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Worm algorithms for classical statistical models

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We show that high-temperature expansions may serve as a basis for the novel approach to efficient Monte Carlo simulations. "Worm" algorithms utilize the idea of updating closed path configurations (produced by high-temperature expansions) through the motion of end points of a disconnected path. An amazing result is that local, Metropolis-type schemes may have dynamical critical exponents close to zero (i.e., their efficiency is comparable to the best cluster methods). We demonstrate this by calculating finite size scaling of the autocorrelation time for various universality classes.

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Metropolis scheme [1] is usually the most universal and easy to program approach to Monte Carlo simulations. However, its advantages are virtually canceled out near phase transition points. It is believed that any scheme based on local [2] Metropolis-type updates connecting system configurations into Markovian chain is inefficient at the transition point because its autocorrelation time, τ , scales as L^z , where L is the system linear dimension and z is the dynamical critical exponent which is close to 2 in most systems [3,4].

An enormous acceleration of simulations at the critical point has been achieved with the invention of cluster algorithms by Swendsen and Wang [5]. However, the original method and its developments (both classical and quantum) [6–8] are essentially non-local schemes, and we are not aware of any exception from this rule.

In this Letter we propose a method which essentially eliminates the critical slowing down problem and yet remains local. The corner stone of our approach is the possibility to introduce the configuration space of closed paths. Closed-path (CP) configurations may be then sampled very efficiently using Worm algorithm (WA) introduced in Ref. [9] for quantum statistical models in which closed trajectories naturally arise from imaginary-time evolution of world lines. In classical models the CP representation derives from high-temperature expansions for a broad class of lattice models (see, e.g. Ref. [10]). In 2D, another family of WA may be introduced by considering domain-wall boundaries as paths.

We note, that our approach is based on principles which differ radically from cluster methods and, most probably, has another range of applicability. For one thing, the CP representation is most suitable for the study of superfluid models by having direct Monte Carlo estimators for the superfluid stiffness (through the histogram of winding numbers [11]) which are not available in the standard site representation.

In what follows we first recall how high-temperature expansions work by employing Ising model as an example (still, trying to keep notations as general as possible). We then explain how WA is used to update the path configuration space. Next, we discuss specific implemen-

tations of WA for $|\psi|^4$ -, XY-, and $q = 3$ Potts models, and comment on the special property of 2D models which allows an alternative CP parameterization of the configuration space. The efficiency of the new method is studied by looking at autocorrelation properties for six different universality classes. It is found that for 2D and 3D Ising models, 2D and 3D XY-models, and Gaussian model the $\tau(L)$ scaling is consistent with the law $\tau(L) = \tau_0 + c \ln(L)$, i.e., its critical exponent is close to zero. For the two-dimensional $q = 3$ Potts model our data are consistent with the power law with $z \approx 0.55$ which means that the Li-Sokal [12] bound $z > \alpha/\nu$ (α and ν are the specific heat and correlation radius critical exponents) derived for the Swendsen-Wang algorithm is seemingly applicable to our method as well.

Since high-temperature expansions for various models can be found in standard texts (see, e.g., Ref. [10]) we briefly remind the procedure for the Ising model

$$-\frac{H}{T} = \beta \sum_{b=\langle ij \rangle} s_i s_j, \quad (1)$$

where $\beta = J/T$ is the dimensionless nearest-neighbor coupling parameter between spin variables $s_i = \pm 1$ and index $b = \langle ij \rangle$ refers to the simple cubic/square lattice bonds (we will also use another notation: $b = (i, \nu)$, in which ν enumerates bonds containing site i). Since H is additive, the corresponding Gibbs exponent factories in terms of exponents for each bond. Expanding each exponent in Taylor series allows one to perform summation over site variables and to arrive at an expansion in powers of β . The partition function, for example, takes the form

$$Z = \sum_{\{s_i\}} \prod_{b=\langle ij \rangle} \left(\sum_{N_b=0}^{\infty} \frac{\beta^{N_b} (s_i s_j)^{N_b}}{N_b!} \right) = \sum_{CP} W_{CP}. \quad (2)$$

Note that summation includes all possible CPs, both connected and disconnected, with self-intersections and overlaps. Graphically, each elementary factor in the order-by-order expansion over the bond Hamiltonian can be represented by a line ascribed to the corresponding bond

[10], and the closed path constraint is imposed by symmetry: the sum $\sum_{s_i} s_i^{k_i}$ is non-zero only if the number of bond lines connected to the site i is even. For future purposes it is convenient to denote the number of bond lines $N_b = 0, 1, 2, \dots$ and call it the “bond state”. Then the “site state” is $k_i = \sum_{\nu} N_{i,\nu}$, and the configuration weight, W_{CP} , is given by

$$W_{CP} = \left(\prod_b \frac{\beta^{N_b}}{N_b!} \right) \left(\prod_i Q(k_i) \right), \quad Q(k) = \sum_{s_i} s_i^k. \quad (3)$$

[$Q(k) \equiv 2$ for the Ising model.]

The spin-spin correlation function $G(i_1 - i_2) = \langle s_{i_1} s_{i_2} \rangle$ (we understand site indices as vectors) by definition equals to $g(i_1 - i_2)/Z$ where $g(i_1 - i_2) = \sum_{\{s_i\}} s_{i_1} s_{i_2} e^{-H/T}$. Configurations for g differ from those contributing to the partition function in only one respect: there are two special sites i_1 and i_2 with odd number of bond lines connected to them, see Fig. 1. The corresponding site states are given by $k_i = 1 + \sum_{\nu} N_{i,\nu}$. These points are the only places where the path may be disconnected. We will abbreviate the configuration space for $g(i)$ as CP_g , and note, that weights W_{CP_g} are given by the same expression (3).

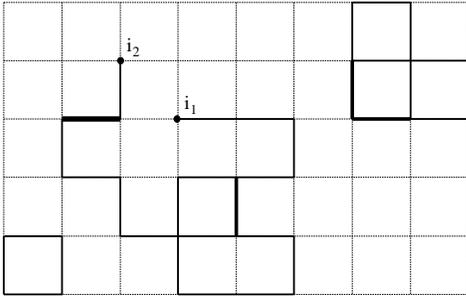


FIG. 1. A typical configuration with the “Worm”. The two circles correspond to the extra s_{i_1} and s_{i_2} variables, and the solid line width is proportional to the bond state number N_b (number of elementary lines); 0-th order terms are shown by dashed lines.

The above consideration is actually a perfect setup for the Monte Carlo simulation since configurations for Z and for $g(0)$ have identical bond elements (for the Ising model they even have equal weights, i.e. $g(0) = Z$). Thus, if an ergodic Metropolis process is sampling g -configurations according to their weights, then the Monte Carlo estimators for $g(i)$ and Z are just

$$g(i|CP_g) = \delta_{i_2 - i_1, i}, \quad Z(CP_g) = \delta_{i_2 - i_1, 0}. \quad (4)$$

The spin susceptibility is given by $\chi = \sum_i g(i)/Z$, and energy may be computed in two ways: (i) as the nearest-neighbor sum $E = (L^d/2)\beta \sum_{|i|=1} g(i)/Z$, and (ii) using direct estimator, $E = \mathcal{E}/Z$, which is non-zero only for the CP configurations contributing to Z :

$$\mathcal{E}(CP) = \beta \sum_b N_b. \quad (5)$$

Our results for τ were obtained using this estimator.

The WA emerges as an idea to update g -configurations through the space motion of the end points i_1 and i_2 only [9]. The algorithm itself is extremely simple and consists of two elementary updates which are proposed in the context of a given configuration: if $i_1 = i_2$, then with probability p_0 we suggest to “move” both end points to site i_0 selected at random among all L^d lattice sites, and with probability $p_1 = 1 - p_0$ to “shift” the end point i_1 to one of the neighboring sites by selecting the direction of the shift at random; if $i_1 \neq i_2$ we always suggest to “shift” i_1 .

For the Ising model the move-update is automatically self-balanced and its acceptance ratio is unity, otherwise it would involve the ratio of Q -functions

$$P_{mv}(i \rightarrow j) = \frac{Q(k_j + 2)}{Q(k_j)} \frac{Q(k_i - 2)}{Q(k_i)}. \quad (6)$$

In contrast, shift-updates also increase/decrease the bond state by “drawing/erasing” bond lines, and we select which way to proceed with probability 1/2. The shifts $i \rightarrow j$ with $N_{b=\langle ij \rangle} \rightarrow N_b + 1$ are balanced by shifts $j \rightarrow i$ with $N_b \rightarrow N_b - 1$. By standard rules [1] we have acceptance ratios as

$$P_{sh}(i \rightarrow j, N_b \rightarrow N_b + 1) = r \frac{\beta}{(N_b + 1)} \frac{Q(k_j + 2)}{Q(k_j)}, \quad (7)$$

$$P_{sh}(i \rightarrow j, N_b \rightarrow N_b - 1) = r \frac{N_b}{\beta} \frac{Q(k_i - 2)}{Q(k_i)}, \quad (8)$$

where

$$r = \begin{cases} 1/(2p_1) & \text{if } i_1 = i_2 = i, \\ 2p_1 & \text{if } i_1 = i, i_2 = j, \\ 1 & \text{otherwise} \end{cases} \quad (9)$$

The Ising model has a special property which can be used in practical applications to enhance the efficiency by truncating the configuration space. Namely, using identity $e^{\beta s_i s_j} \equiv \cosh \beta [1 + \tanh \beta s_i s_j]$ one can restrict the bond summation to include terms $N_b = 0, 1$ only. The corresponding modifications of the scheme are straightforward.

We now turn to the $|\psi|^4$ -model described by the Hamiltonian (ψ_i is a complex variable)

$$-\frac{H}{T} = \sum_{\langle ij \rangle} (\psi_i \psi_j^* + c.c.) + \sum_i [\mu |\psi_i|^2 - U |\psi_i|^4], \quad (10)$$

the two limiting cases of which are the Gaussian model, $U = 0$, and the XY -model, $U = \infty$. The procedure of factorizing the partition function expansion in terms

of the bond Hamiltonian is exactly as before. The only new ingredient which is not present in the Ising model, is that for each bond we have two *different* terms: $\psi_i\psi_j^*$ and $\psi_i^*\psi_j$, and therefore the expansion has to be performed for each of them separately. Graphically, this can be captured by drawing lines with arrows, thus specifying each term by the arrow direction. Correspondingly, the bond state is defined by two numbers $(N_b^{(1)}, N_b^{(2)})$ which tell how many lines and in which direction go along this bond. Since integrals $\int d\psi e^{\mu|\psi|^2 - U|\psi|^4} \psi^m (\psi^*)^{m'} = \delta_{m,m'} Q(k=2m)$ are non-zero only for $m=m'$, we conclude that the configuration space for Z is defined on CP and site states are given by $k_i = \sum_\nu (N_{i,\nu}^{(1)} + N_{i,\nu}^{(2)}) = \text{even}$. [The $Q(k)$ integrals are easily tabulated prior to the simulation.]

In close analogy with the previous case, the configuration space for the two-point correlation function $g(i_1 - i_2) = \int \prod_i d\psi_i \psi_{i_1} \psi_{i_2}^* e^{-H/T}$, is given by CP $_g$ containing two special sites with $k_i = 1 + \sum_\nu (N_{i,\nu}^{(1)} + N_{i,\nu}^{(2)})$. WA updates consist of “moves” which change the location of end points when $i_1 = i_2$ and “shifts” of i_1 which increase/decrease numbers $N_{i_1,\nu}^{(1)}$ and $N_{i_1,\nu}^{(2)}$. Acceptance ratios are given by Eqs. (6-8) where N_b is understood as one of the numbers describing the bond state. An estimator for the winding number (which has exactly the same meaning as in worldline quantum Monte Carlo [11]) of the CP configuration is given by the difference between the bond numbers

$$M_\alpha = L^{-1} \sum_{b_\alpha} (N_{b_\alpha}^{(1)} - N_{b_\alpha}^{(2)}) , \quad (11)$$

where $\alpha = x, y, z, \dots$, and notation b_α is used to specify bonds connecting sites in direction α .

The $q = 3$ Potts model (which we considered to compare with the exhaustive cluster method study by Li and Sokal [12]) is described by

$$-\frac{H}{T} = \beta \sum_{\langle ij \rangle} (\delta_{s_i, s_j} - 1) , \quad s_i = 0, 1, 2 . \quad (12)$$

Introducing phase variable $\varphi_i = (2\pi/3)s_i$ we can rewrite Eq. (12) (up to a constant term) as

$$-\frac{H}{T} = \beta' \sum_{\langle ij \rangle} (e^{i(\varphi_i - \varphi_j)} + c.c.) , \quad \beta' = \beta/3 . \quad (13)$$

With this form one may immediately proceed with the WA along the lines described above for the $|\psi|^4$ -model. However, more efficient scheme results from the identity $e^{2\beta' \cos(\varphi_i - \varphi_j)} = A[1 + \gamma \cos(\varphi_i - \varphi_j)]$, where $A = (e^{2\beta'} + 2e^{-\beta'})/3$ and $\gamma = 2(e^{2\beta'} - e^{-\beta'})/3A$, which allows to restrict summation over bond states to just three values $N_b = (0, 0), (1, 0), (0, 1)$.

We would like to comment that high-temperature expansions are *not* the only procedure to arrive at the CP configuration space and WA. To underline this point we

note that in lattice models with discrete site variables one can unambiguously specify the state of the system (up to symmetry transformations) by drawing domain boundaries, which, in 2D, may be considered as a CP configuration. For the Ising model the configuration weight is simply $W_{CP} = \prod_b e^{\beta(2N_b - 1)}$ where the bond state takes values $N_b = 0, 1$.

To implement WA for efficient sampling of domain boundaries we formally enlarge the configuration space to include CP $_g$ configurations with two end points and proceed exactly as discussed above. The only difference is that now “open” boundaries with $i_1 \neq i_2$ have *no* physical meaning and serve just for updating purposes. Our results for the 2D Ising model in Fig. 2 were obtained using domain-wall representation.

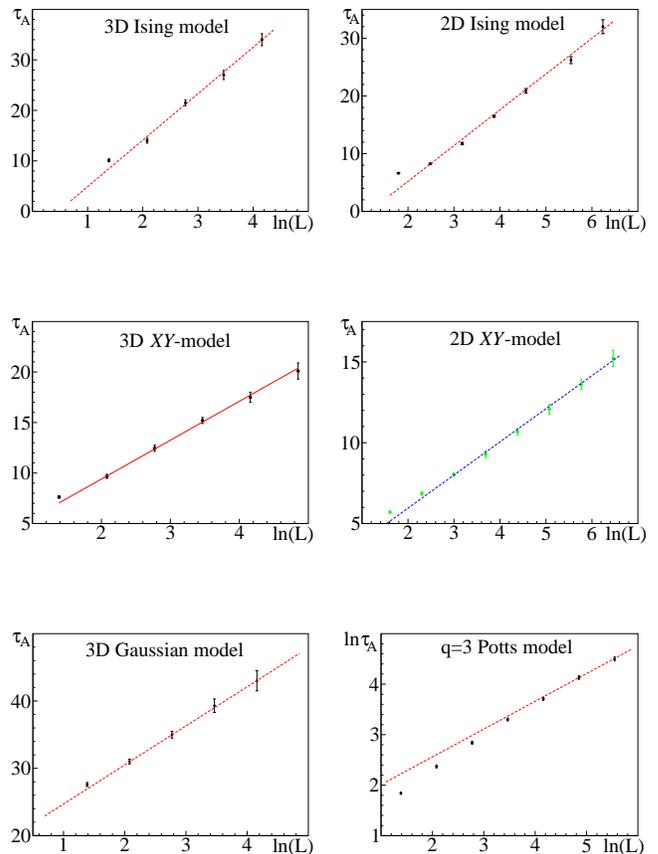


FIG. 2. Autocorrelation times for various universality classes. The 3D Ising model is fitted to $\tau = -4.3 + 9.2 \ln(L)$, and $z(L = 64) = 0.18$ (see text). The 2D Ising model is fitted to $\tau = -7.2 + 6.2 \ln(L)$, and $z(L = 512) = 0.25$. The 3D XY-model is fitted to $\tau = 1.7 + 3.85 \ln(L)$, and $z(L = 128) = 0.2$. The 2D XY-model is fitted to $\tau = 1.85 + 2.05 \ln(L)$, and $z(L = 640) = 0.16$. The 3D Gaussian model is fitted to $\tau = 18.9 + 5.8 \ln(L)$, and $z(L = 64) = 0.17$. The $q = 3$ Potts model in 2D is fitted to the power law $\tau = 4.3L^{0.55}$.

In Fig. 2 we present data for the energy autocorrelation time. In all cases, except $q = 3$ Potts model in 2D, they are consistent with the linear in $\ln L$ behavior. Of course, we may not exclude that logarithmic scaling is actually an intermediate length-scale behavior and at some larger L it crosses over to the power law, $\tau(L) \sim L^z$, with small z . To get an estimate (upper bound) for the possible dynamic exponent we mention in the figure caption the slope $z(L) = d \ln(\tau)/d \ln(L)$ at the largest simulated L . For the $q = 3$ Potts model our data scale as $\tau \sim L^{0.55}$ for $L > 64$, although the dynamic exponent is showing a systematic decrease with L . This has to be compared with the value $z = 0.515$ for the Swendsen-Wong algorithm [12]. It seems that the Li-Sokal lower bound for the dynamic exponent $z > \alpha/\nu$ also applies to our method. For all models discussed here α/ν is very small with exception of the $q = 3$ Potts model where $\alpha/\nu = 0.4$.

To summarize, we found that WA Monte Carlo schemes working with closed path representations of classical statistical models are as efficient as the best cluster methods in reducing the problem of critical slowing down near transition points. The new approach is general enough to find applications other than discussed in this Letter, and may be used to study quantities like superfluid density for which other methods may not have direct estimators.

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