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Simulation of Phase Transition and its Visualization

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CONTANTS

Part I
Basic Concept of Phase transition

Phase Transition

- **Classical Phase Transition**: caused by thermal parameters

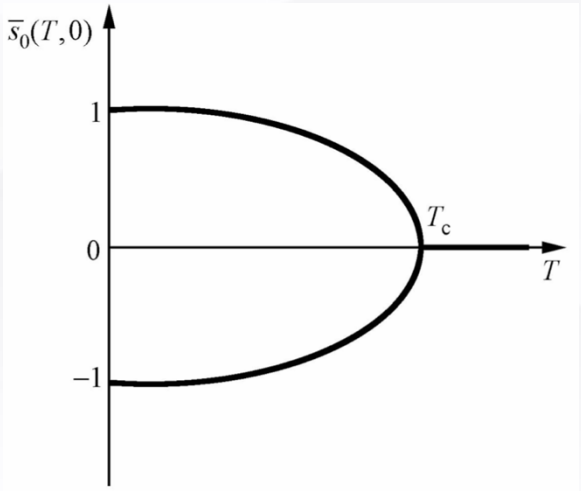
  e.g. water-ice-vapor, superconductor-resistor, Ising Model

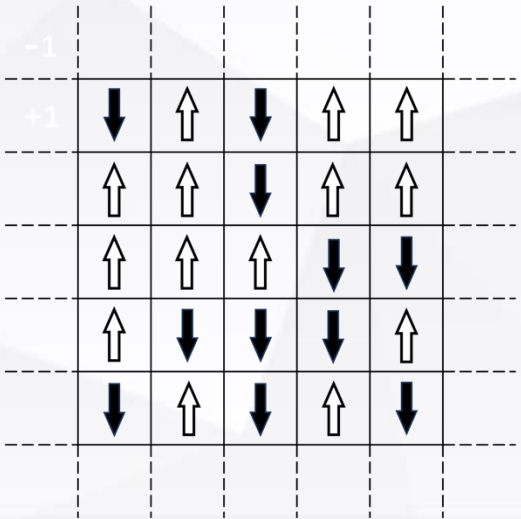
- **Quantum Phase Transition**: adulteration, magnetization

  e.g. Bose-Hubbard Model

2D Ising Model

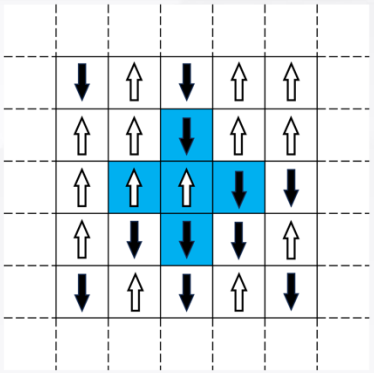
- Paramagnetic-ferromagnetic, T_c : Curie Temperature
- Lenz – Ising : 1D
- Mean field theory: $T_c = 2$
- Ensemble Theory, Onsager, Second-order transition, $\frac{d^2E}{dT^2}$ discontinued
- Landau: Order parameter symmetry breaking theory





$$H = -J \sum_{<i,j>} s_i s_j$$

Part II
Method

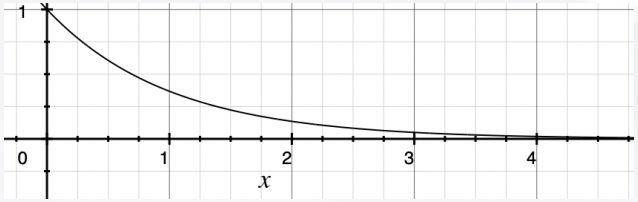


Metropolis Algorithm

1. Give a random spin configuration $\{s_i\} \equiv s_1, s_2 \cdots, s_N$
2. Select a point randomly, calculate the energy change if flip it.

$$\Delta E = (-J\,(-s_m)\sum_n s_n) - (-J\,s_m \sum_n s_n) = 2\,J s_m \sum_n s_n$$

3. If $\Delta E \leq 0$, flip; if $\Delta E > 0$, flip it by a ratio $A = e^{-\Delta E/kT} \in [0, 1]$
4. Repeat 2-3, (Markov chain length)
5. Change the Temperature and repeat 2-4.



Important sample

Markov process

1. **Ergodicity** ✅
2. Detailed Balance:

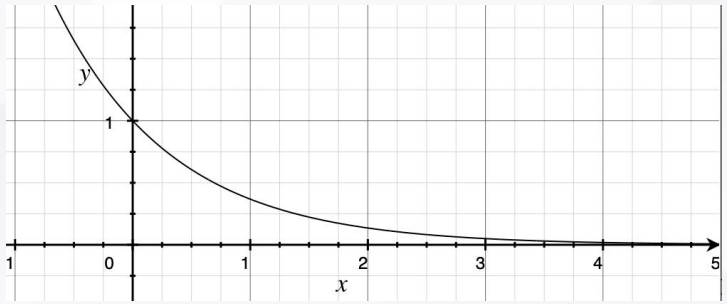
$$p_\mu P(\mu \to \nu) = p_\nu P(\nu \to \mu)$$

$$p_\mu = e^{-\beta E_\mu}, \qquad p_\nu = e^{-\beta E_\nu}$$

$$P(\mu \to \nu) \equiv g(\mu \to \nu) \cdot A(\mu \to \nu)$$

$$g_{\mu \to \nu} = \frac{1}{N}$$

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{g(\mu \to \nu)A(\mu \to \nu)}{g(\nu \to \mu)A(\nu \to \mu)} = \frac{A(\mu \to \nu)}{A(\nu \to \mu)} = e^{-\beta (E_\nu - E_\mu)}$$

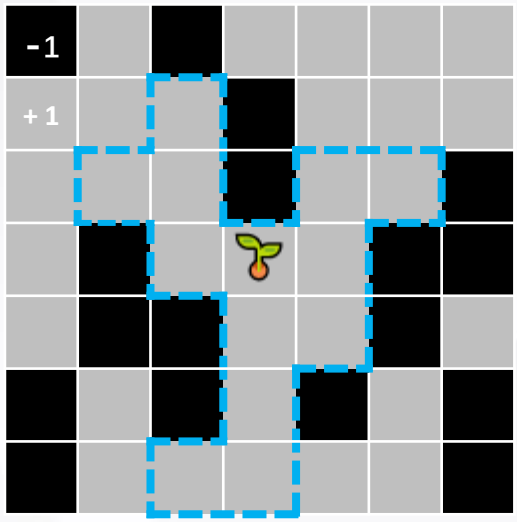


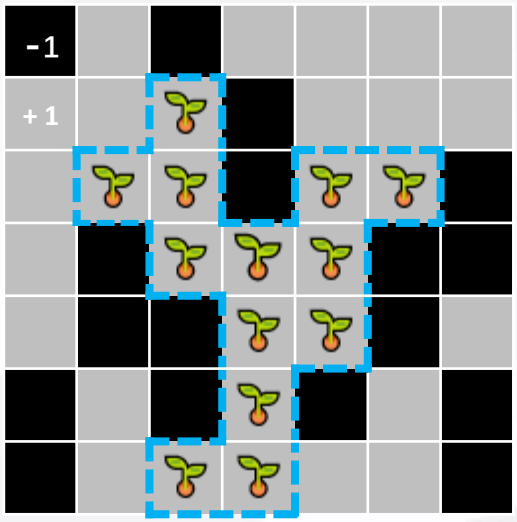
$$A(\mu \to \nu) = \begin{cases} e^{-\beta (E_\nu - E_\mu)}, & \text{if } E_\nu - E_\mu > 0, \\ 1, & \text{others.} \end{cases}$$

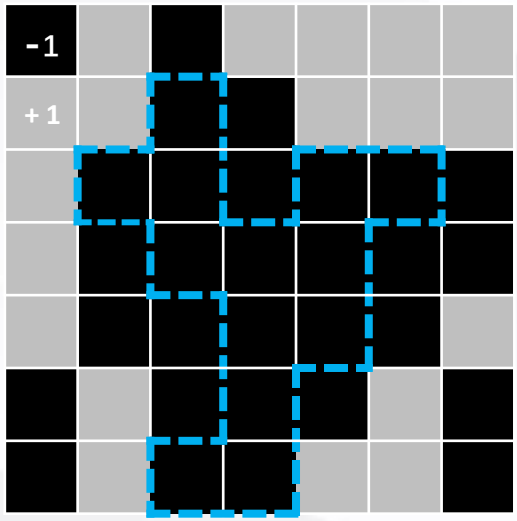
Metropolis's Shortcoming

1. Single-Filp-Dynamics: convergence speed is too slow.
2. Easy to fall into metastable state.

Wolff Algorithm







state μ,
Select a seed

Cluster growth: Add neighbors with a probability P_{add}

Flip the cluster, state ν

Wolff's process

1. Give a random spin configuration $\{s_i\} \equiv s_1, s_2 \cdots, s_N$
2. Select a seed point randomly,
3. Grow the cluster: consider its neighbors, add them to the cluster with $P_{\text{add}} = 1 - e^{2J/kT}$ (use random numbers), until no new members.
4. Flip the cluster.
5. Repeat step 2-4. (called Wolff length)
6. Change T, repeat 2-5.

c: number of added ,
m: number of not added at μ,
n: number of not added at ν.

$$g(\mu \to \nu) = (P_{\text{add}})^c (1 - P_{\text{add}})^m,$$

$$g(\nu \to \mu) = (P_{\text{add}})^c (1 - P_{add})^n$$

$$e^{-\beta\,(E_\nu\, -E_\mu)} = \frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{g(\mu \to \nu)A(\mu \to \nu)}{g(\nu \to \mu)A(\nu \to \mu)} = (1 - P_{\text{add}})^{m-n} \frac{A(\mu \to \nu)}{A(\nu \to \mu)}$$

$$\Delta E = E_\nu - E_\mu = 2J(m - n)$$

$$\Rightarrow \quad \frac{A(\mu \to \nu)}{A(\nu \to \mu)} = e^{\beta 2J(m-n)} (1 - P_{\text{add}})^{m-n}$$

$$\text{Wolff}: \quad P_{\text{add}} = 1 - e^{-2\beta J}$$

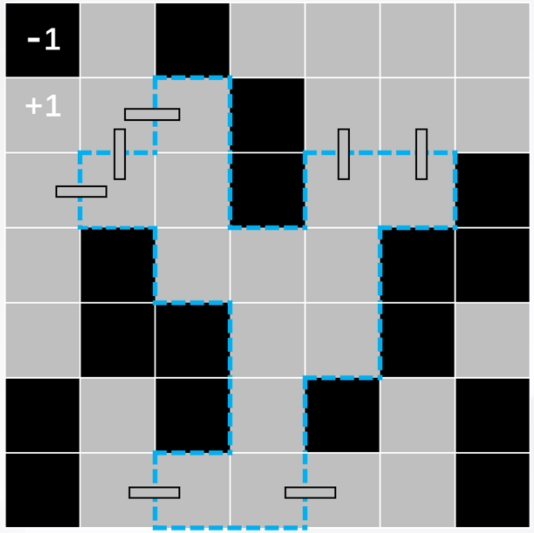
$$\Rightarrow A_w(\nu \to \mu) = A_w(\mu \to \nu) = 1$$

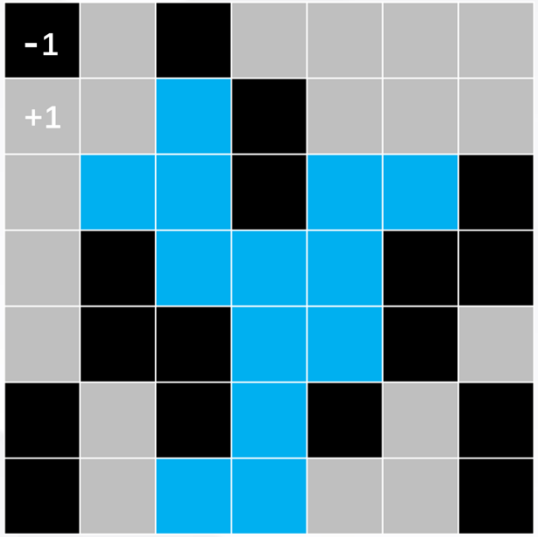
- **Accepted ratio: Wolff > Metropolis** $A_m(\mu \to \nu) = \begin{cases} e^{-\beta\,(E_\nu\, -E_\mu)}, & \text{if } E_\nu - E_\mu > 0, \\ 1, & \text{others.} \end{cases}$
- A sample process will definitely bring a flip: **A higher efficiency.**

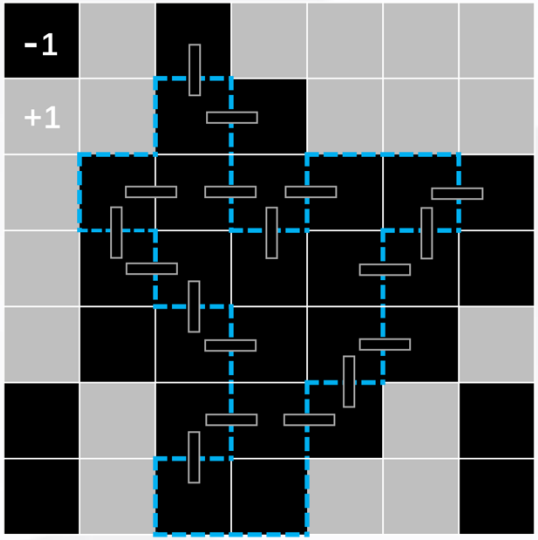
$$\Delta E = E_\nu - E_\mu = 2J(m-n)$$

$$E = -J\sum_{<i,j>} s_i s_j$$

$$\Delta E = 2Js_m\sum_n s_n$$







Gray bond: $m = 7$

Cluster

Black bond: $n = 18$

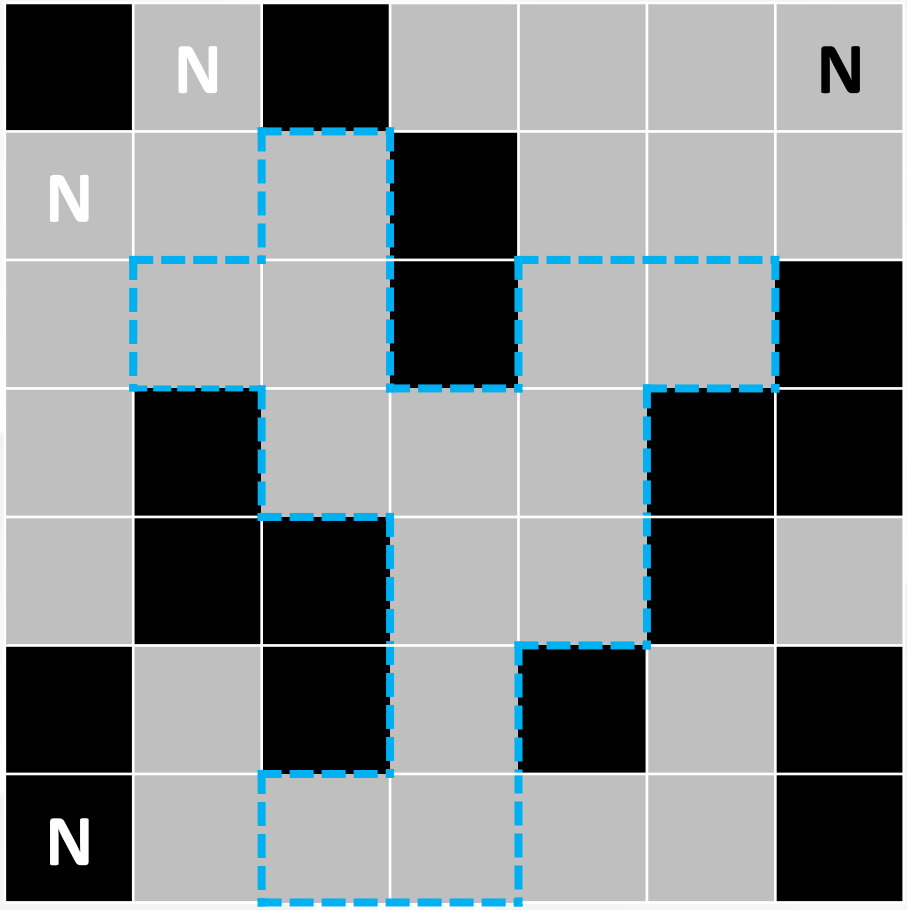
$$E(\mu) = E_{gg} + E_{gb}$$
$$= -J(1\times 1)\times 7 - J[(1)\times(-1)]\times 18$$

$$E(\nu) = E_{bb} + E_{gb}$$
$$= -J[(-1)\times(-1)]\times 18 - J[(-1)\times 1]\times$$

7

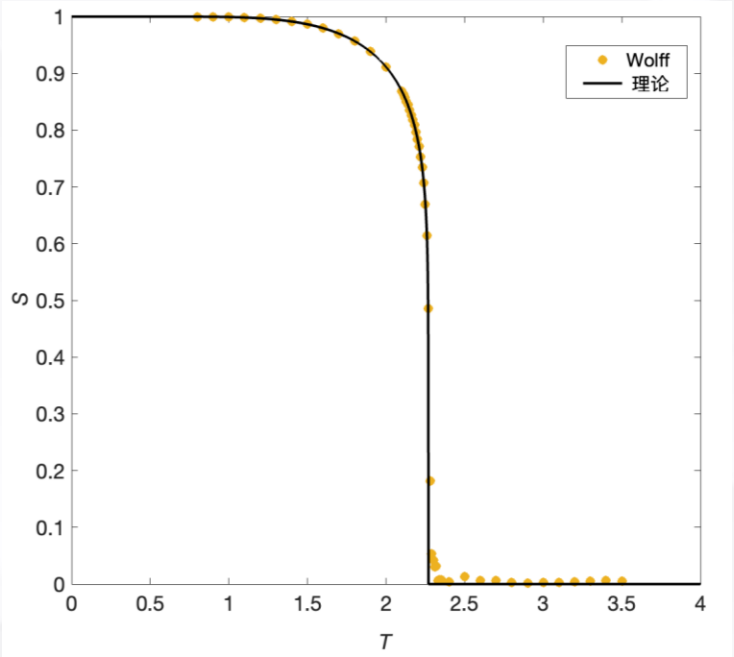
$$\Delta E = E(\nu) - E(\mu) = 2J(7-18) = -22J$$

Periodical Boundary Condition



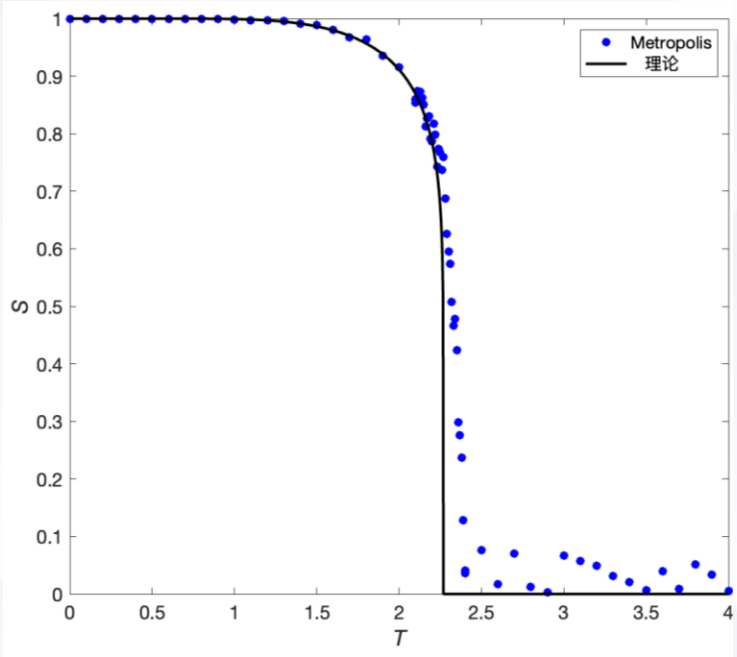
Part III
Result and Discussion

1. Order parameter $\bar{s}$-- the best result



Wolff

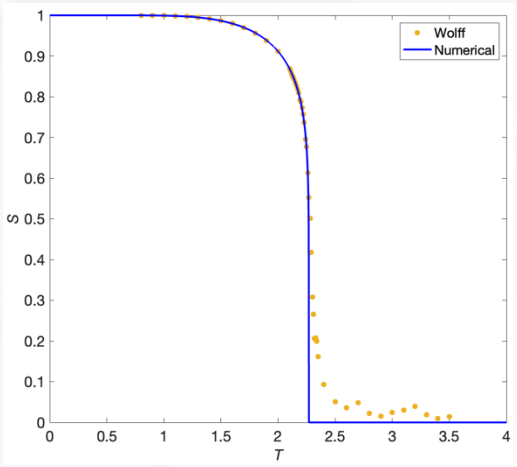
$L = 400, l_w = 1000, t = 20$ hours



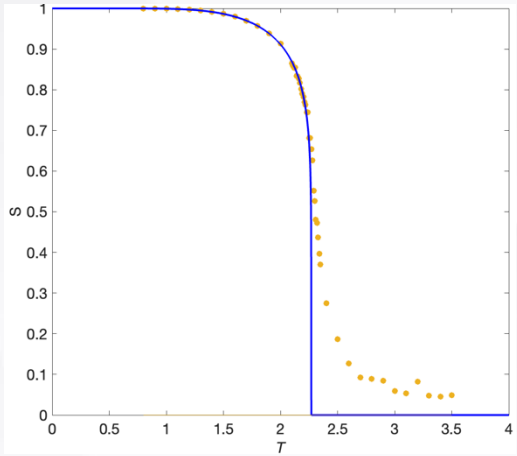
Metropolis

$L = 100, l_m = 500\text{k}, t = 159\text{s}$

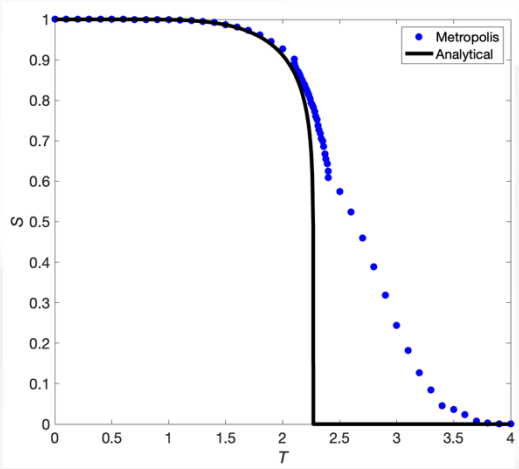
- Reduce/enlarge the system's size: **Metropolis is fast but worsen.**



Wolff, $L = \mathbf{100}, l_w = 1000, t = 690$ s

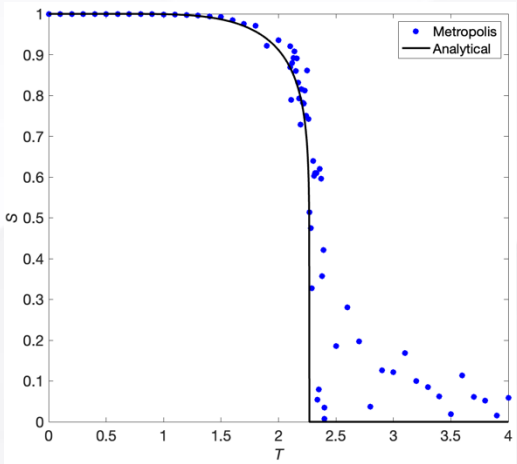


Wolff, $L = \mathbf{40}, l_w = 1000, t = 109$ s



Metorpolis, $L = \mathbf{400}, l_m = 500\text{k}, t = 159$ s

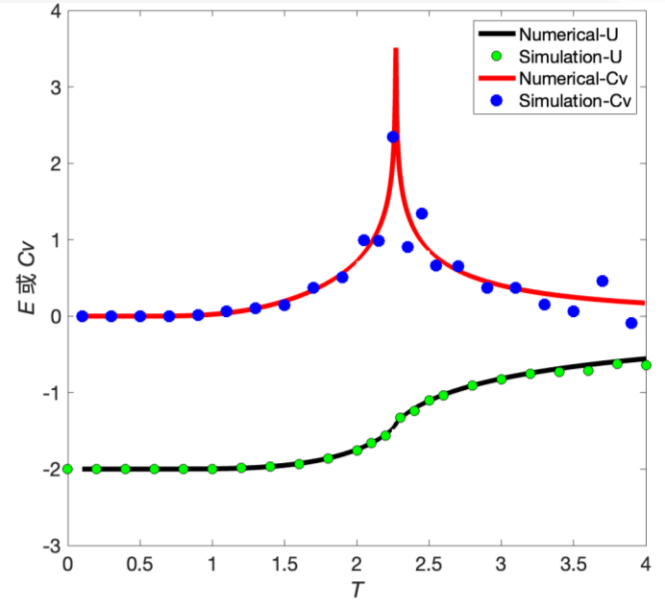
$$p_\mu = e^{-\beta E_\mu}$$



Metorpolis, $L = \mathbf{40}, l_m = 500\text{k}, t = 44$ s

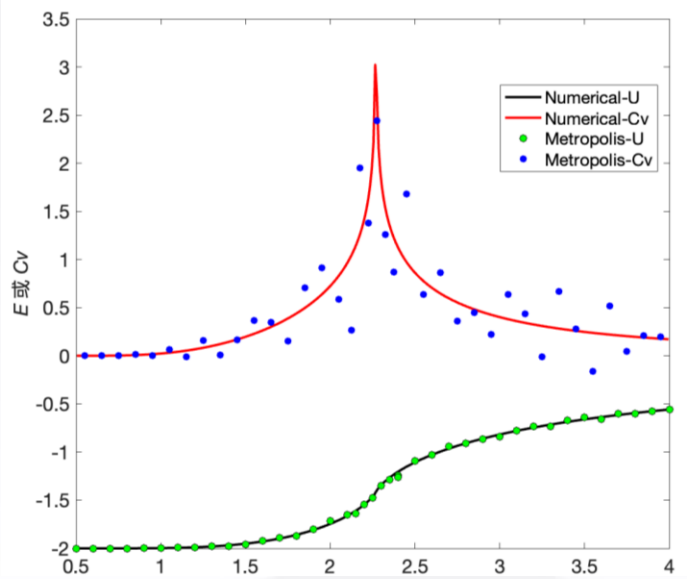
- Enlarge the size,
  - Wolff have a higher precision (sacrifice time)
  - Metropolis could not find all of the states, faster but larger errors.
  - If approaching to the Thermodynamics limit: Wolff ~ Idea Ising Model.

2. Energy & Specific heat capacity 2th phase transition



Wolff

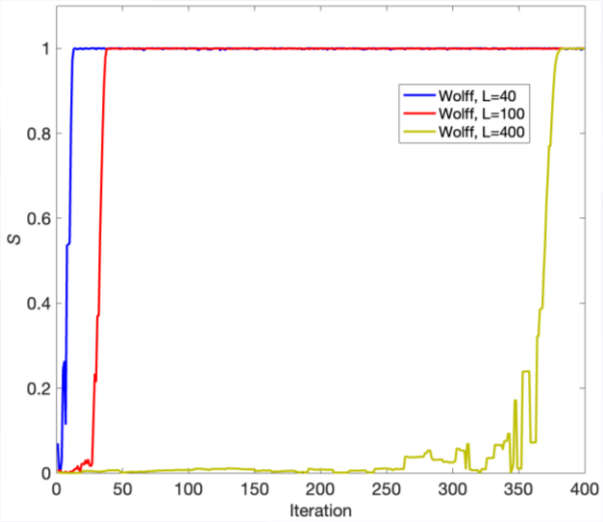
$L = 100, l_w = 2000, t = 190\ \mathrm{s}$



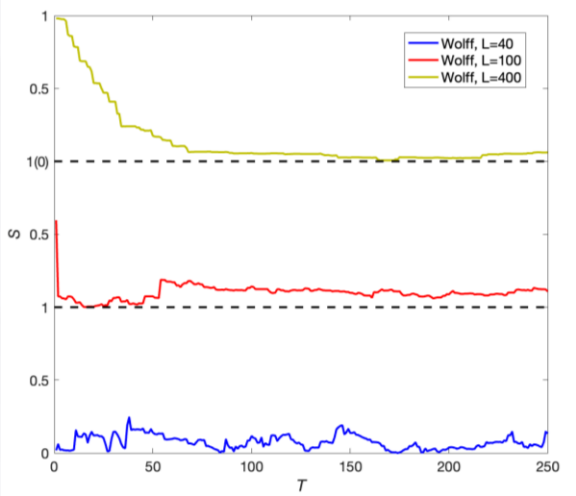
Metropolis

$L = 100, l_m = 500\mathrm{k}, t = 108\mathrm{s}$

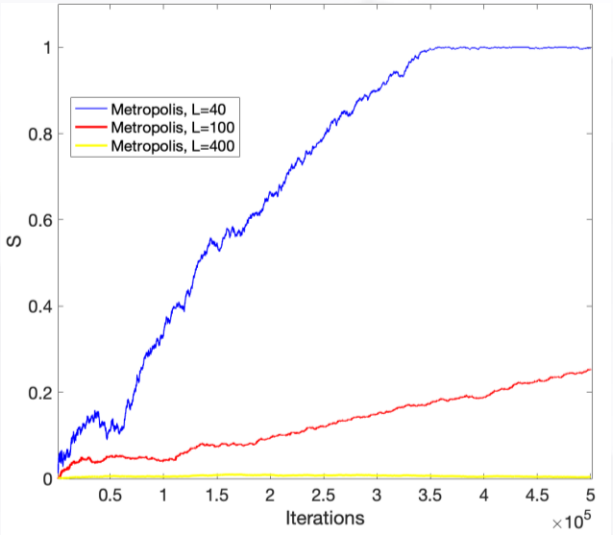
3. Convergence speeds of the algorithms (when away from T_c)



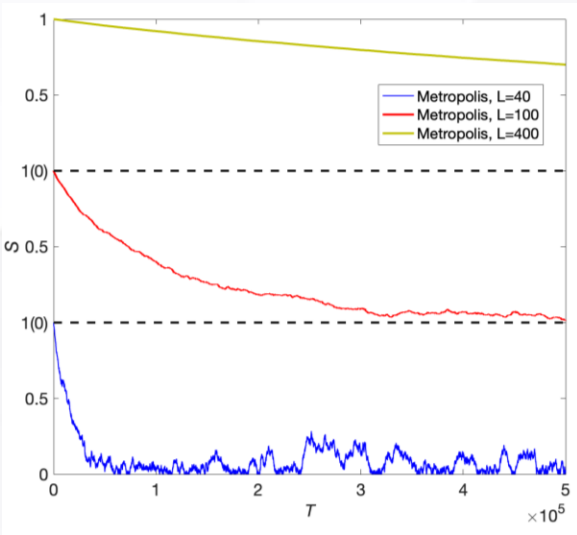
$T = 1,\ \ L = 40,100,400,\ \ t = 76$ s



$T = 3, L = 40,100,400, t = 0.9$ s



$T = 1,\ \ L = 40,100,400,\ \ t = 44$ s



$T = 3, L = 40,100,400, t = 46$ s

- Convergence speed at low/high T
  - Metropolis is slower, need more sampling steps.

    In larger size it has a probability of unconverging.

4. Near T_c

Analytical

$\bar{s} = 0.6134$

表 1 $T_c = 2.26$ 下两种算法的误差对比

	1	2	3	4	5	平均值	标准差	相对误差
Metropolis	0.7843	0.7469	0.7412	0.7776	0.7719	0.7644	0.0192	0.31%
Wolff	0.6120	0.6207	0.6161	0.6159	0.6119	0.6153	0.0036	24.6%

- Wolff‘s result is more stable and more precise
- Metropolis’s single-flip strategy is hard to simulate all states of the system.

Part IV
Conclusion

- Metropolis, low efficiency, needs more samples (longer markov chains) ,

  imprecise, can not improved by only increase the size.

  just use as an approximation.

  In certain size it is acceptable.
- Wolff is faster in high temperature. Near critical point, the result is stable because of finding out more possible state.

Visualization of Ising model's phase transition process

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THANKS

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