# Cluster simulations of loop models on planar lattices.

Youjin Deng New York University

#### **OUTLINE**

- Swendsen-Wang simulation of the Potts model
- Cluster simulation of the O(N) loop model on Honeycomb lattice
- ullet Cluster simulation of the N-component cornercubic model
- ullet Cluster simulation of the N-component facecubic model

In cooperation with

Alan D Sokal (New York Univ.)
Henk W.J. Blöte (Delft Univ. of Tech.; Leiden Univ.)
Wenan Guo (Beijing Normal Univ.)

Thanks to

Jesus Salas, Tim Garoni, Andrea Sportiello

#### Cluster method for the Potts model

Potts model

$$\mathcal{H}_{\mathsf{Potts}}(q,K) = -K \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j} \quad (\sigma = 1, 2, \dots, q)$$

- Metropolis Method
  - $\star$  Integrated autocorrelation time  $\tau \propto L^z$ .
  - $z\sim 2.2$ : severe critical slowing down
- Swendsen-Wang (SW) Method
  - \* Map onto random-cluster model

$$\begin{split} \mathcal{Z}_{\text{Potts}}(q, v) &= \sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + v \delta_{\sigma_i, \sigma_j}) \\ &= \sum_{\{b_{ij}\}} v^{\text{\#bonds}} q^{\text{\#clusters}} \end{split}$$

 $(v = e^K - 1)$ ; bond variable:  $b_{ij} = 0, 1$ 

\* A Swendsen-Wang step:

Start from bond configuration  $\{b_{ij}\}$ :

- (1): Identify Fortuin-Kasteleyn clusters for bond configuration  $\{b_{ij}\}$ .
- (2): Randomly and independently assign for each cluster all spin values to be  $\sigma \in (1,2,\cdots,q)$

(3) For each edge  $\langle ij \rangle$ , set  $b_{ij}=1$  with probability

$$p = \begin{cases} 1 - e^{-K} & \text{if } \sigma_i = \sigma_j \\ 0 & \text{if } \sigma_i \neq \sigma_j \end{cases}$$

• Chayes-Machta (CM) Method (for any real value  $q \ge 1$ )

Start from bond configuration  $\{b_{ij}\}$ :

- (1): Identify Fortuin-Kasteleyn clusters for bond configuration  $\{b_{ij}\}$ .
- (2): Randomly and independently set for each cluster all spin values to be 'active', with probability p=1/q, 'inactive', with p=1-1/q
- (3) For each edge  $\langle ij \rangle$ , update  $b_{ij}$  only if  $\sigma_i$  and  $\sigma_j$  are both ''active''.
  - \* Critical slowing down is strongly suppressed in SW and CM cluster methods. Exponent z satisfies Li-Sokal bound:  $z \geq \alpha/\nu$

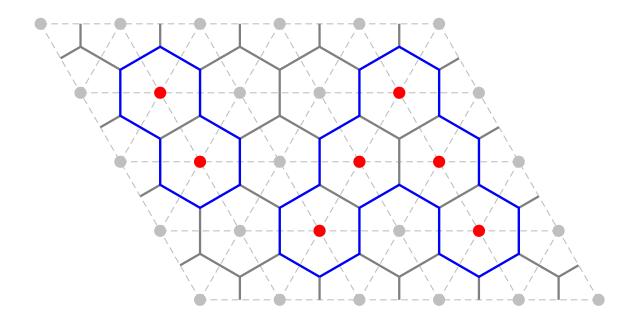
# Honeycomb-lattice O(N) loop model

 $\bullet$  O(N) loop model

$$\mathcal{Z}_{\text{loop}}(\lambda, N) = \int \prod_{k} d\vec{S}_{k} \prod_{\langle ij \rangle} (1 + \lambda N \vec{S}_{i} \cdot \vec{S}_{j}) ,$$

On Honeycomb lattice:

$$\mathcal{Z}_{\text{loop}}(\lambda, N) = \sum_{\{b_{ij}\}: \text{Eulerian}} \lambda^{\text{\#bonds}} N^{\text{\#loops}}$$



\*: critical line

$$\lambda_c(N) = \left(2 + \sqrt{2 - N}\right)^{-1/2}$$

 $\star$ : Universality: a critical O(N) loop model corresponds with a tricritical  $N^2$ -state Potts model

#### • Cluster Simulation

Start from spin configuration  $\{s\}$  on  $\mathcal{T}$ :

- (1): Construct loops on  $\mathcal{H}$  based on  $\{s\}$ : low-temperature graph of spin config. $\{s\}$ .
- (2): For each loop, set it to be 'active'' with probability p=1/N, and to be 'inactive'' with p=1-1/N.
- (3): For each edge  $\langle ij \rangle$ , place bond with probability

$$p = \begin{cases} 1 - \lambda & \text{if } s_i = s_j \\ 1 & \text{if } s_i \neq s_j \text{ and } \langle ij \rangle \text{ is inactive} \\ 0 & \text{if } s_i \neq s_j \text{ and } \langle ij \rangle \text{ is active} \end{cases}$$

- (4) Identify clusters for spins s; randomly flip for each cluster all spins s with probability 1/2.
  - \* Why does it work?

• N-color Ashkin-Teller (AT) model

On triangular lattice T:

$$\mathcal{H}_{AT}(J_2, J_4, N) = -J_2 \sum_{m=1}^{N} \sum_{\langle ij \rangle} \sigma_i^{(m)} \sigma_j^{(m)}$$
$$-J_4 \sum_{m>n} \sum_{\langle ij \rangle} \sigma_i^{(m)} \sigma_j^{(m)} \sigma_i^{(n)} \sigma_j^{(n)}$$

Let  $J_2 \to \infty$ ,  $J_4 \to -\infty$ , but  $J_2 + (N-1)J_4 = J$  held finite.

For edge  $\langle ij \rangle$ , let k denote the number of pairs of unequal Ising spins  $\sigma_i^{(m)} \neq \sigma_j^{(m)}$ , the statistical weight of  $\langle ij \rangle$  is

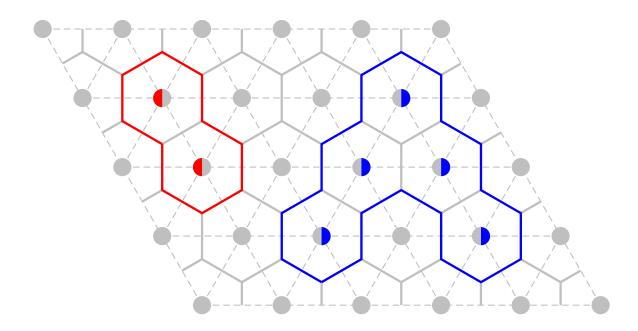
Configuration	Normalized weight
k = 0	1
k = 1	$e^{-2[J_2 + (N-1)J_4]} \equiv e^{-2J}$
$k \geq 2$	$e^{-2kJ} \cdot e^{k(k-1)J_4} \to 0$

In words, an edge can be occupied by at most one pair of unequal Ising variable  $\sigma_i^{(m)} \neq \sigma_j^{(m)}$ .

Low-temperature expansion of  $\mathcal{Z}_{AT}$  leads to:

$$\mathcal{Z}_{\mathrm{AT}}(\lambda,N) = N^2 \sum_{\{b_{ij}\} : \mathrm{Eulerian}} \lambda^{\mathrm{\#bonds}} N^{\mathrm{\#loops}}$$

\*: the N=2 case at criticality is equivalent with the *critical* Baxter-Wu model with 3-spin interactions.



• Cluster Simulation of the N-color AT model

Effective Hamiltonian for variable  $\sigma^{(m)}$ :

$$\mathcal{H}_{\text{eff}}(J_2, J_4, N; \sigma^{(m)}) = -J_{\text{eff}} \sum_{\langle ij \rangle} \sigma_i^{(m)} \sigma_j^{(m)},$$

with

$$J_{\text{eff}} = J_2 + J_4 \sum_{n \neq m} \sigma_i^{(n)} \sigma_j^{(n)}$$
.

 $\sigma^{(m)}$  can be updated by an embedding SW method:

Start from spin config.  $\sigma^{(m)}$  and  $\sigma^{(n)}$  for  $n \neq m$ .

(1) Place bonds with probability

$$p = \begin{cases} 1 - e^{-2J} & \text{if } \sigma_i^{(m)} = \sigma_j^{(m)} \text{ and } \sigma_i^{(n)} = \sigma_j^{(n)} \\ 1 & \text{if } \sigma_i^{(m)} = \sigma_j^{(m)} \text{ and } \sigma_i^{(n)} \neq \sigma_j^{(n)} \\ 0 & \text{if } \sigma_i^{(m)} \neq \sigma_j^{(m)} \end{cases}.$$

- (2) Identify clusters for spins  $\sigma^{(m)}$ .
- (3) For each cluster, independently flip for each cluster all spins  $\sigma^{(m)}$  with 1/2.

#### Reformulation

Define Ising variable  $s = \prod_m \sigma^{(m)}$ . Keep colors of loops in computer memory  $\{loops\}$ .

Start from spin config.  $\{s\}$  and loop config.  $\{\text{loops}\}$ 

(1) Place bonds with probability

$$p = \left\{ \begin{array}{ll} 1 - e^{-2J} & \text{if } s_i = s_j \\ 1 & \text{if } s_i \neq s_j \text{ and } ij \text{ is of color } n \neq m \\ 0 & \text{if } s_i \neq s_j \text{ and } ij \text{ is of color } m \end{array} \right.$$

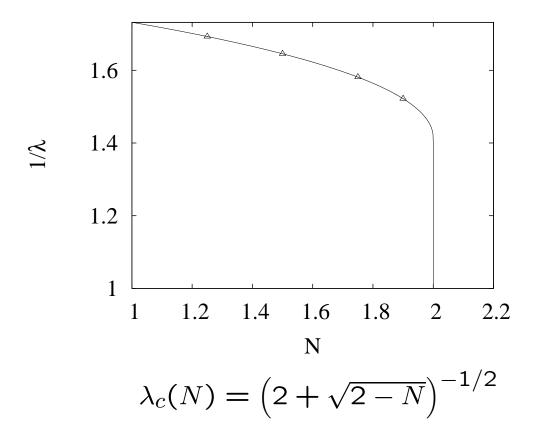
- (2) Identify clusters for  $\{s\}$ . Randomly flip for each cluster all spins with probability 1/2.
- (3) Update loop information for color m (loops of color  $n \neq m$  are frozen).

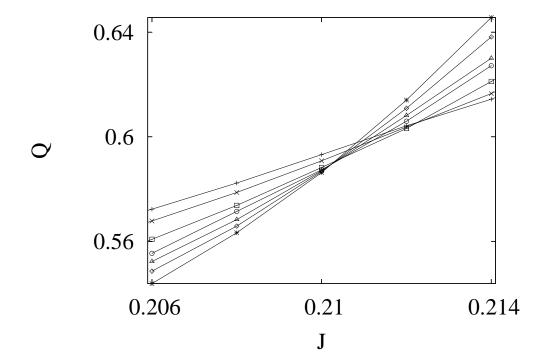
# Static and Dynamic Critical Behavior

# • Sampled Quantities

Specific heat C, susceptibility  $\chi$ , and Binder ratio Q etc.

## • Critical Line





$$\lambda_c(N=1.9)=1.521899 \Rightarrow J_c=0.20998.$$

# • Critical Exponent

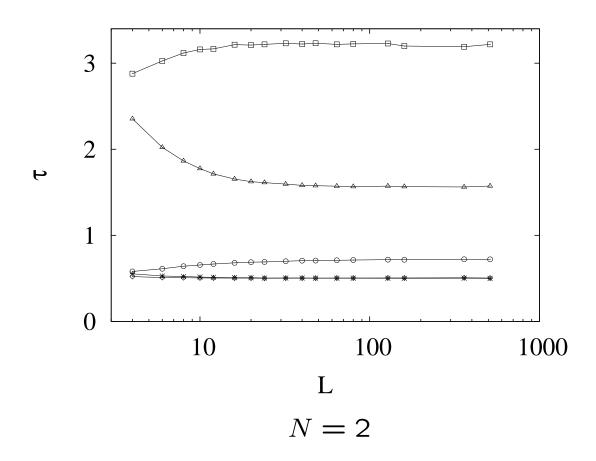
$\overline{}$		$y_{t1}$	$y_{t2}$	$y_h$
4 0 -				1 00 10
1.25	Exact	1.8327	0.8873	1.9343
	Num.	1.8327(2)	0.887(2)	1.9342(2)
1.50	Exact	1.7805	0.7481	1.9198
	Num.	1.7801(4)	0.745(4)	1.9199(2)
1.75	Exact	1.7078	0.5542	1.9034
	Num.	1.7079(4)	0.54(1)	1.9032(2)
2.00	Exact	1.5	0	1.875
	Num.	1.5002(4)	0.1(2)	1.8751(1)

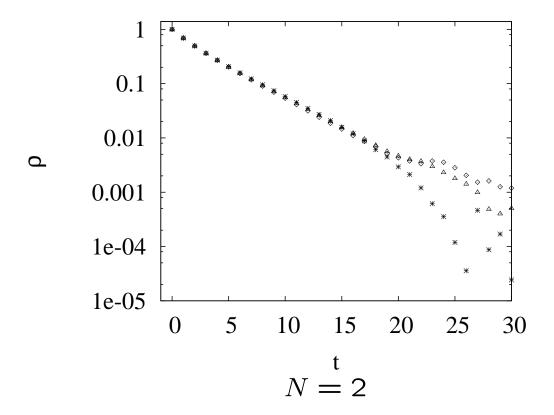
# • Dynamic Critical Behavior

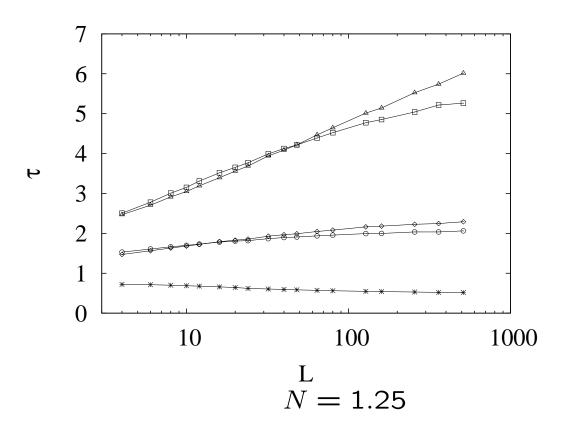
For quantity f, integrated autocorrelation time  $\tau$ :

$$\tau_{int,f} = \frac{1}{2} \sum_{t=-\infty}^{\infty} \rho_f(t) = \frac{1}{2} + \sum_{t=1}^{\infty} \rho_f(t)$$

 $ho_f$ : normalized autocorrelation function







Critical slowing down hardly exits!

### N-component Corner-Cubic Model

• N-component corner-cubic model

O(N) model:

$$\mathcal{Z}_{\text{loop}}(\lambda, N) = \int \prod_{k} d\vec{S}_{k} \prod_{\langle ij \rangle} (1 + \lambda N \vec{S}_{i} \cdot \vec{S}_{j}) ,$$

Approximate  $\vec{S}$  by corner-cubic spin:

$$\begin{aligned} \mathcal{Z}_{\text{CC}} &= \sum_{\{\sigma^{(m)}\}} \prod_{\langle ij \rangle} [1 + \lambda (\sigma_i^{(1)} \sigma_j^{(1)} + \cdots \sigma_i^{(N)} \sigma_j^{(N)})] \\ &= \sum_{\text{Loop colors}} \dots \sum_{\text{Colors}} \lambda^{\text{\#bonds}} \end{aligned}$$

# N-color Ashkin-Teller (AT) model

On each site, put N independent copies of Ising spins  $\sigma^{(m)}$ . Let f be the number of pairs of unequal spins, the normalized weight is

Configuration	Normalized weight
k = 0	1
k = 1	$\lambda$
$k \geq 2$	0

In words, an edge can be occupied at most one pair of unequal Ising variable  $\sigma_i^{(m)} \neq \sigma_j^{(m)}$ .

Low-temperature expansion of  $\mathcal{Z}_{AT}$  leads to:

$$\mathcal{Z}_{\mathsf{AT}}(\lambda,N) \propto \underbrace{\sum \sum \cdots \sum}_{\mathsf{Loop\ colors}} \lambda^{\mathsf{\#bonds}}$$

# Embedding SW method

Start from spin config.  $\sigma^{(m)}$  and  $\sigma^{(n)}$  for  $n \neq m$ .

(1) Place bonds with probability

$$p = \begin{cases} 1 - \lambda & \text{if } \sigma_i^{(m)} = \sigma_j^{(m)} \text{ and } \sigma_i^{(n)} = \sigma_j^{(n)} \\ 1 & \text{if } \sigma_i^{(m)} = \sigma_j^{(m)} \text{ and } \sigma_i^{(n)} \neq \sigma_j^{(n)} \\ 0 & \text{if } \sigma_i^{(m)} \neq \sigma_j^{(m)} \end{cases}.$$

(2) Construct clusters for  $\{\sigma^{(m)}\}$ ; randomly flip for each cluster all spins with 1/2.

• Special Symmetries for N=2

Ising domains: Areas enclosed by loops

Given spin config.  $\sigma^{(1)}$  and  $\sigma^{(2)}$ 

- (1) Calculate  $s=\sigma^{(1)}\cdot\sigma^{(2)}$ , and Construct Ising domains for s.
- (2) For each domain, randomly set  $\sigma^{(1)}=\pm 1$ , let  $\sigma^{(2)}=s\cdot\sigma^{(1)}$ .
  - \* Random swapping between  $\sigma^{(1)}$  and  $\sigma^{(2)}$
- Embedding SW method with Random Swapping (integer  $N \ge 2$ )
- (1) Randomly choose a pair of spins  $\sigma^{(m)}$  and  $\sigma^{(n)},$  and carry out random swapping.
  - (2) Update spins  $\sigma^{(m)}$ .

• Embedding SW method with Random Swap*ping* (noninteger  $N = k/2^l$ )

Example for N=3/2. On each site, put 3 independent spins  $\sigma^{(1)}$ ,  $\sigma^{(2)}$ , and  $\sigma^{(3)}$ .

- (1) Randomly choose a pair of spins  $\sigma^{(i)}$  and  $\sigma^{(j)}$ ; the third copy of spin is  $\sigma^{(k)}$ . Calculate  $s = \sigma^{(i)} \cdot \sigma^{(j)}$ .
- (2) Update spins s by the embedding SW method.

Bond probability is: 
$$p = \begin{cases} 1 - \lambda & \text{if } s_i = s_j \text{ and } \sigma_i^{(k)} = \sigma_j^{(k)} \\ 1 & \text{if } s = s_j \text{ and } \sigma_i^{(k)} \neq \sigma_j^{(k)} \\ 0 & \text{if } s_i \neq s_j \end{cases}.$$

- (3) For each Ising domain of s, randomly set  $\sigma^{(i)} = \pm 1$ , and set  $\sigma^{(j)} = s \cdot \sigma^{(j)}$ .
- $\star$  For noninteger N, the corner-cubic model has not yet been well defined.
- \* The embedding SW method with random swapping suffers little from critical slowing down on the square lattice for N < 2.

### N-component Face-Cubic Model

# Embedding SW method

O(N) model:

$$\mathcal{Z}_{\text{loop}}(\lambda, N) = \int \prod_{k} d\vec{S}_{k} \prod_{\langle ij \rangle} (1 + \lambda N \vec{S}_{i} \cdot \vec{S}_{j}) ,$$

Approximate  $\vec{S}$  by face-cubic spin:

$$\mathcal{Z}_{fC} = \sum_{\{\sigma^{(m)}\}} \prod_{\langle ij \rangle} [1 + \lambda(\sigma_i^{(1)}\sigma_j^{(1)} + \cdots \sigma_i^{(N)}\sigma_j^{(N)})]$$

$$= \sum_{\{s,\tau\}} \prod_{\langle ij \rangle} (1 + \lambda s_i s_j \delta_{\tau_i,\tau_j}) \qquad (1)$$

$$\sigma^{(m)} = 0, \pm 1, \ s = \pm 1, \ \text{and} \ \tau = 1, 2, \cdots N.$$

Expansion of Eq. (1) leads to

$$\mathcal{Z}_{\text{fC}} = \sum_{\text{Eulerian}} \lambda^{\text{\#bonds}} N^{\text{\#clusters}}$$
 
$$\propto \sum_{\text{Eulerian}} \lambda^{\text{\#bonds}} N^{\text{\#domains}}$$

# • SW-type simulation

Let loop config. on lattice  $\mathcal L$  be the low-temperature graph of Ising spins s on the dual lattice  $\mathcal L^*$ .

- (1) Construct Ising domains for s. For each domain, let it be 'active" with probability p=1/N and be 'inactive" with p=1-1/N.
  - (2) Update spins s by SW method. Bond probability is

$$p = \left\{ \begin{array}{ll} 1 - \lambda & s_i = s_j \text{; both } s_i, s_j \text{ are active} \\ 1 & s_i \text{ or } s_j \text{ is inactive} \\ 0 & s_i \neq s_j \text{; both } s_i, s_j \text{ are active} . \end{array} \right.$$

- $\star$  Simulation results for  $N \leq 2$  agree with those by transfer-matrix techniques.
  - \* Suffers little from critical slowing down

#### Conclusions

- A set of cluster methods is developed for some loop models
- Little critical slowing down is observed for  $1 < N \le 2$ .

#### Work to be done

- Directly prove the validity of the cluster methods
- Some versions of cluster methods may be improved
- ullet Develop cluster method for O(N) loop model on square lattice
- Explore new physics.