# 多体問題の計算科学

# Computational Science for Many-body problems
## 2023.4.25
## #3: 古典モンテカルロ法の基礎

## Classical Monte Carlo method

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・ This class is from 14:55 to 16:40 (105 min.)

# Today

Classical

Quantum

# Outline

- Standard Monte Carlo method

  - Monte Carlo integration

  - Importance sampling and Markov Chain Monte Carlo (MCMC)

  - Examples of MCMC

    - Metropolis-Heisting sampling

    - Heat-bath sampling (Gibbs sampling)

- Application to classical spin systems

  - Local update by using Metropolis sampling

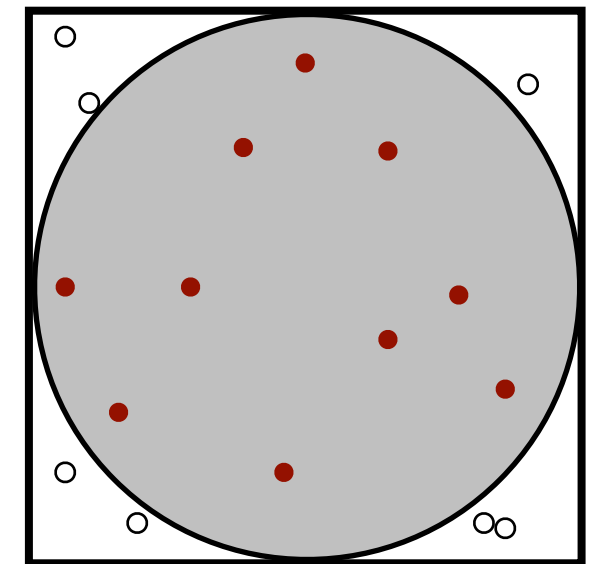  - Global update as the cluster update

# Standard Monte Carlo method

# Monte Carlo method: Randomized algorithm

**Randomized algorithm:** It changes its behavior depending on (psuedo) random numbers on execution.

Example :

**Area of a circle:** $\displaystyle\int_{x^2+y^2\leq 1} dxdy$



**Algorithm (rejection sampling)**

$N_a \leftarrow 0, N_s \leftarrow 0$     initialize

loop $i$

    $x_i \in [-1, 1]$    take uniform

    $y_i \in [-1, 1]$   random numbers

   $N_s \leftarrow N_s + 1$

     if   $x_i^2 + y_i^2 \leq 1$   then $N_a \leftarrow N_a + 1$

end loop

$$\lim_{N_s \to \infty} \frac{N_a}{N_s} = \frac{\pi}{4}$$

With statistical error proportional to $\dfrac{1}{\sqrt{N_s}}$

# Monte Carlo Integration: General aspect

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**Monte Carlo Integration**

$$\int d\Gamma f(\Gamma) = \int d\Gamma \frac{f(\Gamma)}{P(\Gamma)} P(\Gamma) = \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle$$

$P(\Gamma)$ : probability distribution
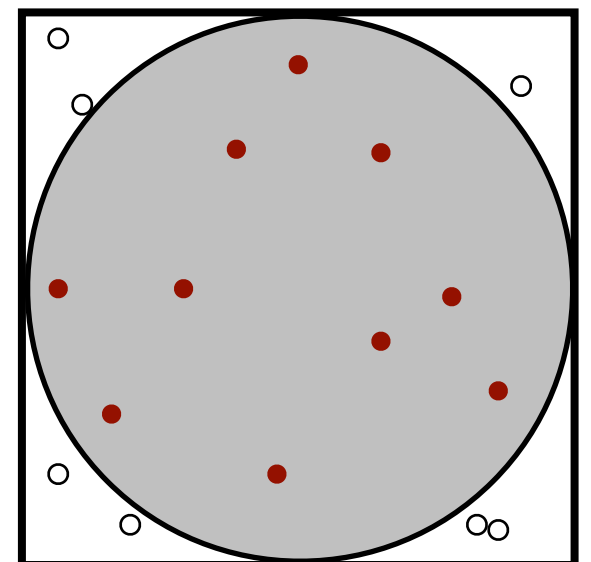
Estimate an integral as an expectation value under $P(\Gamma)$

Previous example:

$$\Gamma = \{(x, y); -1 \leq x \leq 1, -1 \leq y \leq 1\}$$

$$f(\Gamma) = \begin{cases} 1 & \sqrt{x^2 + y^2} \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

$$P(\Gamma) = \text{const.} \quad \text{(Uniform distribution)}$$

# Monte Carlo Integration: General aspect

**Merit of Monte Carlo Integration**

The error is (usually) independent on the dimension of $\Gamma$.

$$\epsilon \sim \sqrt{\frac{\sigma_f^2}{N_s}} \propto O(N_s^{-1/2})$$

$N_s$ : sampling number

$\sigma_f^2$ : Variance

$$\sigma_f^2 = \left\langle \left[ \frac{f(\Gamma)}{P(\Gamma)} \right]^2 \right\rangle - \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle^2$$

The error of usual numerical quadrature,
(eg. trapezoidal formula（台形公式）),

exponentially increases as we increase the dimension of $\Gamma$.

eg. trapezoidal formula $\quad \epsilon \propto O(N_s^{-2/d})$

# Application to higher dimensions:
# The curse of dimensionality(次元の呪い)

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**Rejection sampling** is inefficient for higher dimensions

**Volume ratio** between "*d*-dimensional hyper cubic" (with L=2) and
    "*d*-dimensional hyper sphere" (with r=1)

**Asymptotic form of *Γ*-function**

$$r = \frac{V_\circ}{V_\square} = \frac{\pi^{d/2}/\Gamma(\frac{d}{2}+1)}{2^d} \sim \left(\frac{e\pi}{2d}\right)^{d/2} \qquad \Gamma(x) \sim \left(\frac{x}{e}\right)^x$$

For larger *d*, the ratio exponentially decreases!

And, $\quad \sigma_f^2 = \left\langle \left[\frac{f(\Gamma)}{P(\Gamma)}\right]^2 \right\rangle - \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle^2 = V_\circ^2 \left(\frac{1}{r}-1\right) \sim O(r^{-1})$

(Relative) Error of the rejection sampling increases exponentially.

$$\epsilon \sim O((rN_s)^{-1/2}) = O\left(\left(\frac{2d}{e\pi}\right)^{d/4} N_s^{-1/2}\right)$$

**More efficient way?**

Sample points where |*f*(Γ)| takes large value!
(eg. points within the sphere)

**Importance sampling**

# Importance sampling and Markov Chain Monte Carlo
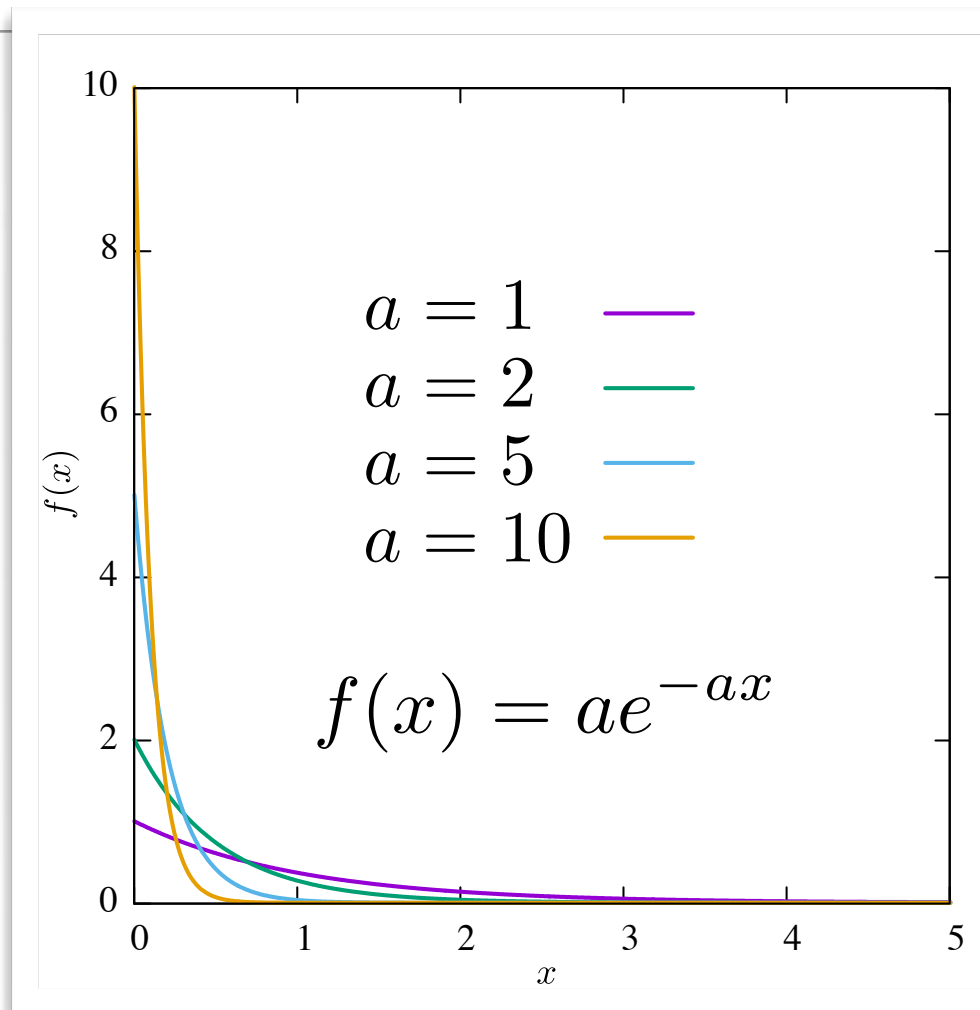
# Sampling with uniform distribution

$$\int d\Gamma f(\Gamma) = \int d\Gamma \frac{f(\Gamma)}{P(\Gamma)} P(\Gamma) \quad \text{with } P(\Gamma) = \text{const.}$$

When $f(\Gamma)$ is "narrow", the sampling becomes inefficient, as like the rejection sampling.

For example, $f(x) = ae^{-ax}$, $x \in [0, l]$

$$\implies \sigma_f^2 \sim \frac{la}{2} \sim O(la) \implies \epsilon \sim O\left(\sqrt{la/N_s}\right)$$

The error increases as the parameter $a$ increases.



$$a = 1$$
$$a = 2$$
$$a = 5$$
$$a = 10$$

$$f(x) = ae^{-ax}$$

This situation typically occurs in a sampling for statistical mechanics.

$$\langle \hat{O} \rangle \equiv \int d\Gamma \hat{O}(\Gamma) \underline{P_{\text{eq}}(\Gamma)}$$

It corresponds to $f(\Gamma) = \hat{O}(\Gamma) P_{\text{eq}}(\Gamma)$

Equilibrium distribution, e.g.,
$$P_{\text{eq}}(\Gamma) \propto e^{-\beta \mathcal{H}(\Gamma)}$$
$$\mathcal{H}(\Gamma) = O(N)$$
$N$: number of particles or spins

# Importance Sampling

### Importance sampling

Chose $P(\Gamma)$ close to $f(\Gamma)$. (e.g. $P(\Gamma) \propto f(\Gamma)$)

➡ $\sigma_f^2 = \left\langle \left[ \dfrac{f(\Gamma)}{P(\Gamma)} \right]^2 \right\rangle - \left\langle \dfrac{f(\Gamma)}{P(\Gamma)} \right\rangle^2$  Becomes small!

**However it is not so easy, in practice!**
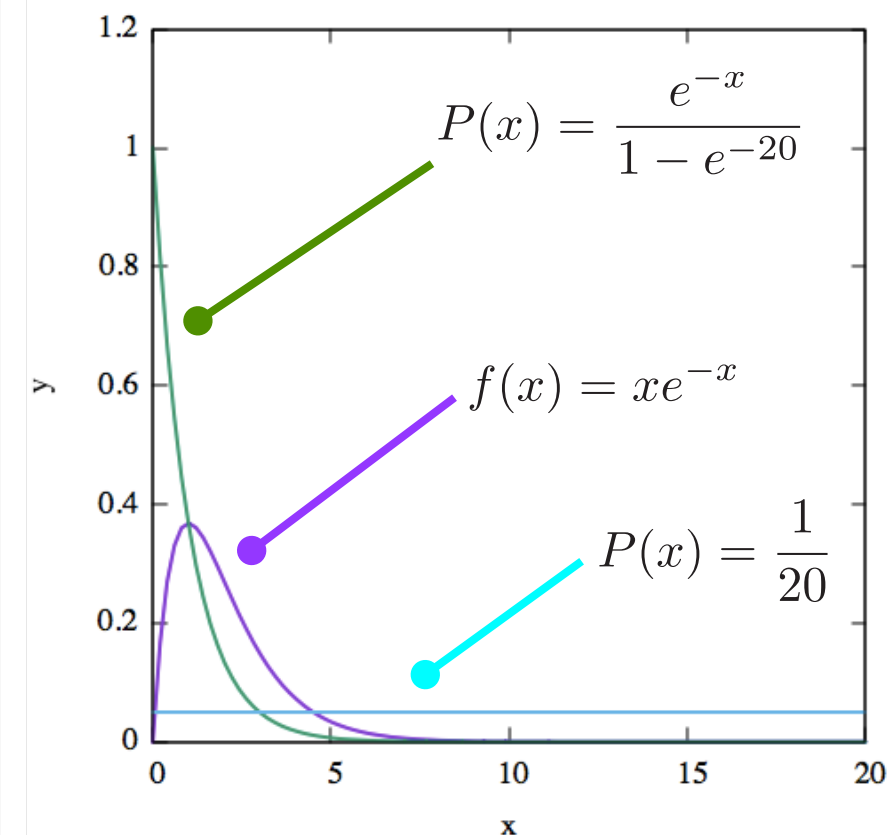
In order to perform Monte Carlo sampling,
$P(\Gamma)$ must be easily generated from pseudo random numbers.

➡ $P_{\text{eq}}(\Gamma) \propto e^{-\beta \mathcal{H}(\Gamma)}$

- We do not know the normalization constant
- It is too complex

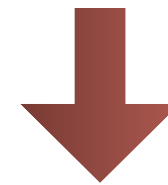**How can we perform the importance sampling?**

**Example of importance sampling**



$P(x) = \dfrac{e^{-x}}{1 - e^{-20}}$

$f(x) = xe^{-x}$

$P(x) = \dfrac{1}{20}$

# Markov Chain Monte Carlo (MCMC)

We might generate a $P(\Gamma)$ as the steady state of a stochastic process.

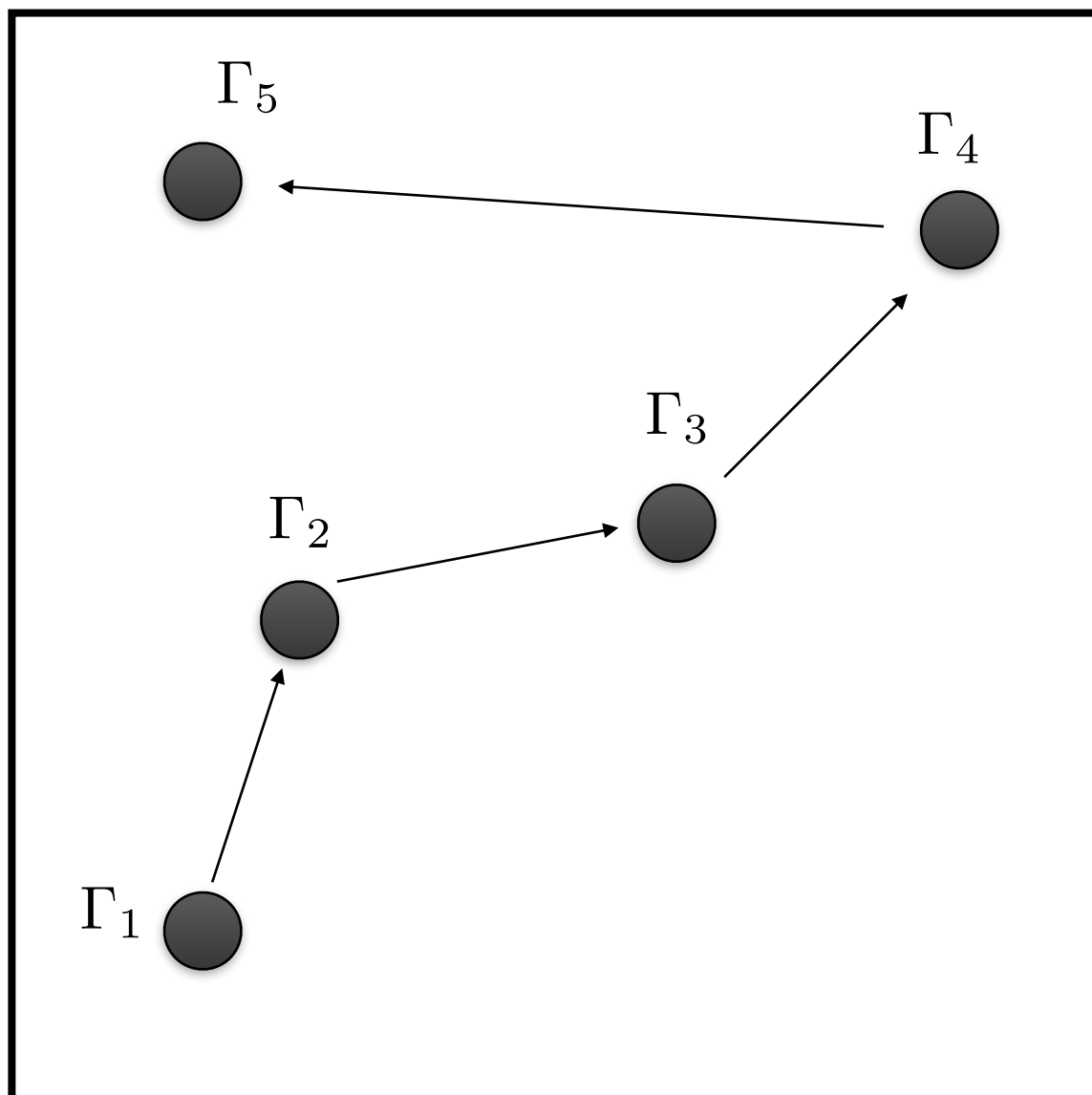A sampling point move in $\Gamma$ "randomly".



**Markov process:**

The next move depends only on the present state and independent of the past states.

The **transition probability** to $\Gamma_{t+1}$ depends on $\Gamma_t$.

$W_{\Gamma \to \Gamma'}$ :transition probability from $\Gamma$ to $\Gamma'$

$$\sum_{\Gamma'} W_{\Gamma \to \Gamma'} = 1$$

# Typical procedure in MCMC

Step 0:  Prepare an initial state $\Gamma_0 \in \{\Gamma\}$

  loop $t$

    1.  Make next candidate state $\Gamma''$ from the transition probability $W_{\Gamma_t \to \Gamma'}$.
    2.  Change the state as $\Gamma_{t+1} = \Gamma''$.

Sequence of the realizations:

$$\Gamma_0 \to \Gamma_1 \to \cdots \to \Gamma_t \to \Gamma_{t+1} \to \dots$$

✳    We may use $\{\Gamma_t\}$ to calculate long-time average of observables.

$$\langle O \rangle = \frac{1}{T} \sum_{t=t_0}^{T+t_0-1} \hat{O}(\Gamma_t)$$

✳ Here, $t_0$ is introduced to reduce the initial state dependence.
✳ $\Gamma_t$ s become stochastic variables. Thus, the above long-time average will be a random average over a certain probability distribution.

Can we describer the dynamics of a probability distribution?

# Master equation of MCMC

**Master equation** for a general Markov process

$\rho_t(\Gamma)$ : probability for appearance of $\Gamma$ at time $t$

$$\sum_{\Gamma'} W_{\Gamma \to \Gamma'} = 1$$
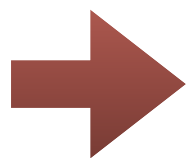
$$\rho_{t+1}(\Gamma) = \rho_t(\Gamma) + \sum_{\Gamma'} W_{\Gamma' \to \Gamma} \rho_t(\Gamma') - \sum_{\Gamma'} W_{\Gamma \to \Gamma'} \rho_t(\Gamma)$$

$$\sum_{\Gamma} \rho_t(\Gamma) = 1$$

$W_{\Gamma \to \Gamma'}$ :transition probability from $\Gamma$ to $\Gamma'$

When a Markov process becomes **a steady state** in the long time limit,

$$\lim_{t \to \infty} \rho_t(\Gamma) = P(\Gamma)$$

We can sample points with distribution $P(\Gamma)$
as the long time average along this stochastic process.

# Markov Chain Monte Carlo: convergence condition

Conditions for transition probability for converging to a given $P(\Gamma)$.

1. "**Ergodicity**"
   - Any two states $\Gamma$ and $\Gamma'$ are connected by $W$ with finite steps.
     - If we regard $W$ as a matrix, this condition means

$$^{\exists}T > 0, ^{\forall}(\Gamma, \Gamma'), \quad [(W)^t]_{\Gamma, \Gamma'} > 0, (^{\forall}t \geq T)$$

2. "**Balance Condition**"
   - The "flows" of probabilities are balanced for $P(\Gamma)$.

$$^{\forall}\Gamma, \quad \sum_{\Gamma'} W_{\Gamma \to \Gamma'} P(\Gamma) = \sum_{\Gamma'} W_{\Gamma' \to \Gamma} P(\Gamma')$$
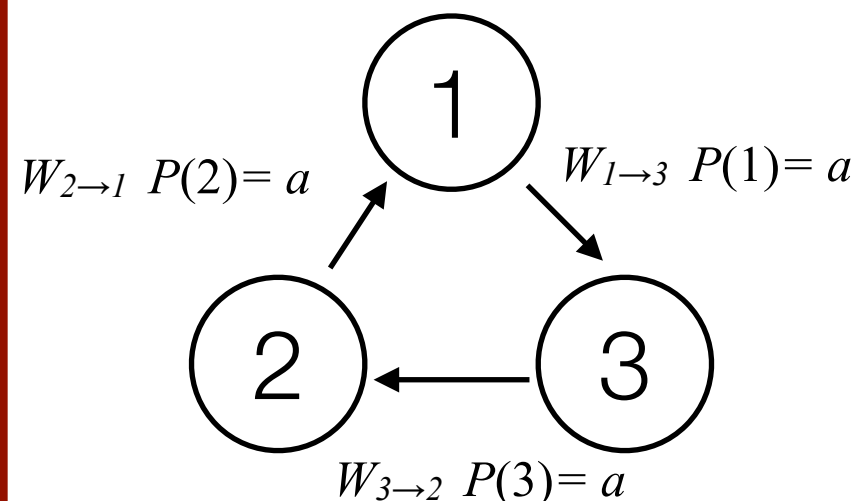
**Special case:**

**Detailed balance condition**
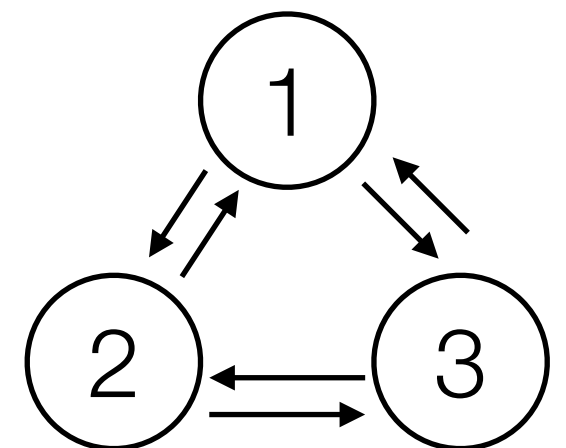
$$W_{\Gamma \to \Gamma'} P(\Gamma) = W_{\Gamma' \to \Gamma} P(\Gamma')$$

No microscopic flow
in the steady state



**Balance condition with flow**     **Detailed balance condition**

$W_{2 \to 1}\ P(2) = a$     $W_{1 \to 3}\ P(1) = a$

$W_{3 \to 2}\ P(3) = a$

# Examples of MCMC

# Example: Metropolis-Heisting sampling

Step 0: Prepare an initial state $\Gamma_0 \in \{\Gamma\}$

loop $t$

1. Make next candidate state $\Gamma"$ randomly from a proposal distribution $q(\Gamma'|\Gamma_t)$
2. Make a uniform random number $r \in [0,1]$
3. Select the next state $\Gamma_{t+1}$ based on $r$ as

$$\Gamma_{t+1} = \begin{cases} \Gamma', & r \le a(\Gamma_t \to \Gamma') \\ \Gamma_t, & \text{otherwise} \end{cases}$$

Acceptance probability: $a(\Gamma_t \to \Gamma') = \min\left(1, \dfrac{P(\Gamma')q(\Gamma_t|\Gamma')}{P(\Gamma_t)q(\Gamma'|\Gamma_t)}\right)$

When $q(\Gamma_t|\Gamma') = q(\Gamma'|\Gamma_t)$ ➡ $a(\Gamma_t \to \Gamma') = \min\left(1, \dfrac{P(\Gamma')}{P(\Gamma_t)}\right)$ | Metropolis sampling |

(example) $\Gamma = x \in (-\infty, \infty)$

$x' = x_t + \epsilon \quad , \epsilon \in [-\sigma, \sigma]$ ➡ $q(x'|x_t) = q(x_t|x')$

# Metropolis-Heisting sampling: Detailed balance

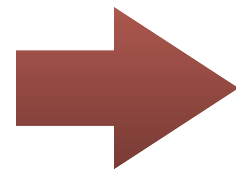Transition probability = (proposal probability) × (Acceptance probability)

$$W_{\Gamma \to \Gamma'} = q(\Gamma'|\Gamma)a(\Gamma \to \Gamma')$$

$$a(\Gamma \to \Gamma') = \min\left(1, \frac{P(\Gamma')q(\Gamma|\Gamma')}{P(\Gamma)q(\Gamma'|\Gamma)}\right)$$

* When $P(\Gamma')q(\Gamma|\Gamma') > P(\Gamma)q(\Gamma'|\Gamma)$

$$W_{\Gamma \to \Gamma'} = q(\Gamma'|\Gamma)$$

$$W_{\Gamma' \to \Gamma} = \frac{q(\Gamma'|\Gamma)P(\Gamma)}{P(\Gamma')}$$

**It satisfies the detailed balance condition.**

$$W_{\Gamma \to \Gamma'} P(\Gamma) = W_{\Gamma' \to \Gamma} P(\Gamma')$$

Thus, by using Metropolis-Heisting sampling,
we can calculate an ensemble average!

$$\langle O \rangle \equiv \int d\Gamma O(\Gamma)P(\Gamma)$$

$$= \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} O(\Gamma_t)$$

**Note:**

We do not need to know the normalization constant.

# Example: Heat-bath sampling (Gibbs sampling)

Suppose we only change a part of variables in $\Gamma$

$$\Gamma = (\Gamma^1, \Gamma^2, \Gamma^3, \cdots, \Gamma^N) \quad\blacktriangleright\quad \Gamma' = (\Gamma^{1\prime}, \Gamma^2, \Gamma^3, \cdots, \Gamma^N)$$

In this case, we may calculate "conditional" probability distribution of $\Gamma^1$,

$$P(\Gamma^1 | \Gamma^2, \Gamma^3, \ldots, \Gamma^N) = \frac{P(\Gamma)}{\int d\Gamma^1 P(\Gamma^1, \Gamma^2, \ldots, \Gamma^N)}$$

Then we can chose a transition probability satisfying the detailed balance condition:

$$W_{\Gamma \to \Gamma'} = P(\Gamma^{1\prime} | \Gamma^2, \Gamma^3, \cdots \Gamma^N)$$

$$\boxed{\begin{aligned} W_{\Gamma \to \Gamma'} P(\Gamma) &= \frac{P(\Gamma')P(\Gamma)}{\int d\Gamma^{1\prime} P(\Gamma^{1\prime}, \Gamma^2, \ldots, \Gamma^N)} \\ &= W_{\Gamma' \to \Gamma} P(\Gamma') \end{aligned}}$$

We generate the next $\Gamma'$ directly from the conditional probability!

- The transition probability is independent on the present $\Gamma^1$.
- In general, it is not easy to produce the conditional probability distribution from uniform random numbers.
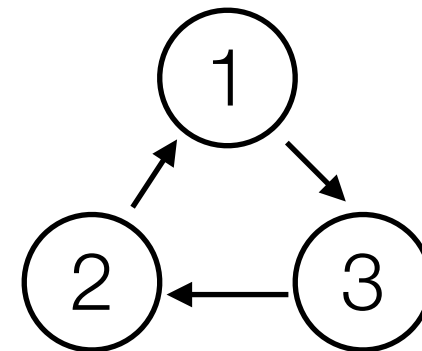
# Sampling based on the balance condition

We do not necessarily use the detailed balance condition.
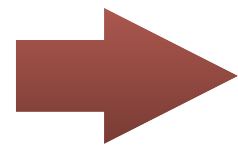
➡️ By using more general balance condition,
we can make "rejection free" transition probabilities.

$W_{\Gamma \to \Gamma} = 0$:The state necessarily changes to another state.

**e.g. Suwa-Todo method**

H. Suwa, and S. Todo, Phys. Rev. Lett. **105**, 120603 (2010).

"詳細釣り合いを満たさないモンテカルロ法"

諏訪秀麿, 藤堂眞治, 日本物理学会誌, **66**, 370 (2011).

"確率の流れをあやつるモンテカルロ法－詳細釣り合いの破れとリフティング"

諏訪秀麿, 藤堂眞治, 日本物理学会誌, **77**, 731 (2022).

# Application to Classical spin system

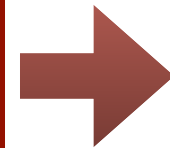# Local update

# Classical spin system

## Model Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i^z$$

Nearest Neighbor interaction

e.g.

Ising spin: $S_i = \pm 1$

Heisenberg spin: $S_i = (S_i^x, S_i^y, S_i^z)$

## MCMC method:

Target steady state is $P(\Gamma) = \dfrac{1}{Z} e^{-\beta \mathcal{H}(\Gamma)}$

$$\langle \hat{O} \rangle = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} \hat{O}(\Gamma_t)$$

$\Gamma_t$: sampling points along Markov chain

## Calculate expectation values under Canonical Ensemble

$$\langle \hat{O} \rangle = \frac{1}{Z} \int d\Gamma \, \hat{O}(\Gamma) e^{-\beta \mathcal{H}(\Gamma)}$$
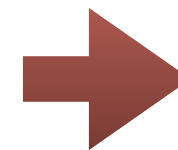
e.g.

**Energy:** $\hat{E}(\Gamma) = \mathcal{H}$

**Squared Energy:** $\hat{E}^2(\Gamma) = (\mathcal{H})^2$

**Heat capacity:**

$$\frac{\langle \hat{E}^2 \rangle - \langle \hat{E} \rangle^2}{k_B T^2}$$

**Squared Magnetization:** $\hat{M}_z^2(\Gamma) = \left( \dfrac{1}{N} \sum_i S_i^z \right)^2$

# Local update

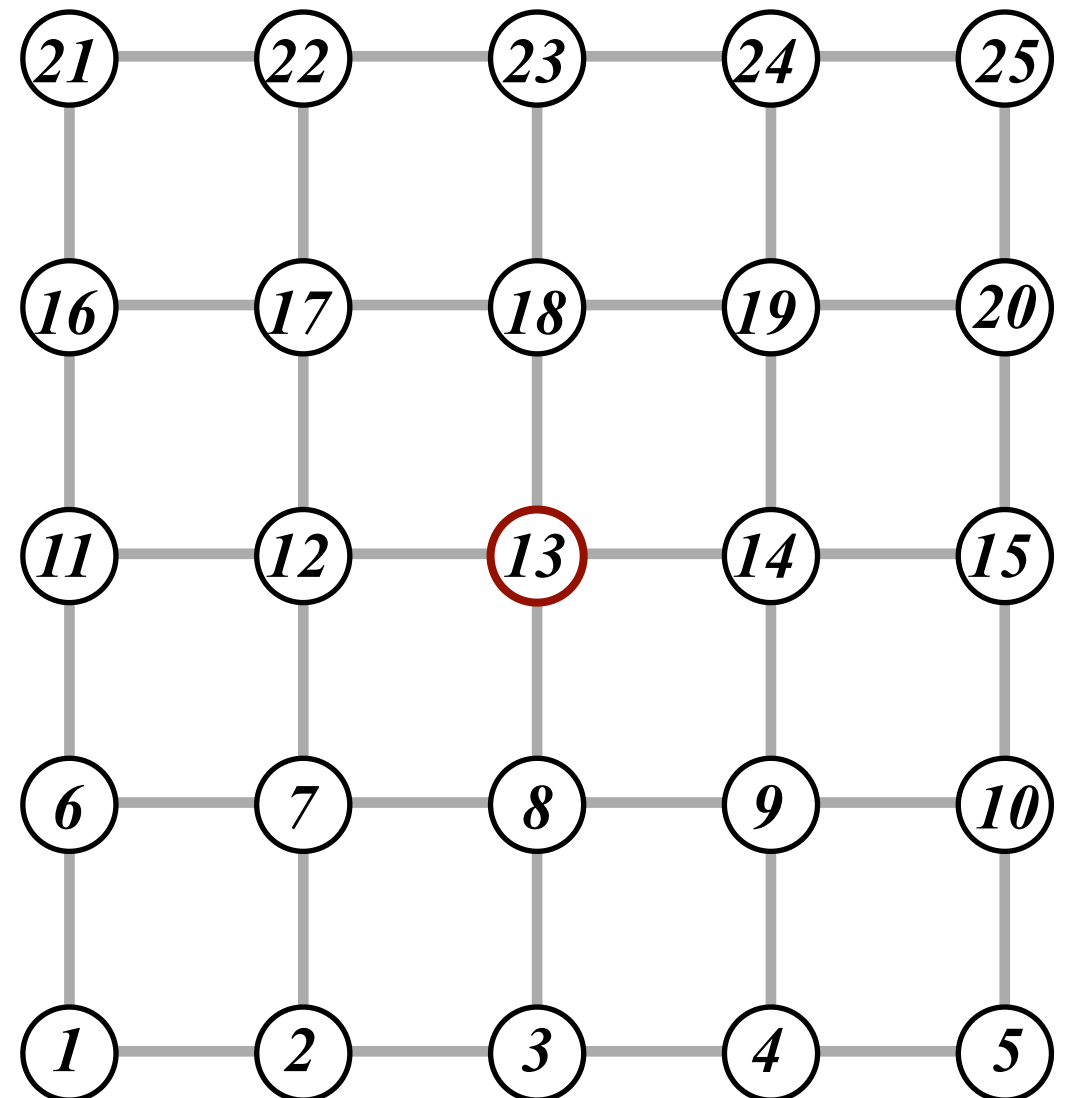**Local update:** We try to change a part of spins (typically single spin) at transitions along Markov chain

$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

➡️ $$\Gamma' = (S_1, S_2, \cdots, S'_{13}, \cdots, S_{25})$$

From $\Gamma$ to $\Gamma'$, we fix $S_1, S_2, .. S_{12}, S_{14}, S_{15}, ... , S_{25}$, and try to change only $S_{13}$.

In this local update, we can easily estimate the transition probability $W$ because the change of Hamiltonian (Energy) is determined only locally.

\* If the Hamiltonian contains long range interactions, the energy estimation becomes more costful.

# Metropolis method:

$$a(\Gamma \to \Gamma') = \min\left(1, \frac{P(\Gamma')}{P(\Gamma)}\right)$$

$$\frac{P(\Gamma')}{P(\Gamma)} = e^{-\beta[\mathcal{H}(\Gamma') - \mathcal{H}(\Gamma)]} = e^{-\beta \Delta E}$$
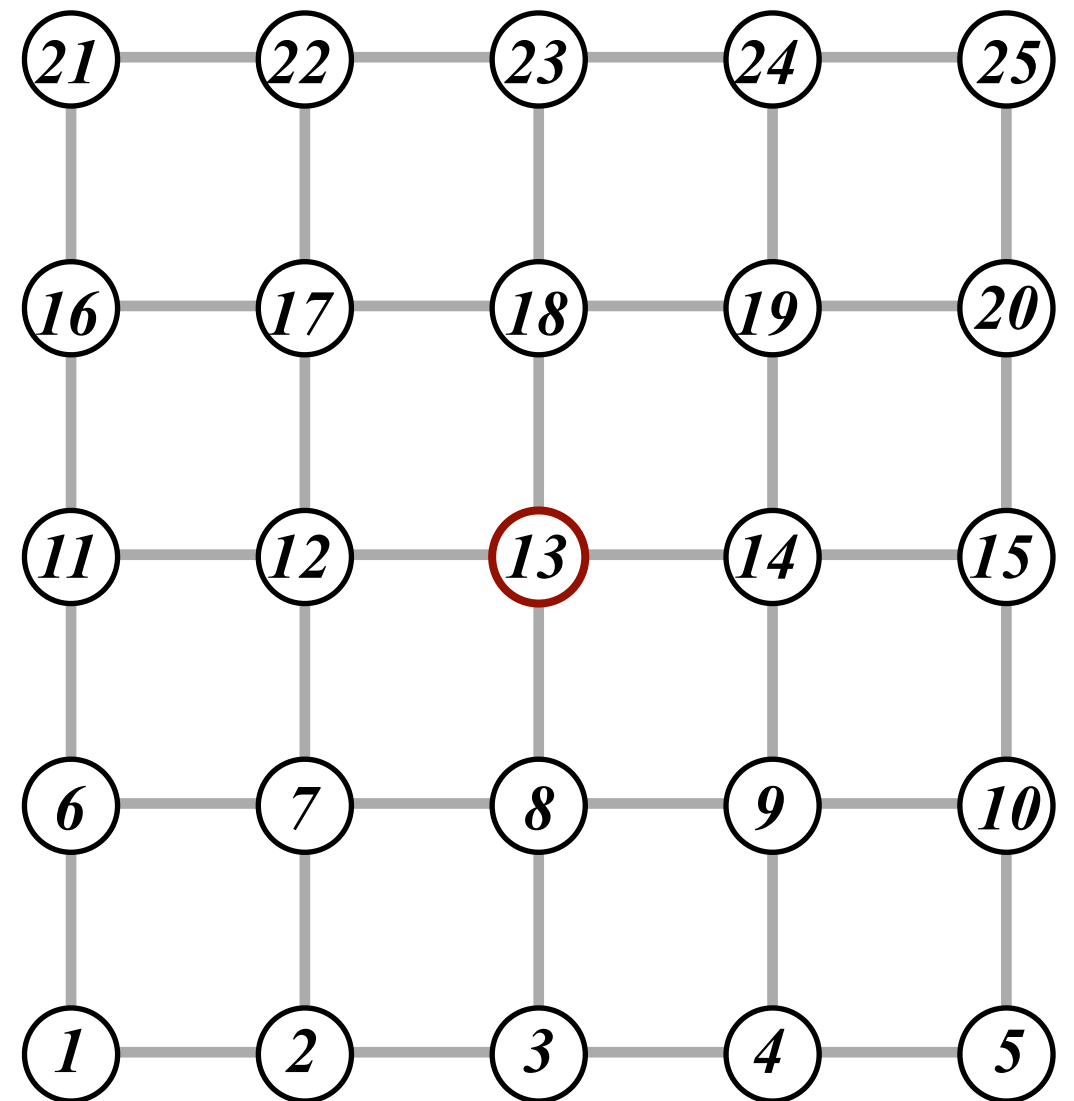
\* We don't need partition function $Z$!

For local update on the square lattice,

$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

$$\Gamma' = (S_1, S_2, \cdots, S_{13}', \cdots, S_{25})$$

$$\Delta E = -J(S_8 + S_{12} + S_{14} + S_{18})(S_{13}' - S_{13})$$
$$- h[(S_{13}^z)' - S_{13}^z]$$

# Metropolis method with local update: summary

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \cdots, S_N)$

loop $t$

  select $i$-th site

1. Make next candidate state $\Gamma'$ by changing $S_i$
   - Ising : $S_i' = -S_i$
   - XY, Heisenberg: $S_i' = S_{i + \delta S}$
     or random unit vector
2. Calculate $\Delta E = \mathcal{H}(\Gamma') - \mathcal{H}(\Gamma)$
3. Make random number $r \in [0, 1]$
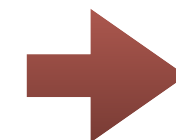4. Select the next state $\Gamma_{t+1}$ based on $r$ as

$$\Gamma_{t+1} = \begin{cases} \Gamma' & r \leq e^{-\beta \Delta E} \\ \Gamma_t & \text{otherwise} \end{cases}$$

Calculate O($\Gamma_t$)

Typically we choose
- random state ($T{\to}\infty$)
- ordered state ($T{\to}0$)

If energy decreases (ΔE < 0), we "accept" new state with probability 1.

It tends to sample low energy states.
**Importance sampling in the canonical ensemble!**

Usually, we observe quantities at least after N-spins are tried to change

# Heat-bath method:

$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$

$\Gamma' = (S_1, S_2, \cdots, S'_{13}, \cdots, S_{25})$

$W_{\Gamma \to \Gamma'} = P(S'_{13} | S_1, S_2, \cdots S_{12}, S_{14}, \cdots, S_{25})$

$\qquad = \dfrac{P(\Gamma')}{\int dS_{13} P(\Gamma)}$

$\qquad = \dfrac{e^{\beta[J(S_8 + S_{12} + S_{14} + S_{18})S'_{13} + h(S^z_{13})']}}{\int dS_{13} e^{\beta[J(S_8 + S_{12} + S_{14} + S_{18})S'_{13} + h(S^z_{13})']}}$

In the case of Ising or Heisenberg spins,
we can easily generate this probability distribution

Ising: $\quad W_{\Gamma \to \Gamma'} = \dfrac{e^{\beta h_{\text{eff}} S'_{13}}}{e^{\beta h_{\text{eff}} S'_{13}} + e^{-\beta h_{\text{eff}} S'_{13}}}$
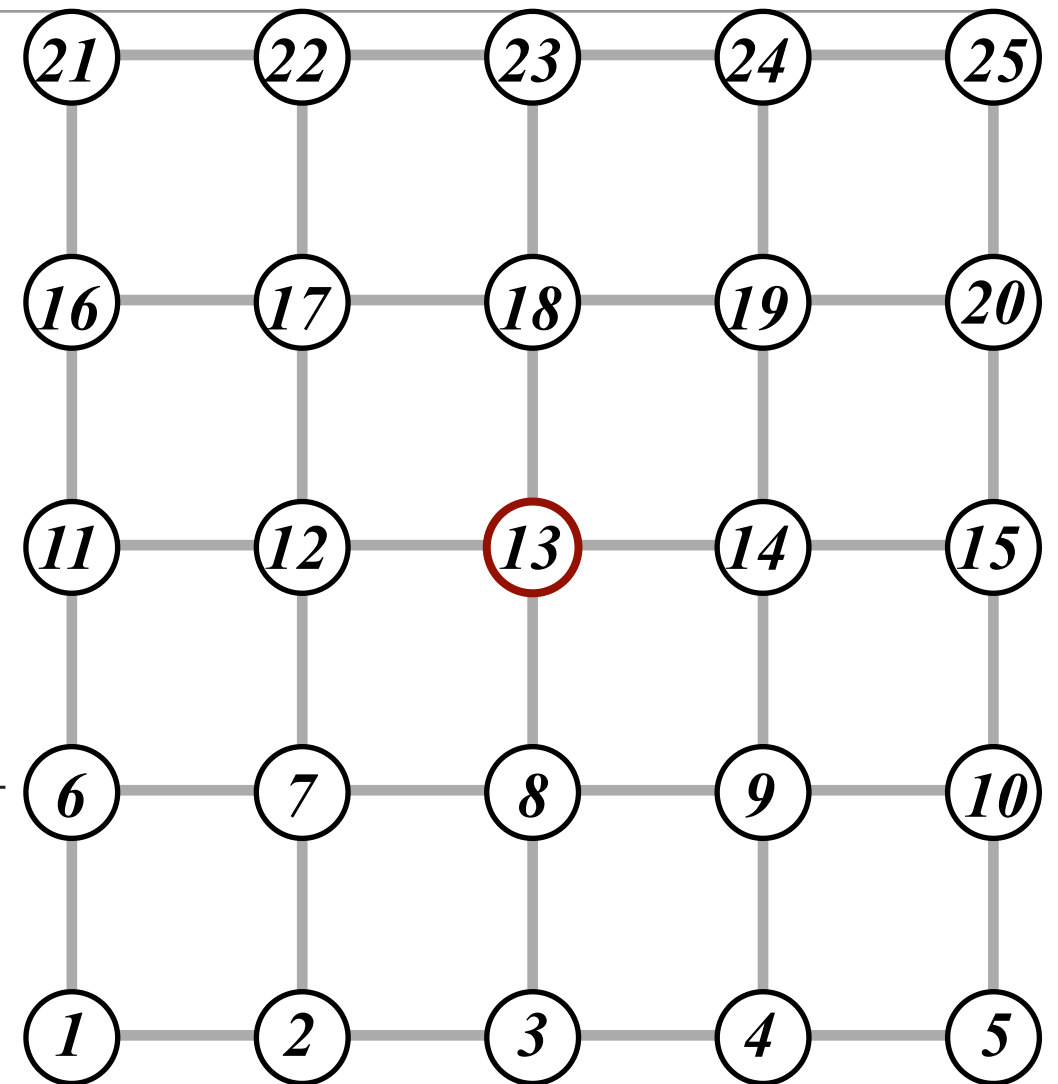
Heisenberg: $\quad W_{\Gamma \to \Gamma'} = \dfrac{(\beta |h_{\text{eff}}|) e^{\beta h_{\text{eff}} \cdot S'_{13}}}{[e^{\beta |h_{\text{eff}}|} - e^{-\beta |h_{\text{eff}}|}]}$

Scaler value

$h_{\text{eff}} \equiv J(S_8 + S_{12} + S_{14} + S_{18}) + h$

Three component vector

$h_{\text{eff}} \equiv J(S_8 + S_{12} + S_{14} + S_{18}) + h\hat{e}_z$

# Heat-bath method with local update: summary

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \cdots, S_N)$

loop $t$

select $i$-th site

1. Calculate effective field $h_{\text{eff}}$
2. Generate S'$_i$ based on the probability
$$P(S_i') \propto e^{\beta h_{\text{eff}} S_i'}$$
(for Ising and Heisenberg spins, it can be generated from uniform random number)
3. The next state $\Gamma_{t+1}$ is $\Gamma'$

Calculate O($\Gamma_t$)

Typically we choose
- random state ($T \to \infty$)
- ordered state ($T \to 0$)

$r \in [0, 1]$ :uniform random number

Ising : $S_i' = \begin{cases} 1 & r \leq P(1) \\ -1 & \text{otherwise} \end{cases}$

Heisenberg:
(in polar co-ordinate with $z \mathbin{/\!/} h_{\text{eff}}$)
$$S_x' = \sin\theta\cos\phi$$
$$S_y' = \sin\theta\sin\phi$$
$$S_z' = \cos\theta$$

$r_1, r_2 \in [0, 1]$:uniform random number

$$\phi = 2\pi r_1$$
$$\cos\theta = -1 + \frac{1}{\beta|h_{\text{eff}}|}$$
$$\times \ln[r_2 + (1 - r_2)e^{2\beta|h_{\text{eff}}|}]$$

Usually, we observe quantities at least after N-spins are tried to change

# Problems in local update

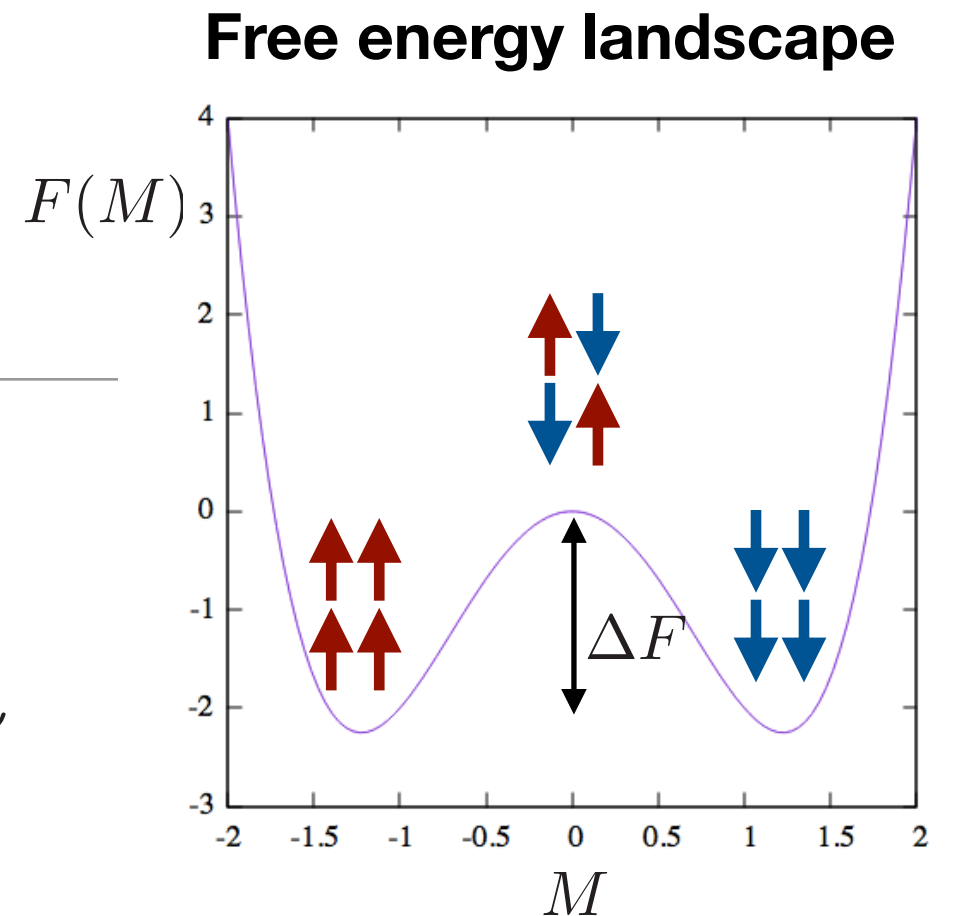Sampling efficiency largely decreases for

1. Critical phenomena

   - Divergence of relaxation time: $\tau \propto |T - T_c|^{-z\nu}$

2. 1st order phase transition (phase coexistence)

3. Low temperature phase with discrete symmetry (e.g. Ising model)

   - Exponentially small probability to move other local minima: $\tau \propto \exp\left[\dfrac{\Delta F}{T}\right]$

Part of these difficulties can be reduced by using "global update".

Simultaneous change of spins in "large cluster"

# Cluster update

# Cluster update method

## Idea of cluster updates

- From a spin configuration $\Gamma$, we can define "reasonable" clusters $G$.

- When we "flip" all spins on a cluster $G$ and make new configuration $\Gamma'$, the free energy difference between $\Gamma$ and $\Gamma'$ is not so large.

- We can change the configuration drastically with higher probability.



$S_i = 1$ ●
$S_i = -1$ ●

**"reasonable" clusters**
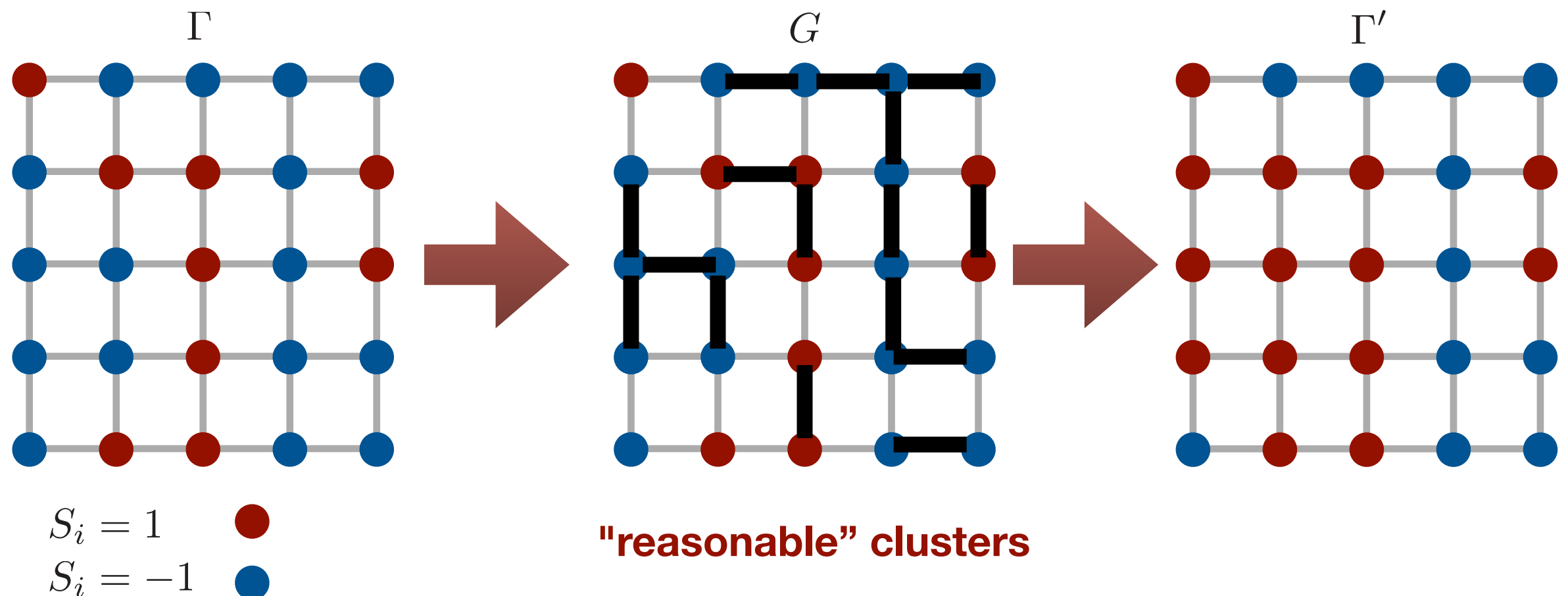
# How to make a cluster configuration?
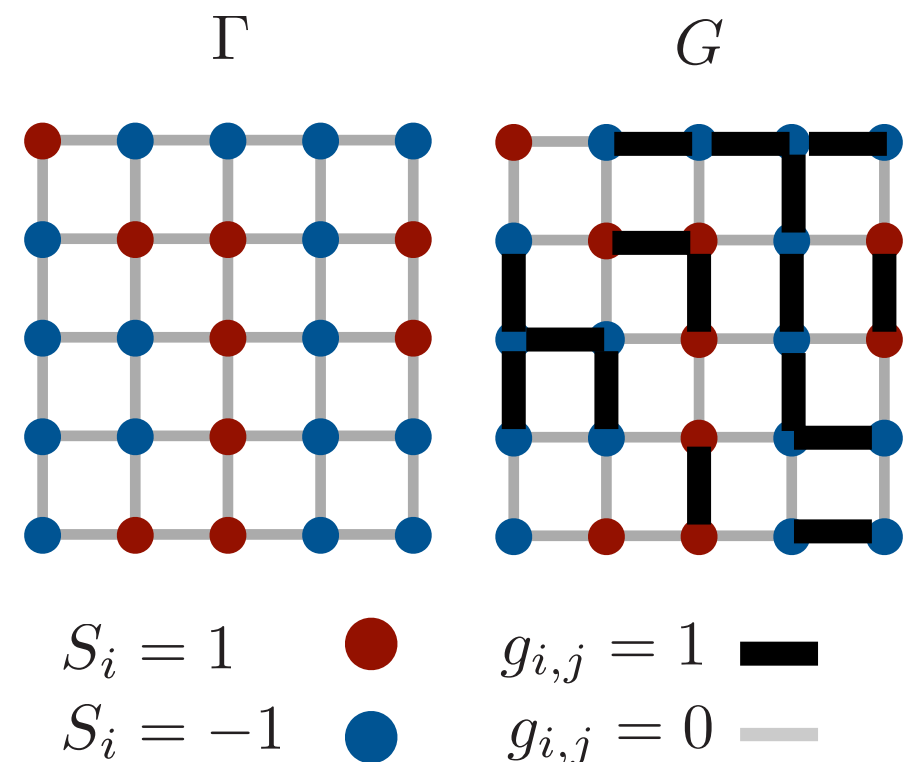
**Fortuin-Kasteleyn mapping** (for Ising model)

P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn, Suppl. **26**, 11 (1969).

C. M. Fortuin and P. W. Kasteleyn, Physica **57**, 536 (1972).

**Ising model**

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j \ , S_i = \pm 1$$

$$e^{\beta J S_i S_j} = \underbrace{e^{-\beta J}}_{g=0} + \underbrace{\delta_{S_i,S_j}(e^{\beta J} - e^{-\beta J})}_{g=1} = \sum_{g=0,1} w(g, S_i, S_j)$$

$$Z = \sum_{\Gamma} e^{\beta J \sum_{\langle i,j \rangle} S_i S_j}$$

$$= \sum_{G} \sum_{\Gamma} \prod_{\langle i,j \rangle} w(g_{i,j}, S_i, S_j)$$

$$G = \{g_{i,j}\} \qquad \Gamma = \{S_i\}$$



$\Gamma$   $G$

$S_i = 1$  ● (red)   $g_{i,j} = 1$ ▬ (black)
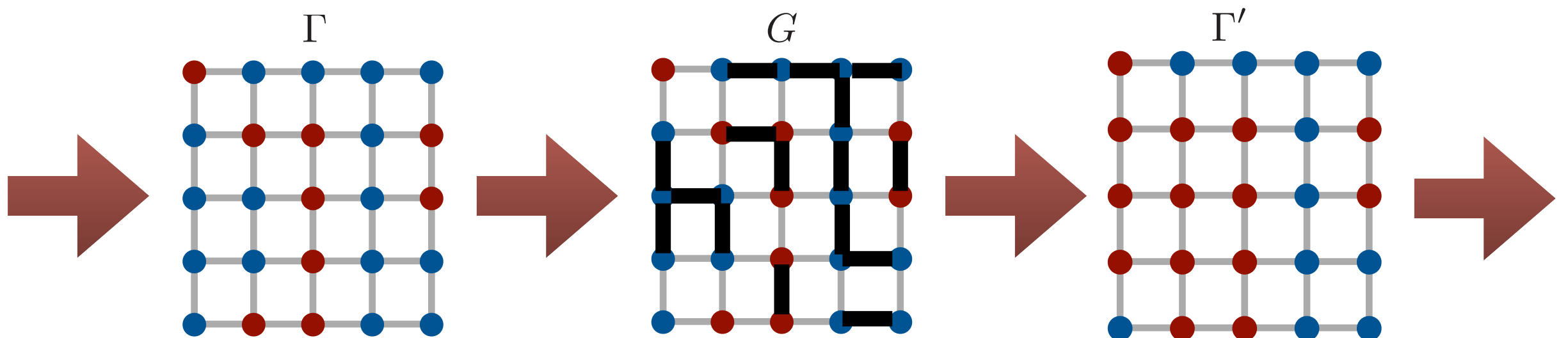$S_i = -1$ ● (blue)  $g_{i,j} = 0$ ▬ (grey)

# Markov chain in extended (G, Γ) space

$$Z = \sum_G \sum_\Gamma \prod_{\langle i,j \rangle} w(g_{i,j}, S_i, S_j) = \sum_G \sum_\Gamma W(G, \Gamma)$$

We consider to update $\Gamma$ and $G$ alternatively:

$$\cdots \rightarrow (G_{t-1}, \Gamma_t) \rightarrow ({\color{red}G_t}, \Gamma_t) \rightarrow (G_t, {\color{red}\Gamma_{t+1}}) \rightarrow ({\color{red}G_{t+1}}, \Gamma_{t+1}) \rightarrow \cdots$$

This update can be symbolically written as

$$\cdots \rightarrow \Gamma_t \rightarrow G_t \rightarrow \Gamma_{t+1} \rightarrow G_{t+1} \rightarrow \cdots$$

# Markov chain in extended $(G, \Gamma)$ space

We assign the transition probabilities as follows:

$$w_{(S_i, S_j) \to 0} = \begin{cases} 1 & (S_i \neq S_j) \\ e^{-2\beta J} & (S_i = S_j) \end{cases}$$
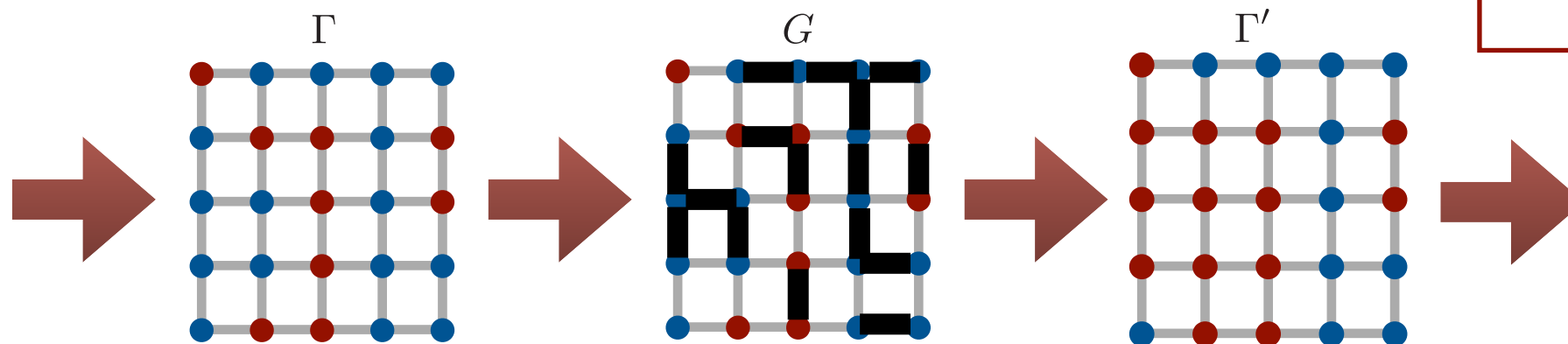
**Transition probabilities (as like the heat bath)**

$$\Gamma \to G' : \ W_{(G,\Gamma) \to (\textcolor{red}{G'},\Gamma)} = \frac{W(G',\Gamma)}{\sum_{G''} W(G'',\Gamma)} = \prod_{\langle i,j \rangle} w_{(S_i,S_j) \to g_{ij}}$$

$$G \to \Gamma' : \ W_{(G,\Gamma) \to (G,\textcolor{red}{\Gamma'})} = \frac{W(G,\Gamma')}{\sum_{\Gamma''} W(G,\Gamma'')} = \prod_{C_j} P(\{S_i \in C_j\})$$

cluster formed from g=1 links

$$P(\{S_i \in C_j\}) = 1$$

(If all spin in cluster is pointing same direction)



$\Gamma$        $G$        $\Gamma'$

# Swendsen-Wang algorithm

**Swendsen-Wang algorithm**

Step 0:  Prepare an initial state  $\Gamma_0 = (S_1, S_2, \cdots, S_N)$

  loop $t$
    loop <i,j>

        · if $S_i = S_j$, generate a random number
          · if $r \leq 1 - e^{-2\beta J}$   connects $i$ and $j$ ($g_{ij}=1$)

     end loop <i,j>

 · Make clusters using algorithms (e.g. union find)
 · Change spins on the same clusters simultaneously
      with probability 1/2 (using random number)

        (Under a finite magnetic field, we need to modify the probability.)
Calculate O($\Gamma_t$)

# Merits of cluster update

1. For low temperature phase, the system easily moves to other minima.

   - Minima are related to the symmetry of the Hamiltonian.

2. For critical phenomena, the dynamical critical exponent becomes much smaller.

   - Swendsen-Wang : $z \simeq 0$    $\tau \propto |T - T_c|^{-z\nu}$

3. Graph representation is closely related to physics

   - e.g. Magnetic susceptibility in SW: $\chi = \dfrac{\beta}{N} \left\langle \sum_C \left( \sum_{i \in C} S_i \right)^2 \right\rangle$

   - By using observable based on graph, statistical error is largely reduced: "Improved estimator"
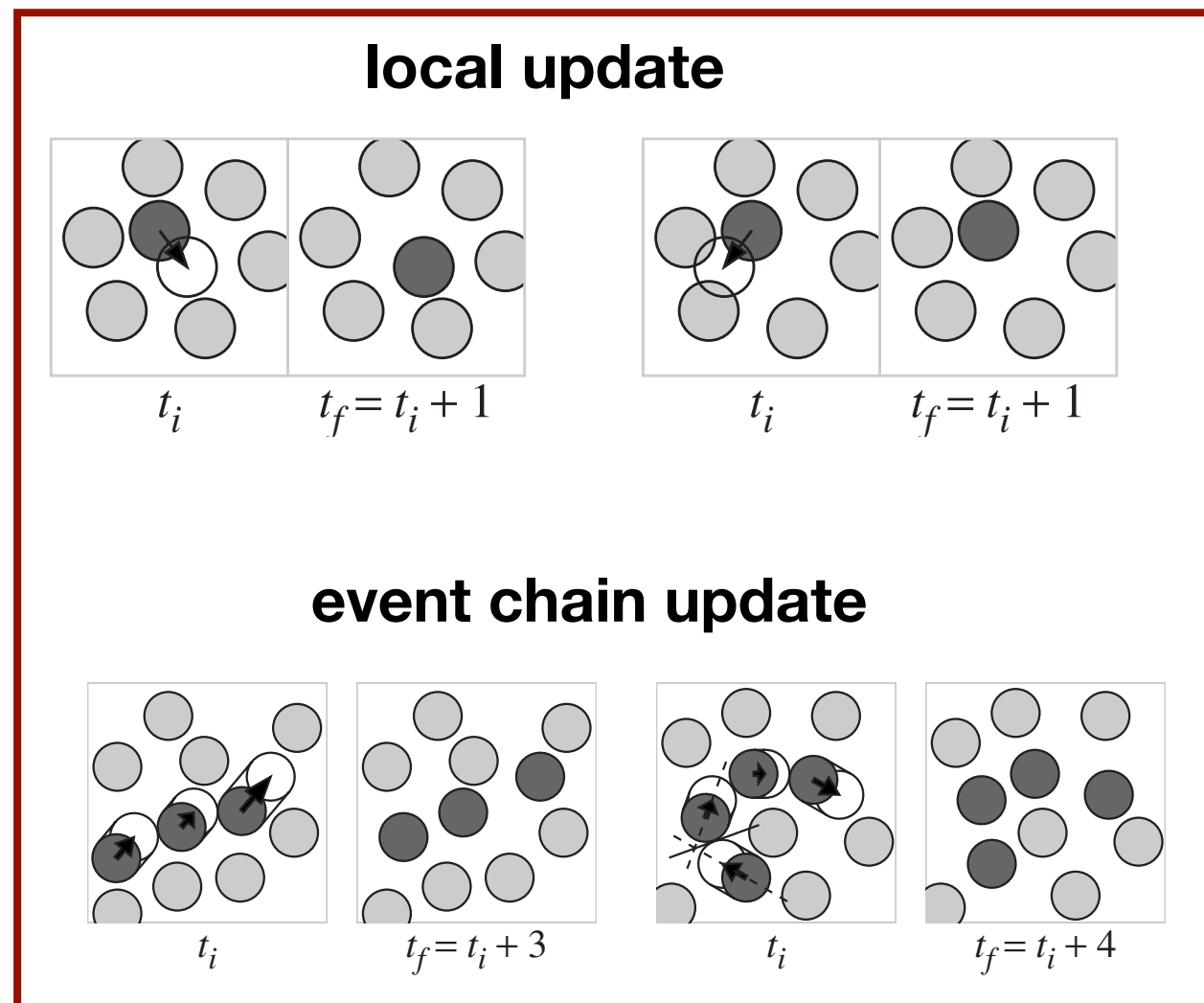
**Free energy landscape**



$F(M)$

$M$

direct change
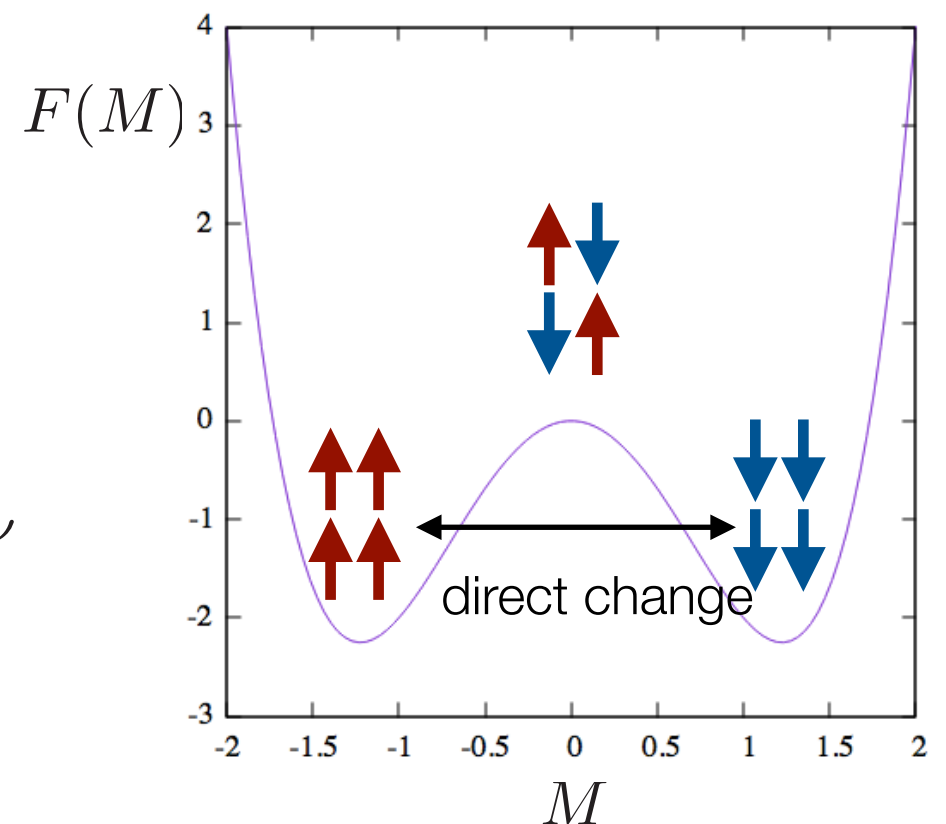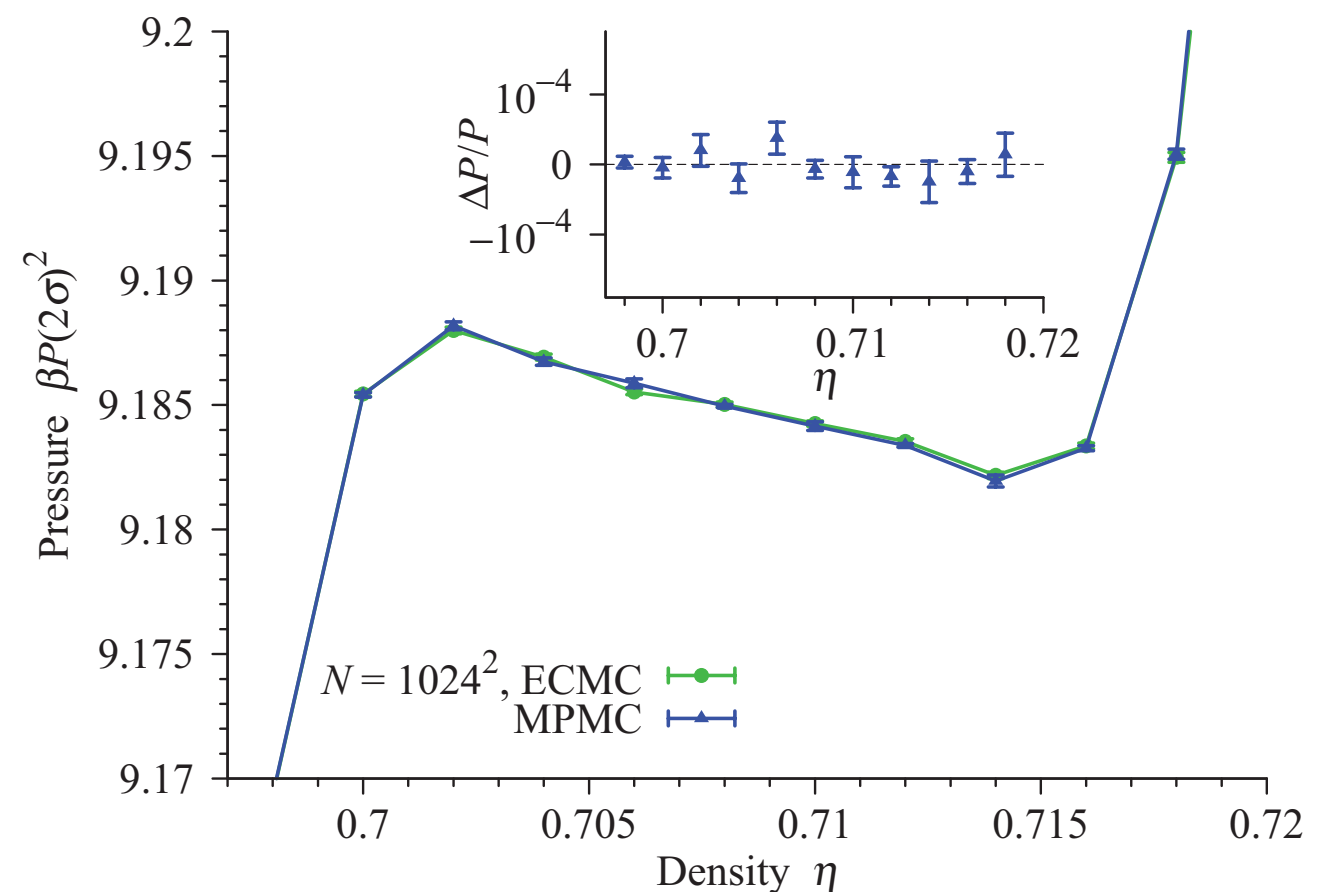
\*Linear size of cluster ~ $\xi$

# Event-chain Monte Carlo

A "global" update for particle system (hard spheres)

E. P. Bernard, W. Krauth, and D. B. Wilson, Phys. Rev. E **80**, 056704 (2009)



**local update**

$t_i$      $t_f = t_i + 1$      $t_i$      $t_f = t_i + 1$

**event chain update**

$t_i$      $t_f = t_i + 3$      $t_i$      $t_f = t_i + 4$

**Application to 2d melting**

M. Engel *et al*, Phys. Rev. E **87**, 042134 (2013)



$N = 1024^2$, ECMC
MPMC

Pressure $\beta P(2\sigma)^2$

Density $\eta$

*Application of the event-chain MC to classical spin systems:

M. Michel, J. Mayer, and W. Krauth, Euro Phys. Lett. **112**, 20003 (2015).

Y. Nishikawa, M. Michel, W. Krauth, and K. Hukushima, Phys. Rev. E **92**, 063306 (2015).

# Next week (5/2)