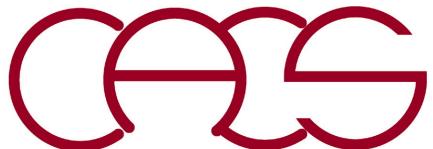


Monte Carlo Simulation of Spins

Aiichiro Nakano

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Department of Computer Science
Department of Physics & Astronomy
Department of Quantitative & Computational Biology
University of Southern California*

Email: anakano@usc.edu



Markov Chains for Complex Dynamics

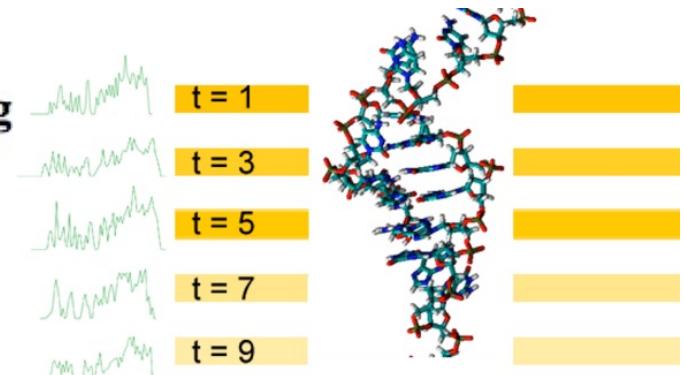
- Hidden Markov model — Viterbi algorithm (*cf.* dynamic programming)
- Perron-Frobenius eigenvalue cluster analysis

DNA Sequencing via Quantum Mechanics and Machine Learning

Int'l J. Comput. Sci. **4**, 352 ('10)

Henry Yuen¹, Fuyuki Shimojo^{1,2}, Kevin J. Zhang^{1,3}, Ken-ichi Nomura¹, Rajiv K. Kalia¹, Aichihiro Nakano^{1*}, Priya Vashishta¹

cf. Henry's historical breakthrough



A Tutorial on Hidden Markov Models and Selected Applications in Speech Recognition

LAWRENCE R. RABINER, FELLOW, IEEE

Proc. IEEE, **77**, 257 ('89)

Implementing the Viterbi Algorithm

Fundamentals and real-time issues for processor designers

HUI-LING LOU

IEEE Signal Processing Mag., **12**(5), 42 ('95)



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Available online at www.sciencedirect.com



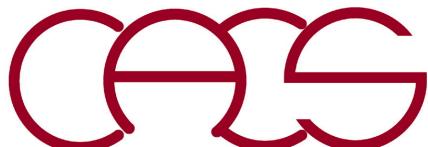
Linear Algebra and its Applications 398 (2005) 161–184

LINEAR ALGEBRA
AND ITS
APPLICATIONS

www.elsevier.com/locate/laa

Robust Perron cluster analysis in conformation dynamics [☆]

Peter Deuflhard, Marcus Weber*

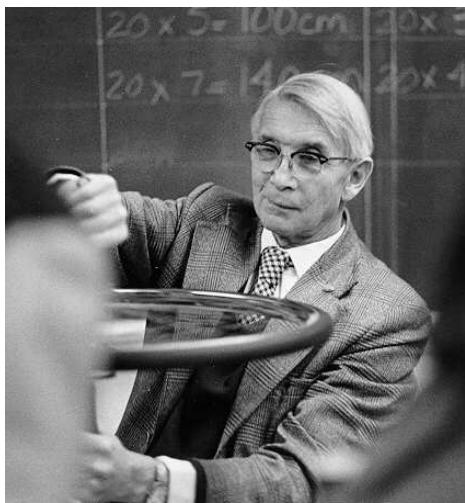


Ising Model

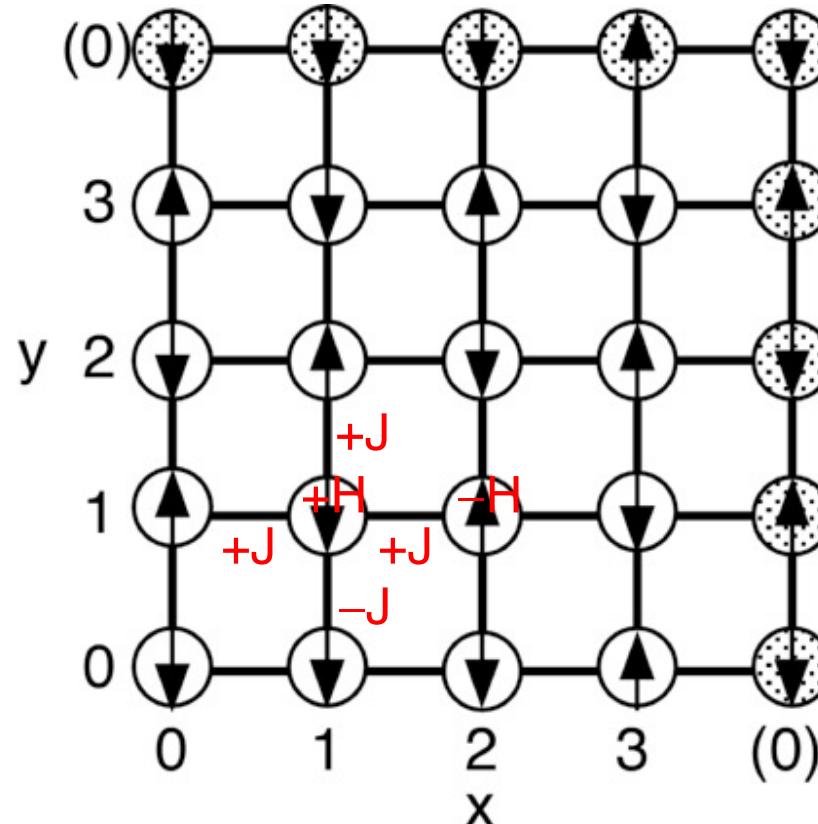
- Ising model: A collection of spins on a lattice, $\{s_k \mid s_k = \pm 1\}$
- Potential energy

$$V(s^N) = -J \sum_{(k,l)} s_k s_l - H \sum_k s_k, \quad s_k = \pm 1$$

where J is the exchange coupling, H is the magnetic field, & (k, l) are nearest-neighbor pairs of lattice sites

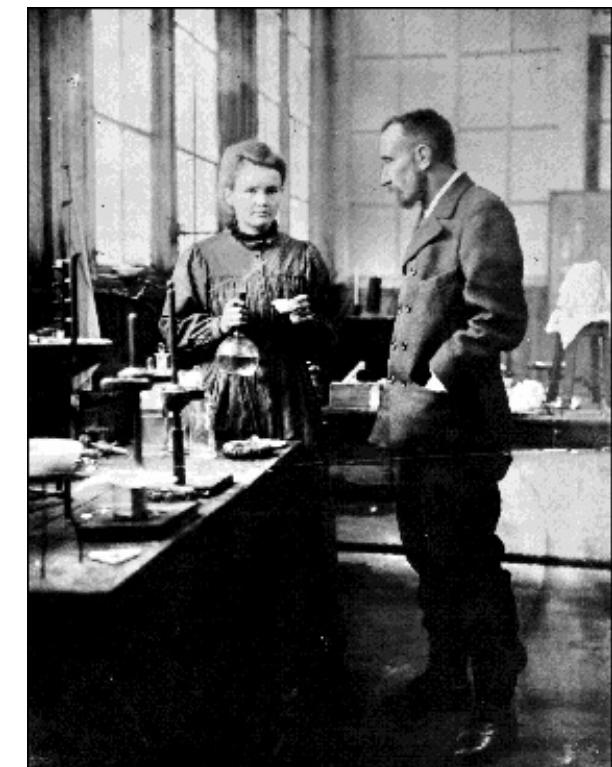


Ernst Ising



- Periodic boundary condition: Wrapping around the lattice

Curie temperature





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News

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Lindsay Bassman Awarded Prestigious Marie Curie Fellowship

APRIL 12, 2022

By Linda Vu

Contact: cscomms@lbl.gov

<https://crd.lbl.gov/news-and-publications/news/2022/lindsay-bassman-awarded-prestigious-marie-curie-fellowship/>

When Lindsay Bassman began her postdoctoral fellowship in the Applied Computing for Scientific Discovery group at Berkeley Lab, she had a Ph.D. in physics, was an experienced programmer, and was skilled at running scientific supercomputer simulations. She hoped the Lab could help her find some good applications for these talents.

She soon found a collaborator in fellow postdoc Katie Klymko (now staff at NERSC), who had a background in statistical mechanics. Together they worked on creating novel quantum algorithms to extract materials and chemical properties from simulations on quantum computers. For example, they developed a new algorithm to compute a material's free energy on a quantum computer.



Now Bassman has been awarded one of Europe's most competitive and prestigious postdoctoral fellowships — [the Marie Skłodowska-Curie Actions](#) — to continue this work in quantum thermodynamics with Michele Campisi at the [CNR Istituto Nanoscienze](#) in Pisa, Italy.

Exotic Magnets

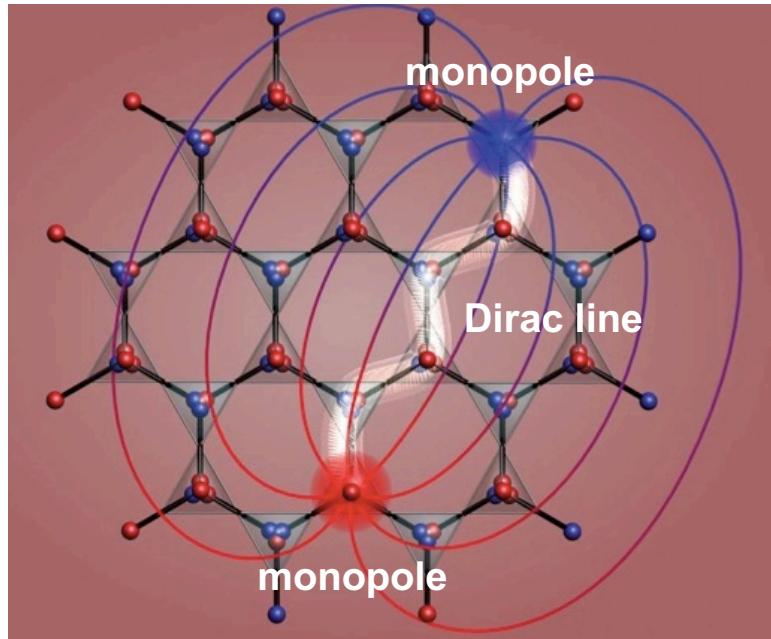
nature

Vol 451 | 3 January 2008 | doi:10.1038/nature06433

LETTERS

Magnetic monopoles in spin ice

C. Castelnovo¹, R. Moessner^{1,2} & S. L. Sondhi³



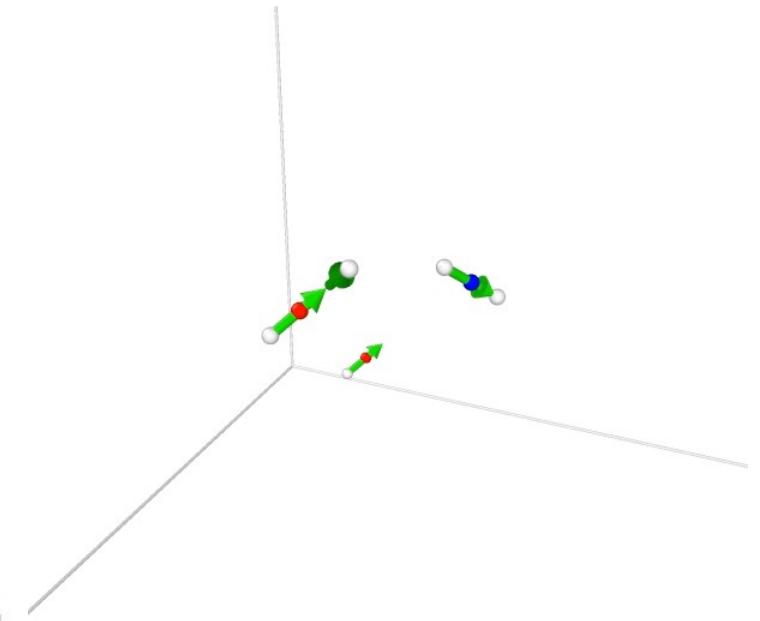
$$H = \frac{J}{3} \sum_{\langle ij \rangle} S_i S_j + D a^3 \sum_{\langle ij \rangle} \left[\frac{\hat{e}_i \cdot \hat{e}_j}{|\mathbf{r}_{ij}|^3} - \frac{3(\hat{e}_i \cdot \mathbf{r}_{ij})(\hat{e}_j \cdot \mathbf{r}_{ij})}{|\mathbf{r}_{ij}|^5} \right] S_i S_j$$

MAGNETISM

Qubit spin ice

Andrew D. King^{1*}, Cristiano Nisoli^{2*}, Edward D. Dahl^{1,3},
Gabriel Poulin-Lamarre¹, Alejandro Lopez-Bezanilla²

Science 373, 576–580 (2021)



Monte Carlo simulation

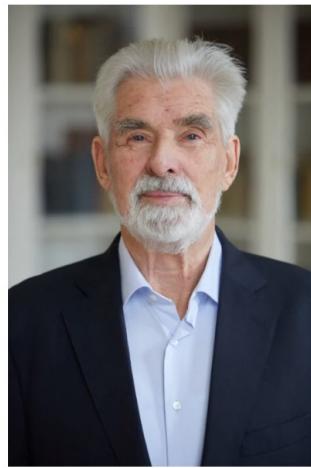
The Nobel Prize in Physics 2021



© Nobel Prize Outreach. Photo:
Risdon Photography

Syukuro Manabe

Prize share: 1/4



© Nobel Prize Outreach. Photo:
Bernhard Ludewig

Klaus Hasselmann

Prize share: 1/4



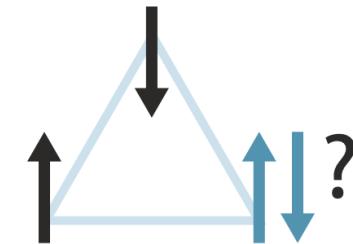
© Nobel Prize Outreach. Photo:
Laura Sbarboli
Giorgio Parisi
Prize share: 1/2

[book] **Spin glass theory and beyond: An Introduction to the Replica Method and Its Applications**

M Mézard, G Parisi, MA Virasoro - 1987 - books.google.com

... In the first part on **spin glass** theory we present a rather ... of the ideas and techniques of **spin glass** theory in two other ... ideas and analogies inspired by **spin glasses** that we present will ...

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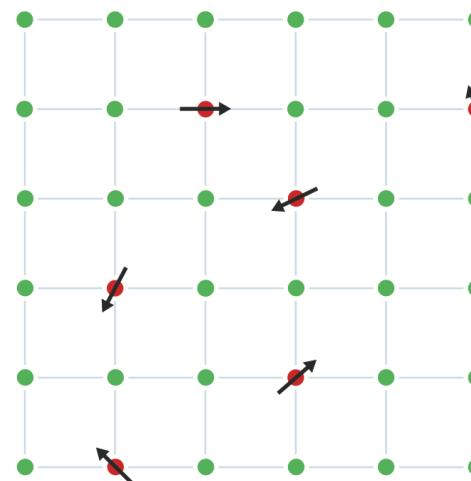


Frustration

When one spin points upward and the other downward, the third one cannot satisfy them both at the same time, because neighbouring spins want to point in different directions. How do the spins find an optimal orientation? Giorgio Parisi is a master at answering these questions for many different materials and phenomena.

The Nobel Prize in Physics 2021 was awarded "for groundbreaking contributions to our understanding of complex physical systems" with one half jointly to Syukuro Manabe and Klaus Hasselmann "for the physical modelling of Earth's climate, quantifying variability and reliably predicting global warming" and the other half to Giorgio Parisi "for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales".

Screenshot



Spin glass

A spin glass is a metal alloy where iron atoms, for example, are randomly mixed into a grid of copper atoms. Each iron atom behaves like a small magnet, or spin, which is affected by the other magnets around it. However, in a spin glass they are frustrated and have difficulty choosing which direction to point. Using his studies of spin glass, Parisi developed a theory of disordered and random phenomena that covers many other complex systems.

● Iron
● Copper

3D Ising Problem Is NP-Complete

PHYSICAL REVIEW VOLUME 65, NUMBERS 3 AND 4 FEBRUARY 1 AND 15, 1944

Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition

LARS ONSAGER

Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut

(Received October 4, 1943)

The partition function of a two-dimensional "ferromagnetic" with scalar "spins" (Ising model) is computed rigorously for the case of vanishing field. The eigenwert problem involved in the corresponding computation for a long strip crystal of finite width (n atoms), joined straight to itself around a cylinder, is solved by direct product decomposition; in the special case $n = \infty$ an integral replaces a sum. The choice of different interaction energies ($\pm J, \pm J'$) in the $(0\ 1)$ and $(1\ 0)$ directions does not complicate the problem. The two-way infinite crystal has an order-disorder transition at a temperature $T = T_c$ given by the condition

$$\sinh(2J/kT_c) \sinh(2J'/kT_c) = 1.$$

The energy is a continuous function of T ; but the specific heat becomes infinite as $-\log |T - T_c|$. For strips of finite width, the maximum of the specific heat increases linearly with $\log n$. The order-converting dual transformation invented by Kramers and Wannier effects a simple automorphism of the basis of the quaternion algebra which is natural to the problem in hand. In addition to the thermodynamic properties of the massive crystal, the free energy of a $(0\ 1)$ boundary between areas of opposite order is computed; on this basis the mean ordered length of a strip crystal is

$$(\exp(2J/kT) \tanh(2J'/kT))^n.$$

Statistical Mechanics, Three-Dimensionality and NP-completeness *

I. Universality of Intractability for the Partition Function of the Ising Model Across Non-Planar Lattices

[Extended Abstract]

Sorin Istrail

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Applied Mathematics Department, MS 1110
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scistra@cs.sandia.gov

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STOC 2000 Portland Oregon USA
1-58113-184-4/00/5

Nobel laureate Richard Feynman wrote in 1972 of the three-dimensional Ising model that "the exact solution for three dimensions has not yet been found."

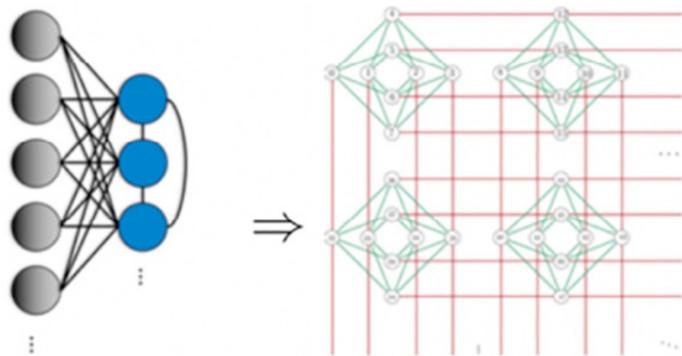
Other researchers who have tried read like a roll call of famous names in science and mathematics: Onsager, Kac, Feynman, Fisher, Kasteleyn, Temperley, Green, Hurst, and more recently Barahona.

Says Istrail, "What these brilliant mathematicians and physicists failed to do, indeed cannot be done."

Ising Model in Machine Learning

Physically very appealing methods for unsupervised learning are the so-called **Boltzmann machines** (BM). A BM is basically an *inverse Ising model* where the data samples are seen as samples from a Boltzmann distribution of a pairwise interacting Ising model. The goal is to learn the values of the interactions and magnetic fields so that the likelihood (probability in the Boltzmann measure) of the observed data is large.

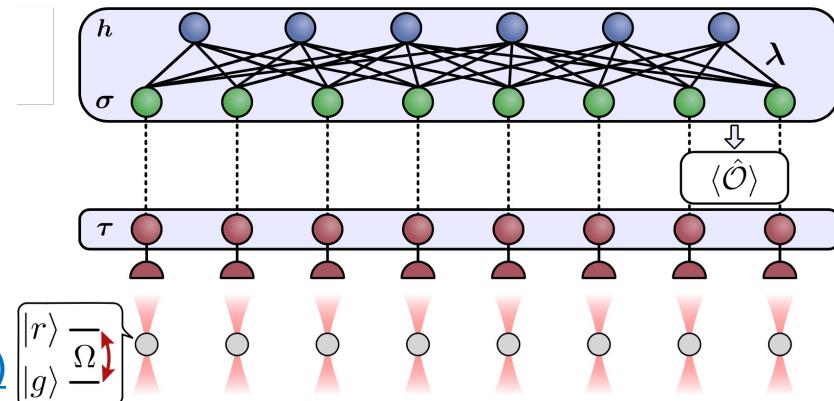
Machine Learning and the Physical Sciences
G. Carleo et al., *Rev. Mod. Phys.* **91**, 045002 ('19)



Quantum-neural nexus?

Quantum-annealing Boltzmann machine
J. Liu et al., *Comput. Mater. Sci.* **173**, 109429 ('20)

Hybrid BM-quantum circuit
G. Torlai et al., *Phys. Rev. Lett.* **123**, 230504 ('19)



MC Algorithm for 2D Ising Model

```

initialize the spins, s[i][j] (0 ≤ i,j ≤ L-1)
Sum_A = 0
for step = 1 to maximum_step
    randomly select a grid point, (i,j)
    compute the change in potential energy, dV, with a single spin
    flip, si,j → -si,j //Attempt
    if dV < 0 accept the flip, si,j ← -si,j
    else if random() ≤ exp(-dV/kBT) then // 0 < random() < 1
        accept the flip, si,j ← -si,j
    endif
    Sum_A = Sum_A + A(sN) // Sample physical quantity A(sN)
endfor
Average_A = Sum_A/maximum_step Mean

```

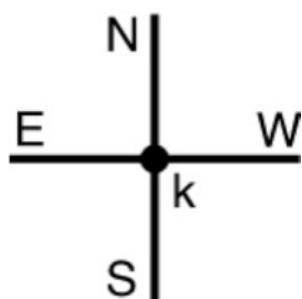
$$\pi_{mn} = \overbrace{\min(\rho_m/\rho_n, 1)}^{\text{accept/reject}} \overbrace{\tilde{\alpha}_{mn}}^{\text{attempt}}$$

} Accept/reject

$$\delta V = V(\dots, s_k', \dots) - V(\dots, s_k, \dots) \quad \frac{P(\dots, s_k', \dots)}{P(\dots, s_k, \dots)} = \frac{e^{-V(\dots, s_k', \dots)/k_B T}}{e^{-V(\dots, s_k, \dots)/k_B T}} = \exp\left(-\frac{\delta V}{k_B T}\right)$$

$$= -J \sum_{l \in n.n.(k)} (s_k' - s_k) s_l - H(s_k' - s_k)$$

$$= -2s_k' \left(J \sum_{l \in n.n.(k)} s_l + H \right)$$



`i = L*(rand()/(double)RAND_MAX);
j = L*(rand()/(double)RAND_MAX);`

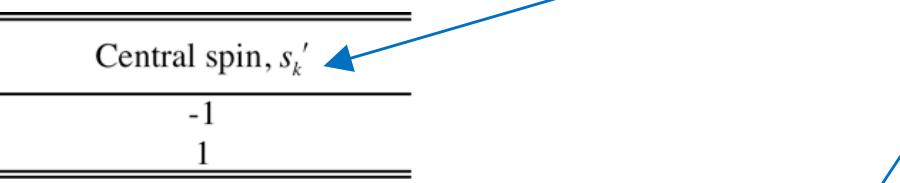
`i = rand()%L;
j = rand()%L;`

$$V(s^N) = -J \sum_{(k,l)} s_k s_l - H \sum_k s_k, \quad s_k = \pm 1$$

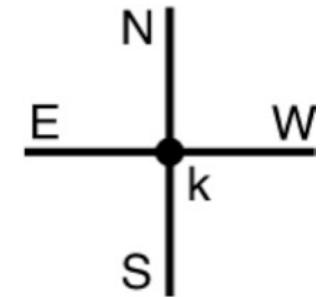
State Transition

Spin flip: $s_k \rightarrow s'_k = -s_k$

- double exp_dV[2][5]: $\exp(-\delta V / k_B T) = \exp\left(2s'_k \left(\frac{J}{k_B T} \sum_{l \in n.n.(k)} s_l + \frac{H}{k_B T}\right)\right)$

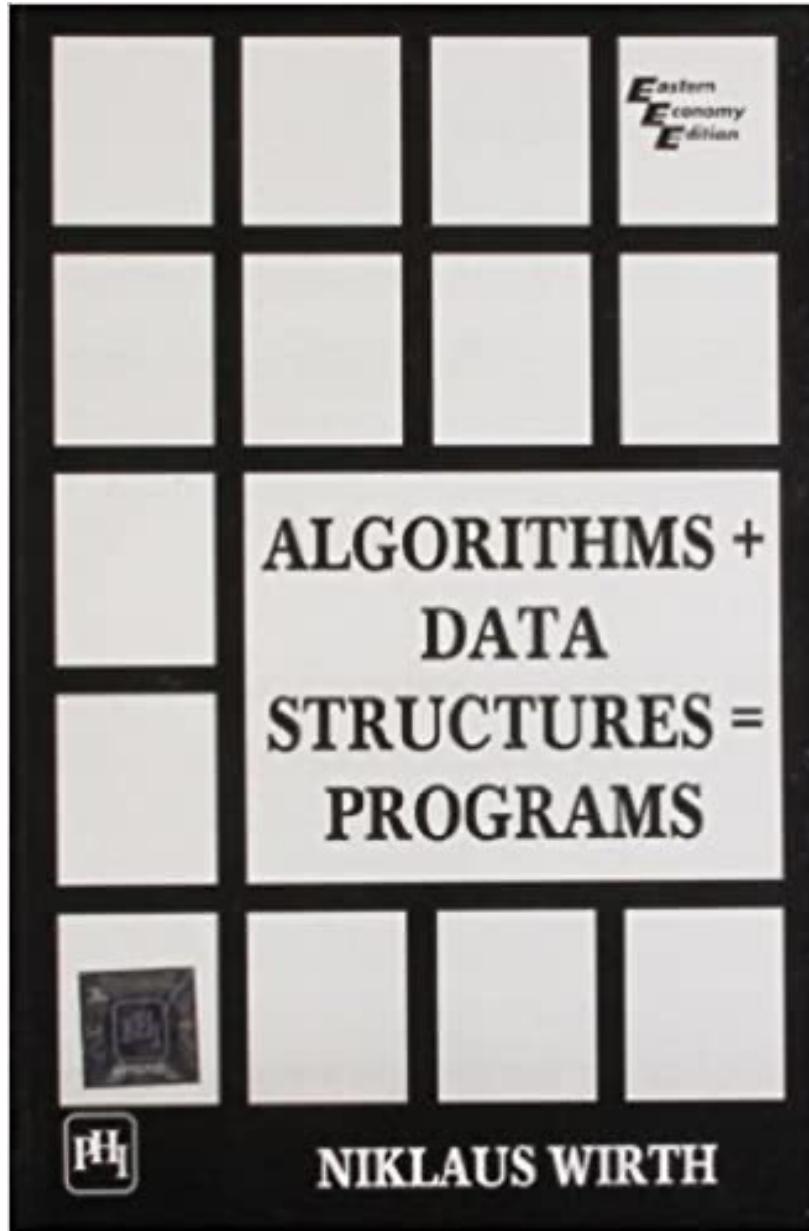


Neighbor spins				Sum
-1	-1	-1	-1	-4
-1	-1	-1	1	-2
-1	-1	1	1	0
-1	1	1	1	2
1	1	1	1	4

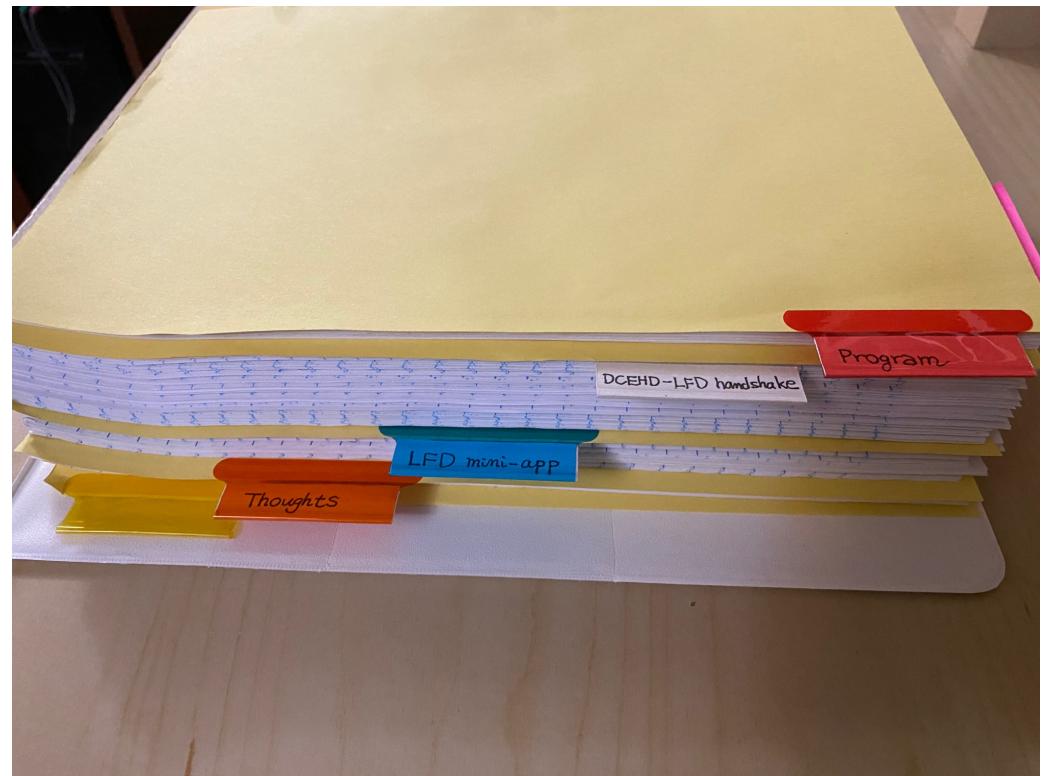


Pre-compute & store transition probability in a table
Note exp() function is compute-intensive

Now, How to Code?



Life of a computational physicist: Concept to algebra to program (= data structure—define & algorithm—pseudocode)



<https://github.com/USCCACS/DCMESH>

Data Structures

- `#define L 20 //Lattice size
int s[L][L]; //Spins s[i][j] = ±1`
- **Periodic boundary condition:** The west, east, south, north neighbors of site (i, j) are (im, j) , (ip, j) , (i, jm) , (i, jp) , where
 $im = (i + L - 1) \% L$
 $ip = (i + 1) \% L$
 $jm = (j + L - 1) \% L$
 $jp = (j + 1) \% L$
- **Transition probability:** `double exp_dV[2][5]`

$$\exp_{dV}[k][l] = \exp\left(-\frac{\delta V}{k_B T}\right) = \exp\left(2s\left[\frac{J}{k_B T} \sum_{s' \in n.n.(s)} s' + \frac{H}{k_B T}\right]\right)$$

where

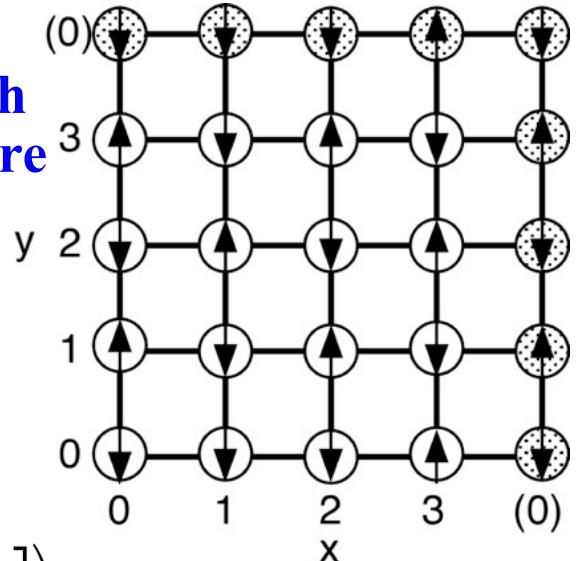
$$k = (1 + s)/2 \quad (k = 0,1; s = -1,1)$$

$$l = (4 + S)/2 \quad (l = 0,1,2,3,4; S = \sum_{\text{neighbor}} s' = -4, -2, 0, 2, 4)$$

- **Ising model parameters**

$$\text{double JdivT} = J/k_B T$$

$$\text{double HdivT} = H/k_B T$$



Spin→array-index transformation

$k=(1+s)/2$	s
0	-1
1	1

$l=(4+S)/2$	S
0	-4
1	-2
2	0
3	2
4	4

Physical Quantities

- double runM;
 - > **Running value of magnetization**, $M = \sum_k s_k$
 - > **To update**, $M += 2s'_k$
- double sumM = 0.0, sumM2 = 0.0; // double type to avoid overflow
 - > **To calculate the mean & variance of the magnetization at the end**
 - > **After each MC step**

```
    sumM += runM;
    sumM2 += runM*runM;
```
- int Sta_step;
 - > **# of MC steps to be performed**
 - > **Mean & standard deviation of the magnetization**

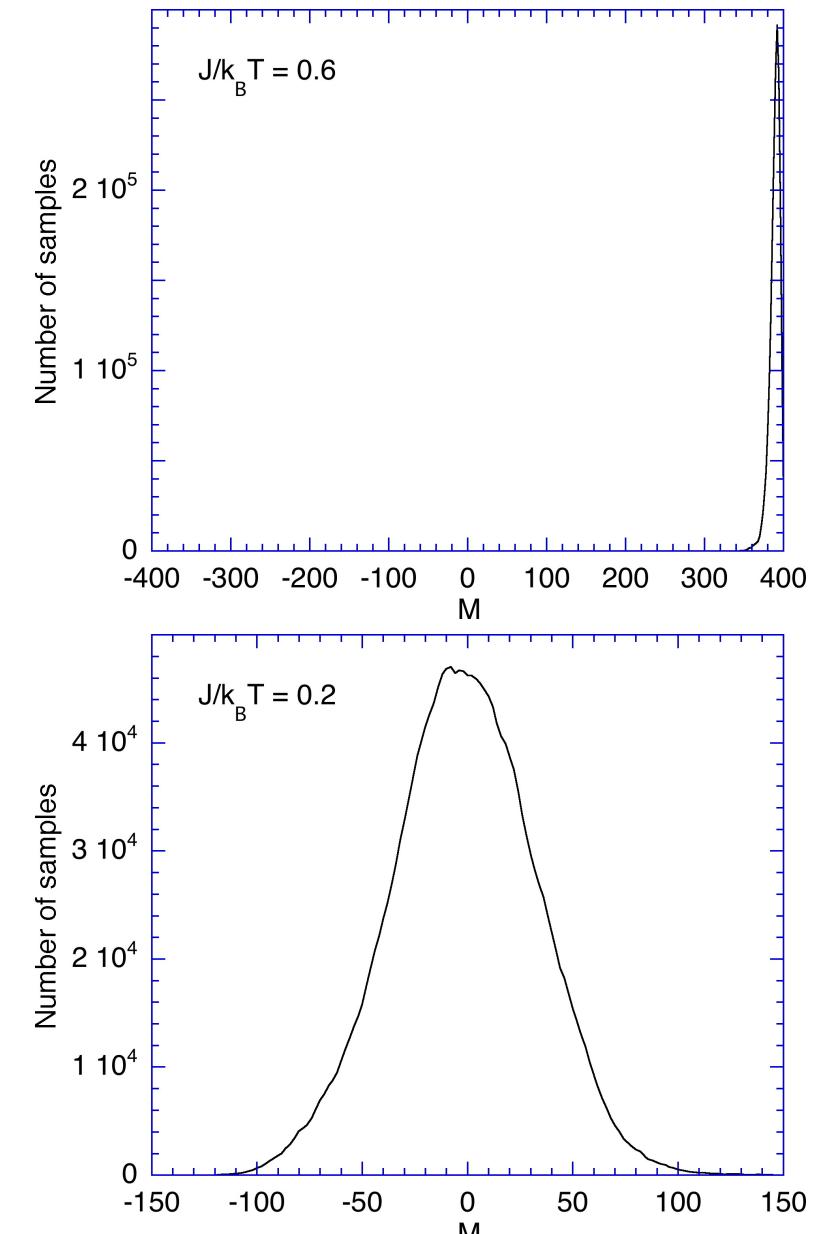
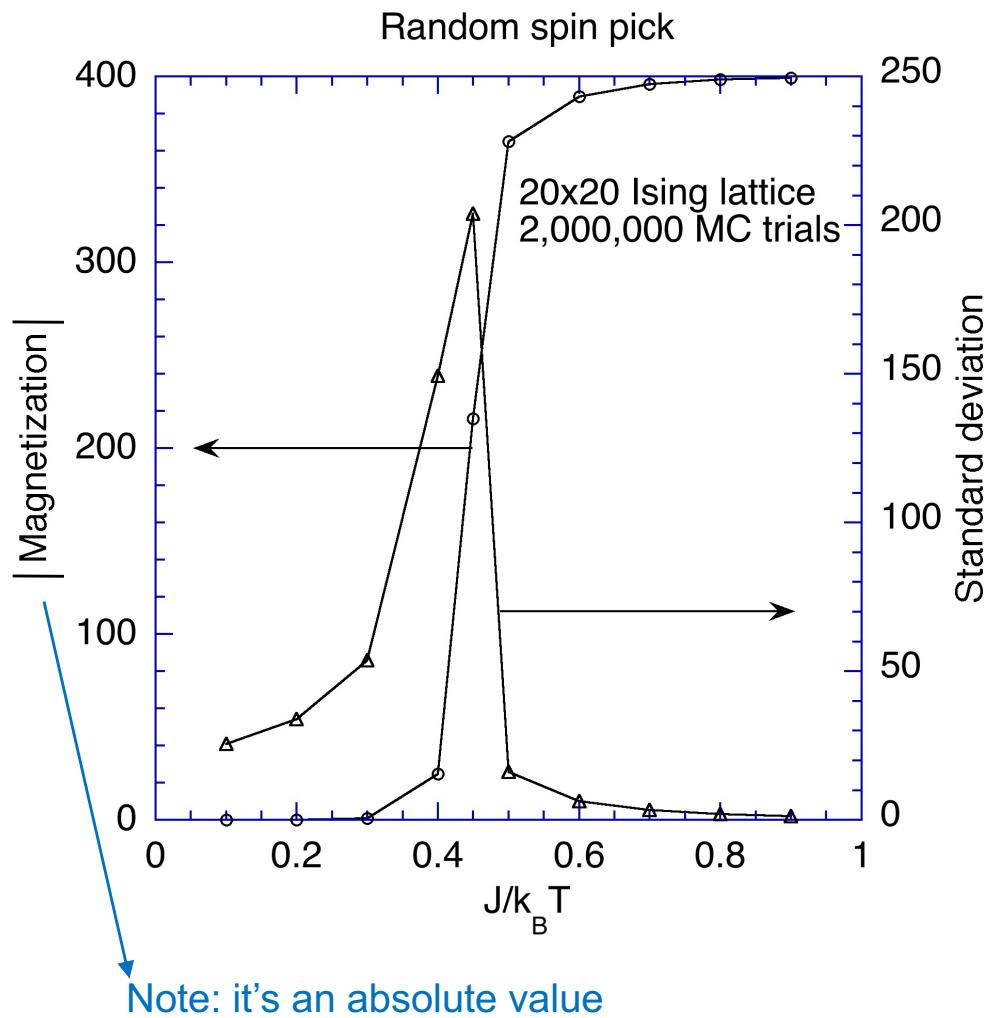
$$avgM = sumM/Sta_step$$

$$sigM = \sqrt{\frac{sumM2}{Sta_step} - avgM^2}$$

```
double avgM, sigM;
```

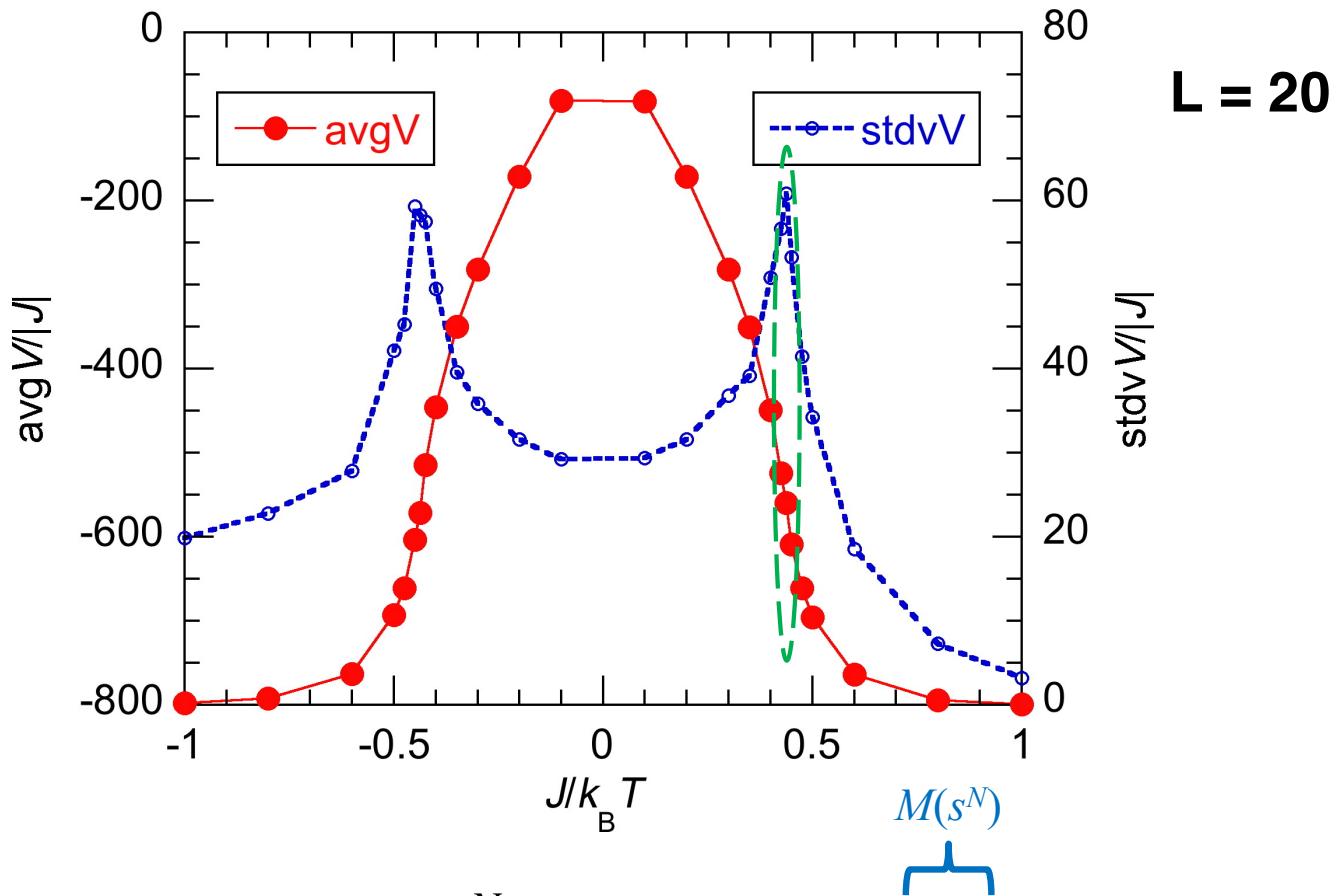
Magnetization & Its Fluctuation

$L = 20$



Histogram for 2 million MC steps

Energy & Its Fluctuation

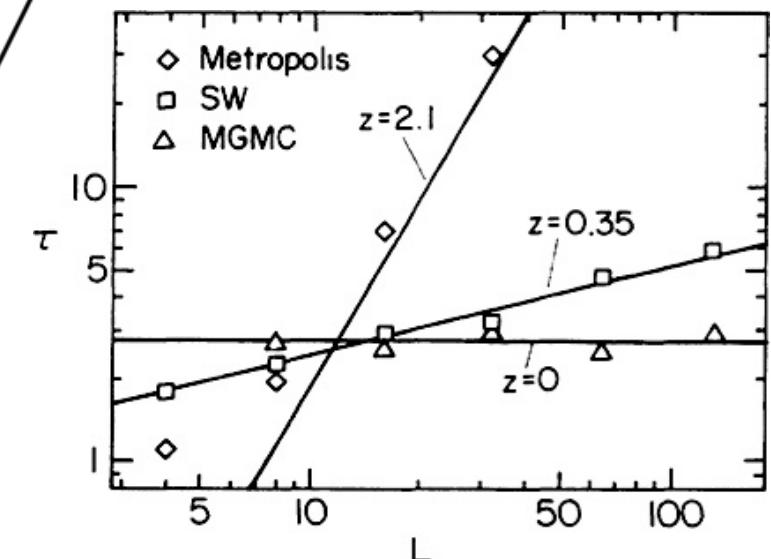
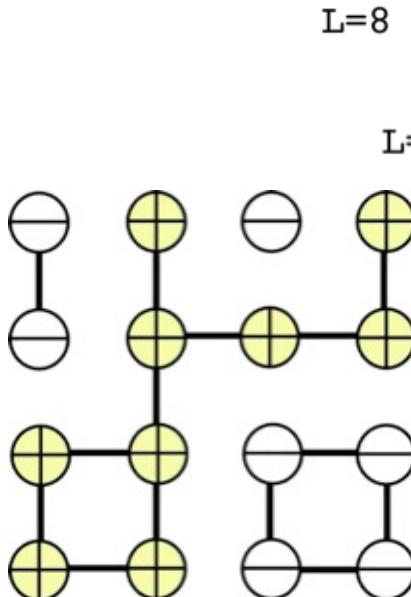


Rich physics: (1) ferro-to-para-to-antiferromagnetic phase transitions;
(2) nucleation growth; (3) fluctuation-dissipation theorem

See notes on (1) [fluctuation-dissipation theorem](#), (2) [unitary time propagation](#)
& (3) [linear response](#)

Cluster MC Algorithms

- **Cluster MC:** Speed up the convergence of MC simulations by introducing collective motions of the degrees-of-freedom, e.g., flipping a cluster of spins at a time
- **Correlation time, τ :** The number of MC steps before two states become uncorrelated, $\langle \delta M(t + t_0)\delta M(t_0) \rangle_{t_0} = \langle (\delta M)^2 \rangle \exp(-t/\tau)$
- **Dynamic critical exponent, z :** Near the critical temperature for magnetic-to-nonmagnetic phase transition, $\tau \sim L^z$ (L : system size)
 - > $z = 2.125$ for 2D Ising model
 - > $z = 0.35$ for Swendsen-Wang cluster MC ('87)
 - > $z \sim 0$ for multigrid (hierarchical cluster) MC (Kandel *et al.*, '88)



Cluster MC Algorithm—Wolff

Algorithm: Single step of Wolff's cluster flip

1. Choose a seed spin at random from the lattice.
2. Look in turn at each of the neighbors of that spin. If they are pointing in the same direction as the seed spin, add them to the cluster with probability $P_{\text{add}} = 1 - \exp(-2J/k_B T)$.
3. For each spin that was added in step 2, examine each of its neighbors to find the ones pointing in the same direction & add each of them to the cluster with probability P_{add} . Repeat this step as many times as necessary until there are no spins left in the cluster whose neighbors have not been considered for inclusion in the cluster.
4. Flip the cluster

U. Wolff, *Phys. Rev. Lett.* **62**, 361 ('89)

<https://aiichironakano.github.io/phys516/Phys516-MCred.pdf>

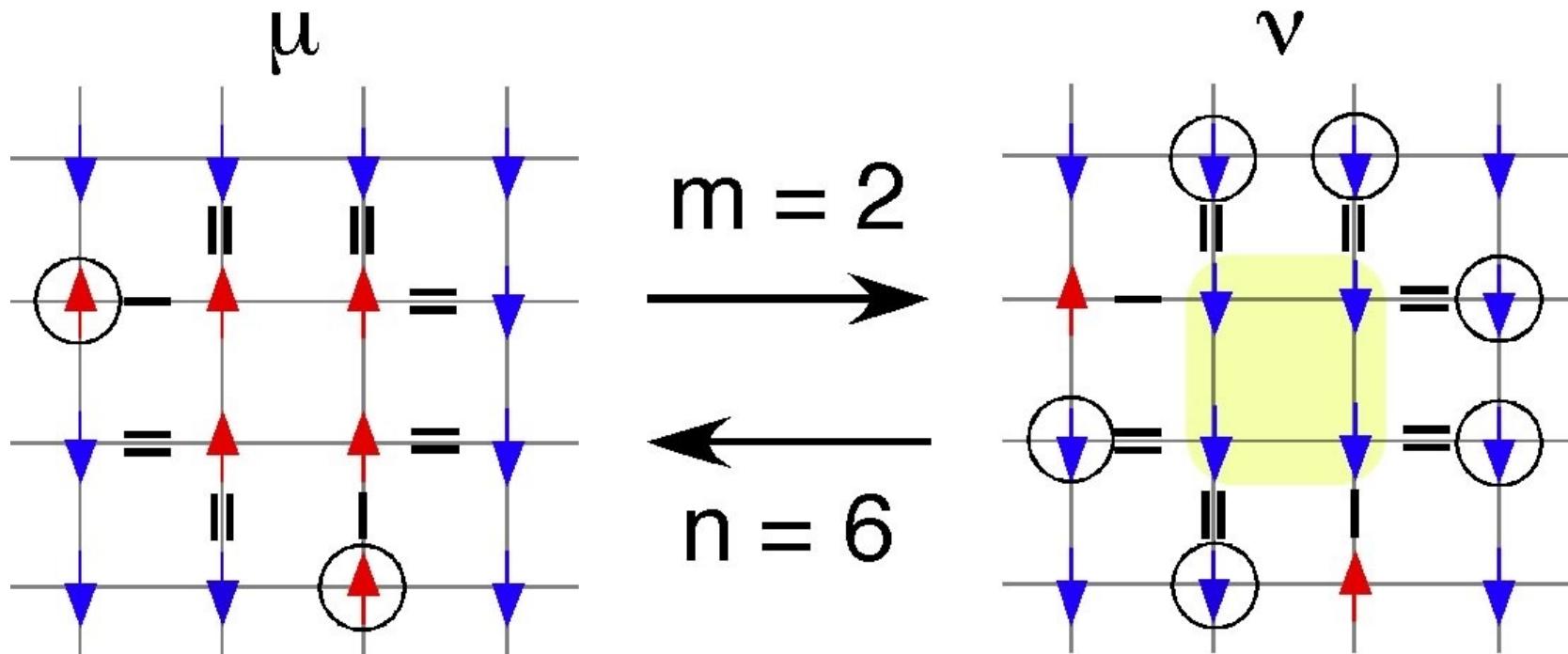
Detailed Balance in Wolff Algorithm

- Key to detailed balance, $\pi_{mn}\rho_n = \pi_{nm}\rho_m$: $P_{\text{add}} = 1 - \exp(-2J/k_B T)$
- Detailed balance for a cluster flip:
 $\mu \rightarrow \nu$ (**m bonds broken**); $\nu \rightarrow \mu$ (**n bonds broken**)

$$(1 - P_{\text{add}})^m P(\mu) = (1 - P_{\text{add}})^n P(\nu)$$

or

$$(1 - P_{\text{add}})^{m-n} = P(\nu)/P(\mu)$$



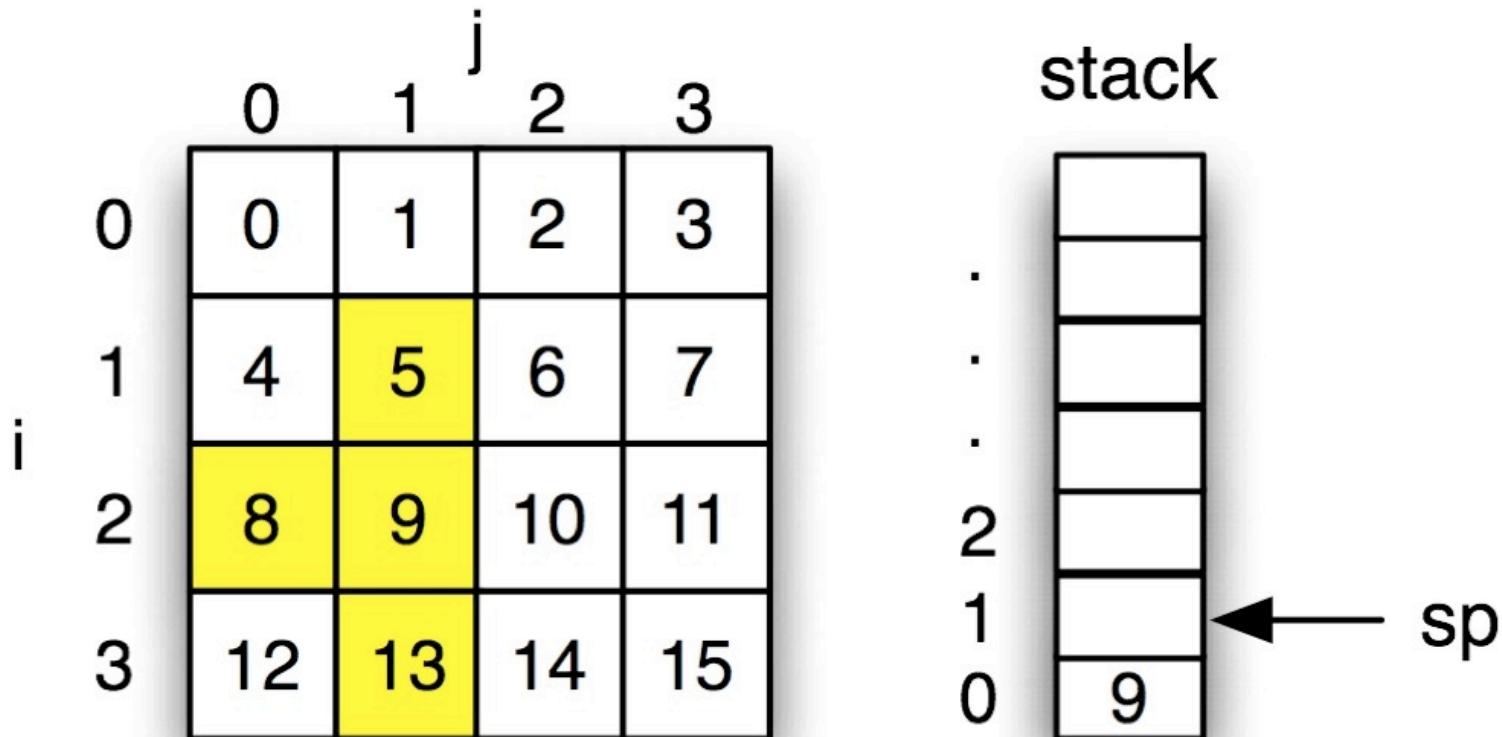
$$(1 - P_{\text{add}})^{m-n} = \exp(-2J[m-n]/k_B T) = \exp(-[E_\nu - E_\mu]/k_B T) = P(\nu)/P(\mu)$$

Wolff Cluster MC Program

Initiate a cluster-flip step using a stack

```
/* Put a random seed spin site onto a stack */
i = rand()%L; j = rand()%L;
stack[0] = i*L + j; // 1D site index put in a stack
sp = 1; // Stack pointer

/* Flip the seed and remember the old & new spins */
oldspin = s[i][j]; newspin = -s[i][j];
s[i][j] = newspin;
```



Cluster Flip

```

while (sp) {
    /* Pop a site off the stack */
    current = stack[--sp]; i = current/L; j = current%L;

    /* Check the neighbors */
    if ((nn=i+1) >= L) nn -= L; /* South neighbor */
    if (s[nn][j] == oldspin)
        if (rand()/(double)RAND_MAX < padd) {
            stack[sp++] = nn*L + j; s[nn][j] = newspin;
        }

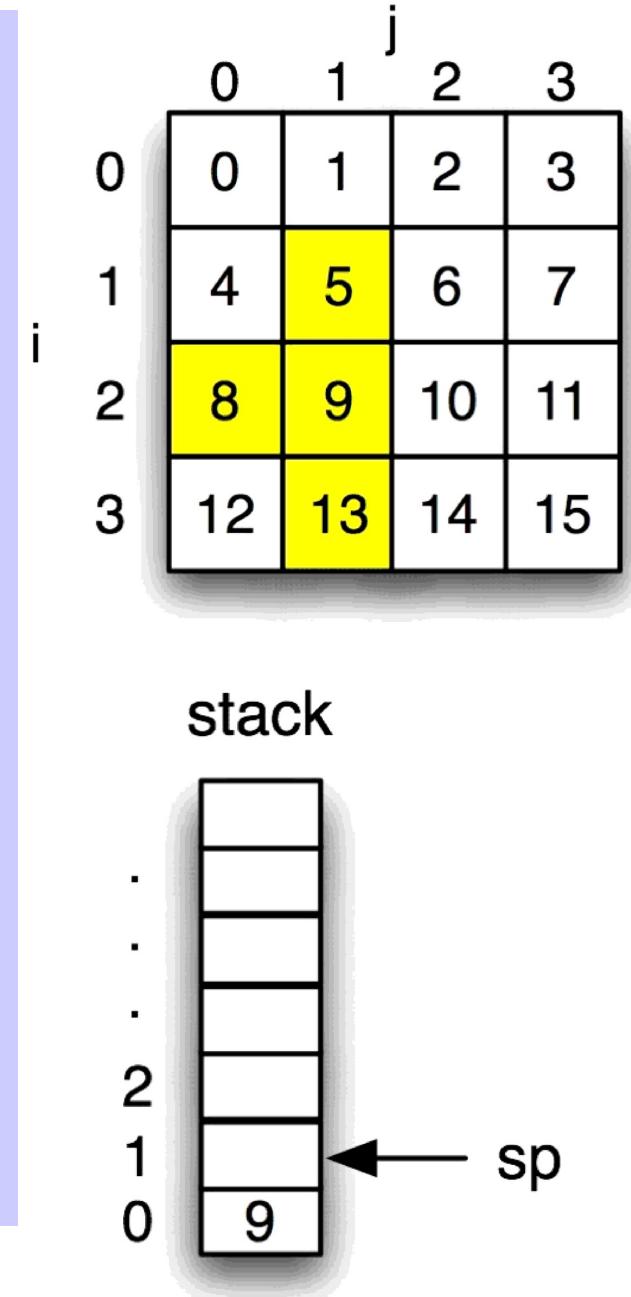
    if ((nn=i-1) < 0) nn += L; /* North neighbor */
    if (s[nn][j] == oldspin)
        if (rand()/(double)RAND_MAX < padd) {
            stack[sp++] = nn*L + j; s[nn][j] = newspin;
        }

    if ((nn=j+1) >= L) nn -= L; /* East neighbor */
    if (s[i][nn] == oldspin)
        if (rand()/(double)RAND_MAX < padd) {
            stack[sp++] = i*L + nn; s[i][nn] = newspin;
        }

    if ((nn=j-1) < 0) nn += L; /* West neighbor */
    if (s[i][nn] == oldspin)
        if (rand()/(double)RAND_MAX < padd) {
            stack[sp++] = i*L + nn; s[i][nn] = newspin;
        }
} /* End while stack is not empty */

```

$$padd = 1 - \exp(-2J/k_B T)$$



Sample Run

