Loop-Cluster Coupling and Algorithm for Classical Statistical Models

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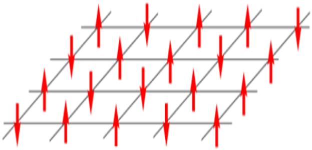
Reference

- **Lei Zhang**, Manon Michel, Eren M. Elçi and Youjin Deng, Phys. Rev. Lett. **125**, 200603 (2020).

Representations of the Potts model

spin representation



- Defined on $G = (V, E)$
- Hamiltonian

$$H_{\text{spin}} = - \sum_{(ij)\in E} J_{ij} \delta_{\sigma_i \sigma_j}$$

  - $\sigma_i \in \{0, 1, ..., q-1\}$, $i \in V$

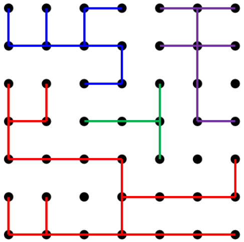
- Counting measure $\left(p_{ij} = 1 - \exp(-J_{ij})\right)$

$$d\mu_{\text{spin}}(\{\sigma\}) = \mathcal{Z}_{\text{spin}}^{-1} \prod_{(ij)} \exp\left[J_{ij}(\delta_{\sigma_i,\sigma_j} - 1)\right] d\mu_0(\{\sigma\})$$

$$= \mathcal{Z}_{\text{spin}}^{-1} \prod_{(ij)} \left[p_{ij}\delta_{\sigma_i,\sigma_j} + (1 - p_{ij})\right] d\mu_0(\{\sigma\})$$

Representations of the Potts model

Fortuin-Kasteleyn (FK) representation



- Bond variable $b \in \{0,1\}$ on each edge (ij)
  - $b = 1$: (ij) is occupied
  - $b = 0$: (ij) is unoccupied
- Configuration space: all possible $\{b\}$
- $G_\mathsf{b} = (V, E_\mathsf{b})$ E_b: set of occupied edges

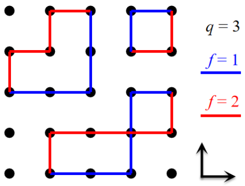
- Counting measure $\left(p_{ij} = 1 - \exp(-J_{ij})\right)$

$$d\mu_{\mathrm{FK}}(\{b\}) = \mathcal{Z}_{\mathrm{FK}}^{-1} q^{k(G_\mathsf{b})} \prod_{(ij)\in E_\mathsf{b}} p_{ij} \prod_{(ij)\notin E_\mathsf{b}} (1 - p_{ij}) d\mu_0(\{b\})$$

  - $k(G_\mathsf{b})$: number of clusters in G_b
  - $q > 0$ is real

Representations of the Potts model

q-flow representation



- Choose an orientation for each (ij)
  - sgn$(i \to j) = -$sgn$(j \to i) \in \{\pm 1\}$
- Flow variable $f_{ij} \in \{0, 1, ..., q-1\}$
- Conservation law

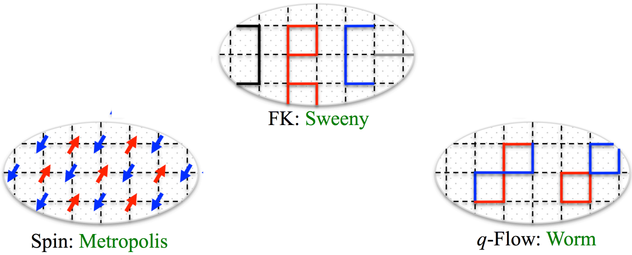
$$\sum_{j:(ij)\in E} \text{sgn}(i \to j) f_{ij} = 0 \mod q$$

- Counting measure $\left(p_{ij} = 1 - \exp(-J_{ij})\right)$

$$d\mu_{\text{qFlow}}(\{f\}) = \mathcal{Z}_{\text{qFlow}}^{-1}\, \delta_{\partial G=\varnothing} \prod_{(ij)\in E_{\text{f}}} \frac{p_{ij}}{q} \prod_{(ij)\notin E_{\text{f}}} (1 - \frac{q-1}{q} p_{ij}) d\mu_0(\{f\})$$

  - ∂G: vertices breaking the conservation law
  - E_{f}: set of edges with non-zero flows
- It is known that $\mathcal{Z}_{\text{spin}} = \mathcal{Z}_{\text{FK}} = q^{|V|} \mathcal{Z}_{\text{qFlow}}$

Algorithms for Potts model



- Spin: Metropolis Alg. [J. Chem. Phys. 21, 1087 (1953)]
- FK: Sweeny Alg. [Phys. Rev. B 27, 4445 (1983)]
- q-flow: Worm Alg. [Phys. Rev. Lett. 87, 160601 (2001)]

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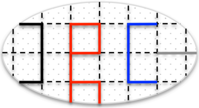
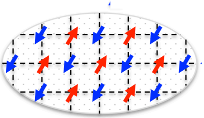
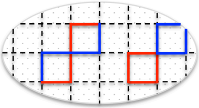


FK: Sweeny



Spin: Metropolis



q-Flow: Worm

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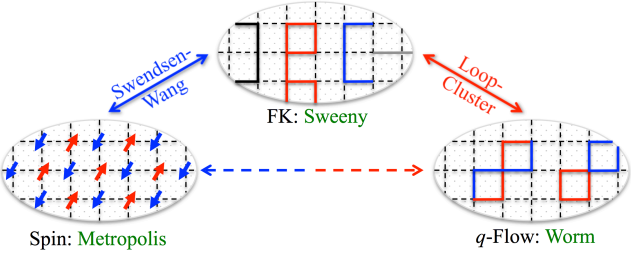
Limit: simulations and measurements are constricted in the same representation

Algorithms for Potts model



- Spin & FK: Swendsen-Wang (SW) Alg. [PRL 58, 86 (1987)]
- q-flow & FK[1]:Loop-Cluster (LC) Alg. [PRL: 125, 200603 (2020)]
- q-flow & Spin: Combination of SW Alg. and LC Alg.

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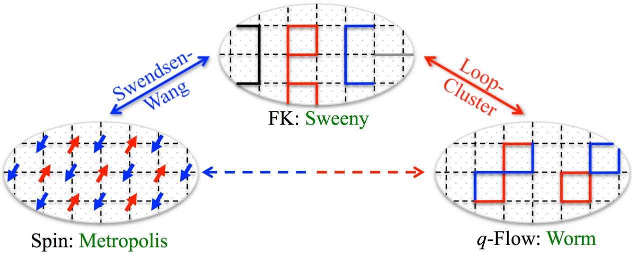
Algorithms for Potts model



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A single Markov-chain simulation can simultaneously sample physical quantities in any representation!

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How to couple different representations?

General idea [PRD 38,2009 (1988)]: define a joint model $d\mu(\{f\},\{b\})$ so that

- Marginal measure of $\{f\}$ is precisely the q-flow measure
- Marginal measure of $\{b\}$ is precisely the FK measure

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- Marginal measure of $\{f\}$ is precisely the q-flow measure
- Marginal measure of $\{b\}$ is precisely the FK measure

Then

- Given $\{f\}$, FK configurations are generated according to conditional measure $d\mu(\cdot|\{f\})$
- Given $\{b\}$, q-flow configurations are generated according to conditional measure $d\mu(\cdot|\{b\})$

Loop-Cluster Joint Model

- Definition

$$d\mu_{\rm jLC}(\{f\},\{b\}) = \mathcal{Z}_{\rm jLC}^{-1}\ \delta_{\partial G=\varnothing} \prod_{(ij)} \left[\frac{p_{ij}}{q} \delta_{f_{ij}\neq 0}\delta_{b_{ij},1} + \frac{p_{ij}}{q}\delta_{f_{ij}=0}\delta_{b_{ij},1} + (1-p_{ij})\delta_{f_{ij}=0}\delta_{b_{ij},0} \right] d\mu_0(\{f\})d\mu_0(\{b\})$$

- Given $\{f\}$, conditional measure $d\mu(\cdot|\{f\})$ is obtained as:
  - independently for each (ij)
    $p(b_{ij}=1|f_{ij}>0)=1$; $p(b_{ij}=1|f_{ij}=0)=\frac{p_{ij}}{p_{ij}+q(1-p_{ij})}=t_{ij}$
- Given $\{b\}$, conditional measure $d\mu(\cdot|\{b\})$ is obtained as:
  - for subset of flow variables $\{f\}_{\rm b}$ on $G_{\rm b}$
    $p(\{f\}_{\rm b}|G_{\rm b}) = q^{-c(G_{\rm b})}\delta_{\partial G_{\rm b}=\varnothing}$
  - for subset of flow variables on $(ij)\notin E_{\rm b}$
    $p(f_{ij}=0|b_{ij}=0)=1$

Loop-Cluster Algorithm

- From q-flow to FK
  - For each $f_{ij} \neq 0$, set $b_{ij} = 1$
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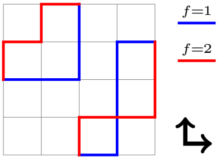

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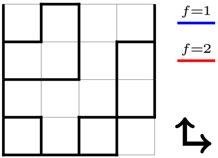

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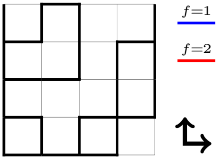

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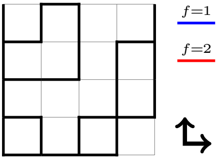

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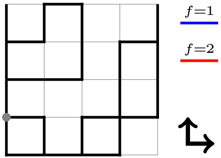

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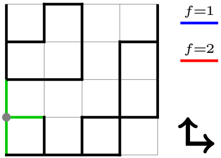

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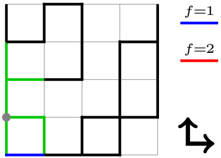

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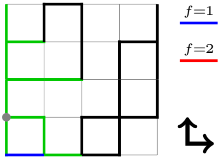

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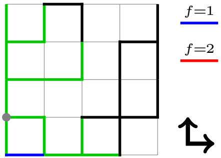

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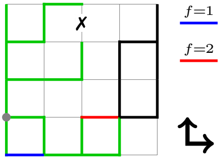

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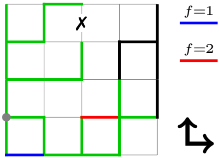

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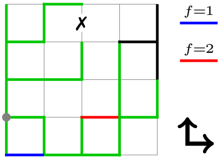

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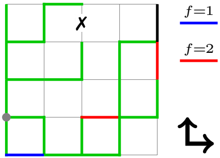

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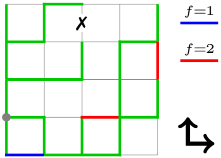

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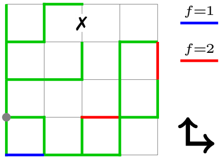

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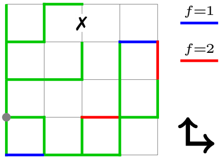

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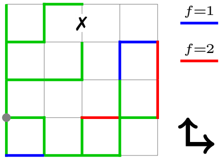

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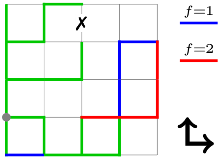

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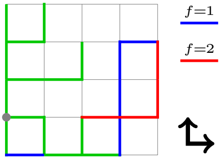

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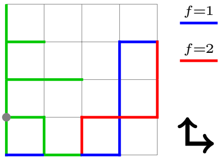

- From q-flow to FK
  - For each $f_{ij} \neq 0$, set $b_{ij} = 1$
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    (i) Search: construct a spanning tree from a root vertex; uniformly assign a flow value $f \in \{0, 1, ..., q-1\}$ to each missing edge
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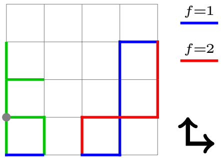

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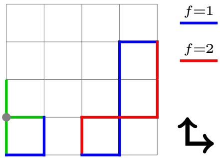

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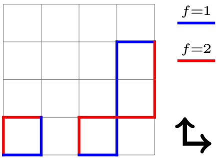

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Loop-Cluster Algorithm

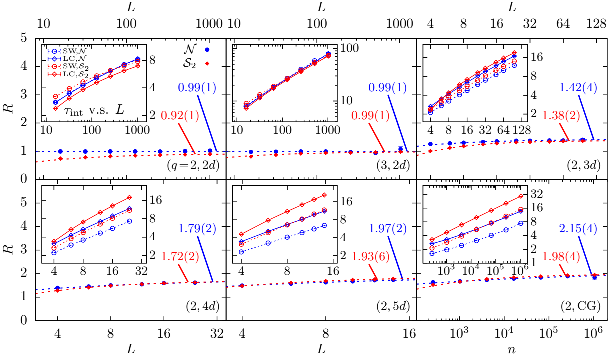
Extension

- Real $q \geq 1$ version for FK representation
  - Starting from $\{b\}$, choose an integer $1 \leq m \leq q$
  - Activate each cluster with probability m/q
  - Update active partition with LC algorithm for $q' = m$
- Single-cluster version for q-flow representation
  - Begin with $\{f\}$
  - Grow a cluster by Loop-to-Cluster process until it can not become larger
  - Update this cluster by Cluster-to-Loop process

Monte Carlo simulations

Efficiency

- Comparison of LC & SW

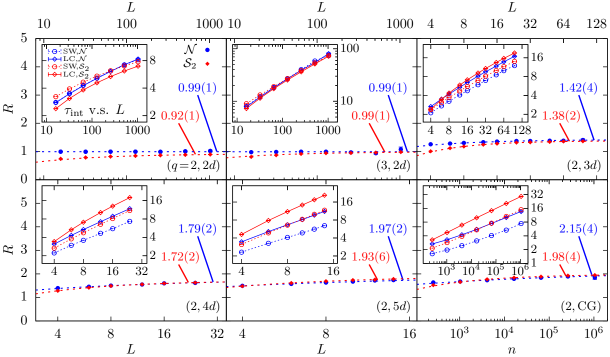


  - $\mathcal{N}$: # of occupied bonds
  - $\mathcal{S}_2$: second moment of FK cluster sizes
  - $R = \tau_{\rm int}^{\rm (LC)}/\tau_{\rm int}^{\rm (SW)}$, $\tau_{\rm int}$: integrated autocorrelation time

Monte Carlo simulations

Efficiency

- Comparison of LC & SW: in same dynamic universality class



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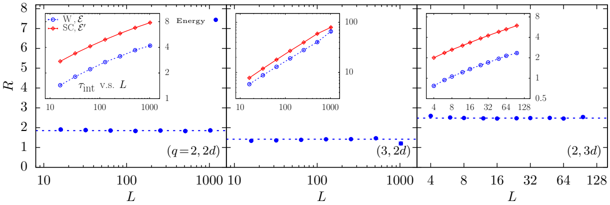
Monte Carlo simulations

Efficiency

- Comparison of single-cluster version & Wolff Alg



  - $\mathcal{E} = \sum_{(ij)\in E} \delta_{\sigma_i,\sigma_j}$, $\mathcal{E}' = \sum_{(ij)\in E} \delta_{f_{ij}\neq 0}$
  - $R = \tau^{(\text{SC})}_{\text{int},\mathcal{E}'} / \tau^{(\text{W})}_{\text{int},\mathcal{E}}$
- Also in the same dynamic universality class

Monte Carlo simulations

New family of fractal objects

- For q-flow, backbone and FK clusters: $D_{\rm qF} \leq D_{\rm bb} \leq D_{\rm FK}$
- Construct a hierarchy of $q_{\sf F}$-flow clusters
  - For FK configuration with real q, do Cluster-to-Loop updates with $q_{\sf F}$
  - For $q_{\sf F} = 2$, the results are
    - $D_{q{\sf F}} = 1.3333(2) \approx 4/3$ for $q = 1$
    - $D_{q{\sf F}} = 1.3754(12) \approx 11/8$ for $q = 2$
    - $D_{q{\sf F}} = 1.417(2) \approx 17/12$ for $q = 3$
    - $D_{q{\sf F}} = 1.464(6) \approx 35/24$ for $q = 2 + \sqrt{3}$
  - All are consistent with $D_{\sf EP} = 1 + g/8$
  - We conjecture $D_{q{\sf F}}(q_{\sf F} = 2) = D_{\sf EP}$

Summary

- We present the Loop-Cluster joint model to couple the FK and q-flow representations of the Potts model
- Loop-Cluster algorithm is proposed, lifting the limitation of performing both simulations and measurements in a given representation
- LC algorithm and its single-cluster version belong to the same dynamic class as the SW and the Wolff algorithm, respectively
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Thanks!