Computational Science for many-body problems

- This class is from 15:10 to 16:40 (90 min.)

- The recordings of the previous lectures have been uploaded on ITC-LMS.

- Lecture slides are also available on ITC-LMS and github: https://github.com/compsci-alliance/many-body-problems

古典モンテカルロ法の基礎

Classical Monte Carlo method

理学系研究科　大久保毅

Graduate school of science, **Tsuyoshi Okubo**

Next (5/10)

Classical

1st: Many-body problems in physics and why they are hard to solve

2nd: Classical statistical models and numerical simulation

3rd: Classical Monte Carlo method

4th: Applications of classical Monte Carlo method

5th: Molecular dynamics simulation and its applications

6th: Extended ensemble method for Monte Carlo methods

Quantum

7th: Quantum lattice models and numerical simulation

8th: Quantum Monte Carlo methods

9th: Applications of quantum Monte Carlo methods

10th: Linear algebra of large and sparse matrices for quantum many-body problems

11th: Krylov subspace methods and their applications to quantum many-body problems

12th: Large sparse matrices, and quantum statistical mechanics

13th: Parallelization for many-body problems

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

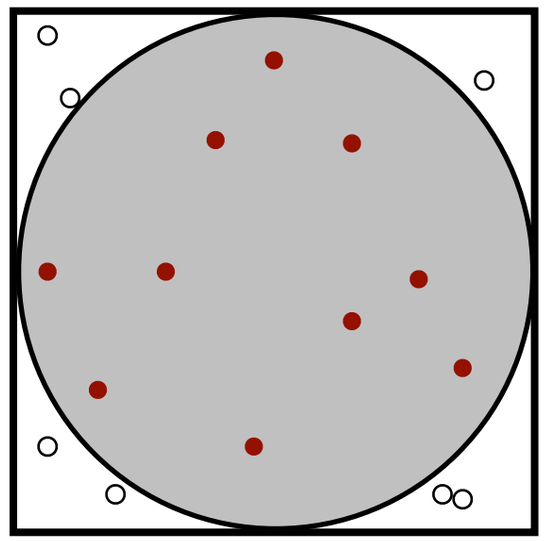
Standard Monte Carlo method

Monte Carlo method: Randomized algorithm

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

Example :

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



Algorithm (rejection sampling)

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

loop i

$x_i \in [-1,1]$

$y_i \in [-1,1]$ take uniform 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 $\frac{1}{\sqrt{N_s}}$

Monte Carlo Integration: General aspect

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

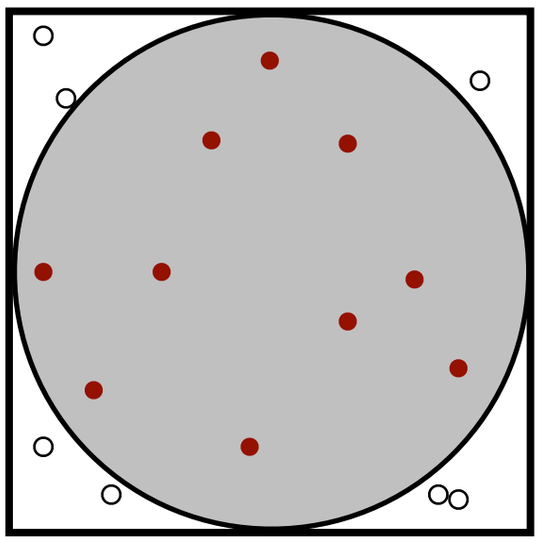
Estimate an integral as an expectation value under $P(\Gamma)$

Previous example:

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

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

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



Monte Carlo Integration: General aspect

Merit of Monte Carlo Integration

The error is (usually) independent on the dimension of Γ.

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

N_s : sampling number

σ_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 increase the dimension of Γ.

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

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

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)

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

Asymptotic form of *Γ*-function

$$\Gamma(x) \sim \left(\frac{x}{e}\right)^x$$

For larger *d*, the ratio exponentially decreases!

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

→ (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 $|f(\Gamma)|$ takes large value!
(eg. points within the sphere)

→ **Importance sampling**

Importance sampling and Markov Chain Monte Carlo

Sampling with uniform distribution

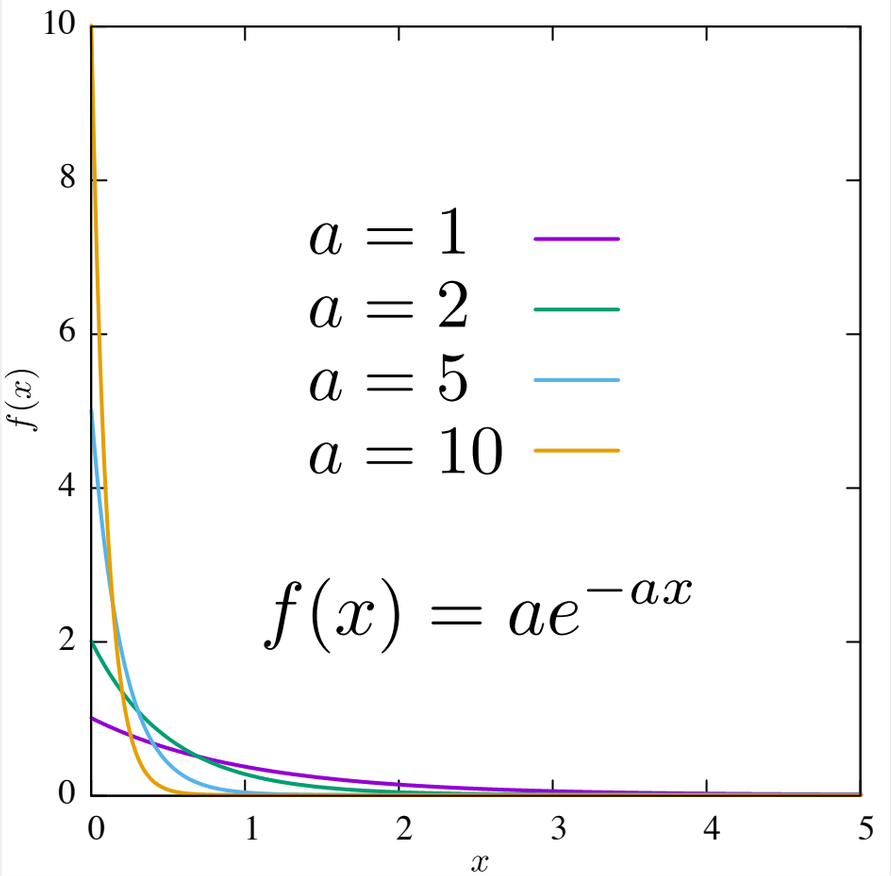
$$\int d\Gamma f(\Gamma) = \int d\Gamma \frac{f(\Gamma)}{P(\Gamma)} P(\Gamma) \quad \text{with } P(\Gamma) = \text{const.}$$

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

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

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

The error increases as the parameter a increases.



This situation typically occurs in a sampling for statistical mechanics.

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

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

Equilibrium distribution, e.g.,

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

$$\mathcal{H}(\Gamma) = O(N)$$

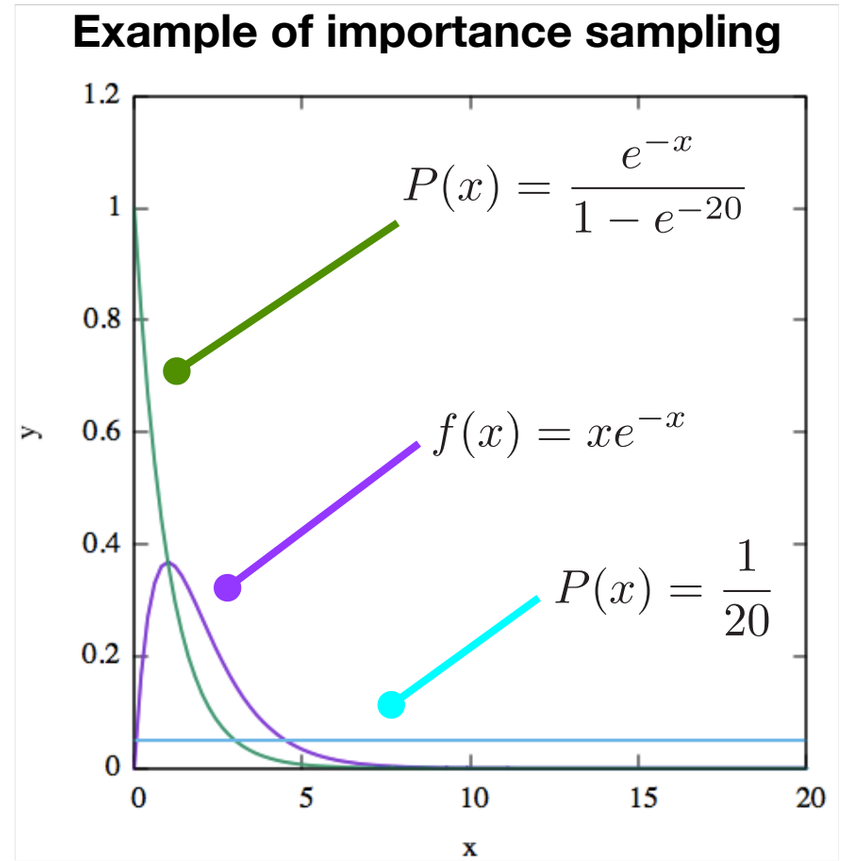
N: number of particles or spins

Importance Sampling

Importance sampling

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

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

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

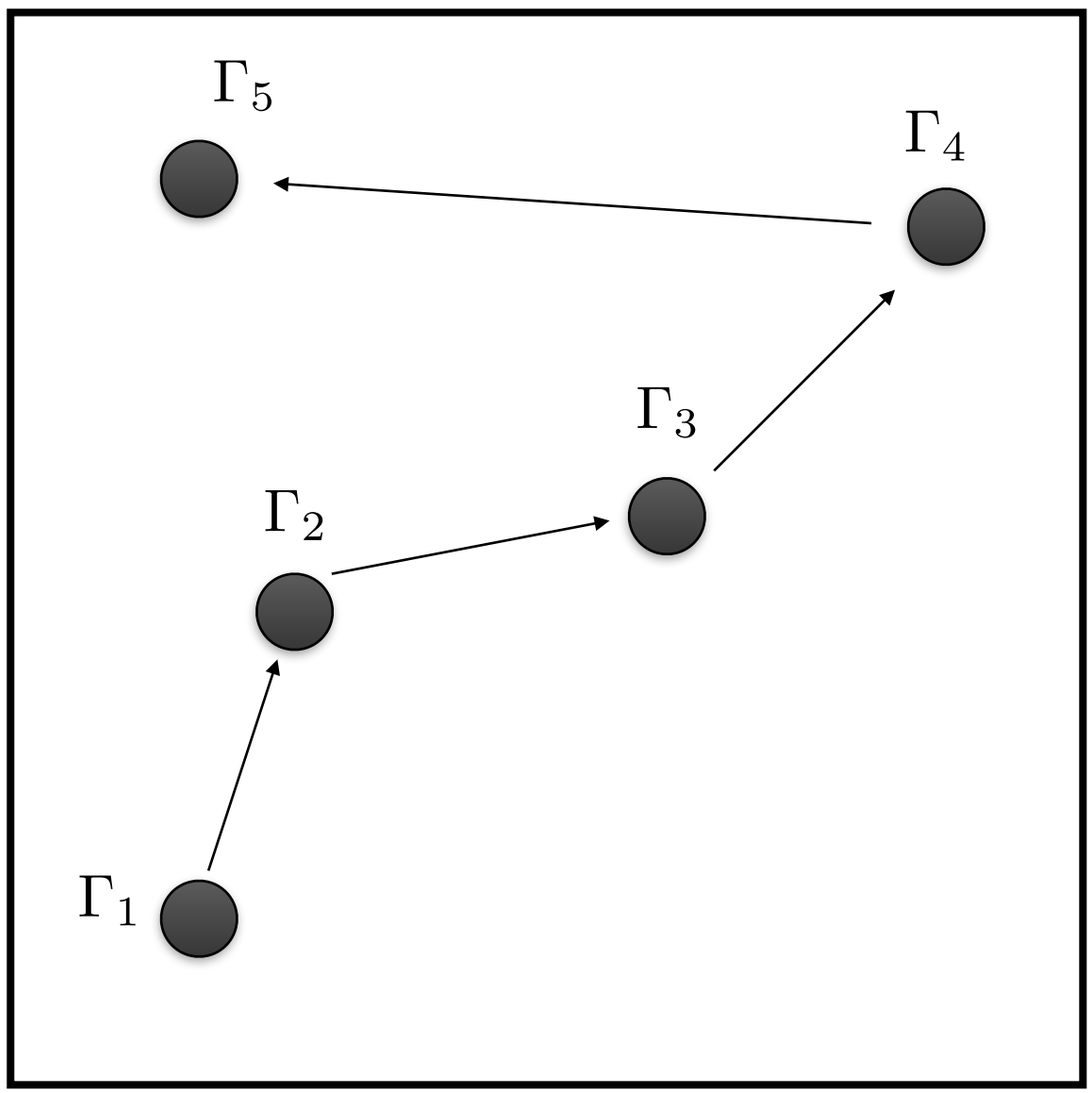
- We do not know the normalization constant
- It is too complex

How can we perform the importance sampling?

Markov Chain Monte Carlo (MCMC)

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

A sampling point move in Γ "randomly".



Markov process:

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

The **transition probability** to Γ_{t+1} depends on Γ_t.

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

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

Typical procedure in MCMC

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

loop t

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

Sequence of the realizations:

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

✶ 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.

✶ Γ_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 Γ at time t

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

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

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

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

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 Γ and Γ' 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 $P(\Gamma)$.

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

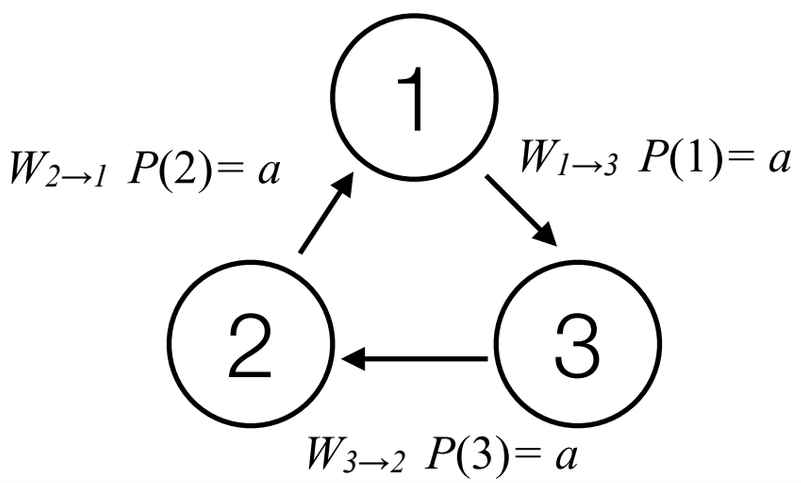
Special case:

Detailed balance condition

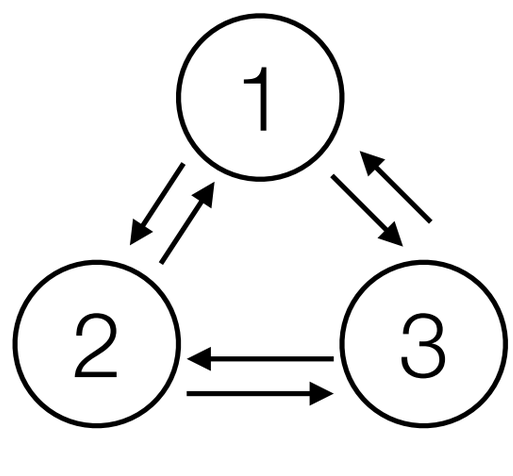
$$W_{\Gamma\to\Gamma'} P(\Gamma) = W_{\Gamma'\to\Gamma} P(\Gamma')$$

No microscopic flow
in the steady state

Balance condition with flow



Detailed balance condition



Examples of MCMC

Example: Metropolis-Heisting sampling

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

loop t

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

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

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

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

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

In this case, we may calculate "conditional" probability distribution of Γ^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:

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

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

We generate the next Γ' directly from the conditional probability!

- The transition probability is independent on the present Γ^1.
- In general, it is not easy to produce the conditional probability distribution from uniform random numbers.

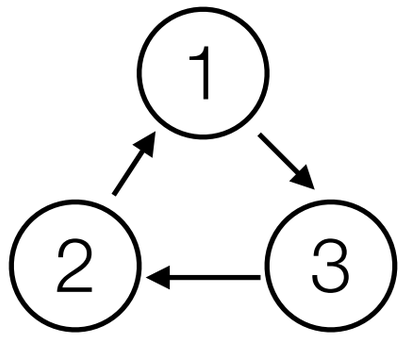
Sampling based on the balance condition

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).

Application to replica exchange Monte Carlo for molecular dynamics simulation

S. G. Itoh and H. Okumura, J. Chem. Theory Comput. **9**, 570 (2013).

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 $P(\Gamma) = \frac{1}{Z} e^{-\beta \mathcal{H}(\Gamma)}$

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

Γ_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: $\hat{M}_z^2(\Gamma) = \left(\frac{1}{N} \sum_i S_i^z \right)^2$

Local update

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

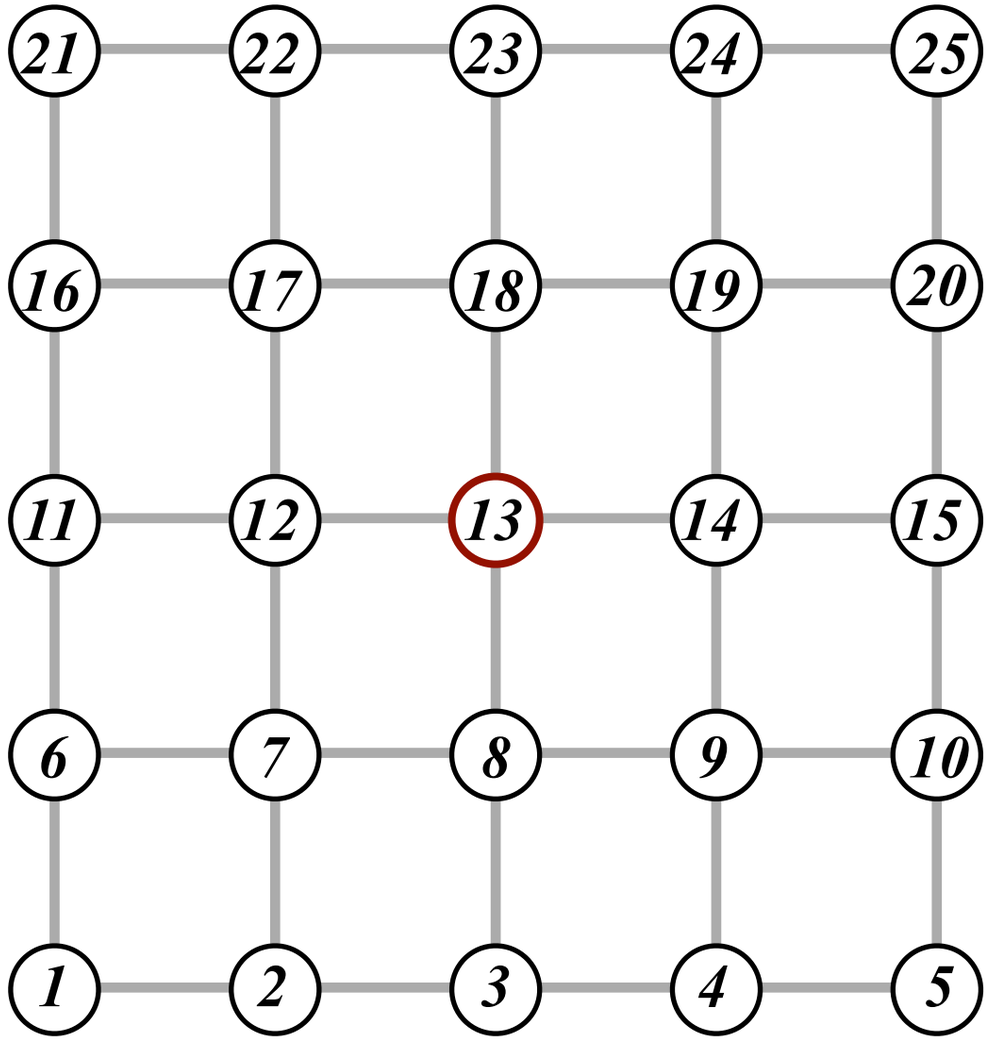
$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

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

From Γ to Γ', we fix $S_1, S_2, .. S_{12}, S_{14}, S_{15}, \ldots, S_{25}$, 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:

*Proposal probability satisfies

$$q(\Gamma|\Gamma') = q(\Gamma'|\Gamma).$$

eg. $S_i' = -S_i$ for Ising spin.

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

$$\frac{P(\Gamma')}{P(\Gamma)} = e^{-\beta[\mathcal{H}(\Gamma')-\mathcal{H}(\Gamma)]} = e^{-\beta\Delta E}$$

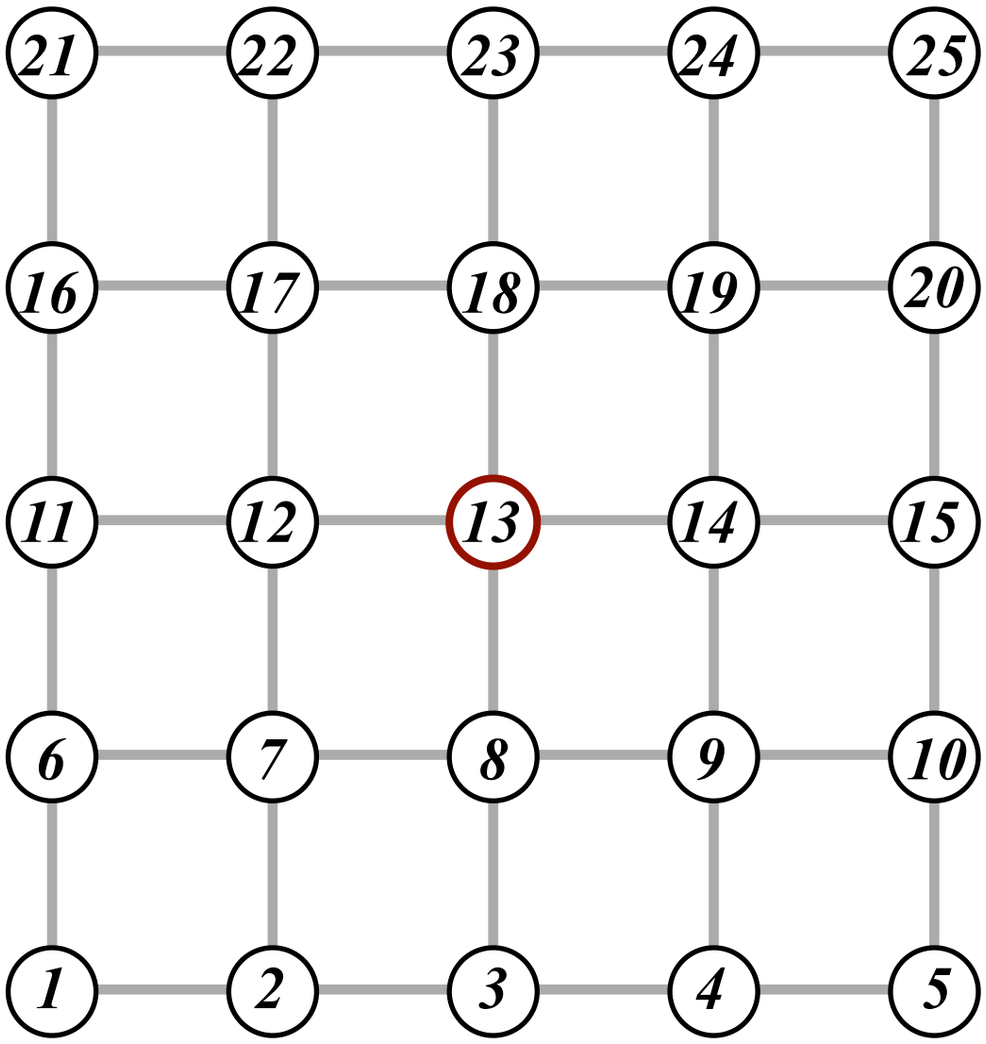
* We don't need partition function Z!

For local update on the square lattice,

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

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

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



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 Γ' 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 Γ_{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 ($\Delta E < 0$), 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:

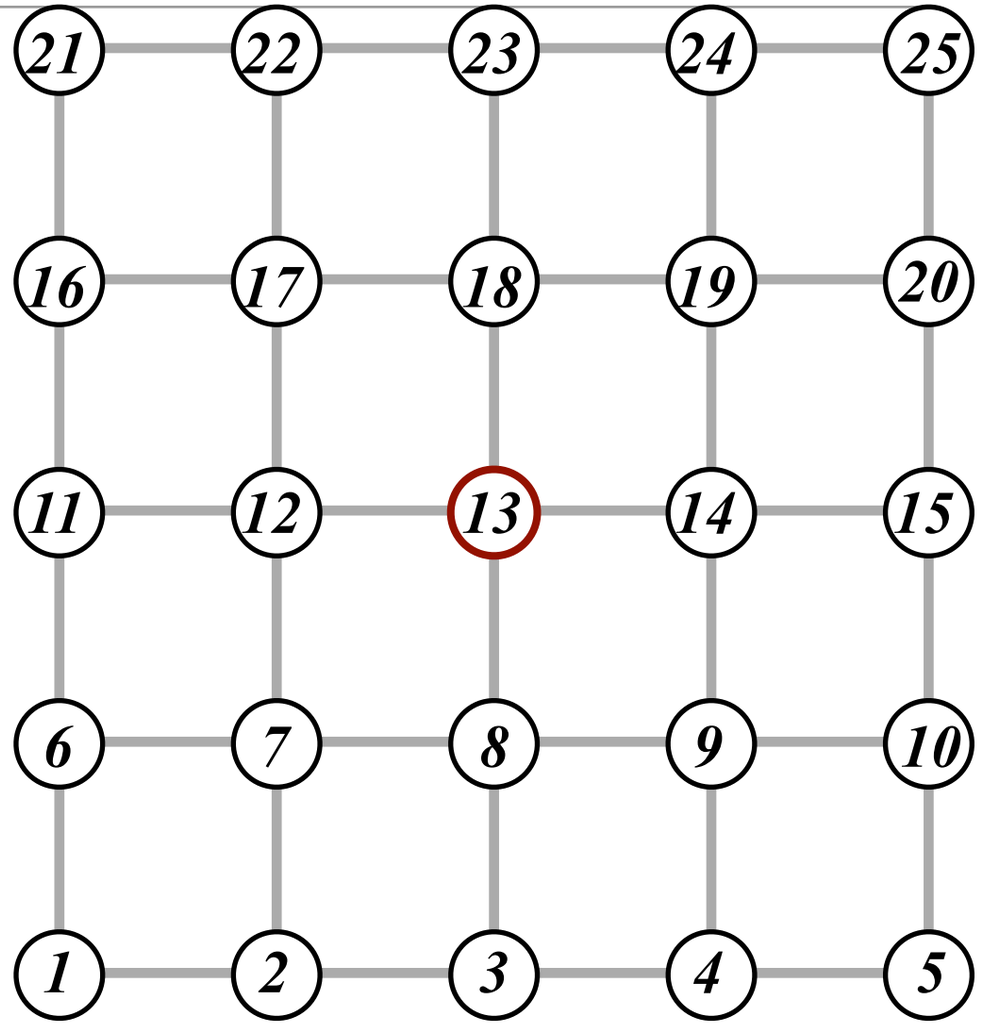
$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

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

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

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

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



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

Ising: $W_{\Gamma\to\Gamma'} = \dfrac{e^{\beta h_{\rm eff} S'_{13}}}{e^{\beta h_{\rm eff} S'_{13}} + e^{-\beta h_{\rm eff} S'_{13}}}$

Scaler value

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

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

Three component vector

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

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_{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 Γ_{t+1} is Γ'

Calculate O(Γ_t)

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

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

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

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

Heisenberg:
(in polar co-ordinate with z // h_{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

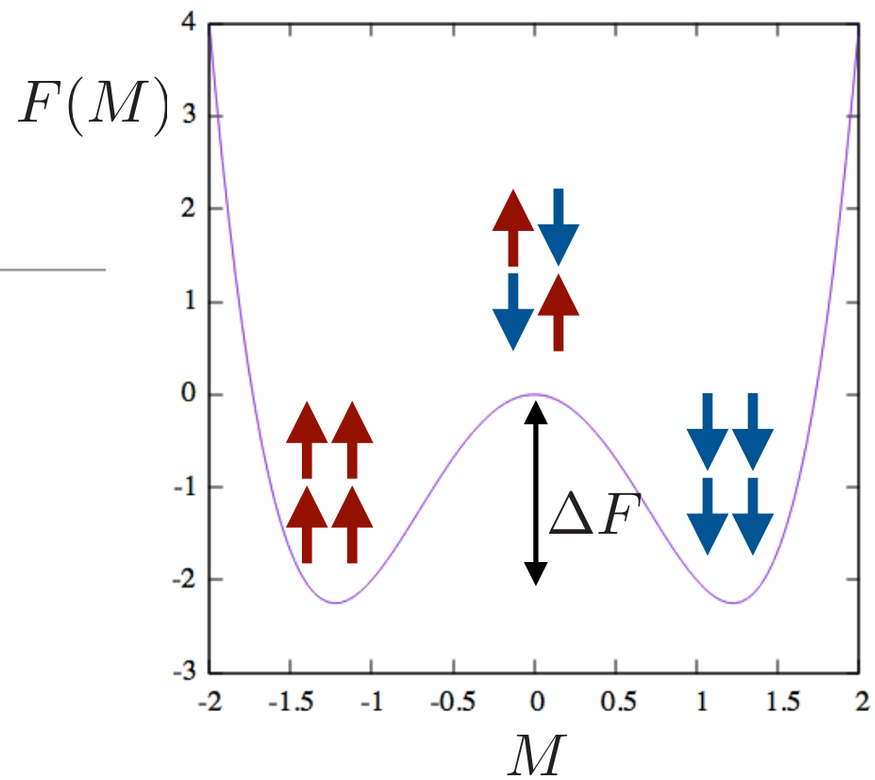
$$\phi = 2\pi r_1$$
$$\cos\theta = -1 + \frac{1}{\beta|h_{\text{eff}}|} \times \ln[r_2 + (1 - r_2)e^{2\beta|h_{\text{eff}}|}]$$

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: $\tau \propto \exp\left[\frac{\Delta F}{T}\right]$

Free energy landscape



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

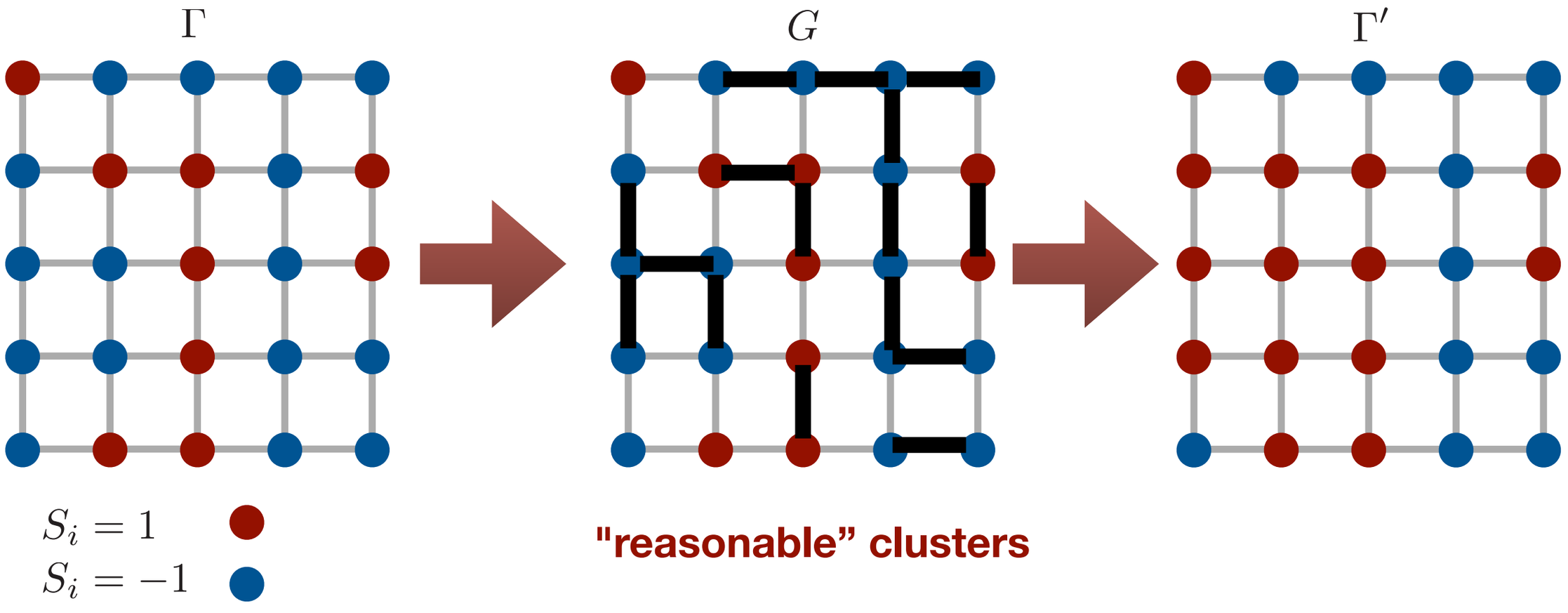
Simultaneous change of spins in "large cluster"

Cluster update

Cluster update method

Idea of cluster updates

- From a spin configuration Γ, we can define "reasonable" clusters G.
- When we "flip" all spins on a cluster G and make new configuration Γ', the free energy difference between Γ and Γ' is not so large.
- We can change the configuration drastically with higher probability.



How to make a cluster configuration?

Fortuin-Kasteleyn mapping (for Ising model)

Ising model

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

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

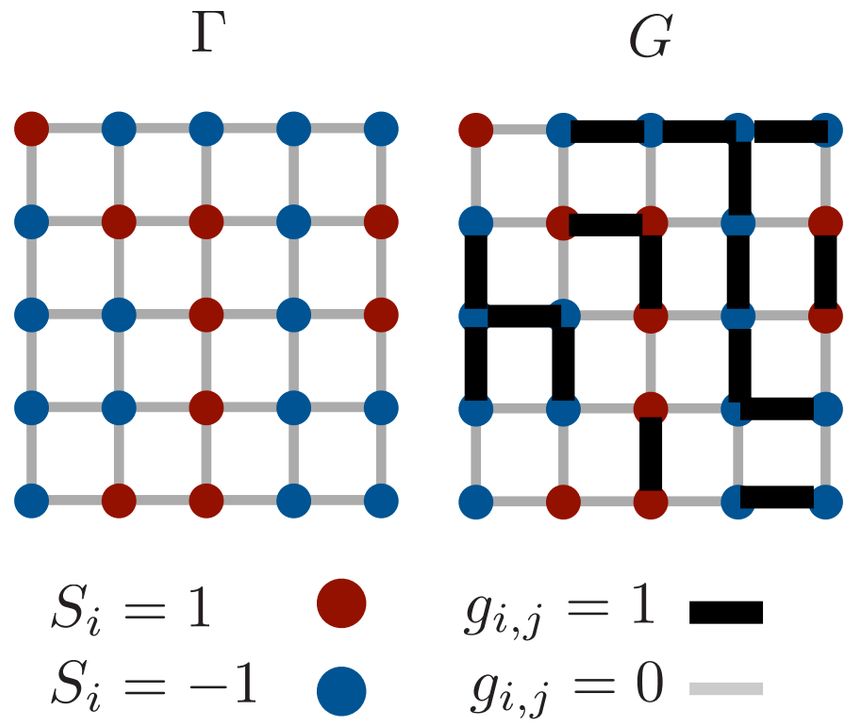
C. M. Fortuin and P. W. Kasteleyn, Physica **57**, 536 (1972).

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

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

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

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



Markov chain in extended $(\mathbf{G}, \mathbf{\Gamma})$ space

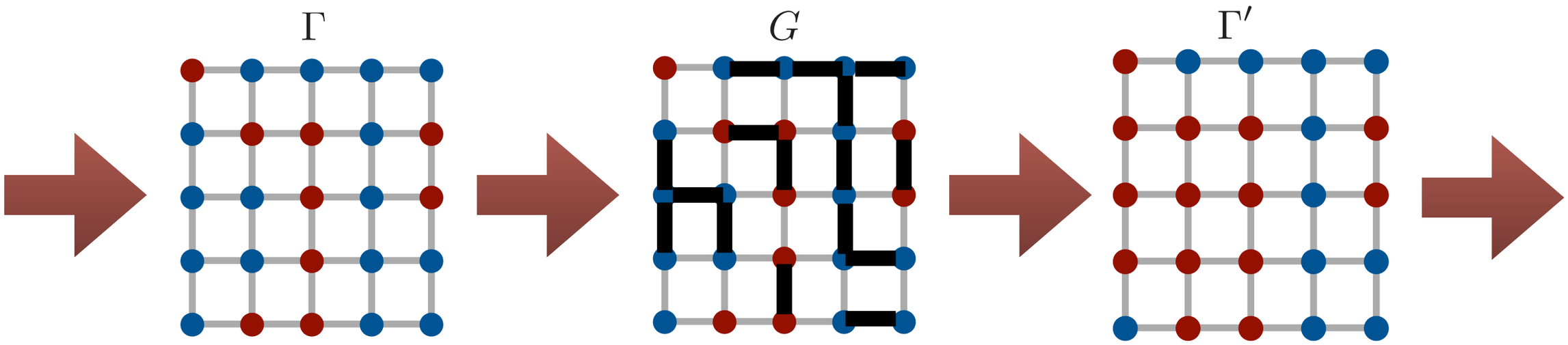
$$Z = \sum_{G} \sum_{\Gamma} \prod_{\langle i,j \rangle} w(g_{i,j}, S_i, S_j) = \sum_{G} \sum_{\Gamma} W(G, \Gamma)$$

We consider to update Γ and G alternatively:

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

This update can be symbolically written as

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



Markov chain in extended (G, Γ) space

We assign the transition probabilities as follows:

$$w_{(S_i,S_j)\to 0} = \begin{cases} 1 & (S_i \neq S_j) \\ e^{-2\beta J} & (S_i = S_j) \end{cases}$$

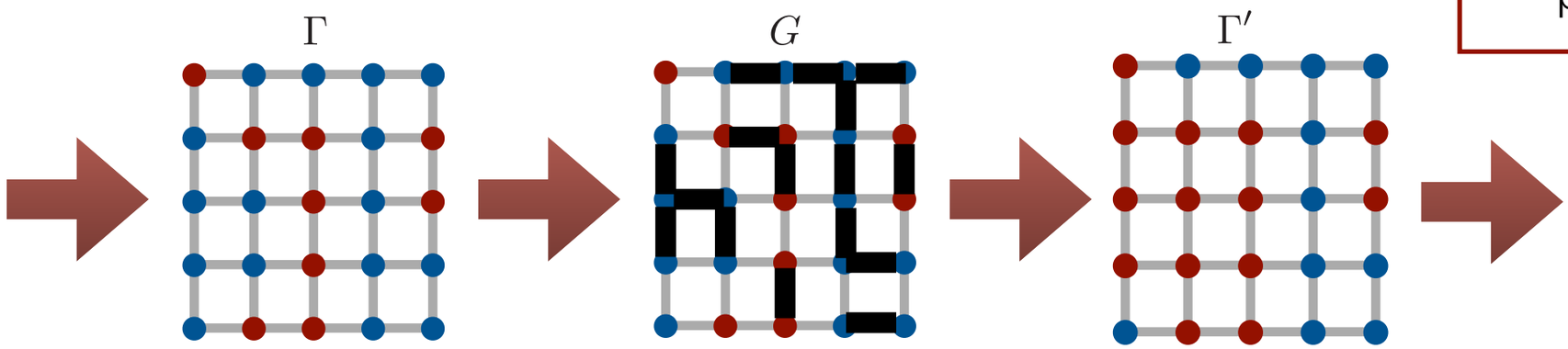
Transition probabilities (as like the heat bath)

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

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

cluster formed from g=1 links

$P(\{S_i \in C_j\}) = 1$
(If all spin in cluster is pointing same direction)



Swendsen-Wang algorithm

Swendsen-Wang algorithm

R. H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58**, 86 (1987)

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>

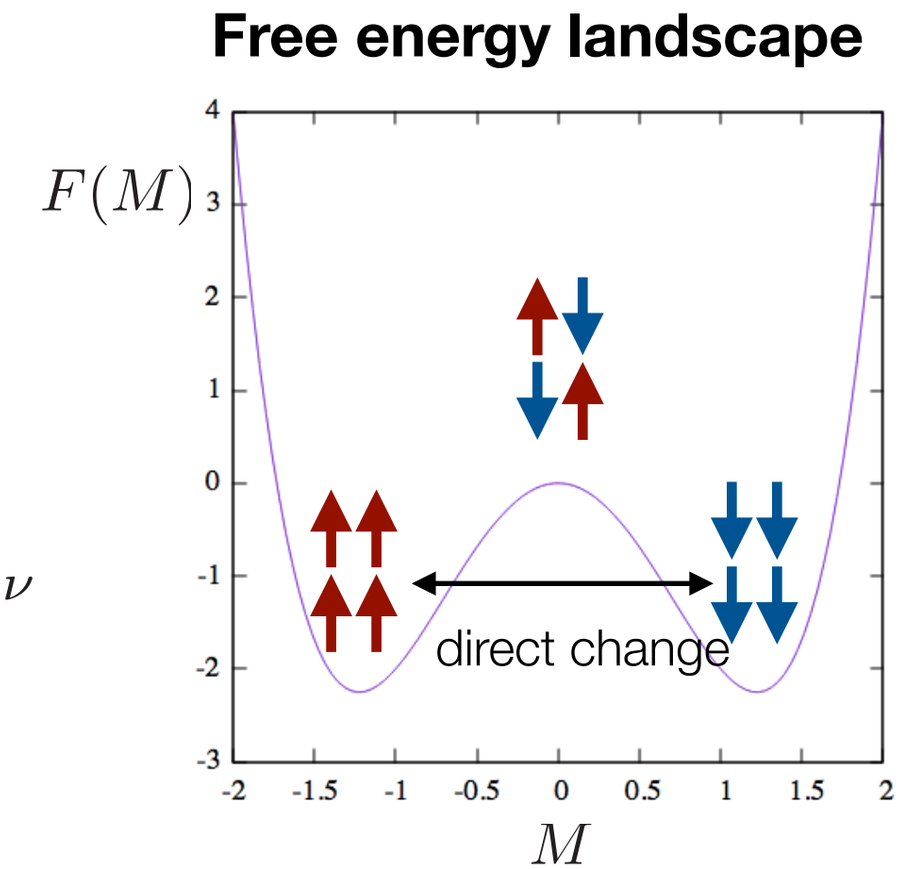
- Make clusters using algorithms (e.g. union find)
- Change spins on the same clusters simultaneously with probability 1/2 (using random number)

(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 : $z \simeq 0 \quad \tau \propto |T - T_c|^{-z\nu}$
3. Graph representation is closely related to physics
   - e.g. Magnetic susceptibility in SW: $\chi = \frac{\beta}{N} \left\langle \sum_C \left(\sum_{i \in C} S_i \right)^2 \right\rangle$
   - By using observable based on graph, statistical error is largely reduced: "Improved estimator"



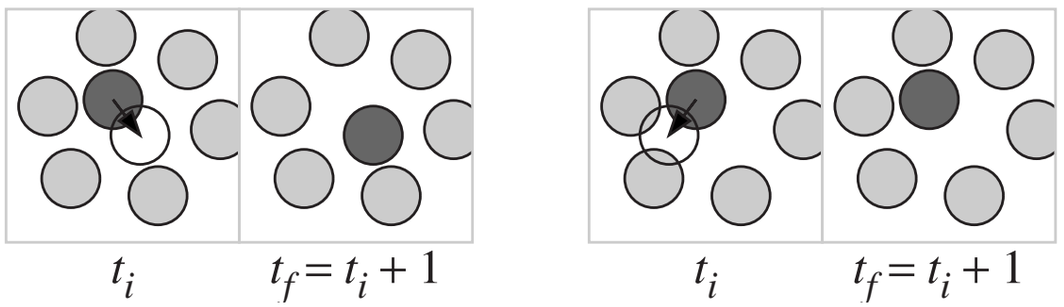
*Linear size of cluster ~ ξ

Event-chain Monte Carlo

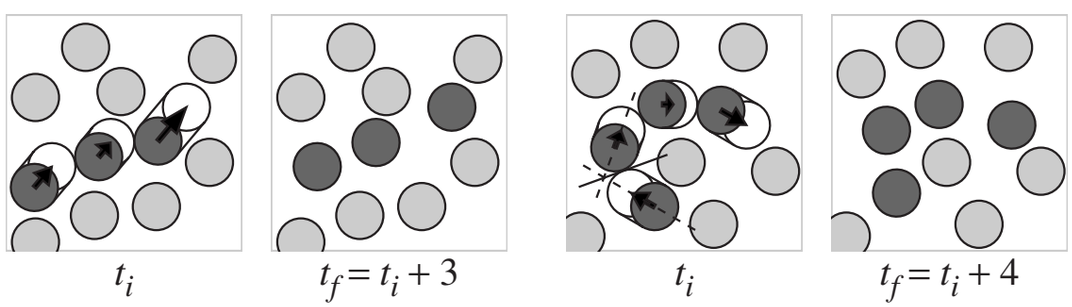
A "global" update for particle system (hard spheres)

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

local update

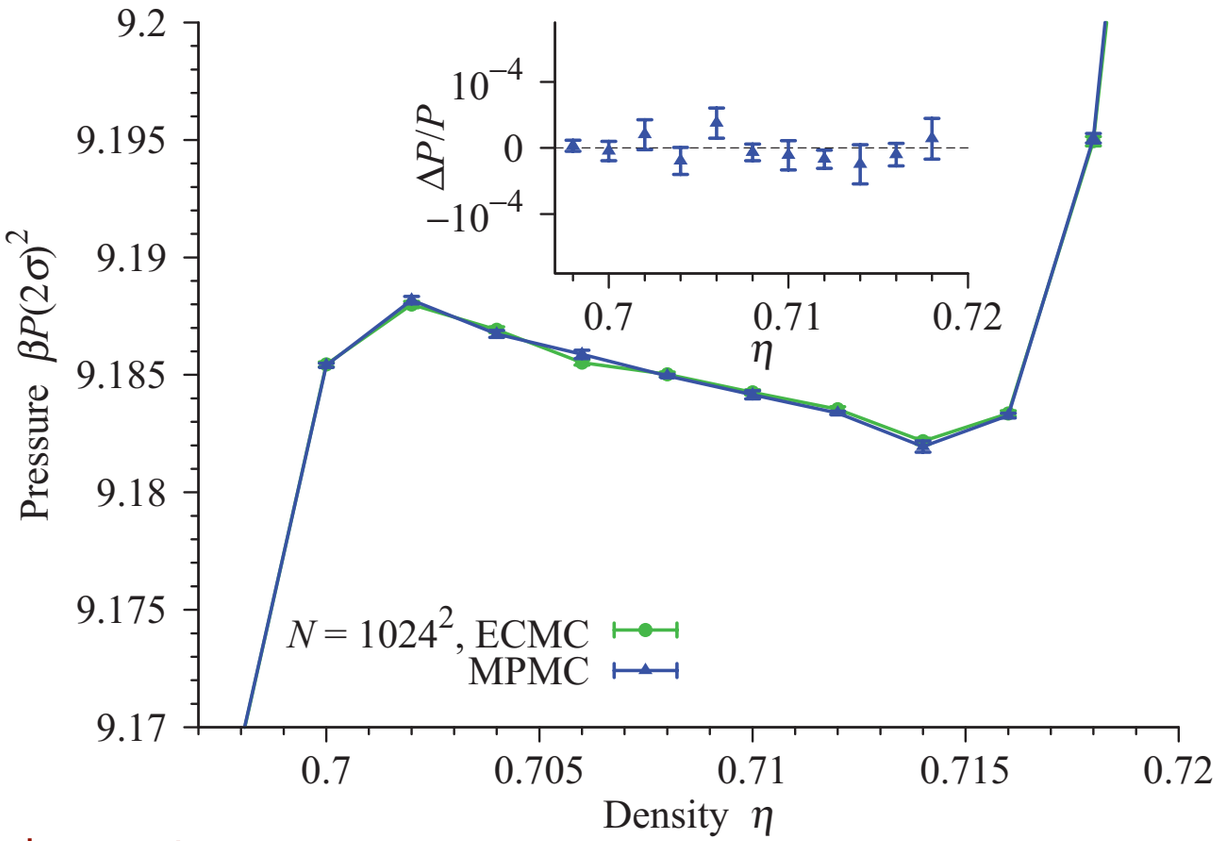


event chain update



Application to 2d melting

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



*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 (5/10)

Classical

1st: Many-body problems in physics and why they are hard to solve

2nd: Classical statistical models and numerical simulation

3rd: Classical Monte Carlo method

4th: Applications of classical Monte Carlo method

5th: Molecular dynamics simulation and its applications

6th: Extended ensemble method for Monte Carlo methods

Quantum

7th: Quantum lattice models and numerical simulation

8th: Quantum Monte Carlo methods

9th: Applications of quantum Monte Carlo methods

10th: Linear algebra of large and sparse matrices for quantum many-body problems

11th: Krylov subspace methods and their applications to quantum many-body problems

12th: Large sparse matrices, and quantum statistical mechanics

13th: Parallelization for many-body problems