Loop-Cluster Monte Carlo Algorithm for Classical Statistical Models

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We introduce a joint model of bond-occupation variables interacting with so-called q-flow variables. It leads us to formulate a Loop-Cluster (LC) Monte Carlo algorithm which passes back and forth between the Fortuin-Kasteleyn (FK) bond representation of the q-state Potts model and the so-called q-flow representation. Together with the Swendsen-Wang (SW) cluster method, the LC algorithm couples the spin, FK and q-flow representations of the Potts model. As a result, a single Markov-chain simulation can use an arbitrary combination of the SW, worm, LC and other algorithms, and simultaneously sample physical quantities in any representation. Generalizations to real value q ≥ 1 and to a single-cluster version are also obtained. Investigation of dynamic properties is performed for q = 2, 3 on both the complete graph and toroidal grids of dimension 2 ≤ d ≤ 5. Our numerical results suggest that the LC algorithm and its single-cluster version are in the same dynamic universality class as the SW and the Wolff algorithm, respectively. Finally, it is shown, for the Potts model undergoing continuous phase transition, the q-flow clusters, defined as sets of vertices connected via non-zero flow variables, are fractal objects.

INTRODUCTION

The understanding of critical phenomena is now strongly intertwined with the study of the rich behavior of the q-state Potts model [1]. Aside from the historical spin representation [2, 3], two other representations of the Potts model have played a central role: the q-flow [4, 5] and Fortuin-Kasteleyn (FK) bond representations [6, 7], the latter of which is also known as the random-cluster (RC) model. On one hand, theoretical advances were achieved thanks to the geometric and probabilistic interpretations they brought, as well as the extension to positive real q values [8–10]. For instance, they play an important role in conformal field theory [11] by their connection with stochastic Loewner evolution [12–16]. On the other hand, numerical Monte Carlo (MC) methods, detrimental in the study of not-exactly soluble models, have massively gained from these insights. Indeed, in the spin representation, the Metropolis [17] or heat-bath schemes rely on single-spin moves and often suffer from severe critical slowing-down near the critical point, resulting in low computational efficiency [18, 19]. By summing out the spin degree of freedom, these alternative representations yield MC schemes prone to relieve or even eliminate the critical slowing-down [20–23].

In the FK representation, random clusters can be sampled through local-bond updates as in the Sweeny algorithm [20] or cluster updates as in the Swendsen-Wang (SW) algorithm [21], by switching between spin and FK representations. As for the q-flow representation, one can apply the Prokof’ev-Svistunov worm algorithm, which exhibits broad applications in both classical and quantum systems [23–26]. The worm algorithm has proven to be particularly efficient at computing the magnetic susceptibility [27], the second-moment correlation length [27] and the spin-spin correlation function [28]. However, the q-flow representation was still lacking a general mapping to the spin or FK representations which could allow to compute observables independently in these representations.

Recently, Grimmett and Janson [29] successfully build a coupling between the q-flow and FK representations of the Ising model. In this Letter, by the introduction of a joint model of FK bond variables interacting with q-flow variables, we give a simple explanation of the coupling for the Ising model [29] and further generalize it to the Potts model of any integer q ≥ 1. The joint model also provides a setup for the construction of a new MC algorithm, which we call the Loop-Cluster (LC) method. As a consequence, applications of algorithms are no longer restricted to one particular representation, and one can apply the most efficient algorithm to update in one representation and use the LC and/or SW algorithm to measure observables in other representations, as illustrated in Fig. 1. With the induced-subgraph scheme [9], the LC algorithm is generalized to any real value q ≥ 1, which for 2 ≥ q > 1, reduces to the Chayes-Machta algorithm [8]. A single-cluster version is also proposed. The dynamic properties of the LC scheme and its single-cluster version are investigated over the complete graph and toroidal grids and are shown to be in the same universality class as their respective cluster-scheme counterparts. Finally, with the joint model, q-flow clusters, defined by sets of vertices connected by non-zero flow variables, can
be proven to be smaller than those of the backbones of FK clusters and thus to have at criticality a fractal dimension smaller than the backbone dimension for the Potts model of continuous phase transition.

Now, we can assign to each edge \((ij)\) of the graph \(G\) a \(q\)-flow variable \(f_{ij} \in \{0, 1, \cdots, q - 1\}\), and denote by \(G_{\ell} \equiv (V, E_{\ell}) \subseteq G\) the subgraph of edges \((ij)\) with nonzero flows \(f_{ij} > 0\). Further, we introduce symbol \(\partial G\) to represent the set of vertices that do not satisfy the conservation condition given by the \(q\)-modular Kirchhoff conservation law as

\[
\sum_{j:(i,j) \in E} \text{sgn}(i \rightarrow j) f_{ij} = 0 \mod q, \quad \text{for any } i \in V \tag{3}
\]

where \(\text{sgn}(i \rightarrow j) = -\text{sgn}(j \rightarrow i) \in \{\pm 1\}\) arises from the orientation of edge \((ij)\). For any configuration \(\{f\}\), the \(q\)-flow model is described by the probability distribution,

\[
d\mu_{\text{qFlow}}(\{f\}) = Z_{\text{qFlow}}^{-1} \delta_{\partial G = \emptyset} \prod_{(ij) \in E} (1 - \frac{q}{q-1} p_{ij}) d\mu_0(\{f\}) \tag{4}
\]

where \(\delta_{\partial G = \emptyset}\) means an empty set for \(\partial G\), i.e., no vertex breaks the conservation law. The orientation of each edge \((ij) \in E\) plays no physical role and can be randomly chosen, as reversing an edge \((ij)\) orientation can be counterbalanced by mapping the flow variable \(f_{ij}\) to \(q - f_{ij} \mod q\).

Using high-temperature expansion [4–7, 30], duality relations [1, 31] or low-temperature expansion for 2d-planar graphs, one can show that \(Z_{\text{spin}} = Z_{\text{FK}} = q^{|V|} Z_{\text{qFlow}}\). Thus, apart from an unimportant constant \(q^{|V|}\), the Potts (1), the RC (6) and the \(q\)-flow models (4) are equivalent to each other.

**JOINT MODELS.**

In 1988, Edwards and Sokal defined a joint model [32], having the \(q\)-state Potts spin \(\sigma_i\) at the vertices and occupation variable \(b_{ij}\) on the edges, with probability distribution

\[
d\mu_{\text{SW}}(\{\sigma\}, \{b\}) = Z_{\text{SW}}^{-1} \prod_{(ij) \in E_{\text{b}}} p_{ij} \delta_{b_{ij}, 1} \delta_{\sigma_i, \sigma_j} + (1 - p_{ij}) \delta_{b_{ij}, 0} d\mu_0(\{\sigma\}) d\mu_0(\{b\}) \tag{5}
\]

On this basis, the SW cluster algorithm can be easily understood as passing back and forth between the spin and FK representations, via the joint model (5). Given a spin configuration, a random FK configuration is generated as the following: independently for each edge \((ij)\), one sets \(b_{ij} = 0\) for \(\sigma_i \neq \sigma_j\), and sets \(b_{ij} = 1\) (resp. 0) with probability \(p_{ij}\) (resp. \((1 - p_{ij})\)), for \(\sigma_i = \sigma_j\). The reverse process starts with a FK bond configuration. One picks up equiprobably a \(\sigma_i\) variable from the set \(\{0, 1, \cdots, q-1\}\) for each connected cluster and assigns the \(\sigma\) value to all the spins in this cluster.
We shall formulate an algorithm which passes back and forth between the FK bond and the q-flow configurations. We first remark that, using the Euler formula $k(G_b) = |V| - |E_b| + c(G_b)$ where $c(G_b)$ is the number of independent loops (cycles) in $G_b$, we can rewrite the RC model as

$$d\mu_{\text{FK}}(\{b\}) = Z_{\text{FK}} q^{|V|+c(G_b)} \prod_{(ij) \in E_b} \prod_{(ij) \notin E_b} (1-p_{ij})d\mu_0(\{b\}).$$

Further, the simple decomposition in the q-flow model leads to

$$d\mu_{\text{qFlow}}(\{f\}) = Z_{\text{qFlow}}^{-1} \delta_{\partial G = \emptyset} \prod_{(ij) \in E} \prod_{(ij) \notin E} \left( \frac{p_{ij}}{q} + (1-p_{ij}) \right) d\mu_0(\{f\}).$$

Analogously to [32], we define a joint model, having both the bond variable $b_{ij}$ and the flow variable $f_{ij}$ on each edge, with the probability distribution

$$d\mu_{\text{JLC}}(\{f\}, \{b\}) = Z_{\text{JLC}}^{-1} \delta_{\partial G = \emptyset} \prod_{(ij) \in E} \prod_{(ij) \notin E} \left( \frac{p_{ij}}{q} \delta_{f_{ij} = 0} \delta_{b_{ij} = 1} + \frac{\nu}{q} \delta_{f_{ij} = 0} \delta_{b_{ij} = 0} \right) \times d\mu_0(\{f\})d\mu_0(\{b\}).$$

As the edge state $(f_{ij} \neq 0, b_{ij} = 0)$ is forbidden i.e., has zero probability, it yields $G_1 \subseteq G_b \subseteq G$. By explicitly performing the summation over either the $\{b\}$ or the $\{f\}$ variables, it is easy to verify the following facts about the joint model (8):

(i) The marginal probability of the flow variables $\{f\}$ is precisely the q-flow model (7), since, after summation over the bond states $b_{ij} = 0, 1$, an edge with the flow state $f_{ij} = 0$ has the statistical weight $\frac{p_{ij}}{q}$, and one with $f_{ij} = 0$ a statistical weight of $(1-p_{ij}) + \frac{\nu}{q}$, as in (7).

(ii) The marginal probability of the bond variables $\{b\}$ is precisely the RC model (6). The summation over the flow variables $\{f\}$ involves the number of choices of assigning the flow variables under the constraints that $\partial G = \emptyset$ and the state $(f_{ij} \neq 0, b_{ij} = 0)$ is forbidden. This number identifies with the number of possible flow configurations on the subgraph of occupied bonds, i.e., the flow configurations satisfying $\partial G_b = \emptyset$. This number amounts to $q^{c(G_b)}$, by considering the decomposition of the Kirchhoff law (3) into the loop flows on the graph $G_b$. Indeed, once the flow variable of an unshared edge of a loop is determined among the $q$ possible values, it must be propagated along the loop, defining the loop flow. The final flow for a given edge is the sum of the loop flows it is contained in. Thus, any bridge edge, i.e., not contained in any loop and increasing the number of clusters if deleted, is assigned a flow zero.

(iii) Given the flow variables $\{f\}$, the conditional distribution of the bond variables $\{b\}$ is $p(b_{ij} = 1 | f_{ij} > 0) = 1$ for any edge $(i, j)$ with a non-zero flow and $p(b_{ij} = 1 | f_{ij} = 0) = \frac{\nu}{1-p_{ij} + \nu} = t_{ij}$ otherwise.

(iv) Given the bond variables $\{b\}$, the conditional distribution of the flow variables $\{f\}$ is, for any cluster $G_c \subseteq G$, $p(\{f_{ij}\}| (i,j) \in E_c) = q^{-c(G_c)} \delta_{\partial G_c = \emptyset}$ and $p(f_{ij} = 0 | b_{ij} = 0) = 1$ for all edges with unoccupied bonds.

(v) The joint model (8) highlights the fundamental relationship between the FK and q-flow representations as both can be understood as the result of a high-temperature expansion over $\frac{p_{ij}}{1-p_{ij}}$ and $t_{ij}$, respectively, revealing either the connected-cluster or flow structure. Furthermore $t_{ij}$ identifies with the thermal transmissivity arising in the renormalization group [5, 33].

(vi) As in the FK representation, clusters can also be defined for a given flow configuration as sets of vertices connected via edges of non-zero flow variables. As $G_1 \subseteq G_b$, a FK cluster may contain more than one q-flow cluster while the reverse cannot occur. Further, since any bridge edge in the FK configuration has a zero flow, the q-flow clusters actually live on top of the backbones of the FK clusters, i.e., sets of vertices connected via non-bridge edges. Finally, since any loop can have a flow zero with probability $1/q$, q-flow clusters are generally smaller than the backbone clusters and, therefore, for the Potts model with continuous phase transition, one has $D_{\text{qFlow}} \leq D_{bb} \leq D_{FK}$, where $D_{\text{qFlow}}$, $D_{bb}$, $D_{FK}$ are the fractal dimensions of the q-flow, backbone, and FK clusters, respectively.

**LOOP-CLUSTER ALGORITHM**

We are now ready to formulate a Monte Carlo method which simulates the joint model (8) through a Gibbs/heat-bath sampling approach. To be specific, we alternatively generate new bond variables, independent of the old ones, given the flows following (iii), and new flow variables, independent of the old ones, given the bonds following (iv). The marginal distribution $d\mu_{\text{FK}}$ in (6) ($d\mu_{\text{qFlow}}$ in (7)) from the joint model (8) is then simply obtained by erasing the flow variables $\{f\}$ (bond variables $\{b\}$), as stated in (i,ii). This sampling procedure is a generalization of the mapping method proposed in [29] for the Ising case. We call this method the **Loop-Cluster** algorithm:

(A) Given a q-flow configuration, generating a random FK bond configuration is a straightforward local process given in (iii): for each non-zero flow $f_{ij} \neq 0$, one sets $b_{ij} = 1$; for each edge with empty flow $f_{ij} = 0$, one independently sets $b_{ij} = 1$ with probability $t_{ij}$, and $b_{ij} = 0$, otherwise. The number of operations in this step equals the number of edges of the original graph, $|E|$.

(B) Given a FK bond configuration, generating a q-flow configuration follows from (iv) and depends on the subgraph-$G_b$ topology: For all the non-occupied edges $b_{ij} = 0$, one sets $f_{ij} = 0$; the edges in $E_b$ are assigned
flow variables \{f\} as described in (ii), once a set of independent loops have been defined.

In more details, we first construct a spanning tree for each connected cluster by a rooted procedure, either the breadth-first or the depth-first search. Any occupied edge of the graph \( G_b \) missing from the tree defines a loop by the symmetric sum of the tree paths from the pair of ending vertices of the missing edge to the root vertex. Each of these occupied bonds is uniformly assigned a flow variable \( f_{ij} \in \{0, 1, \cdots, q - 1\} \) on the fly. Then, we backtrack the tree and calculate the flow variables for all its edges by applying the \( q \)-modular Kirchhoff conservation law to each vertex. The number of operations is twice the number of edges in the original graph, \( 2|E| \). Figure 2 illustrates an example of “constructing-tree” and “backtracking” processes for \( q = 3 \).

In comparison with the SW cluster algorithm, of which the number of operations is at least \( 2|E| \), the total number of operations \( 3|E| \) for the LC algorithm is slightly larger.

We remark that for \( q = 1 \), the RC model is just the standard bond percolation. In this case, the set of flow variables \( \{0, \cdots, q - 1\} \) reduces to \( \{0\} \), and the zero-flow configuration \( \{f_{ij} = 0\} \) becomes the only valid \( q \)-flow configuration. As a result, the LC algorithm is equivalent to the conventional strategy for updating a bond percolation model.

**Extension.**—The LC algorithm can be extended to sample from the RC model of real value \( q \geq 1 \), via the induced-subgraph decomposition [9]. Starting with a FK bond configuration and setting an integer \( 1 \leq m \leq q \) and \( q/m \) or sampled as “inactive”. One obtains then an effective RC model with \( q' = m \) on the subgraph defined by active vertices and edges and a model with \( q' = q - m \) on the complementary inactive subgraph. The active partition can then be updated through any valid MC algorithms, while the inactive one is left unchanged. For \( 2 \geq q \geq 1 \), with the unique choice \( m = 1 \), one can apply the conventional percolation strategy for any active edge, corresponding to the Chayes-Machta algorithm [8]. For \( q \geq 2 \), one can choose integer \( m \geq 2 \) and apply the LC algorithm on the active subgraph, leading to an extended LC algorithm.

Moreover, a single-cluster version can be formulated to sample from the \( q \)-flow model. Starting from a \( q \)-flow configuration, one randomly chooses a root vertex and grows a cluster by Step (A) until it cannot become larger, i.e. all the boundary edges have been sampled as unoccupied; then a new \( q \)-flow configuration can be sampled through Step (B). Like the Wolff algorithm, the single-cluster LC algorithm is more likely to update larger clusters [22], which on average contain larger loops, and to show higher efficiency.

**DYNAMICAL BEHAVIOR**

We study the dynamics of the LC algorithm and compare it to the SW scheme for both “energy-” and “susceptibility-like” quantities in the FK representation, i.e. respectively the total number \( \mathcal{N} \) of occupied bonds and the second moment of FK cluster sizes, defined as \( \mathcal{S}_2 = \sum_C |C|^2 \) with \( |C| \) the size of cluster \( C \). Simulations are performed on toroidal grids for \( 2 \leq d \leq 5 \) and on finite complete graphs (CG) with \( n \) vertices. The critical coupling strengths are \( J_c = \ln(\sqrt{q} + 1) \) for \( q = 2, 3, d = 2 \), \( 0.443 \ 309 \ 262(16) \) for \( q = 2, d = 3 \) [34, 35], \( 0.299 \ 389 \ 4(10) \) for \( q = 2, d = 4 \) [36], \( 0.227 \ 830 \ 0(8) \) for \( q = 2, d = 5 \) [37], and \( 2/n \) for \( q = 2 \), CG.

For an observable \( \mathcal{O} \), we calculate the normalized autocorrelation function \( \rho_{\mathcal{O}}(t) = \langle \mathcal{O}|(\mathcal{O})^2 \rangle / \langle (\mathcal{O})^2 \rangle - \langle \mathcal{O} \rangle^2 \rangle \) and the integrated autocorrelation time \( \tau_{\text{int}, \mathcal{O}} = \frac{1}{2} + \sum_{t=1}^{\infty} \rho_{\mathcal{O}}(t) \). In practice, we have \( 5 \times 10^7 \) to \( 10^8 \) samples for each \( (q, d, L) \) or \( (q, n) \), and thus use the windowing method [38] to truncate the summation for \( \tau_{\text{int}} \).

The results are summarized in Fig. 3, which shows the ratio \( R = \tau_{\text{int}, \text{LC}} / \tau_{\text{int}, \text{SW}} \) and the \( \tau_{\text{int}} \) values in the inset plots. It is clear that for both energy- and susceptibility-like quantities \( \mathcal{N} \) and \( \mathcal{S}_2 \), the ratio \( R \) converges to a constant as system size increases. In two dimensions, it is interesting to observe that \( R_{\mathcal{N}} \) is consistent with 1, ir-
FIG. 3: Ratios of integrated autocorrelation times \( R = \frac{\tau_{\text{int,LC}}}{\tau_{\text{int,SW}}} \) for the LC and the SW algorithm, with \( q = 2 \) in dimensions \( 2 \leq d \leq 5 \) and on the complete graph (CG), as well as with \( (q=3, d=2) \). The values of \( \tau_{\text{int}} \) are shown in the inset plots and the asymptotic fitted values for \( R \) are indicated in each subplot.

respective of system size \( L \) and the \( q \) value. For each \( (q, d, L) \), the \( R \) values can be well described by ansatz \( R_{\text{inf}} + B L^{-\Delta} \), with \( \Delta \) a correction exponent. The results, shown in Fig. 3, displays an increase of the \( R_{\text{inf}} \) with \( d \), up to a value slightly larger than 2 for CG (effectively \( d \to \infty \)). Therefore, it is strongly suggested that the LC and the SW algorithm belong to the same dynamic universality class.

Our numerical results confirm that the single-cluster LC algorithm and the Wolff method have the same average sizes of the updated cluster and belong to the same dynamic class.

CONCLUSION

We introduce a joint model of the FK and \( q \)-flow representations of the Potts model, bridging the gap between its three standard representations and generalizing previous work for the Ising case. An important application is the design of a LC algorithm based on the conditional probabilities drawn from the joint model, which overcomes the previous limitation of performing both the simulations and measurements in a given representation. Generalization to real value of \( q \geq 1 \) and a single-cluster version of the LC method is obtained. Numerical results suggest that the LC method and its single-cluster version belong to the same dynamical class as the SW and the Wolff algorithm, respectively. Finally, we show that for the Potts model of continuous phase transition, the random clusters in the \( q \)-flow representation are fractal objects, with a fractal dimension not larger than the backbone one of the FK clusters.

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