

# Using Sequential Importance Sampling for Nonequilibrium Reweighting

Hwee Kuan Lee and Yutaka Okabe  
*Department of Physics, Tokyo Metropolitan University*

We present a reweighting method for nonequilibrium Markov processes. With nonequilibrium Monte Carlo simulations at one temperature, one calculates the averages of time dependent physical quantities for a range of temperatures. We propose that reweighting for nonequilibrium is most useful when combined with dynamical finite size scaling. The procedure is demonstrated for the Ising model and the driven diffusive lattice gas model in this paper.

## I. BACKGROUND

Most phenomena occurring in nature are in nonequilibrium states and models for nonequilibrium systems have captured a lot of attention. Monte Carlo simulation has been a standard tool in scientific computing, and advanced simulation methods have been developed. However, many advanced Monte Carlo methods are not applicable to nonequilibrium systems. Efficient Monte Carlo algorithms for nonequilibrium simulation are highly demanded.

Quite recently, the present authors [1, 2] have proposed a reweighting method for nonequilibrium systems based on the Sequential Importance Sampling (SIS) [3, 4]. With reweighting, only simulation at a single temperature is required to obtain information for a range of temperatures. Moreover, the nonequilibrium relaxation method has been successfully applied to the study of critical phenomena [5, 6]. In the nonequilibrium relaxation method, simulations were performed for several temperatures; the critical temperature, the dynamical exponent and other quantities are estimated using the scaling behavior of nonequilibrium process. If we combine the strength of nonequilibrium relaxation method with a reweighting technique, we can expect an effective method of simulation.

## II. METHOD

In a Monte Carlo simulation, a sequence of points in the phase space  $\sigma_i$  are visited. Consider a simulation up to  $t$ th Monte Carlo steps and define a path as the points in phase space being visited from the 1st Monte Carlo step to the  $t$ th Monte Carlo steps as,

$$\vec{x}_t = (\sigma_1, \sigma_2, \dots, \sigma_t) \quad (1)$$

where  $\sigma_t$  is the system configuration at time  $t$ . Hereafter, we refer to the Monte Carlo step simply as the time of simulation. Such a path  $\vec{x}_t$  can be generated using any Monte Carlo method at a temperature  $T$ . Suppose many simulations were performed at an inverse temperature  $\beta = 1/k_B T$  to obtain a set of paths  $\vec{x}_t^j$ ,  $j = 1, \dots, n$  (From now on,  $\beta$  shall be referred to as temperature). The dynamical thermal average of some quantity  $Q(t)$  can be calculated by  $\langle Q(t) \rangle_\beta = (1/n) \sum_{j=1}^n Q(\vec{x}_t^j)$ . Our objective is to calculate the thermal average of  $Q(t)$  at another temperature  $\beta'$ . This can be achieved by reweighting  $Q(\vec{x}_t^j)$  with a set of weights  $w_t^j$ . For the same set of paths  $\vec{x}_t^j$ , the thermal average at  $\beta'$  is,

$$\langle Q(t) \rangle_{\beta'} = \frac{\sum_{j=1}^n w_t^j Q(\vec{x}_t^j)}{\sum_{j=1}^n w_t^j} \quad (2)$$

Although not labeled explicitly in Eq. (2), the set of weights  $w_t^j$  depend on the simulation temperature  $\beta$  and the new temperature  $\beta'$ . As presented in Lee and Okabe [1, 2], the weights can be calculated using the following algorithm,

1. Assume that the Monte Carlo simulation is carried out at a temperature  $\beta$  and a path  $\vec{x}_t^j$  for some arbitrary time  $t$  is sampled.
2. To go from time  $t$ , let  $\sigma'^j$  be a trial configuration and  $T(\sigma'^j | \sigma_t^j)$  be the probability to select this configuration. If the trial move is accepted with the acceptance probability  $A_\beta(\sigma'^j | \sigma_t^j)$ , then the new configuration at  $t+1$  becomes  $\sigma_{t+1}^j = \sigma'^j$ . If the move is not accepted,  $\sigma_{t+1}^j = \sigma_t^j$ .

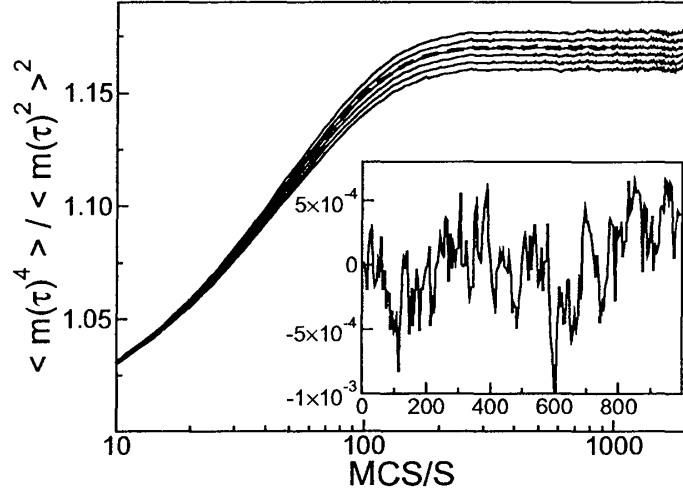


FIG. 1: Values of  $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$  for several reweighted temperatures from simulations at  $T = 2.270$ . From top to bottom,  $T = 2.272, 2.271, 2.270, 2.269, 2.268, 2.267$ . To check the range of reweighting, an additional simulation was performed at  $T = 2.268$  and reweighted to  $T = 2.270$ . Dashed line shows  $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$  at  $T = 2.270$  reweighted from  $T = 2.268$ . Insert shows that the difference between the dashed line and solid line is about  $5 \times 10^{-4}$  while error bars on  $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$  are of the order  $10^{-3}$ . The system size is  $L = 32$ .

3. In terms of transition probability  $P_\beta(\sigma_{t+1}^j | \sigma_t^j)$ , we write it as  $P_\beta(\sigma_{t+1}^j | \sigma_t^j) = T(\sigma^j | \sigma_t^j) A_\beta(\sigma_t^j | \sigma_t^j)$  if the move is accepted.  $P_\beta(\sigma_{t+1}^j | \sigma_t^j) = T(\sigma^j | \sigma_t^j) [1 - A_\beta(\sigma_t^j | \sigma_t^j)]$  if the move is not accepted.
4. We can now define an incremental weight as,  $\delta w_{t+1}^j = P_{\beta'}(\sigma_{t+1}^j | \sigma_t^j) / P_\beta(\sigma_{t+1}^j | \sigma_t^j)$  and the required weights are,

$$w_{t+1}^j = w_t^j (\delta w_{t+1}^j) \quad (3)$$

5. Repeat steps 2 to 4 until  $t$  reaches some predetermined maximum simulation time.

For each path  $\vec{x}_t^j, j = 1, \dots, n$ , these steps are repeated. The observant reader may notice that in this method, essentially the usual Monte Carlo update is carried out, and at the same time, the weights are updated.

### III. THE ISING MODEL

To illustrate how this method can be implemented, we use the ferromagnetic Ising model on a square lattice. Its Hamiltonian is given by,

$$\mathcal{H} = - \sum_{\langle kl \rangle} s_k s_l \quad (4)$$

where the sum is over nearest neighbors and  $s_k$  takes the values  $\pm 1$ . Periodic boundary conditions are used on a  $L \times L$  lattice. We use the single spin-flip update with the Metropolis acceptance rate. The simulation is performed at a temperature  $\beta$  and reweighted to several temperatures  $\beta_1, \beta_2, \dots$ . The initial system configuration at time  $t = 1$  is set to  $s_k = 1$  for all  $k = 1, \dots, N$ . Where  $N$  is the total number of lattice sites. The ratio of the moments of the order parameter is used for the analysis of the phase transition. Fig. 1 shows plots of  $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$  for several reweighted temperatures from simulations at  $T = 2.270$ . From top to bottom,  $T = 2.272, 2.271, 2.270, 2.269, 2.268, 2.267$ . The lattice size was  $L = 32$  and accuracy of reweighting was checked by performing an additional simulation at  $T = 2.268$ . This simulation was then reweighted to  $T = 2.270$  and compared to the curve from the original simulation. The dashed line in Fig. 1 shows  $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$  at  $T = 2.270$  reweighted from  $T = 2.268$ . Insert shows that the difference between the dashed line and solid line is about  $5 \times 10^{-4}$  while error bars of  $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$  are of the order  $10^{-3}$ . Averages were taken with  $1.28 \times 10^6$  samples. The systematic errors due to reweighting are smaller than the statistical errors for this temperature shift.

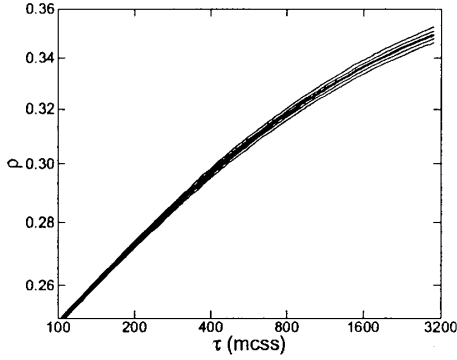


FIG. 2: Plot of order parameter with infinite drive for  $64 \times 32$  lattice with actual simulation performed at  $T = 3.160$  shown with a bold line. From top to bottom values of  $T$  are 3.150, 3.155, 3.160, 3.165, 3.170. Averages were taken over  $4.096 \times 10^6$  samples.

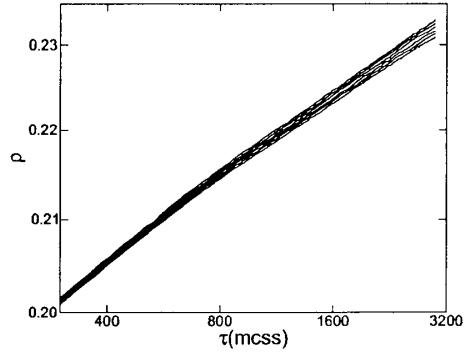


FIG. 3: Plot of order parameter with finite drive for  $32 \times 32$  lattice with actual simulation performed at  $(T, E) = (2.765, 0.515)$  and  $(T, E) = (2.780, 0.500)$ . From top to bottom values of  $T$  and  $E$  are  $(T, E) = (2.760, 0.520)$ ,  $(2.765, 0.515)$ ,  $(2.770, 0.510)$ ,  $(2.775, 0.505)$ ,  $(2.780, 0.500)$ ,  $(2.785, 0.495)$ .

#### IV. DRIVEN DIFFUSIVE LATTICE GAS

To illustrate reweighting for a perpetually nonequilibrium system, we use the driven diffusive lattice gas. This model was proposed by Katz, Lebowitz and Spohn (KLS) [7] as a model for super-ionic conductors. It is constructed as a  $L_x \times L_y$  square lattice with *half-filled* lattice sites having periodic boundary conditions. Its Hamiltonian is given by,

$$\mathcal{H} = -4 \sum_{\langle kl, k'l' \rangle} n_{kl} n_{k'l'} \quad (5)$$

where the summation is over nearest lattice sites. The variable  $n_{kl} = 1$  when the site is filled and  $n_{kl} = 0$  otherwise. The probabilities for each particle to jump to an empty nearest neighbor site are given by,

$$A_\beta = \min[1, \exp(-\beta(\Delta\mathcal{H} - \epsilon E))] \quad (6)$$

$\Delta\mathcal{H}$  represents the change in energy due to the jump,  $E$  is a constant driving force,  $\epsilon = -1, 0$  or  $1$  depending on whether the jump is against, orthogonal or along the direction of the drive, and  $\beta$  is the inverse temperature of the thermal bath. The KLS model exhibits an order-disorder second order phase transition. In the ordered phase, strips of high- and low-density domains are formed along the direction of the drive. In the final steady state, the particles are condensed into a single strip parallel to the direction of the drive. Hence the order parameter can be defined as the density profile along the direction of the drive, and moments of the order parameters are given by

$$\rho^k = \frac{1}{(L_x/2)} \sum_{j=1}^{L_x} \left| \frac{1}{L_y} \sum_{i=1}^{L_y} n_{ij} - \frac{1}{2} \right|^k, \quad (7)$$

where  $n_{ij} = 0$  or  $1$  as defined in Eq. (5), and  $k = 1, 2, 4$  represents the first, second and fourth moments of the order parameter, respectively.

We make a comment on the technical detail of calculating the weights. For case of infinite drive ( $E = \infty$ ), possible values of incremental weights  $\delta w_i$  are,

$$\begin{aligned} \delta w_0 &= 1, \\ \delta w_1 &= \exp(-12(\beta' - \beta)), \\ \delta w_2 &= \exp(-8(\beta' - \beta)), \\ \delta w_3 &= \exp(-4(\beta' - \beta)) \\ \delta w_4 &= (1 - \exp(-12\beta')) / (1 - \exp(-12\beta)), \\ \delta w_5 &= (1 - \exp(-8\beta')) / (1 - \exp(-8\beta)), \\ \delta w_6 &= (1 - \exp(-4\beta')) / (1 - \exp(-4\beta)). \end{aligned} \quad (8)$$

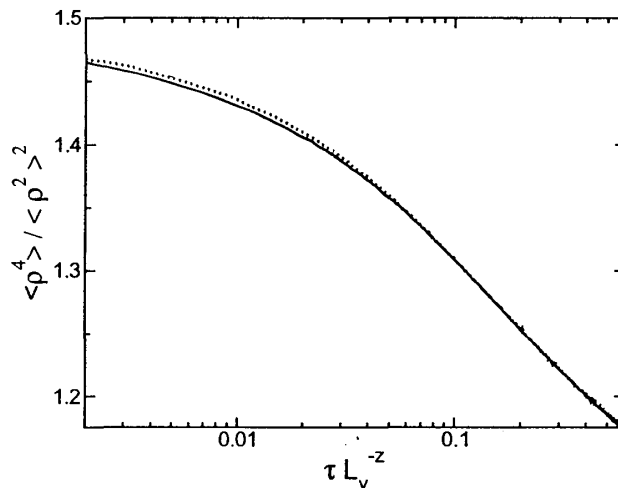


FIG. 4: Scaling plot of  $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$  versus  $\tau L_y^{-z}$  for  $z = 2.09$ ,  $L_y = 64$  (solid line) and  $L_y = 128$  (dotted line) at  $T = 3.175$ . Initial system configurations were prepared with  $\rho_0 = 0$ .

The weights can then be written as a product of incremental weights,

$$w_t^j = (\delta w_1)^{h_1^j(t)} (\delta w_2)^{h_2^j(t)} \dots (\delta w_6)^{h_6^j(t)}. \quad (9)$$

where  $h_1^j(t) \dots h_6^j(t)$  are the number of hits on the incremental weights  $\delta w_1 \dots \delta w_6$  during the course of simulation from time 1 to  $t$ . Note that  $\delta w_0$  is irrelevant in Eq. (9). Generalization of this counting method to the case of finite  $E$  is trivial. Since the calculation of weights has been reduced to accumulating a histogram, the multi-spin coding technique can be implemented not only for the spin update process but also for the calculation of histogram of incremental weights. Once the histogram  $h_1^j(t) \dots h_6^j(t)$  is obtained, using Eq. (9) allows us to reweight to a large number of temperatures (drives) with negligible extra computational efforts.

For dynamical scaling, we use the scaling relation [2] which is valid at  $T_c$ ,

$$\frac{\langle \rho^4 \rangle}{\langle \rho^2 \rangle^2} = g(\tau^{-1/z} L_y) \quad (10)$$

where  $g$  is the scaling function,  $\tau$  is Monte Carlo steps,  $z$  is the dynamical exponent and  $L_y$  is the lattice size in the direction of the drive.

We now show the results of the Monte Carlo simulation for the KLS model. We first illustrate the reweighting for the order parameter, and then show how reweighting can be combined with dynamical finite-size scaling (Eq. (10)) to calculate the critical temperature and dynamical exponent. Figure 2 shows how data over a range of temperatures can be extracted from simulations at a single temperature. The temporal evolution of the order parameter  $\rho$  for the infinite drive ( $E = \infty$ ) was investigated for  $64 \times 32$  lattice. Simulations were performed at  $T = 3.160$ , and data were reweighted to nearby temperatures,  $T = 3.150, 3.155, 3.165, 3.170$  (from top to bottom). Averages were taken over  $4.096 \times 10^6$  samples. We made independent calculations directly at  $T = 3.150$ , for example, to check the effectiveness of the reweighting. The deviation of the data between the reweighted ones from  $T = 3.160$  and the direct ones at  $T = 3.150$  are found to be the same within statistical errors.

We also made simulations for the finite drive ( $E \approx 0.5$ ). We illustrate the reweighting over both  $E$  and  $T$ . We performed two simulations at  $(T, E) = (2.765, 0.515)$  and  $(2.780, 0.500)$  for  $32 \times 32$  lattice. The combination of the order parameter is made by using  $\bar{\rho} = (\sum_{k=1}^2 \rho_k / \Delta_k^2) / (\sum_{k=1}^2 1 / \Delta_k^2)$ , where  $\rho_{1,2}$  and  $\Delta_{1,2}$  are the order parameter and error estimates from the first and second simulations, respectively. Figure 3 shows the temporal evolution of the order parameter for several temperatures and drives. Data was reweighted to several values at  $(T, E) = (2.760, 0.520), (2.770, 0.510), (2.775, 0.505), (2.785, 0.495)$ . Averages were taken over  $2.048 \times 10^6$  samples for each simulation. Generally, we found that reweighting is effective when the distributions  $P_{\beta, E}(\vec{x}_t^j)$  and  $P_{\beta', E'}(\vec{x}_t^j)$  have sufficient overlaps. Error bars and fluctuations of weights can also be used as quantitative measures on the effective range of reweighting.

To determine  $T_c$ , we use the dynamical finite-size scaling of the ratio-of-moments (Eq. (10)). Here we concentrate on the infinite drive ( $E = \infty$ ). We simulated  $64 \times 64$  and  $64 \times 128$  lattices, and calculated

the ratio of the moments,  $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$ . Fitting was performed for several temperatures near  $T_c$ , which were reweighted from the data obtained at a single temperature, and for each temperature we adjusted the value of  $z$ . The best fit was found to be at  $T = 3.175$  and  $z = 2.09$ . Figure 4 shows the scaling plot of  $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$  as a function of  $\tau L_y^{-z}$  for  $64 \times 64$  (solid line) and  $64 \times 128$  (dotted line) lattice sizes at  $T = 3.175$  and  $z = 2.09$ . The curves are almost indistinguishable at this scale although some corrections to scaling can be observed below  $\tau L_y^{-z} = 0.02$ . To study the corrections to scaling, similar fitting procedure was performed for  $64 \times 32$  and  $64 \times 64$  lattices. The best fit occurs at  $T = 3.155 \pm 0.005$  with  $z = 2.23 \pm 0.03$ . The estimate for  $T_c$  increases with the system size, whereas that for  $z$  decreases. Our estimates of  $T_c$  and  $z$  are compatible with the recent estimates for infinite lattice,  $T_c = 3.1980 \pm 0.0002$  [8],  $T_c = 3.200 \pm 0.010$  [9],  $z = 2.016 \pm 0.040$  [9]. A more systematic analysis of the corrections to scaling to get a precise estimate of  $T_c$  and several critical exponents for infinite lattice will be left to a separate publication. Before closing we show the actual procedure of the reweighting for each system size. For  $64 \times 32$  lattice,  $4.096 \times 10^6$  samples were used for the simulation at  $T = 3.16$ . For  $64 \times 64$  lattice,  $8.19 \times 10^5$  samples were used for each simulation at  $T = 3.174$  and  $3.180$ . Results were then reweighted to other temperatures and combined using weighted mean,  $\bar{r} = (\sum_{k=1}^2 r_k / \Delta_k^2) / (\sum_{k=1}^2 1 / \Delta_k^2)$ . Here  $r_{1,2}$  and  $\Delta_{1,2}$  are the ratio-of-moments and error estimates from the first and second simulations, respectively. For  $64 \times 128$  lattice size,  $1.64 \times 10^5$  samples were used for each simulation at  $T = 3.174, 3.177$  and  $3.180$ , and reweighted results were combined using the same procedure.

## V. DISCUSSIONS

We have shown how reweighting can be done on nonequilibrium systems and presented two examples of its applications. We propose that the nonequilibrium reweighting method is most effective when combined with finite size scaling of the nonequilibrium relaxation process.

Finally, we make a remark on possible applications. The nonequilibrium reweighting method should be applicable with other Monte Carlo updates, such as cluster updates and N-fold way. The nonequilibrium reweighting method has very interesting properties. For example, for nonequilibrium systems, the derivatives of thermodynamic quantities cannot be calculated using the fluctuation-dissipation theorem. With reweighting, the derivatives can be calculated directly by differentiating the weights explicitly, that is,

$$\frac{d\langle Q(t) \rangle_{\beta'}}{d\beta'} = \frac{\sum_{j=1}^n Q(\vec{x}_t^j) \frac{dw_t^j}{d\beta'}}{\sum_{j=1}^n w_t^j} - \langle Q(t) \rangle_{\beta'} \frac{\sum_{j=1}^n \frac{dw_t^j}{d\beta'}}{\sum_{j=1}^n w_t^j}. \quad (11)$$

Here,  $dw_t^j/d\beta'$  can be obtained by differentiating Eq. (9) with respect to  $\beta'$ . We believe that the nonequilibrium reweighting method would have several directions for applications.

This work is supported by a Grant-in-Aid for Scientific Research from the Japan Society for the Promotion of Science. The computation of this work has been done using computer facilities of the Supercomputer Center, Institute of Solid State Physics, University of Tokyo.

- 
- [1] H. K. Lee and Y. Okabe, Phys. Rev. Lett. **71**, 015102R (2005).
  - [2] H. K. Lee and Y. Okabe, J. Phys. A: Math. Gen. **38**, L241 (2005).
  - [3] A. Doucet, N. De Freitas and N. Gordon, *Sequential Monte Carlo Methods in Practice*, (Springer, New York, 2001).
  - [4] J. L. Zhang and J. S. Liu, J. Chem. Phys. **117**, 3492 (2002); A brief introduction of the SIS method is given in the appendix.
  - [5] H. J. Luo, L. Schülke and B. Zheng, Phys. Rev. Lett. **81**, 180 (1998).
  - [6] N. Ito, K. Hukushima, K. Ogawa and Y. Ozeki, J. Phys. Soc. Jpn. **69**, 1931 (2000).
  - [7] S. Katz, J. L. lebowitz and H. Sophn, Phys. Rev. B **28**, 1655 (1983).
  - [8] S. Caracciolo, A. Gambassi, M. Gubinelli and A. Pelissetto, J. Phys. A **36**, L315 (2003).
  - [9] G. P. Saracco and E. V. Albano, J. Chem. Phys. **118**, 4157 (2003).