(Pseudo) random number generator

linear congruential generator $$X_{n+1} = (aX_n + b) \bmod m$$

(Pseudo) random number generator

linear congruential generator

$$X_{n+1} = (aX_n + b) \bmod m$$

Lagged Fibonacci generator

$$S_n \equiv S_{n-j} \star S_{n-k} \pmod{m}, 0 < j < k$$

(Pseudo) random number generator

linear congruential generator

$$X_{n+1} = (aX_n + b) \bmod m$$

Lagged Fibonacci generator

$$S_n \equiv S_{n-j} \star S_{n-k} \pmod{m}, 0 < j < k$$

Discussions:

- ✓ Results can be repeated (controlled by the seed): helpful to debug code.

(Pseudo) random number generator

linear congruential generator $X_{n+1} = (aX_n + b) \bmod m$

Lagged Fibonacci generator $S_n \equiv S_{n-j} \star S_{n-k} \pmod{m}, 0 < j < k$

Discussions:

- Results can be repeated (controlled by the seed): helpful to debug code.
- Before using a generator, make sure you know the period length.

(Pseudo) random number generator

linear congruential generator

$$X_{n+1} = (aX_n + b) \bmod m$$

Lagged Fibonacci generator

$$S_n \equiv S_{n-j} \star S_{n-k} \pmod{m}, 0 < j < k$$

Discussions:

- Results can be repeated (controlled by the seed): helpful to debug code.
- Before using a generator, make sure you know the period length.
- In parallel calculation (MPI, for example), the generators need to be independent for each process.

(Pseudo) random number generator

linear congruential generator

$$X_{n+1} = (aX_n + b) \bmod m$$

Lagged Fibonacci generator

$$S_n \equiv S_{n-j} \star S_{n-k} \pmod{m}, 0 < j < k$$

Discussions:

- Results can be repeated (controlled by the seed): helpful to debug code.
- Before using a generator, make sure you know the period length.
- In parallel calculation (MPI, for example), the generators need to be independent for each process.
- Use tested library.

Error estimation

Consider N successive observations A_μ, with = 1,…,N, consider the expectation value of the square of the statistical error:

$$\langle (\delta A)^2 \rangle = \left\langle \left[\frac{1}{\mathcal{N}} \sum_{\mu=1}^{\mathcal{N}} (A_\mu - \langle A \rangle) \right]^2 \right\rangle$$

Error estimation

Consider N successive observations A_μ, with = 1,…,N, consider the expectation value of the square of the statistical error:

$$\langle(\delta A)^2\rangle = \left\langle \left[\frac{1}{\mathcal{N}} \sum_{\mu=1}^{\mathcal{N}} (A_\mu - \langle A \rangle) \right]^2 \right\rangle$$

$$= \frac{1}{\mathcal{N}^2} \sum_{\mu=1}^{\mathcal{N}} \langle (A_\mu - \langle A \rangle)^2 \rangle + \frac{2}{\mathcal{N}^2} \sum_{\mu_1=1}^{\mathcal{N}} \sum_{\mu_2=\mu_1+1}^{\mathcal{N}} \left(\langle A_{\mu_1} A_{\mu_2} \rangle - \langle A \rangle^2 \right)$$

Error estimation

Consider N successive observations A_μ, with = 1,…,N, consider the expectation value of the square of the statistical error:

$$\left\langle (\delta A)^2 \right\rangle = \left\langle \left[\frac{1}{\mathcal{N}} \sum_{\mu=1}^{\mathcal{N}} (A_\mu - \langle A \rangle) \right]^2 \right\rangle$$

$$= \frac{1}{\mathcal{N}^2} \sum_{\mu=1}^{\mathcal{N}} \left\langle (A_\mu - \langle A \rangle)^2 \right\rangle + \frac{2}{\mathcal{N}^2} \sum_{\mu_1=1}^{\mathcal{N}} \sum_{\mu_2=\mu_1+1}^{\mathcal{N}} \left(\langle A_{\mu_1} A_{\mu_2} \rangle - \langle A \rangle^2 \right)$$

We take the samples after equilibrium which means a translational invariance with “time” :

$$\langle A_{\mu_1} A_{\mu_2} \rangle = \langle A_0 A_{\mu_2 - \mu_1} \rangle$$

Error estimation

Consider N successive observations A_μ, with = 1,…,N, consider the expectation value of the square of the statistical error:

$$\left\langle (\delta A)^2 \right\rangle = \left\langle \left[\frac{1}{\mathcal{N}} \sum_{\mu=1}^{\mathcal{N}} (A_\mu - \langle A \rangle) \right]^2 \right\rangle$$

$$= \frac{1}{\mathcal{N}^2} \sum_{\mu=1}^{\mathcal{N}} \left\langle (A_\mu - \langle A \rangle)^2 \right\rangle + \frac{2}{\mathcal{N}^2} \sum_{\mu_1=1}^{\mathcal{N}} \sum_{\mu_2=\mu_1+1}^{\mathcal{N}} \left(\langle A_{\mu_1} A_{\mu_2} \rangle - \langle A \rangle^2 \right)$$

We take the samples after equilibrium which means a translational invariance with “time” :

$$\langle A_{\mu_1} A_{\mu_2} \rangle = \langle A_0 A_{\mu_2 - \mu_1} \rangle$$

We have

$$\left\langle (\delta A)^2 \right\rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 + 2 \sum_{\mu=1}^{\mathcal{N}} \left(1 - \frac{\mu}{\mathcal{N}} \right) \left(\langle A_0 A_\mu \rangle - \langle A \rangle^2 \right) \right]$$

Error estimation

Suppose the time interval between two measurements is δt , the time at each measurement is $t = \delta t\, \mu$, we can change the summation into an integration with $t = \delta t\, N$ (if *N* >> 1):

$$\langle (\delta A)^2 \rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \left[\langle A(0) A(t') \rangle - \langle A \rangle^2 \right] dt' \right]$$

Error estimation

Suppose the time interval between two measurements is δt , the time at each measurement is $t = \delta t\, \mu$, we can change the summation into an integration with $t = \delta t\, N$ (if *N* >> 1):

$$\left\langle (\delta A)^2 \right\rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \left[\langle A(0) A(t') \rangle - \langle A \rangle^2 \right] dt' \right]$$

$$= \frac{1}{\mathcal{N}} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \left[1 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \phi_A(t')\, dt' \right]$$

Error estimation

Suppose the time interval between two measurements is δt, the time at each measurement is $t = \delta t\, \mu$, we can change the summation into an integration with $t = \delta t\, N$ (if *N* >> 1):

$$\left\langle (\delta A)^2 \right\rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \left[\langle A(0) A(t') \rangle - \langle A \rangle^2 \right] dt' \right]$$

$$= \frac{1}{\mathcal{N}} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \left[1 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \phi_A(t')\, dt' \right]$$

Where we define:

$$\phi_A(t) = \frac{\left[\langle A(0) A(t) \rangle - \langle A \rangle^2 \right]}{\left[\langle A^2 \rangle - \langle A \rangle^2 \right]}$$

Error estimation

Suppose the time interval between two measurements is δt, the time at each measurement is $t = \delta t\, \mu$, we can change the summation into an integration with $t = \delta t\, N$ (if *N* >> 1):

$$\left\langle (\delta A)^2 \right\rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \left[\langle A(0) A(t') \rangle - \langle A \rangle^2 \right] dt' \right]$$

$$= \frac{1}{\mathcal{N}} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \left[1 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \phi_A(t')\, dt' \right]$$

Where we define:

$$\phi_A(t) = \frac{\left[\langle A(0) A(t) \rangle - \langle A \rangle^2 \right]}{\left[\langle A^2 \rangle - \langle A \rangle^2 \right]}$$

$$\phi_A(t = 0) = 1$$

$$\phi_A(t \to \infty) = 0$$

Error estimation

Suppose the time interval between two measurements is δt , the time at each measurement is $t = \delta t\, \mu$, we can change the summation into an integration with $t = \delta t\, N$ (if *N* >> 1):

$$\left\langle (\delta A)^2 \right\rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \left[\langle A(0) A(t') \rangle - \langle A \rangle^2 \right] dt' \right]$$

$$= \frac{1}{\mathcal{N}} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \left[1 + \frac{2}{\delta t} \int_0^t \left(1 - \frac{t'}{t} \right) \phi_A(t')\, dt' \right]$$

Where we define:

$$\phi_A(t) = \frac{\left[\langle A(0) A(t) \rangle - \langle A \rangle^2 \right]}{\left[\langle A^2 \rangle - \langle A \rangle^2 \right]}$$

$$\phi_A(t = 0) = 1$$

$$\phi_A(t \to \infty) = 0$$

Suppose the integral of $\phi_A(t)$ exists (relaxation time):

$$\tau_A \equiv \int_0^\infty \phi_A(t)\, dt$$

Error estimation

Since $\phi_A(t)$ is essentially non-zero only for $t' \leq \tau_A$, and at the same time t'/t is small when $t' \leq \tau_A$ if *N* >> 1, we have

$$\left\langle (\delta A)^2 \right\rangle = \frac{1}{\mathcal{N}} \left[\langle A^2 \rangle - \langle A \rangle^2 \right] \left(1 + 2\, \frac{\tau_A}{\delta t} \right)$$

Error estimation

Since $\phi_A(t)$ is essentially non-zero only for $t' \leq \tau_A$, and at the same time t'/t is small when $t' \leq \tau_A$ if N >> 1, we have

$$\langle(\delta A)^2\rangle = \frac{1}{\mathcal{N}}[\langle A^2\rangle - \langle A\rangle^2]\left(1 + 2\,\frac{\tau_A}{\delta t}\right)$$

If $\tau_A \gg \delta t$ $\quad \langle(\delta A)^2\rangle = [\langle A^2\rangle - \langle A\rangle^2](2\tau_A/t)$ because $N\delta t = t$

Error estimation

Since $\phi_A(t)$ is essentially non-zero only for $t' \leq \tau_A$, and at the same time t'/t is small when $t' \leq \tau_A$ if N >> 1, we have

$$\langle(\delta A)^2\rangle = \frac{1}{\mathcal{N}}\left[\langle A^2\rangle - \langle A\rangle^2\right]\left(1 + 2\,\frac{\tau_A}{\delta t}\right)$$

If $\tau_A \gg \delta t$ $\quad \langle(\delta A)^2\rangle = [\langle A^2\rangle - \langle A\rangle^2](2\tau_A/t)$ because $N\delta t = t$

irrelevant to δt !!!

Error estimation

Since $\phi_A(t)$ is essentially non-zero only for $t' \leq \tau_A$, and at the same time t'/t is small when $t' \leq \tau_A$ if *N* >> 1, we have

$$\langle(\delta A)^2\rangle = \frac{1}{\mathcal{N}}[\langle A^2\rangle - \langle A\rangle^2]\left(1 + 2\,\frac{\tau_A}{\delta t}\right)$$

If $\tau_A \gg \delta t$ $\quad \langle(\delta A)^2\rangle = [\langle A^2\rangle - \langle A\rangle^2](2\tau_A/t)$ because $N\delta t = t$

irrelevant to δt !!!

Discussion:

- What if $\tau_A \ll \delta_t$?

Error estimation

Since $\phi_A(t)$ is essentially non-zero only for $t' \leq \tau_A$, and at the same time t'/t is small when $t' \leq \tau_A$ if *N* >> 1, we have

$$\langle(\delta A)^2\rangle = \frac{1}{N}[\langle A^2\rangle - \langle A\rangle^2]\left(1 + 2\,\frac{\tau_A}{\delta t}\right)$$

If $\tau_A \gg \delta t$ $\quad \langle(\delta A)^2\rangle = [\langle A^2\rangle - \langle A\rangle^2](2\tau_A/t)$ because $N\delta t = t$

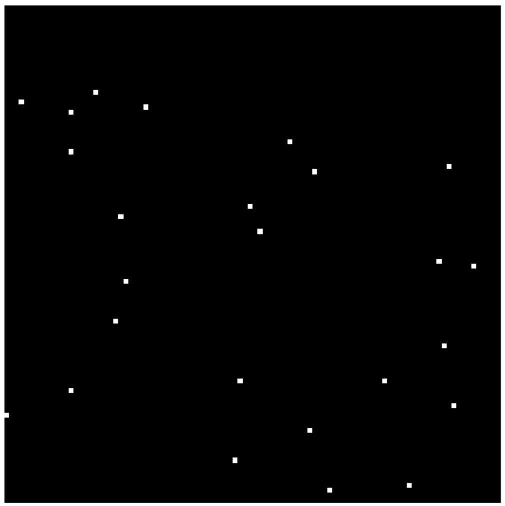
irrelevant to δt !!!

Discussion:

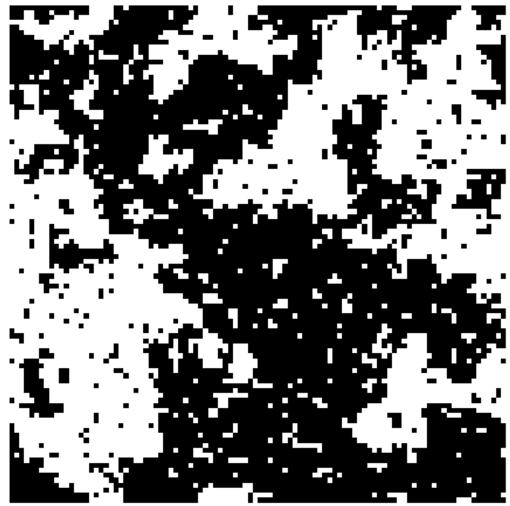
- What if $\tau_A \ll \delta_t$?
- How to calculate the relaxation time?

Critical slowing down

Snapshots of the 2D Ising model for three temperature



$T \ll T_c$

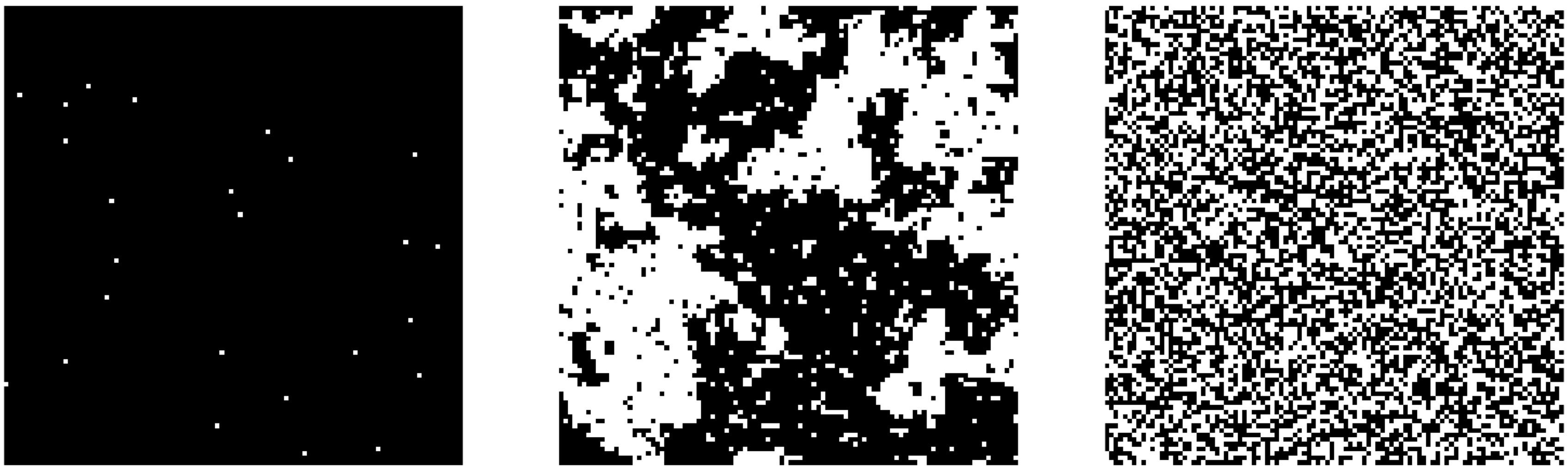


$T \approx T_c$

$T \gg T_c$

Critical slowing down

Snapshots of the 2D Ising model for three temperature

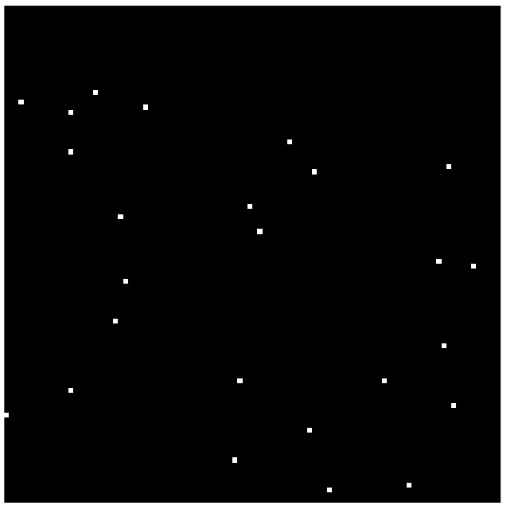


$T \ll T_c$ $\quad$ $T \approx T_c$ $\quad$ $T \gg T_c$

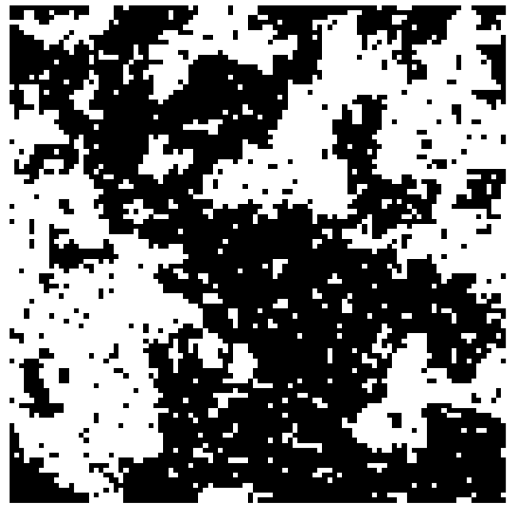
Recall the metropolis algorithm $A_{\text{met}}(A \to B) = \text{Min}\,[1, P_B/P_A] = \text{Min}\,[1, \exp(-\beta(E_B - E_A)]$

Critical slowing down

Snapshots of the 2D Ising model for three temperature



$T \ll T_c$



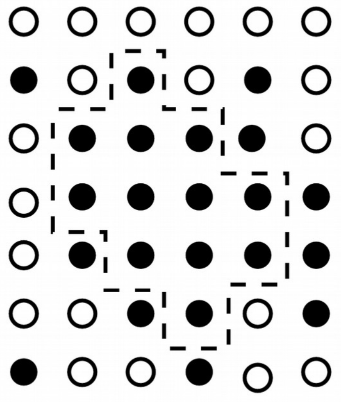
$T \approx T_c$

$T \gg T_c$

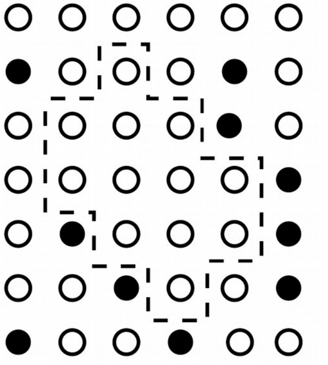
Recall the metropolis algorithm $A_{\text{met}}(A \to B) = \text{Min}\left[1, P_B/P_A\right] = \text{Min}\left[1, \exp(-\beta(E_B - E_A)\right]$

At the critical point, the relaxation time diverges with system size: $\tau \propto L^z$ z: dynamic exponent

Cluster updating: Wolff algorithm as an example

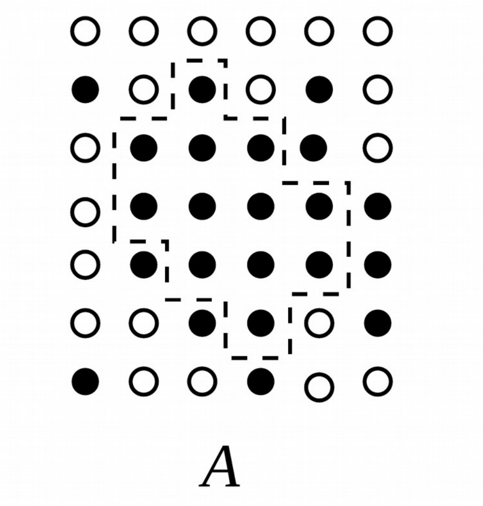


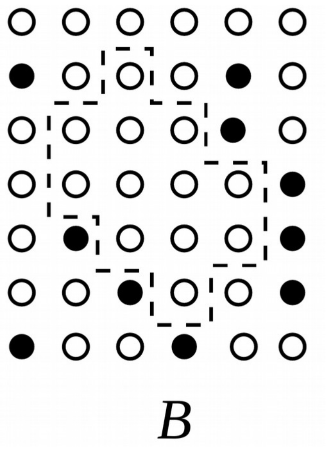
A



B

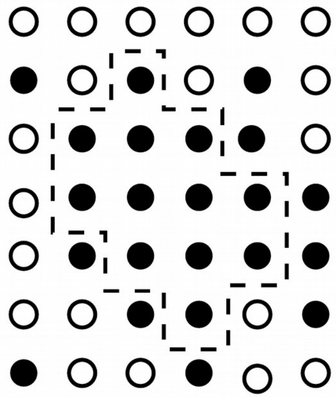
Cluster updating: Wolff algorithm as an example



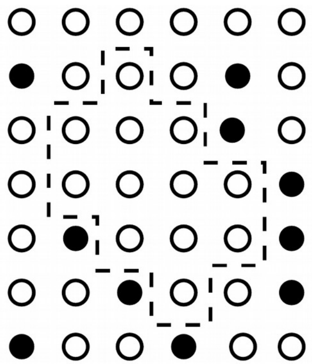


- Randomly choose an initial site (the seed).

Cluster updating: Wolff algorithm as an example



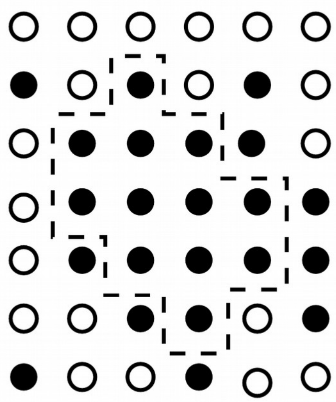
A



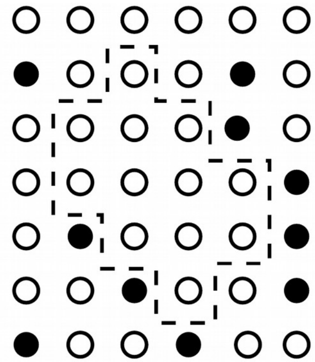
B

- Randomly choose an initial site (the seed).
- Add each neighboring spin, provided it is aligned with the seed, with probability p_{add}. If the neighboring spin is not aligned with the seed, it can't be added to the cluster.

Cluster updating: Wolff algorithm as an example



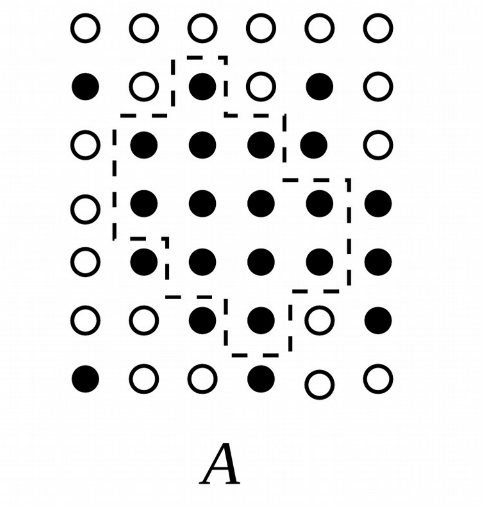
A

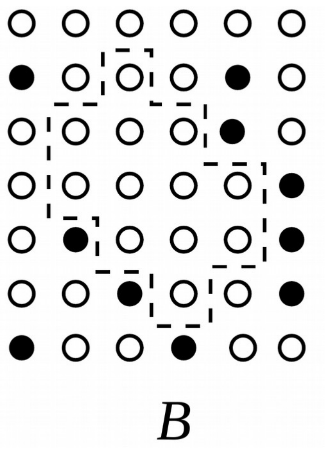


B

- Randomly choose an initial site (the seed).
- Add each neighboring spin, provided it is aligned with the seed, with probability p_{add}. If the neighboring spin is not aligned with the seed, it can't be added to the cluster.
- Repeat above process for each of the added spins.

Cluster updating: Wolff algorithm as an example





- Randomly choose an initial site (the seed).
- Add each neighboring spin, provided it is aligned with the seed, with probability p_{add}. If the neighboring spin is not aligned with the seed, it can't be added to the cluster.
- Repeat above process for each of the added spins.
- When no neighbor can be added to the cluster anymore, flip all the spins in the cluster.

Cluster updating: Wolff algorithm as an example

Trial probability:

$$T(A \to B)/T(B \to A) = (1 - P_{\mathrm{add}})^{m-n}$$

m(n) the number of spins not added to the cluster in the boundary:

Cluster updating: Wolff algorithm as an example

Trial probability:

$$T(A \to B)/T(B \to A) = (1 - P_{\text{add}})^{m-n}$$

m(n) the number of spins not added to the cluster in the boundary:

Detailed balance condition requires:

$$\frac{T(A \to B) \cdot A(A \to B)}{T(B \to A) \cdot A(B \to A)} = (1 - P_{\text{add}})^{m-n} \frac{A(A \to B)}{A(B \to A)} = e^{-\beta(E_B - E_A)}$$

Cluster updating: Wolff algorithm as an example

Trial probability:

$$T(A \to B)/T(B \to A) = (1 - P_{\text{add}})^{m-n}$$

m(n) the number of spins not added to the cluster in the boundary:

Detailed balance condition requires:

$$\frac{T(A \to B) \cdot A(A \to B)}{T(B \to A) \cdot A(B \to A)} = (1 - P_{\text{add}})^{m-n} \frac{A(A \to B)}{A(B \to A)} = e^{-\beta(E_B - E_A)}$$

Because:

$$E_A - E_B = 2J(n - m)$$

Cluster updating: Wolff algorithm as an example

Trial probability:

$$T(A \to B)/T(B \to A) = (1 - P_{\text{add}})^{m-n}$$

m(n) the number of spins not added to the cluster in the boundary:

Detailed balance condition requires:

$$\frac{T(A \to B) \cdot A(A \to B)}{T(B \to A) \cdot A(B \to A)} = (1 - P_{\text{add}})^{m-n} \frac{A(A \to B)}{A(B \to A)} = e^{-\beta(E_B - E_A)}$$

Because:

$$E_A - E_B = 2J(n - m)$$

Detailed balance condition is now

$$\frac{A(A \to B)}{A(B \to A)} = \left[(1 - P_{\text{add}})e^{2\beta J}\right]^{n-m}$$

Cluster updating: Wolff algorithm as an example

Trial probability:

$$T(A \to B)/T(B \to A) = (1 - P_{\text{add}})^{m-n}$$

m(n) the number of spins not added to the cluster in the boundary:

Detailed balance condition requires:

$$\frac{T(A \to B) \cdot A(A \to B)}{T(B \to A) \cdot A(B \to A)} = (1 - P_{\text{add}})^{m-n} \frac{A(A \to B)}{A(B \to A)} = e^{-\beta(E_B - E_A)}$$

Because:

$$E_A - E_B = 2J(n - m)$$

Detailed balance condition is now

$$\frac{A(A \to B)}{A(B \to A)} = \left[(1 - P_{\text{add}})e^{2\beta J}\right]^{n-m}$$

What will happen if we choose?

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

Cluster updating: Wolff algorithm as an example

$$A(A \to B) = A(B \to A) = 1$$

This is why we can flip all the spins in the cluster after it is formed.

Cluster updating: Wolff algorithm as an example

$$A(A \to B) = A(B \to A) = 1$$

This is why we can flip all the spins in the cluster after it is formed.

Dynamic exponent in Wolff algorithm is

$$z_c^W \approx 0$$

Cluster updating: Wolff algorithm as an example

$$A(A \to B) = A(B \to A) = 1$$

This is why we can flip all the spins in the cluster after it is formed.

Dynamic exponent in Wolff algorithm is

$$z_c^W \approx 0$$

Compared to Metropolis algorithm

$$z_c^M = 2.1665(12)$$

Error estimation: binning/ blocking

Average over two consecutive measures: $A_i^{(l)} := \frac{1}{2}(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)})$

Error estimation: binning/ blocking

Average over two consecutive measures:

$$A_i^{(l)} := \frac{1}{2}(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)})$$

Calculate the variance as if the measurements are independent:

$$\Delta_A^{(l)} \approx \sqrt{\frac{1}{M_l(M_l - 1)} \sum_{i=1}^{M_l} (A_i^{(l)} - \overline{A^{(l)}})^2}$$

Error estimation: binning/ blocking

Average over two consecutive measures: $$A_i^{(l)} := \frac{1}{2}\left(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)}\right)$$

Calculate the variance as if the measurements are independent: $$\Delta_A^{(l)} \approx \sqrt{\frac{1}{M_l(M_l - 1)} \sum_{i=1}^{M_l} \left(A_i^{(l)} - \overline{A^{(l)}}\right)^2}$$

Repeat the binning process, the calculated (incorrect) variance converges to the correct value: $$\Delta_A = \lim_{l \to \infty} \Delta_A^{(l)}$$

Error estimation: binning/ blocking

Average over two consecutive measures:

$$A_i^{(l)} := \frac{1}{2}(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)})$$

Calculate the variance as if the measurements are independent:

$$\Delta_A^{(l)} \approx \sqrt{\frac{1}{M_l(M_l-1)}\sum_{i=1}^{M_l}(A_i^{(l)} - \overline{A^{(l)}})^2}$$

Repeat the binning process, the calculated (incorrect) variance converges to the correct value:

$$\Delta_A = \lim_{l\to\infty} \Delta_A^{(l)}$$

The relaxation time can be estimate using:

$$\tau_A = \frac{1}{2}\left[\left(\frac{\Delta_A}{\Delta_A^{(0)}}\right)^2 - 1\right]$$

Error estimation: binning/ blocking

Average over two consecutive measures:

$$A_i^{(l)} := \frac{1}{2}(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)})$$

Calculate the variance as if the measurements are independent:

$$\Delta_A^{(l)} \approx \sqrt{\frac{1}{M_l(M_l-1)}\sum_{i=1}^{M_l}(A_i^{(l)} - \overline{A^{(l)}})^2}$$

Repeat the binning process, the calculated (incorrect) variance converges to the correct value:

$$\Delta_A = \lim_{l\to\infty}\Delta_A^{(l)}$$

The relaxation time can be estimate using:

$$\tau_A = \frac{1}{2}\left[\left(\frac{\Delta_A}{\Delta_A^{(0)}}\right)^2 - 1\right]$$

Question: what if the measurements are independent at step 0?

Error estimation: binning/ blocking