A cluster Monte Carlo algorithm with a conserved order parameter

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We propose a cluster simulation algorithm for statistical ensembles with fixed order parameter. We use the tethered ensemble, which features Helmholtz’s effective potential rather than Gibbs’s free energy, and in which canonical averages are recovered with arbitrary accuracy. For the $D = 2, 3$ Ising model our method’s critical slowing down is comparable to that of canonical cluster algorithms. Yet, we can do more than merely reproduce canonical values. As an example, we obtain a competitive value for the 3D Ising anomalous dimension from the maxima of the effective potential.

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Monte Carlo simulations constitute one of the most important modern tools of theoretical physics. In situations that defy an analytical treatment, a Monte Carlo computation succeeds by wandering randomly across the system’s configuration space. Over the years many methods have been proposed in order to optimize this sampling process. Here we combine two: fixing some global parameter, in the first case it outperforms the Metropolis method in the standard benchmark of the dynamical system. This ensemble arises from the canonical development of an efficient cluster method in this situation.

Despite continued research on cluster methods, the de-
celeration of the dynamics in Ising models (\eta is the anomalous dimension) is smaller. Beyond the canonical ensemble setting, considering global conservation laws is often useful (as in micromagnetic or microcanonical ensembles). It is known that $z = 4 - \eta$ for locally conserved order parameter dynamics in Ising models (\eta is the anomalous dimension). For non-local conservation laws $z$ is smaller. Despite continued research on cluster methods, the development of an efficient cluster method in this situation has long been considered somewhat of a challenge.

Here we present a working cluster algorithm with a globally conserved order parameter. We employ the Tethered Monte Carlo (TMC) framework, which we briefly review. TMC is a general approach to reconstruct the effective potential. We demonstrate our cluster method in the standard benchmark of the $D = 2, 3$ Ising model. In the first case it outperforms the Metropolis version of the Swendsen-Wang algorithm.

The tethered ensemble is similar to the micromagnetic one, but instead of fixing the magnetization we couple it to a Gaussian ‘magnetostat’ in order to define a new parameter, \( \hat{m} \). This ensemble arises from the canonical one through a Legendre transformation that replaces the magnetic field \( h \) by \( \hat{m} \). Thus, Helmholtz’s effective potential takes the place of Gibbs’s free energy. The main observable is the tethered magnetic field \( \hat{h} \), considered as a function of \( \hat{m} \).

We shall work on the Ising model in a cubic lattice of size \( N = L^3 \) and periodic boundary conditions, with partition function \( \langle \cdot, \cdot \rangle \); nearest neighbors)

\[
Z = \sum_{\{\sigma_x\}} \exp \left[ \beta \sum_{(x,y)} \sigma_x \sigma_y \right], \quad \sigma_x = \pm 1. \quad (1)
\]

We shall consider its energy and magnetization,

\[
E = N \varepsilon = -\frac{1}{D} \sum_{(x,y)} \sigma_x \sigma_y, \quad M = N m = \sum_x \sigma_x. \quad (2)
\]

We use lower-case for densities so that, for instance, \( \varepsilon \) is the energy per bond. Canonical averages are denoted by \( \langle \cdot \rangle \), as in the specific heat and susceptibility:

\[
C = N \left( \langle e^2 \rangle_{\beta} - \langle e \rangle_{\beta}^2 \right), \quad \chi = N \left( \langle m^2 \rangle_{\beta} - \langle m \rangle_{\beta}^2 \right). \quad (3)
\]

Note that the probability density (pdf) \( p_1(m) \) is the sum of \( N + 1 \) Dirac deltas. We smooth it by coupling \( m \) to \( N \) Gaussian demons to build the tethered ensemble

\[
\hat{M} = N \hat{m} = M + \frac{1}{2} \sum_i \phi_i^2. \quad (4)
\]

As the \( \phi_i \) are independent, \( \hat{m} \simeq m + 1/2 \). The definitions of the pdf \( p(\hat{m}) \) for \( \hat{m} \) and of the effective potential \( \Omega_N(\hat{m}, \beta) \) are straightforward

\[
p(\hat{m}) = e^{\Omega_N(\hat{m}, \beta)} = \frac{1}{Z} \int_{-\infty}^{\infty} \prod_{i=1}^N d\phi_i \sum_{\{\sigma_x\}} e^{-\beta E + \hat{M} - \hat{M}^2} \delta \left( \hat{m} - m - \sum_i \phi_i^2/(2N) \right). \quad (5)
\]

Our use of demons is reminiscent of Creutz’s microcanonical algorithm, but we shall integrate the \( \phi_i \) out in order to define our tethered averages,

\[
\langle O \rangle_{\hat{m}, \beta} = \frac{\sum_{\{\sigma_x\}} O(\hat{m}; \{\sigma_x\}) \omega_N(\beta, \hat{m}; \{\sigma_x\})}{\sum_{\{\sigma_x\}} \omega_N(\beta, \hat{m}; \{\sigma_x\})}, \quad (6)
\]
where $O$ represents a generic observable and
\[
\omega_N(\beta, \hat{m}; \{\sigma_x\}) = e^{-\beta E + M - M (\hat{m} - m)} (N - 2) / 2 \theta(\hat{m} - m),
\]
(7) ($\theta$ is Heaviside’s step function). Then we find that
\[
\hat{h} = -1 + N/2 - 1 \frac{M - M}{M - M}. \quad \langle \hat{h} \rangle_{\hat{m}, \beta} = \frac{\partial \Omega_N(\hat{m}, \beta)}{\partial \hat{m}}.
\]
(8) Therefore, we can construct the effective potential by integrating $\langle \hat{h} \rangle_{\hat{m}, \beta}$ on $\hat{m}$. Once we have $\Omega_N(\hat{m}, \beta)$ we can compute canonical averages for any given value of the external magnetic field $h$ with the formula
\[
\langle O \rangle_{\beta}(h) = \int \frac{d\hat{m}}{\Omega_N(\hat{m}, \beta) \hat{m}} e^{\langle \hat{h} \rangle_{\hat{m}, \beta} + \hat{h} \hat{m}} e^{\Omega_N(\hat{m}, \beta) + \hat{h} \hat{m}}.\]
(9)

The TMC simulation algorithm consists of four steps: (1) Select an appropriate sampling $\hat{m}_i$, $i = 1, \ldots, N_\hat{m}$ for $\hat{m}$, keeping in mind that $\hat{m} \simeq m + 1/2$. (2) Run independent simulations for each $\hat{m}_i$, measuring the tethered averages $\langle O \rangle_{\hat{m}, \beta}$. (3) Integrate (a smooth interpolation of) $\langle \hat{h} \rangle_{\hat{m}, \beta}$ to obtain $\Omega_N(\hat{m}, \beta)$. (4) Use equation (9) to recover the canonical averages. Figure 1 illustrates this process for the 3D Ising model. Let us remark that this is the algorithm for reproducing canonical averages. However, see below, one can also obtain physically relevant results directly from the tethered averages.

In [10] we implemented this algorithm, using Metropolis dynamics for step (2). Surprisingly enough, magnetic observables such as $\hat{h}$ or $m$ presented no critical slowing down (other quantities such as the energy presented the $z \approx 2$ behavior typical of a local update [7]).

Our cluster algorithm, a tethered version of Swendsen-Wang, is best explained using the bond-occupation variables $n_{xy}$ $(= 0, 1)$ and the conditional probability distributions of $[12]$. The lattice bond joining neighboring sites $x$ and $y$ is occupied if $n_{xy} = 1$. The occupied bonds partition the lattice in connected clusters of size $N_i$, $i = 1, \ldots, N_c$. Plugging in (7) the identity
\[
e^{\beta (\sigma_x \sigma_y - 1)} = \sum_{n_{xy} = 0, 1} [((1 - p) \delta_{n_{xy} = 0} + p \delta_{\sigma_x \sigma_y}) \delta_{n_{xy} = 1}],\]
(10) where $p = 1 - e^{-2 \beta}$, we immediately read the conditional probabilities of the spins given the bonds and vice versa: (a) As in a canonical case, given the $\{\sigma_x\}$, bonds are independent and $n_{xy}$ is 1 with probability $p \delta_{\sigma_x \sigma_y}$, (b) Given the $n_{xy}$ the $N_i$ spins within cluster $i$ are equal to $S_i \pm 1$. The probability of the $2^{N_c} \{S_i\}$ configurations depends on $M = \sum_i N_i$ through eq. (11):
\[
p(\{S_i\}) \propto e^{M - 2^{N_c} (M - M) (N - 2) / 2 \theta(M - M)}.
\]
(11)

Our cluster update will consist, then, in a cluster tracing using conditioned probability (a) and in a cluster flipping using (b). For this last step we perform a dynamical Monte Carlo, taking the $S_i$ at $t = 0$ from the initial spin configuration. At each $t$ we select $N'_c \ll N_c$ different clusters. We then use (11) to perform a heat bath among the $2^{N_c}$ configurations with the remaining $N_c - N'_c$ clusters fixed [22]. We take $N'_{rep}$ such steps.

Taking $N'_{rep} > 1$ steps is advantageous because over a large number of repetitions many of the $S_i$ will eventually be flipped, decorrelating the system. Furthermore, it takes much longer to trace the clusters than to flip them once, so $N'_{rep}$ can be made relatively large without noticeably increasing the simulation time. In Figure 2 we

![Figure 1](image1.png)

**FIG. 1:** (color online). Computation of the effective potential $\Omega_N(\hat{m}, \beta)$, eq. [5], for an $L = 128$ Ising 3D lattice. **Top:** We simulate each point independently to measure $\langle \hat{h} \rangle_{\hat{m}, \beta}$, eq. [8], (the lines are cubic splines and the errors are much smaller than the points). **Bottom:** This curve is then integrated to yield $p(\hat{m})$, which we show in a linear (□) and in a logarithmic (○) scale. **Inset:** $\langle \hat{h} \rangle_{\hat{m}, \beta}$ for $\hat{m} \simeq m + 1/2 > 1/2$.

![Figure 2](image2.png)

**FIG. 2:** (color online). Spin overlap, eq. [12], in a 2D critical $L = 512$ Ising model at the central minimum (□) and right maximum (○) of the effective potential [5].
represent the overlap

$$o = \frac{\langle \sum_x \left[ \sigma_{x}^{(t=0)} \sigma_{x}^{(t=N_{rep})} - \langle m \rangle_{m,\beta}^{2} \rangle \rangle_{m,\beta} \rangle_{m,\beta}}{N(1 - \langle m \rangle_{m,\beta}^{2})},$$

which vanishes for completely uncorrelated configurations. Clearly, the configuration can significantly evolve for a fixed distribution of the bonds. A major error reduction (a factor 25 in our largest lattices) is achieved by measuring $h$ at each of the $N_{rep}$ steps.

Naturally, one must eventually refresh the bond configuration. A simulation at fixed $\hat{m}$ then consists of $N_{MC}$ steps where one traces the clusters and performs $N_{rep}$ iterations of the random walk in the $S_{i}$ space. We have empirically found that an $N_{rep}$ that equilibrates the cluster-tracing and cluster-flipping times is close to optimal, and very easy to find (one only has to scale $N_{rep}$ with $N$, as the tracing of clusters is an $O(N\ln N)$ operation). For $N = 256^{3}$ spins, this results in $N_{rep} \approx 5 \cdot 10^{5}$.

The efficiency of a MC method is best assessed through the equilibrium autocorrelation function [13] for an observable $O$, $C_{O}(t) = \langle \left[ O(0) - \langle O \rangle \right] [O(t) - \langle O \rangle] \rangle$. The slowness of the dynamics can be quantified with the integrated autocorrelation time $\tau_{O}$. Defining $\rho_{O}(t) = C_{O}(t)/C_{O}(0)$, $\tau_{O}$ is just the time integral of $\rho_{O}(t)$ in $(0, \infty)$. We estimate it with the self-consistent window method [15] for our numerical estimate $\hat{\rho}_{O}$ of $\rho_{O}$,

$$\tau_{O} = \frac{1}{2} + \sum_{t=1}^{A} \hat{\rho}_{O}(t), \quad A = W \tau_{O}. \tag{13}$$

We typically use $W = 6$, but have checked that the results are consistent for several $W$’s. Since $\tau_{O} \propto L^{\eta_{O}}$, one is interested in the observable with largest $z_{O}$ ($E$ in our case, as is typical for cluster methods).

We have used $\tau_{E}$ to assess our algorithm’s performance for the Ising model in two (at $\beta = \beta_{c} = \ln(1 + \sqrt{2})/2$ and three dimensions (at $\beta = 0.22165459 \approx \beta_{c}$ [10]). For both $D’s$, we find that the $\tau_{E}$ are largest at $\hat{m} = 0.5$ (the central minimum of $p(\hat{m})$), so we report their values at that point in Table I. In 2D we obtain $z_{E} = 0.241(7)$, while in 3D our dynamic exponent is $z_{E} = 0.472(8)$, compatible with the Swendsen-Wang value of $z_{E} = 0.460(5)$ [14]. We also include our results with a slightly modified algorithm, where we take two Metropolis steps each cluster step. This mixed algorithm has significantly smaller $\tau_{E}$ in both dimensions. Paradoxically, in 3D, $z_{E} > z_{E}$ ($z_{E}$ is unmeasurable in 2D), which probably means that larger $L$ would be needed to compute it properly. Since for our lattice sizes the mixed algorithm fares better, we shall use it hereafter.

As a proof of TMC’s accuracy, we have reproduced some of the critical Swendsen-Wang simulations of [14] for the 3D Ising model (Table II). In accordance with our $\tau_{E}$ analysis, the errors with both algorithms are comparable. In 2D, the new cluster algorithm outperforms Metropolis. For instance, for an $L = 1024$ lattice, taking 10 times fewer steps than in [10] and the same $\hat{m}_{\beta}$ grid, cluster errors are 8 times smaller for $E$, 6 times smaller for $C$ and 10 times smaller for $\chi$ and $\xi$.

| $L$ | Cluster | Met. + Cluster | Swendsen-Wang |
|-----|---------|----------------|---------------|
| 16  | 2.310(14) | 0.775(3) | 5.459(3) |
| 24  | 2.440(26) | 0.920(4) | 7.963(9) |
| 32  | 2.758(20) | 1.055(5) | 9.831(9) |
| 64  | 3.347(22) | 1.147(7) | 11.337(12) |
| 128 | 4.11(5) | 1.861(12) | 13.90(3) |
| 256 | 4.87(4) | 2.391(16) | 15.90(5) |
| 512 | 5.79(8) | 3.040(24) | 19.10(9) |
| 1024| 6.78(8) | 3.70(4) | 21.83(10) |

TABLE I: Integrated autocorrelation times for the energy at $\hat{m} = 0.5$ and $\beta = \beta_{c}$, for $D = 2, 3$ Ising model. We compare the cluster and mixed versions of our TMC algorithm. We also include the results of [14] for canonical Swendsen-Wang. Our values for $z_{E}$ are fits to $\tau_{E} = AL^{z_{E}}$, where the smallest lattice in range is $L_{min} = 128$ (2D) and $L_{min} = 32$ (3D).
values of $\hat{m}$ at either side of the peak, and use a linear interpolation. Our 3D results are in Table III.

We have found that eq. (14) yields remarkably good fits for $L_{\text{min}} = 48$. Furthermore, increasing $L_{\text{min}}$ results in compatible values of $\eta$, with growing errors. Our preferred estimate is $\eta = 0.0360(7)$, where we took the central value from $L_{\text{min}} = 48$ and the error from $L_{\text{min}} = 64$ to account for systematic effects. This estimate compares favorably with the best Monte Carlo computation known to us, $\eta = 0.0362(8)$ [18], and is compatible with a high-temperature expansion value of $\eta = 0.0363(15)$ [19] (however, both quoted values [18, 19] were computed with a perfect action, not in the Ising model).

In summary, we have shown how models with conserved order parameter can be efficiently simulated with a cluster method. We work in the tethered ensemble framework, which allows us to compute the Helmholtz effective potential. The method is tested in the $D = 2, 3$ Ising model. For the computation of canonical expectation values in large lattices, our cluster algorithm is no less efficient than a canonical one in 3D (in 2D the dynamical exponent $z \approx 0.24$ is larger than that for the canonical algorithm, but still very small). The tethered ensemble permits a very efficient computation of quantities such as the maxima of the effective potential, which would be extremely costly to reproduce in a canonical setting. Our estimate for the anomalous dimension of the 3D Ising model compares favorably with all previous Monte Carlo computations known to us. We plan to further develop this algorithm to study disordered systems [20] and the condensation transition [21].

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Let $k$ be one of the $2^{N_c}$ assignments, and $f_k$ be its weight [11]. Form the vector $A_k = \sum_{r=1}^{k} f_r / \sum_{r=1}^{N_c} f_r$, with $A_{-1} = 0$. Extract a uniform random number $0 \leq R < 1$. For our chosen $k$, $A_{k+1} \leq R < A_k$.