Accelerating Monte Carlo: Wolff in arbitrary external fields

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We introduce a natural way to extend celebrated spin-cluster Monte Carlo algorithms for fast thermal lattice simulations at criticality, like Wolff, to systems in arbitrary fields. The method relies on the generalization of the 'ghost spin' representation to one with a 'ghost transformation' that restores invariance to spin symmetries at the cost of an extra degree of freedom. The ordinary cluster-building process can then be run on the new representation. For several canonical systems, we show that this extension preserves the scaling of accelerated dynamics in the absence of a field.

Lattice models are important in the study of statistical physics and phase transitions. Rarely exactly solvable, they are typically studied by approximate and numerical methods. Monte Carlo techniques are a common way of doing this, approximating thermodynamic quantities by sampling the distribution of systems states. These Monte Carlo algorithms are better the faster they arrive at a statistically independent sample. This typically becomes a problem near critical points, where critical slowing down [1] results in power-law divergences of dynamic timescales. Celebrated cluster algorithms largely addressed this in the absence of symmetry-breaking fields by using nonlocal updates [2] whose clusters undergo a percolation transition at the critical point of the system [3]. These result in relatively small dynamic exponents for many spin systems [4–7], including the Ising, $O(n)$ [8], and Potts [9, 10] models. These algorithms rely on the natural symmetry of the systems in question under symmetry operations on the spins. Some success has been made in extending these algorithms to systems in certain external fields by adding a 'ghost site' [11] that returns global rotation invariance to spin Hamiltonians at the cost of an extra degree of freedom, allowing the method to be used in a subcategory of interesting fields [12–14]. Static fields have also been applied by including a separate metropolis or heat bath update step after cluster formation [15, 16], and other categories of fields have been applied using replica methods [17–19]. We show that the scaling of correlation time near the critical point of several models suggests that the 'ghost' approach is a natural one, e.g., that it extends the celebrated scaling of dynamics in these algorithms at zero field to various non-symmetric perturbations. We also show, by a redefinition of the spin–spin coupling in a generic class of spin systems, *arbitrary* external fields can be treated using cluster methods. Rather than the introduction of a 'ghost spin,' our representation relies on introducing a 'ghost transformation.'

We will pose the problem in a general way, but several specific examples can be found in Table I for concreteness. Let $G = (V, E)$ be a graph, where the set of vertices $V = \{1, \dots, N\}$ enumerates the sites of a lattice and the set of edges E contains pairs of neighboring sites. Let R be a group acting on a set X, with the action of group elements $r \in R$ on elements $s \in X$ denoted $r \cdot s$. X is the set of states accessible by a spin, and R is the *symmetry group* of X. The set X must admit a measure μ that is invariant under the action of R, e.g., for any $A \subseteq X$ and $r \in R$, $\mu(r \cdot A) = \mu(A)$. This trait is shared by the counting measure on any discrete set, or by any group acting by isometries on a Riemannian manifold, such as $O(n)$ on S^{n-1} in the $O(n)$ model [20]. Finally, the subset of elements in R of order two must act transitively on X. This property, while apparently obscure, is shared by any symmetric space [21] or by any transitive, finitely generated isometry group. In fact, all the examples listed here have spins spaces with natural metrics whose symmetry group is their set of isometries. We put one spin at each site of the lattice described by G, so that the state of the entire spin system is described by elements $\mathbf{s} \in X \times \cdots \times X = X^N$.

The Hamiltonian of this system is a function $\mathcal{H} : X^N \to \mathbb{R}$ defined by

$$\mathcal{H}(\mathbf{s}) = -\sum_{\{i,j\} \in E} Z(s_i, s_j) - \sum_{i \in V} B(s_i), \qquad (1)$$

where $Z : X \times X \to \mathbb{R}$ couples adjacent spins and $B : X \to \mathbb{R}$ is an external field. Z must be symmetric in its arguments and invariant under the action of any element of R applied to the entire lattice, that is, for any $r \in R$ and $s, t \in X$, $Z(r \cdot s, r \cdot t) = Z(s, t)$. One may also allow Z to also be a function of edge—for modelling random-bond, long-range, or anisotropic interactions—or allow B to be a function of site—for applying arbitrary boundary conditions or modelling random fields. The formal results of this paper (that the algorithm obeys detailed balance and ergodicity) hold equally well for these cases, but we will drop the additional index notation for clarity. Statements about efficiency may not.

The goal of statistical mechanics is to compute expectation values of observables $A : X^N \to \mathbb{R}$. Assuming the ergodic hypothesis holds (for systems with broken-symmetry states, it does not), the expected value $\langle A \rangle$ of an observable A is its average over every state $\mathbf{s}$ in the configuration space X^N weighted by the Boltzmann

	Spins (X)	Symmetry (R)	Action ($g \cdot s$)	Coupling ($Z(s,t)$)	Common Field ($B(s)$)
Ising	$\{-1,1\}$	$\mathbb{Z}/2\mathbb{Z}$	$0 \cdot s \mapsto s,\ 1 \cdot s \mapsto -s$	st	Hs
O(n)	S^{n-1}	O(n)	$M \cdot s \mapsto Ms$	$s^{\mathrm{T}} t$	$H^{\mathrm{T}} s$
Potts	$\mathbb{Z}/q\mathbb{Z}$	D_n	$r_m \cdot s = m + s,\ s_m \cdot s = -m - s$	$\delta(s,t)$	$\sum_m H_m \delta(m,s)$
Clock	$\mathbb{Z}/q\mathbb{Z}$	D_n	$r_m \cdot s = m + s,\ s_m \cdot s = -m - s$	$\cos(2\pi \frac{s-t}{q})$	$\sum_m H_m \cos(2\pi \frac{s-m}{q})$
Discrete Gaussian	$\mathbb{Z}$	$D_{\inf}$	$r_m \cdot s = m + s,\ s_m \cdot s = -m - s$	$(s-t)^2$	Hs^2

TABLE I. Several examples of spin systems and the symmetry groups that act on them. Common choices for the spin–spin coupling in these systems and their external fields are also given. Other fields are possible, of course: for instance, some are interested in modulated fields $H \cos(2\pi k \theta(s))$ for integer k and $\theta(s)$ giving the angle of s to some axis applied to the O(2) model [22].

probability of that state appearing, or

$$\langle A \rangle = \frac{\int_{X^N} A(\mathbf{s}) e^{-\beta \mathcal{H}(\mathbf{s})} \, d\mu(\mathbf{s})}{\int_{X^N} e^{-\beta \mathcal{H}(\mathbf{s})} \, d\mu(\mathbf{s})}, \qquad (2)$$

where for $Y_1 \times \cdots \times Y_N = Y \subseteq X^N$ the measure $\mu(Y) = \mu(Y_1) \cdots \mu(Y_N)$ is the simple extension of the measure on X to a measure on X^N. These values are estimated using Monte Carlo techniques by constructing a finite sequence of states $\{\mathbf{s}_1, \ldots, \mathbf{s}_M\}$ such that

$$\langle A \rangle \simeq \frac{1}{M} \sum_{i=1}^{M} A(\mathbf{s}_i). \qquad (3)$$

Sufficient conditions for this average to converge to $\langle A \rangle$ as $M \to \infty$ are that the process that selects $\mathbf{s}_{i+1}$ given the previous states be Markovian (only depends on $\mathbf{s}_i$), ergodic (any state can be accessed), and obey detailed balance (the ratio of probabilities that $\mathbf{s}'$ follows $\mathbf{s}$ and vice versa is equal to the ratio of weights for $\mathbf{s}$ and $\mathbf{s}'$ in the ensemble).

While any of several related cluster algorithms can be described for this system, we will focus on the Wolff algorithm [8]. In the absence of an external field, e.g., B(s)=0, the Wolff algorithm proceeds in the following way.

1. Pick a random site and a random rotation $r \in R$ of order two, and add the site to a stack.

2. While the stack isn't empty,

   (a) pop site m from the stack.

   (b) If site m isn't marked,

      i. mark the site.

      ii. For every j such that $\{m, j\} \in E$, add site j to the stack with probability

$$p_r(s_m, s_j) = \min\{0, 1 - e^{\beta(Z(r \cdot s_m, s_j) - Z(s_m, s_j))}\}. \qquad (4)$$

      iii. Take $s_m \mapsto r \cdot s_m$.

When the stack is exhausted, a cluster of connected spins will have been rotated by the action of r. In order for this algorithm to be useful, it must satisfy ergodicity and detailed balance. Ergodicity is satisfied since we have ensured that the subset of elements in R that are order two acts transitively on K, e.g., for any $s, t \in X$ there exists $r \in R$ such that $r \cdot s = t$. Since there is a nonzero probability that only one spin is rotated and that spin can be rotated into any state, ergodicity follows. The probability $P(\mathbf{s} \to \mathbf{s}')$ that the configuration $\mathbf{s}$ is brought to $\mathbf{s}'$ by the flipping of a cluster formed by accepting rotations of spins via bonds $C \subseteq E$ and rejecting rotations via bonds $\partial C \subset E$ is related to the probability of the reverse process $P(\mathbf{s}' \to \mathbf{s})$ by

$$\frac{P(\mathbf{s} \to \mathbf{s}')}{P(\mathbf{s}' \to \mathbf{s})} = \prod_{\{i,j\} \in C} \frac{p_r(s_i, s_j)}{p_{r^{-1}}(s'_i, s'_j)} \prod_{\{i,j\} \in \partial C} \frac{1 - p_r(s_i, s_j)}{1 - p_{r^{-1}}(s'_i, s'_j)}$$
$$= \prod_{\{i,j\} \in \partial C} e^{\beta(Z(r \cdot s_i, s_j) - Z(s_i, s_j))} = \frac{p_r(s_i, s_j)}{p_r(s_i, s_j)} \frac{e^{-\beta \mathcal{H}(\mathbf{s})}}{e^{-\beta \mathcal{H}(\mathbf{s}')}}, \qquad (5)$$

whence detailed balance is also satisfied.

This algorithm relies on the fact that the coupling Z depends only on relative orientation of the spins—global reorientations do not affect the Hamiltonian. The external field B breaks this symmetry. However, it can be restored. Define a new graph $\tilde{G} = (\tilde{V}, \tilde{E})$, where $\tilde{V} = \{0, 1, \ldots, N\}$ adds the new 'ghost' site 0 which is connected by

$$\tilde{E} = E \cup \big\{ \{0, i\} \mid i \in V \big\} \qquad (6)$$

to all other sites. Instead of assigning the ghost site a spin whose value comes from X, we assign it values in the symmetry group $s_0 \in R$, so that the configuration space of the new model is $R \times X^N$. We introduce the Hamiltonian $\tilde{\mathcal{H}} : R \times X^N \to \mathbb{R}$ defined by

$$\tilde{\mathcal{H}}(s_0, \mathbf{s}) = -\sum_{\{i,j\} \in E} Z(s_i, s_j) - \sum_{i \in V} B(s_0^{-1} \cdot s_i)$$
$$= -\sum_{\{i,j\} \in \tilde{E}} \tilde{Z}(s_i, s_j), \qquad (7)$$

where the new coupling $\tilde{Z} : (R \cup X) \times (R \cup X) \to \mathbb{R}$ is

defined for $s, t \in R \cup X$ by

$$\tilde{Z}(s,t) = \begin{cases} Z(s,t) & \text{if } s, t \in X \\ B(s^{-1} \cdot t) & \text{if } s \in R \\ B(t^{-1} \cdot s) & \text{if } t \in R. \end{cases} \qquad (8)$$

The modified coupling is invariant under the action of group elements: for any $r, s_0 \in R$ and $s \in X$,

$$\begin{aligned} \tilde{Z}(rs_0, r \cdot s) &= B((rs_0)^{-1} \cdot (r \cdot s)) \\ &= B(s_0^{-1} \cdot s) = \tilde{Z}(s_0, s) \end{aligned} \qquad (9)$$

The invariance of $\tilde{Z}$ to rotations given other arguments follows from the invariance properties of Z.

We have produced a system incorporating the field function B whose Hamiltonian is invariant under global rotations, but how does it relate to our old system, whose properties we actually want to measure? If $A : X^N \to \mathbb{R}$ is an observable of the original system, we construct an observable $\tilde{A} : R \times X^N \to \mathbb{R}$ of the new system defined by

$$\tilde{A}(s_0, \mathbf{s}) = A(s_0^{-1} \cdot \mathbf{s}) \qquad (10)$$

whose expectation value in the new system equals that of the original observable in the old system. First, note that $\tilde{\mathcal{H}}(1, \mathbf{s}) = \mathcal{H}(\mathbf{s})$. Since the Hamiltonian is invariant under global rotations, it follows that for any $g \in R$, $\tilde{\mathcal{H}}(g, g \cdot \mathbf{s}) = \mathcal{H}(\mathbf{s})$. Using the invariance properties of the measure on X and introducing a measure ρ on R, it follows that

$$\begin{aligned} \langle \tilde{A} \rangle &= \frac{\int_R \int_{X^N} \tilde{A}(s_0, \mathbf{s}) e^{-\beta \tilde{\mathcal{H}}(s_0, \mathbf{s})} \, d\mu(\mathbf{s}) \, d\rho(s_0)}{\int_R \int_{X^N} e^{-\beta \tilde{\mathcal{H}}(s_0, \mathbf{s})} \, d\mu(\mathbf{s}) \, d\rho(s_0)} \\ &= \frac{\int_R \int_{X^N} A(s_0^{-1} \cdot \mathbf{s}) e^{-\beta \tilde{\mathcal{H}}(s_0, \mathbf{s})} \, d\mu(\mathbf{s}) \, d\rho(s_0)}{\int_R \int_{X^N} e^{-\beta \tilde{\mathcal{H}}(s_0, \mathbf{s})} \, d\mu(\mathbf{s}) \, d\rho(s_0)} \\ &= \frac{\int_R \int_{X^N} A(\mathbf{s}') e^{-\beta \tilde{\mathcal{H}}(s_0, s_0 \cdot \mathbf{s}')} d\mu(s_0 \cdot \mathbf{s}') \, d\rho(s_0)}{\int_R \int_{X^N} e^{-\beta \tilde{\mathcal{H}}(s_0, s_0 \cdot \mathbf{s}')} d\mu(s_0 \cdot \mathbf{s}') \, d\rho(s_0)} \\ &= \frac{\int_R d\rho(s_0)}{\int_R d\rho(s_0)} \frac{\int_{X^N} A(\mathbf{s}') e^{-\beta \mathcal{H}(\mathbf{s}')} d\mu(\mathbf{s}')}{\int_{X^N} e^{-\beta \mathcal{H}(\mathbf{s}')} d\mu(\mathbf{s}')} = \langle A \rangle. \end{aligned} \qquad (11)$$

Using this equivalence, spin systems in a field may be treated in the following way.

1. Add a site to your lattice adjacent to every other site.

2. Initialize a 'spin' at that site whose value is a representation of a member of the symmetry group of your ordinary spins.

3. Carry out the ordinary Wolff cluster-flip procedure on this new lattice, substituting $\tilde{Z}$ as defined in (8) for Z.

Ensemble averages of observables A can then be estimated by sampling the value of $\tilde{A}$ on the new system. In contrast with the simpler ghost spin representation, this form of the Hamiltonian might be considered the 'ghost transformation' representation.

Several specific examples from Table I are described in the following.

The Ising model. In the Ising model spins are drawn from the set $\{1, -1\}$. Its symmetry group is C_2, the cyclic group on two elements, which can be conveniently represented by a multiplicative group with elements $\{1, -1\}$, exactly the same as the spins themselves. The only nontrivial element is of order two. Since the symmetry group and the spins are described by the same elements, performing the algorithm on the Ising model in a field is fully described by just using the 'ghost spin' representation. This algorithm or algorithms based on the same decomposition of the Hamiltonian have been applied by several researchers [12–14]. The algorithm has been implemented by one of the authors in an existing interactive Ising simulator at https://mattbierbaum.github.io/ising.js [23].

The $O(n)$ model. In the $O(n)$ model spins are described by vectors on the $(n-1)$-sphere S^{n-1}. Its symmetry group is $O(n)$, $n \times n$ orthogonal matrices, which act on the spins by matrix multiplication. The elements of $O(n)$ of order two are reflections about hyperplanes through the origin and π rotations about any axis through the origin. Since the former generate the entire group, reflections alone suffice to provide ergodicity. The 'ghost spin' version of the algorithm has been used to apply a simple vector field to the $O(3)$ model [24]. Other fields of interest include $(n+1)$-dimensional spherical harmonics [22] and cubic fields [25, 26], which can be applied with the new method. The method is quickly generalized to spins whose symmetry groups other compact Lie groups

The Potts & clock models. In both the q-state Potts and clock models spins are described by elements of $\mathbb{Z}/q\mathbb{Z}$, the set of integers modulo q. Its symmetry group is the dihedral group $D_q = \{r_0, \dots, r_{q-1}, s_0, \dots, s_{q-1}\}$, the group of symmetries of a regular q-gon. The element r_n represents a rotation by $2\pi n / q$, and the element s_n represents a reflection composed with the rotation r_n. The group acts on spins by permutation: $r_n \cdot m = n + m \pmod{q}$ and $s_n \cdot m = -(n + m) \pmod{q}$. This is the natural action of the group on the vertices of a regular polygon that have been numbered 0 through $q - 1$. The elements of D_q of order 2 are all reflections and $r_{q/2}$ if q is even, though the former can generate the latter. While reflections do not necessarily generate the entire group, their action on $\mathbb{Z}/q\mathbb{Z}$ is transitive and therefore the algorithm is ergodic.

Roughening models. Though not often thought of as a spin model, roughening of surfaces can be described in this framework. Spins are described by integers $\mathbb{Z}$ and their symmetry group is the infinite dihedral group $D_\infty =$

{$r_i, s_i \mid i \in \mathbb{Z}$}, whose action on the spin $j \in \mathbb{Z}$ is given by $r_i \cdot j = i + j$ and $s_i \cdot j = -i - j$. The elements of order two are reflections s_i, whose action on $\mathbb{Z}$ is transitive. The coupling can be any function of the absolute difference $|i - j|$. Because random choice of reflection will almost always result in energy changes so large that the whole system is flipped, it is better to select random reflections about integers close to the average state of the system. A variant of the algorithm has been applied without a field [27].

No algorithm is worthwhile if it doesn't run efficiently. This algorithm, being an extension of the Wolff algorithm into a new domain, should be considered successful if it likewise extends the efficiency of the Wolff algorithm into that domain. Some systems are not efficient under Wolff, and we don't expect this extension to help them. For instance, Ising models with random fields or bonds technically can be treated with Wolff [28], but it is not efficient because the clusters formed do scale naturally with the correlation length [17, 29]. Other approaches, like replica methods, should be relied on instead [17–19].

At a critical point, correlation time τ scales with system size $L = N^{-D}$ as $\tau \sim L^z$. Cluster algorithms are celebrated for their small dynamic exponents z. In the vicinity of an ordinary critical point, the renormalization group predicts scaling behavior for the correlation time as a function of temperature t and field h of the form

$$\tau = h^{-z\nu/\beta\delta} \mathcal{T}(ht^{-\beta\delta}, hL^{\beta\delta/\nu}). \tag{12}$$

If a given dynamics for a system at zero field results in scaling like L^z, one should expect its natural extension in the presence of a field to scale roughly like $h^{-z\nu/\beta\delta}$ and collapse appropriately as a function of $hL^{\beta\delta/\nu}$. We measured the autocorrelation time for the $D = 2$ square-lattice model at a variety of system sizes, temperatures, and fields $B(s) = hs/\beta$ using standard methods [30]. The resulting scaling behavior, plotted in Fig. 1, is indeed consistent with an extension to finite field of the behavior at zero field.

Since the formation and flipping of clusters is the hallmark of Wolff dynamics, another way to ensure that the dynamics with field scale like those without is to analyze the distribution of cluster sizes. The success of the algorithm at zero field is related to the fact that the clusters formed undergo a percolation transition at models' critical point. According to the scaling theory of percolation [31], the distribution of cluster sizes in a full Swendsen–Wang decomposition of the system scales consistently near the critical point if it has the form

$$P_{\mathrm{SW}}(s) = s^{-\tau} f(ts^\sigma, th^{-1/\beta\delta}, tL^{1/\nu}). \tag{13}$$

The distribution of cluster sizes in the Wolff algorithm can be computed from this using the fact that the algorithm selects clusters with probability proportional to
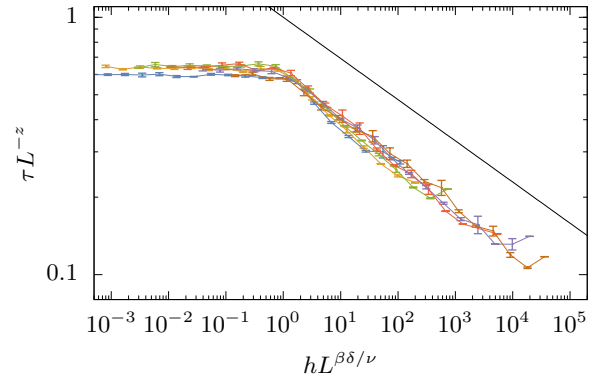

FIG. 1. Collapse of the correlation time τ of the 2D square lattice Ising model along the critical isotherm at various systems sizes $N = L \times L$ for $L = 8, 16, 32, 64, 128,$ and 256 as a function of the renormalization invariant $hL^{\beta\delta/\nu}$. The exponent $z = 0.30$ is taken from recent measurements at zero field [6]. The solid black line shows a plot of $(hL^{\beta\delta/\nu})^{-z\nu/\beta\delta}$.

their size, or

$$\langle s_{1\mathrm{C}} \rangle = \sum_s sP_{1\mathrm{C}}(s) = \sum_s s\frac{s}{N}P_{\mathrm{SW}}(s)$$
$$= L^{\gamma/\nu} g(ht^{-\beta\delta}, hL^{\beta\delta/\nu}). \tag{14}$$

For the Ising model, an additional scaling relation can be written. Since the average cluster size is the average squared magnetization, it can be related to the scaling functions of the magnetization and susceptibility per site by (with $ht^{-\beta\delta}$ dependence dropped)

$$\langle s_{1\mathrm{C}} \rangle = L^D \langle M^2 \rangle = \beta \langle \chi \rangle + L^D \langle M \rangle^2$$
$$= L^{\gamma/\nu} \big[(hL^{\beta\delta/\nu}, ht^{-\beta\delta})^{-\gamma/\beta\delta} \beta \mathcal{Y}(hL^{\beta\delta/\nu, ht^{-\beta\delta}})$$
$$+ (hL^{\beta\delta/\nu}, ht^{-\beta\delta})^{2/\delta} \mathcal{M}(hL^{\beta\delta/\nu}, ht^{-\beta\delta}) \big]. \tag{15}$$

We therefore expect that, for the Ising model, $\langle s_{1\mathrm{C}} \rangle$ should go as $(hL^{\beta\delta})^{2/\delta}$ for large argument. We further conjecture that this scaling behavior should hold for other models whose critical points correspond with the percolation transition of Wolff clusters. This behavior is supported by our numeric work along the critical isotherm for various Ising, Potts, and O(n) models, shown in Fig. 2. Fields for the Potts and O(n) models take the form $B(s) = (h/\beta) \sum_m \cos(2\pi(s - m)/q)$ and $B(s) = (h/\beta)[1, 0, \ldots, 0]s$ respectively. As can be seen, the average cluster size collapses for each model according to the scaling hypothesis, and the large-field behavior likewise scales as we expect from the naïve Ising conjecture.

We have taken several disparate extensions of cluster methods to spin models in an external field and generalized them to work for any model of a broad class. The resulting representation involves the introduction of not a ghost spin, but a ghost transformation. We provided
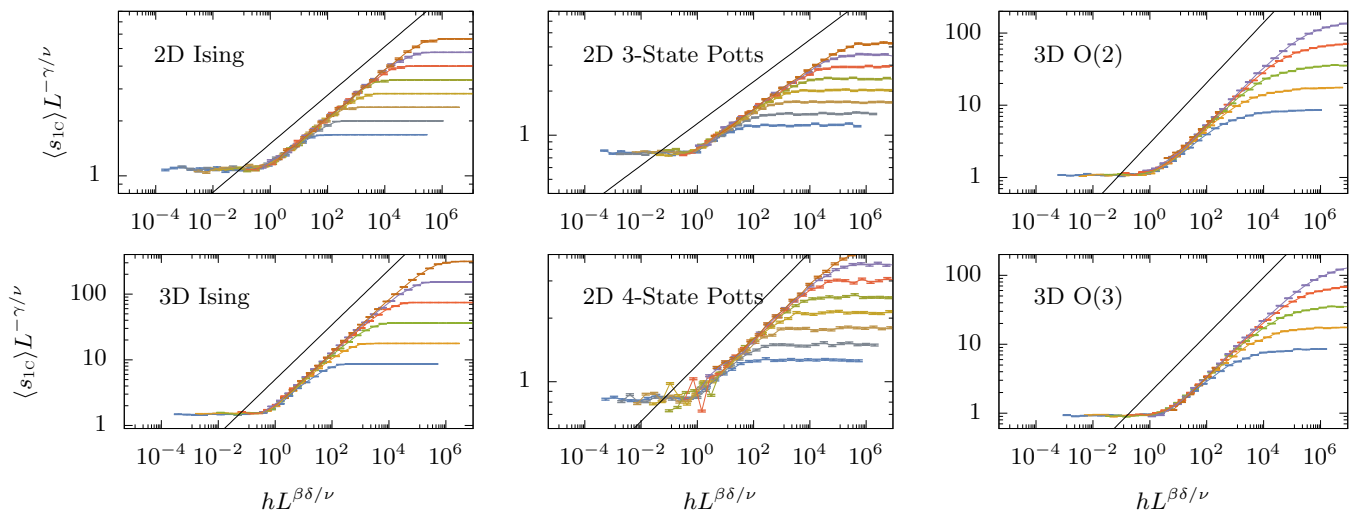
FIG. 2. Collapses of rescaled average Wolff cluster size $\langle s \rangle_{1c} L^{-\gamma/\nu}$ as a function of field scaling variable $hL^{\beta\delta/\nu}$ for a variety of models. Critical exponents γ, ν, β, and δ are model-dependant. Colored lines and points depict values as measured by the extended algorithm. Solid black lines show a plot of $g(0,x) \propto x^{2/\delta}$ for each model.

evidence that algorithmic extensions deriving from this method are the natural way to extend cluster methods in the presence of a field, in the sense that they appear to reproduce the scaling of dynamic properties in a field that would be expected from renormalization group predictions.

In addition to uniting several extensions of cluster methods under a single description, our approach allows the application of fields not possible under prior methods. Instead of simply applying a spin-like field, this method allows for the application of *arbitrary functions* of the spins. For instance, theoretical predictions for the effect of symmetry-breaking perturbations on spin models can be tested numerically [22, 25, 26, 32].

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