. The system on a $11 \times 11 \times 12$ lattice was simulated at the critical temperature. The initial $10^4$ MCS is skipped. The $m$ denotes the number of samples and the magnetization is measured every 50 MCS. Five independent simulations are used to estimate the errors. No correlation is observed in these results.

| $m$   | IRBIT = 16 | IRBIT = 18 | IRBIT = 20 |
|-------|------------|------------|------------|
|       | $c$ | $X$      | $c$ | $X$    | $c$ | $X$     |
| $10^2$| -0.0011 | -0.92     | 0.0002 | 0.17   | -0.0009 | -0.75    |
| $10^3$| 0.00003  | 0.08      | -0.00007 | -0.18 | 0.00028 | 0.72     |
| $10^4$| 0.00016  | 1.33      | 0.00012 | 1.00   | 0.00011 | 0.92     |
| $10^5$| 0.000014 | 0.39      | 0.000052 | 1.44  | 0.000053 | 1.36     |
Figure 1: The values of magnetizations $M_1(t)$ and $M_2(t)$ of two samples with different permutations are plotted. After $10^4$ MCS, the magnetizations were calculated 100 times at every 1000 MCS at the critical temperature. Five independent simulations were made and therefore there are 500 points. No clear correlation is observed. The quantitative analysis of the correlation is given in Table 4.

7 Conclusion and Remarks

It is shown that the random permutation or random shuffling of the numbers in the interval $[0, 1]$ transforms one uniformly distributed random sequences into another statistically almost independent random sequences. Based on this property, a new method named recycle algorithm for random number generation and its usage is proposed. Its efficiency is studied. It is also shown that this algorithm reduces the computational time of long and high-precision Monte Carlo simulation. This algorithm is especially useful in the Ising Monte Carlo simulation with independent-system coding technique. It makes it clear that the random shuffling of the Boltzmann factor tables makes the statistically independent simulation possible for the systems with the same parameters using that coding technique.

This recycle algorithm will be also useful in Monte Carlo simulations with MIMD architecture parallel computer. One processor generates random integers and broadcasts them to all the other processors. Each processor holds one random permutation
and transforms the broadcasted random integers with its table. When the cost for broadcasting is smaller than the generation, this method will be useful.

The automatic optimization of the bit-width of the random numbers and the number of permutation tables is possible by using the results of efficiency analysis in the fourth section. It will be useful for moderate-scale Monte Carlo simulation.

In the very large scale dynamics Monte Carlo simulation, this algorithm is often useful. The number of tables and bit-width can be determined by the necessary accuracy of the simulation and memory capacity of the computer.

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Appendix A—Program for Hypersphere

The FORTRAN programs for the Monte Carlo integration of the volume of five-dimensional hypersphere used in the sixth section are shown. Two kinds of programs are listed in the following. One uses the conventional algorithm and the other uses the recycle algorithm.

Conventional Random Number Use

The simulation parameters are specified in two PARAMETER statements at the beginning. NSIZE and ISAMPL specify the number of trials in one sample and the number of samples, respectively. IRBIT and IRSEED specify the bit-width of the random number and the initial seed. IRSEED should be an odd integer. The random number generation routines are given at the end of this Appendix A.
IMPLICIT REAL*8 (A-H,O-Z)
PARAMETER(NSIZE=10000000,ISAMPL=64)
PARAMETER(IRBIT=16,IRSEED=14643557)
DIMENSION ACC(ISAMPL)

C INITIALIZATION OF RANDOM NUMBER GENERATION ROUTINE
CALL INITTW(IRSEED,IRBIT)

C MONTE CARLO SAMPLING
DO 10 I=1,ISAMPL
   ACC(I)=SPHAMR(NSIZE,IRBIT)
10 CONTINUE

C ERROR ANALYSIS
AAVE=0.0D0
ASQ=0.0D0
DO 20 I=1,ISAMPL
   AAVE=AAVE+ACC(I)
   ASQ=ASQ+ACC(I)*ACC(I)
20 CONTINUE
AAVE=AAVE/DFLOAT(ISAMPL)
ASQ=ASQ/DFLOAT(ISAMPL)
AERR=DSQRT((ASQ-AAVE*AAVE)/DFLOAT(ISAMPL-1))

C OUTPUT
WRITE(6,100)NSIZE,ISAMPL,(NSIZE*ISAMPL)
100 FORMAT(' TRIAL=',I8,' SAMPLE=',I6,' TOTAL TRIAL=',I10)
WRITE(6,110)IRBIT,2.0d0**(-IRBIT)
110 FORMAT(' BIT WIDTH=',I2,' RNG RESOLUTION=',F10.8)
WRITE(6,120)AAVE,AERR
120 FORMAT(' ESTIMATED VOLUME=',F10.8,'+-',F10.8)
STOP
END

FUNCTION SPHAMR(N,IRBIT)
IMPLICIT REAL*8 (A-H,O-Z)
ANORMS=4.0D0**IRBIT
ICNT=0
DO 10 I=1,N
   A1=DFLOAT(IRNDTW())
   A2=DFLOAT(IRNDTW())
   A3=DFLOAT(IRNDTW())
   A4=DFLOAT(IRNDTW())
   A5=DFLOAT(IRNDTW())
   A=A1*A1+A2*A2+A3*A3+A4*A4+A5*A5
   IF(A.LT.ANORMS)ICNT=ICNT+1
10 CONTINUE
SPHAMR=DFLOAT(ICNT)*32.0D0/DFLOAT(N)
RETURN
END

Recycle Algorithm

In the following program, the number of trials of one sample is \( NSIZE \times IREP \). \( ISAMPL \) specifies the number of random permutation tables and the original random
sequence is also used. Therefore the number of sample is ISAMPL+1. The random number generation routine at the end of this Appendix and the subroutine PERM2 in the third section are also necessary.

```
IMPLICIT REAL*8 (A-H,O-Z)
PARAMETER(IRBIT=16,NSIZE=1000000,IREP=10,ISAMPL=63)
PARAMETER(IRSEED=14643557)
PARAMETER(ILIST=2**IRBIT)
DIMENSION IX(0:ILIST-1,ISAMPL),IR(NSIZE,5)
DIMENSION ACC(0:ISAMPL)
CALL INITTW(IRSEED,IRBIT)
DO 10 J=1,ISAMPL
   DO 20 I=0,ILIST-1
      IX(I,J)=I
   CONTINUE
   CALL PERM2(IRBIT,ILIST,IX(0,J))
10 CONTINUE
   DO 30 I=0,ISAMPL
      ACC(I)=0.0D0
30 CONTINUE
   DO 40 I=1,IREP
      CALL ITWDIM(NSIZE*5,IR)
      ACC(0)=ACC(0)+SPHAMC(NSIZE,IR(1,1),IR(1,2),
1 IR(1,3),IR(1,4),IR(1,5),IRBIT)
      DO 50 J=1,ISAMPL
         ACC(J)=ACC(J)+SPHAMD(NSIZE,IR(1,1),IR(1,2),
1 IR(1,3),IR(1,4),IR(1,5),IRBIT,ILIST,IX(0,J))
50 CONTINUE
40 CONTINUE
   AAVE=0.0D0
   ASQ=0.0D0
   DO 70 I=0,ISAMPL
      ACC(I)=ACC(I)/DFLOAT(IREP)
      AAVE=AAVE+ACC(I)
      ASQ=ASQ+ACC(I)*ACC(I)
70 CONTINUE
   AAVE=AAVE/DFLOAT(ISAMPL+1)
   ASQ=ASQ/DFLOAT(ISAMPL+1)
   AERR=DSQRT((ASQ-AAVE*AAVE)/DFLOAT(ISAMPL))
C OUTPUT
   WRITE(6,100)NSIZE*IREP,ISAMPL+1,NSIZE*UREP*(ISAMPL+1)
100 FORMAT(' TRIAL=',I8,' SAMPLE=',I6,' TOTAL TRIAL=',I10)
   WRITE(6,110)IRBIT,2.0D0**(-IRBIT)
110 FORMAT(' BIT WIDTH=',I2,' RNG RESOLUTION=',F10.8)
   WRITE(6,120)AAVE,AERR
120 FORMAT(' ESTIMATED VOLUME=',F10.8,'+-',F10.8)
STOP
END
```

FUNCTION SPHAMC(N,IR1,IR2,IR3,IR4,IR5,IRBIT)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION IR1(N),IR2(N),IR3(N),IR4(N),IR5(N)
**Random Number Generation Routine**

The random number generation routine used in the above two programs is given. The Tausworthe sequence (or Kirkpatrick and Stoll method) is used to generate the pseudo-random integers.

```fortran
SUBROUTINE INILSD(N)
  COMMON /LCSEED/NSEED
  NSEED=N
  RETURN
END

FUNCTION LCARNG()
  INTEGER*4 LCARNG
  DATA MASK31/Z’7FFFFFFF’/
  COMMON /LCSEED/NSEED
  ICNT=0
  DO 10 I=1,N
    A1=DFLOAT(IR1(I))
    A2=DFLOAT(IR2(I))
    A3=DFLOAT(IR3(I))
    A4=DFLOAT(IR4(I))
    A5=DFLOAT(IR5(I))
    A=A1*A1+A2*A2+A3*A3+A4*A4+A5*A5
    IF(A.LT.ANORMS)ICNT=ICNT+1
  10 CONTINUE
  SPHAMD=DFLOAT(ICNT)*32.0D0/DFLOAT(N)
  RETURN
END
```

The random number generation routine used in the above two programs is given. The Tausworthe sequence (or Kirkpatrick and Stoll method) is used to generate the pseudo-random integers.
NSEED = NSEED * 48828125
NSEED = IAND(NSEED, MASK31)
LCARNG = NSEED
RETURN
END
SUBROUTINE INITTW(INSEEK, IRBIT)
PARAMETER (ISELBT = -24)
COMMON /TWSTOR/ IDIM(250), IPL(250), IQL(250), IP
DATA IRCNST/Z'7FFFFFFF'/
CALL INILSD(INSEEK)
DO 10 I = 1, 250
   IDIM(I) = 0
DO 20 J = 1, 32
   ITMP = LCARNG()
   ITMP = ISHFT(ITMP, ISELBT)
   ITMP = IAND(ITMP, 1)
   IDIM(I) = ISHFT(IDIM(I), 1)
   IDIM(I) = IOR(IDIM(I), ITMP)
20  CONTINUE
10  CONTINUE
C BIT MASKING
IRLST = 0
DO 40 I = 1, IRBIT
   IRLST = ISHFT(IRLST, 1)
   IRLST = IOR(IRLST, 1)
40  CONTINUE
DO 30 I = 1, 250
   IDIM(I) = IAND(IDIM(I), IRLST)
30  CONTINUE
IP = 1
DO 50 I = 1, 250
   IPL(I) = I + 1
   IT = I - 103
   IF (IT .LT. 1) IT = IT + 250
   IQL(I) = IT
50  CONTINUE
IPL(250) = 1
RETURN
END
FUNCTION IRNDTW()
COMMON /TWSTOR/ IR(250), IPL(250), IQL(250), IP
IRNDTW = IEOR(IR(IP), IR(IQL(IP)))
IR(IP) = IRNDTW
IP = IPL(IP)
RETURN
END
SUBROUTINE ITWDIM(N, IDIM)
COMMON /TWSTOR/ IR(250), IPL(250), IQL(250), IP
DIMENSION IDIM(N)
DO 10 I = 1, N
Appendix B—Shuffling of Boltzmann-factor Table

The shuffling routine for Boltzmann factor tables (BFT) of Ising Monte Carlo simulation with independent-system coding technique is given. This BFSHUF routine is for the simulation with two BFT and it is easily modified for more BFT simulation. This routine uses vectorized efficient random-number-generation routine RNDO2I of RNDTIK library which generates Kirkpatrick-Stoll type random integers. RNDO2I is assumed to be initialized to generate IRBIT-bit wide random integers.

SUBROUTINE BFSHUF(IX1,IX2,IRBIT,N,IRD)
	PARAMETER(IWIDTH=64,NMAX=30)
	DIMENSION IX1(0:2**IRBIT-1),IX2(0:2**IRBIT-1)
	DIMENSION IRD(N)
	IRPOS=1
	CALL RNDO2I(N,IRD)
	DO 10 I=0,IWIDTH-2
		IRPOS=ISHFT(1,I)
		DO 20 J=1,IRBIT
		IN=2**(IRBIT-J)
		IS=1-J
		DO 30 K=IN*2-1,IN,-1
			IR=ISHFT(IRD(IRPOS),IS)
			IRPOS=IRPOS+1
			IF(IRPOS.GT.N)THEN
				CALL RNDO2I(N,IRD)
			END IF
			IF(IR.LE.K)GO TO 50
			20 CONTINUE
			WRITE(*,*)'ERROR IN BFSHUF! RANDOM NUMBER IS BIASED.'
		STOP
	30 CONTINUE
	40 WRITE(*,*)'ERROR IN BFSHUF! RANDOM NUMBER IS BIASED.'
	STOP
	50 ID=IEOR(IX1(K),IX1(IR))
	ID=IAND(ID,IRPOS)
	IX1(K)=IEOR(IX1(K),ID)

C 1992.10.26. BY NOBUYASU ITO
C BOLTZMANN FACTOR TABLE SHUFFLING ROUTINE
C IX1, IX2 : BOLTZMANN FACTOR TABLE TO BE SHUFFLED
C IRBIT : BIT-WIDTH OF THE RANDOM NUMBER SHOULD BE GIVEN
C THE SIZE OF IX1 AND IX2 IS ASSUMED TO BE
C IX1(0:2**IRBIT-1) IX2(0:2**IRBIT-1).
C IRD(N) : WORK AREA. ANY SIZE N IS GOOD BUT LARGE VALUE
C (MORE THAN SEVERAL THOUSANDS) IS MORE EFFICIENT.
IX1(IR) = IEOR(IX1(IR), ID)
ID = IEOR(IX2(K), IX2(IR))
ID = IAND(ID, IPOS)
IX2(K) = IEOR(IX2(K), ID)
IX2(IR) = IEOR(IX2(IR), ID)

30 CONTINUE
20 CONTINUE
10 CONTINUE
RETURN
END