拡張アンサンブル法によるモンテカルロ計算

Extended Ensemble method for Monte Carlo Methods

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Contents

Back ground

Extended ensemble = general ensemble

In conventional MC or MD simulation:

We try to estimate expectation values under "physically relevant" ensembles.

NVE, NVT, NPT, …

Even if an ensemble is not directly connected to any physical systems, we can use is to enhance the efficiency of numerical calculation (MC, MD) for interested physical system.

Large relaxation time in standard MC and MD

- Critical phenomena
  - $\tau \sim L^z$ with standard algorithm (critical slowing down)
  - z can be significantly reduced by using "global update"
- First order phase transition,Glass transition (structural glass, spin glass), protein folding,
  - $\tau \sim \exp(\Delta E/T)$ or $\exp(\Delta \mathrm{E}/|T\text{-}T_c|)$; Note $\Delta E \propto L^d$!
  - exponential can be reduce to polynomial by using extended ensemble methods

Origin of exponentially long relaxation time

Partition function of the canonical ensemble

$$Z = \int d\Gamma e^{-\beta \mathcal{H}(\Gamma)} = \int dE \underbrace{\rho(E)}_{\text{Density of state}} e^{-\beta E} = \int dE e^{-\underbrace{\beta F(E)}_{\text{“Free energy”}}}$$

Density of state

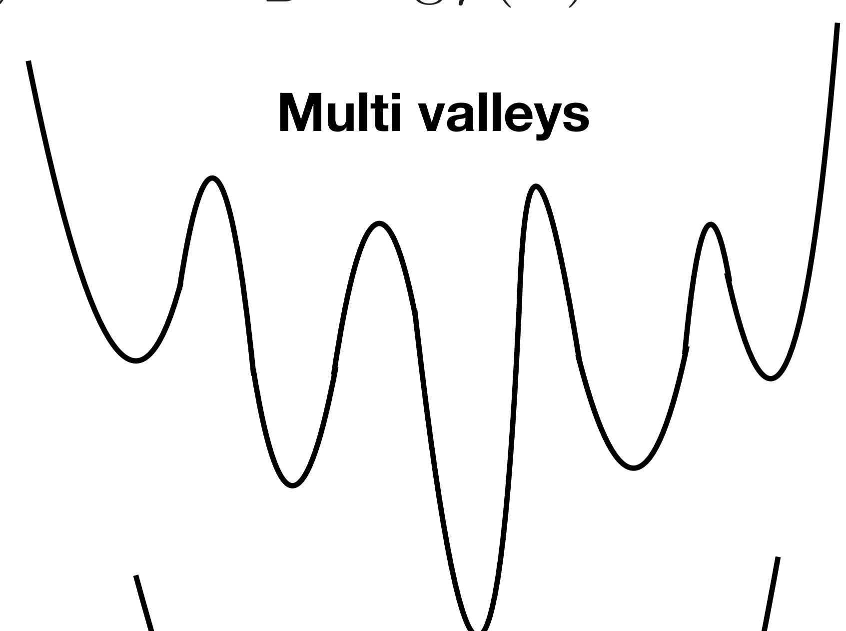
“Free energy”

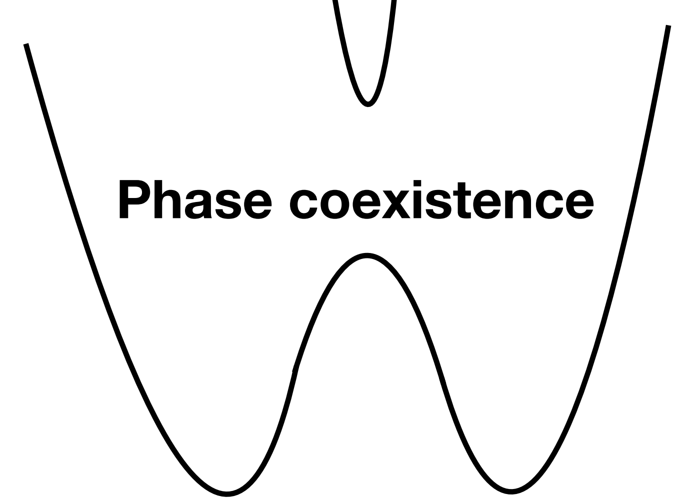
$$F(E) \equiv E - k_B T \log \rho(E)$$

Probability distribution for energy

$$P(E) = \frac{1}{Z} e^{-\beta F(E)}$$

Note! Free energy is extensive: $F(E) \propto N$





- “Transition probability” is proportional to the exponential of Free-energy difference: exp(-ΔF/T)
- Usual algorithm of MC (and MD) changes the state (or the energy) gradually.

If there are local minima, the relaxation time could be exponentially large as the size is increased.

Density of state and standard histogram method

Density of state

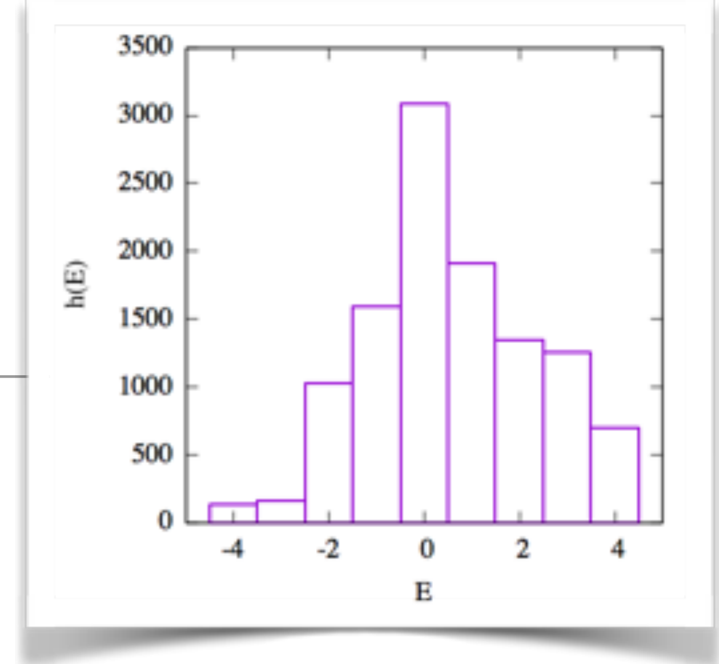
$$Z = \int d\Gamma e^{-\beta \mathcal{H}(\Gamma)} = \int dE \rho(E) e^{-\beta E}$$
$$= \int dE \int dM \rho(E, M) e^{-\beta E}$$

$\int d\Gamma$	~O(N)-dimensional integral
$\int dE$	~1-dimensional
$\int dE \int dM$	~2-dimensional

- If we know the exact $\rho(E)$(or $\rho(E, M)$), the calculation of partition function reduced to 1 or (a few) -dimensional integral.
- Even if we only know an approximate density of state,
$$\tilde{\rho}(E) \simeq \rho(E)$$
we can improve the sampling efficiency by using its information

- Histogram method
- Multi canonical method
- Wang-Landau method

Energy Histogram



Energy histogram:

In MC or MD calculations

$h(E_i)$:# or samples (snap shots) with energy in

$$E_i - \Delta E/2 \leq E < E_i + \Delta E/2$$

$$P(E)\Delta E \simeq \frac{1}{N_h} h(E)$$

Total # of samples

$$N_h \equiv \sum_i h(E_i)$$

For *e.g.* NVT ensemble

$$P(E) = \frac{1}{Z(\beta)} \rho(E) e^{-\beta E} \quad \Rightarrow \quad \rho(E) \simeq \frac{Z(\beta)}{N_h \Delta E} h(E) e^{\beta E}$$

We can calculate (approximate) density of state from usual MC or MD simulations!

Histogram method (reweighting method)

Energy expectation value of different temperature

$$\boxed{\langle E\rangle_{\beta'} = \frac{\displaystyle\int dE\rho(E)Ee^{-\beta' E}}{\displaystyle\int dE\rho(E)e^{-\beta' E}} \simeq \frac{\displaystyle\sum_i E_i h(E_i)e^{-(\beta'-\beta)E_i}}{\displaystyle\sum_i h(E_i)e^{-(\beta'-\beta)E_i}}}$$

Any expectation values can also be calculated by the histogram method

$$\rho(E) \simeq \frac{Z(\beta)}{N_h \Delta E} h(E) e^{\beta E}$$

$$\boxed{\langle O\rangle_{\beta'} \simeq \frac{\displaystyle\sum_i O(E_i)h(E_i)e^{-(\beta'-\beta)E_i}}{\displaystyle\sum_i h(E_i)e^{-(\beta'-\beta)E_i}}}$$

Average at energy E_i

$$O(E_i) \equiv \sum_{E(\Gamma_j)\in E_i} O(\Gamma_j)$$

Limitation of histogram method

Reweighted histogram becomes
less accurate
when T’ is far from the original T.

“Tail” of the original histogram has only small # of snapshots→large noise

Central limit theorem

Width of energy distribution: $\propto \sqrt{N}$

Average of energy: $\propto N$

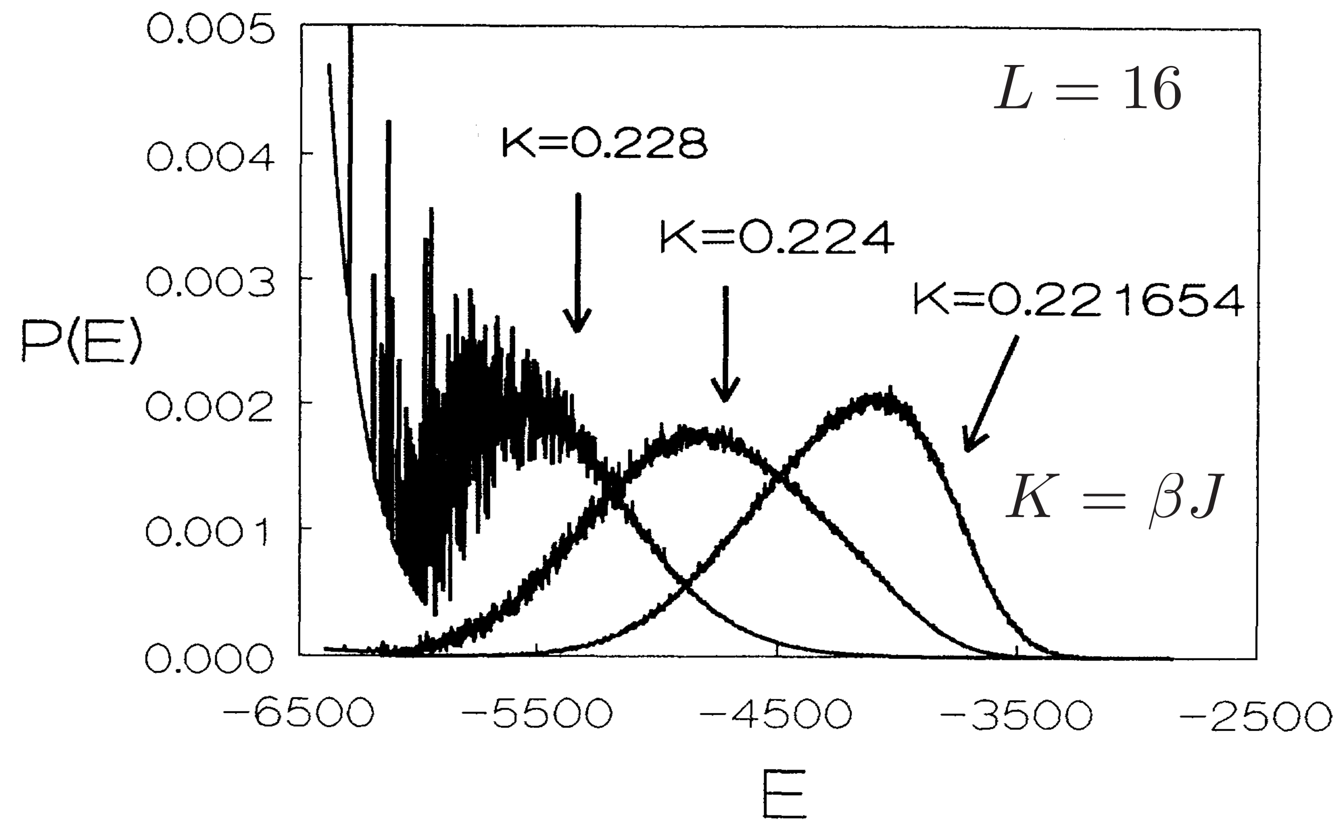
Distribution becomes narrower as N is increased!

Reliable temperature region for reweighting:

$$\Delta T \propto \frac{1}{\sqrt{N}}$$

Energy distribution of 3d-Ising model

A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991)



MC simulation at K=0.221654

Reweighting to K=0.224 and K=0.228

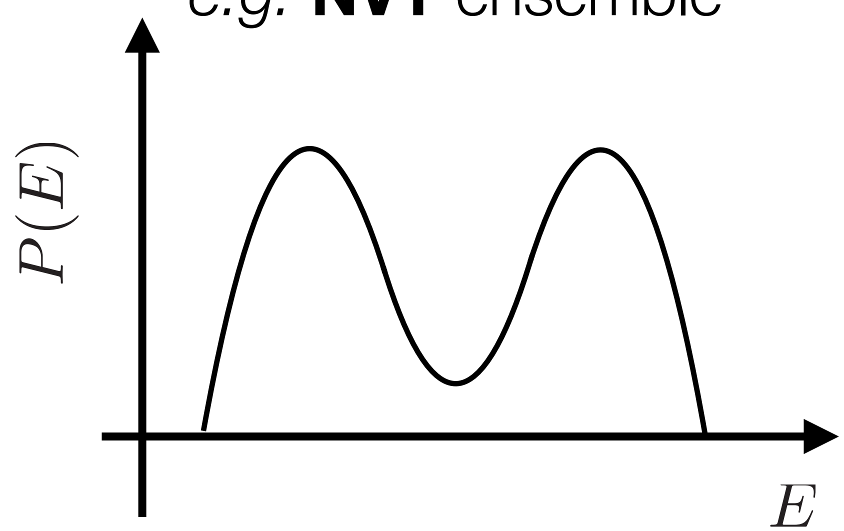
Multi Canonical methods

Idea of Multi-Canonical method

B.A. Berg and T. Neuhaus (1992)

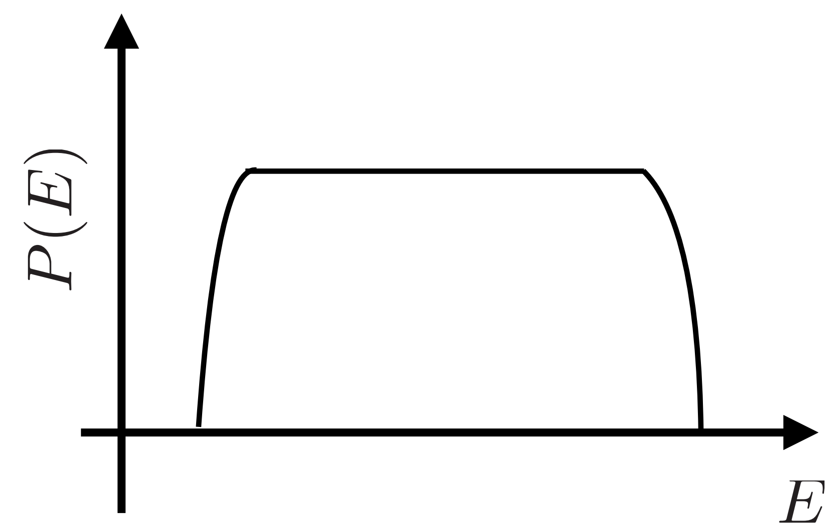
If we can prepare a special ensemble
where the energy distribution is “flat”,
we can efficiently sample all relevant states.

e.g. **NVT** ensemble



$$P(E) \propto \rho(E) e^{-\beta E}$$

“special” ensemble



$$\tilde{P}(E) \propto \rho(E) e^{-S(E)} = \text{const.}$$

Special ensemble is log of DOS!

$$S(E) = \log \rho(E)$$

How to obtain the special ensemble?

Special ensemble is log of DOS!

$$S(E) = \log \rho(E)$$

DOS is unknown!

We can obtain $f(E)$ approximately by iterative calculations.

"Image" of an iterative algorithm

1. Run MC simulation on a temperature and calculate energy histogram

$$\boxed{h(E) \sim \rho(E) e^{-\beta E}}$$

2. Based on the energy histogram, extract approximate $S(E)$

$$\boxed{S^0(E) = \beta E + \log h(E)}$$

3. **Loop** n
   1. Run MC simulation under $S^{(n)}(E)$ and calculate histogram $h^{(n)}(E)$
   2. Calculate next $S^{(n+1)}(E)$ as

$$\boxed{S^{(n+1)}(E) = S^{(n)}(E) + \log h^{(n)}(E)}$$

Detailed algorithm

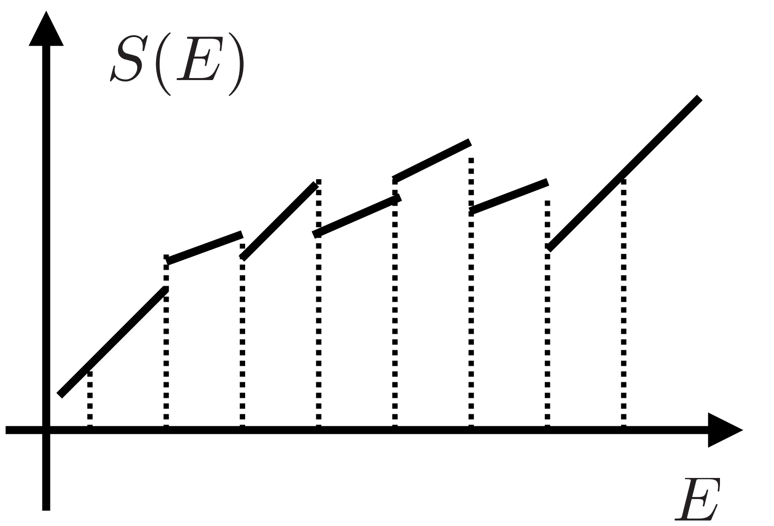
B.A. Berg, Nucl. Phys. B (Proc. Suple.) **63**A-C, 982 (1998)

Suppose $S(E)$ looks like: $S(E) = \beta(E)E - \alpha(E)$

(Energy dependent temperature)

$$S(E) \simeq \beta_i E - \alpha_i$$

for $E_i - \Delta E/2 \leq E \leq E_i + \Delta E/2$



In a specific interval, we want to optimize β and α,
$i.e.$ $P(E)$ becomes flat.

By defining $\beta_i \equiv \dfrac{S(E_{i+1}) - S(E_i)}{\Delta E}$

$$\alpha_{i-1} = \alpha_i + (\beta_{i-1} - \beta_i)E_i$$

We fix $\alpha_{i_{max}} = 0$

Detailed algorithm

B.A. Berg, Nucl. Phys. B (Proc. Suple.) **63**A-C, 982 (1998)

Iteration :how to determine next β and α

In order to make the histogram flat, $\boxed{S^{(n+1)}(E) = S^{(n)}(E) + \log h^{(n)}(E)}$

$$\tilde{\beta}_i^{(n+1)} = \beta_i^{(n)} + \log \frac{h_{i+1}^{(n)}}{h_i^{(n)}}$$

This estimator could be suffered from large statistical error

Gradual change from the previous β

$$\beta_i^{(n+1)} = (1 - c_i)\beta_i^{(n)} + c_i \tilde{\beta}_i^{(n+1)}$$

*For optimal c_i , see the reference

α is calculated from β

$$\alpha_{i-1}^{(n+1)} = \alpha_i^{(n+1)} + (\beta_{i-1}^{(n+1)} - \beta_i^{(n+1)})E_i$$

Example of application

***q*-state Potts model** on the square lattice

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{S_i, S_j} \qquad S_i = 0, 1, 2, \cdots, q-1$$

Phase transition at

$$T_c/J = \frac{1}{\log(1+\sqrt{q})}$$

$q = 2$: Equivalent to Ising model

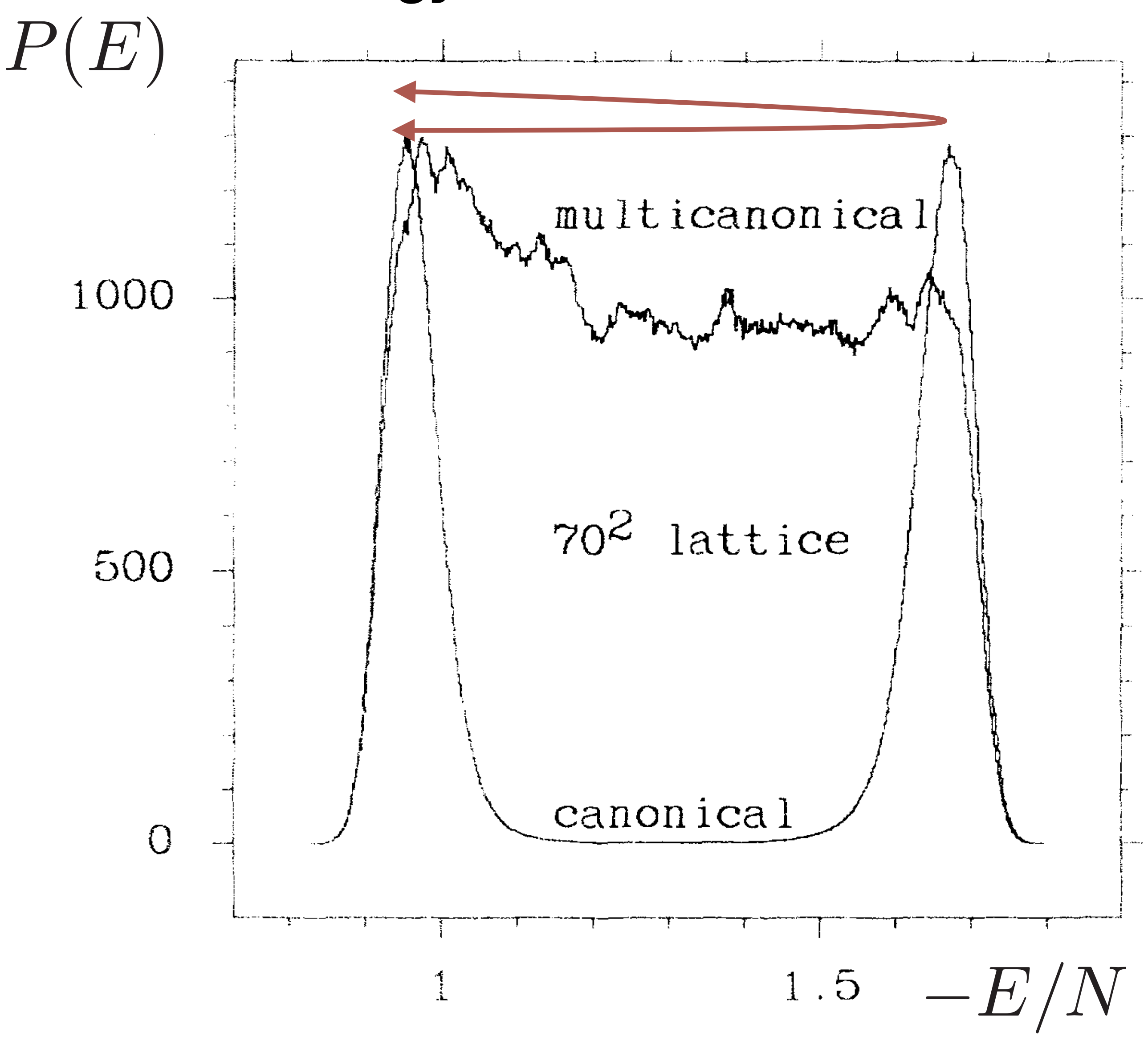
$q \leq 4$: Continuous phase transition

$q > 5$: 1st order phase transition

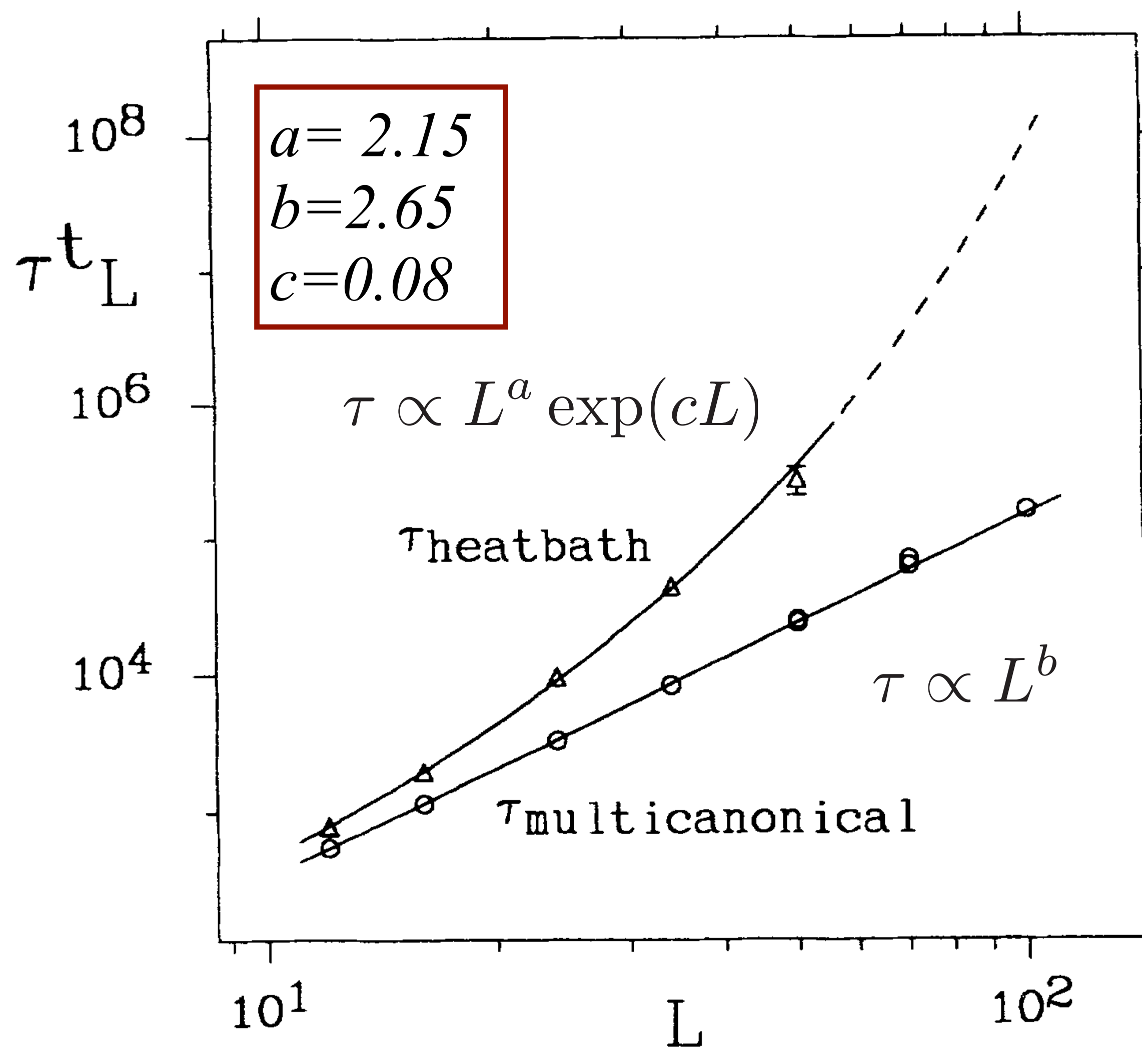
Multi Canonical method for q=10 Potts model

B.A. Berg and T. Neuhaus, Phys. Rev. Lett. **68**, 9 (1992)

Energy distribution around Tc



Tunneling time



By Multi Canonical method, the tunneling time is reduced to the power of L!

Wang-Landau method

F. Wang and D. P. Landau (2001)

Another method to obtain the density of state:

Random walk on the energy space

Markov Chain Monte Carlo with the probability

$$W_{\Gamma \to \Gamma'} = \min\left(\frac{g(E(\Gamma))}{g(E(\Gamma'))}, 1\right)$$

$g(E)$:estimate of DOS

if $g(E) = \rho(E)$ $\Rightarrow$ This MCMC give us completely flat histogram

Wang-Landau method:update of g(E)

F. Wang and D. P. Landau (2001)

Initially, we don't know DOS. ➡ Set an initial guess, e.g. $g(E) = 1$

Along MCMC, we update *g(E)* of the *E(Γ)* as

$$g_{new}(E) = g(E) \times f$$

If the multiplication factor is "gradually" reduced to f=1,

***g(E)* eventually converges to *ρ*(*E*).**

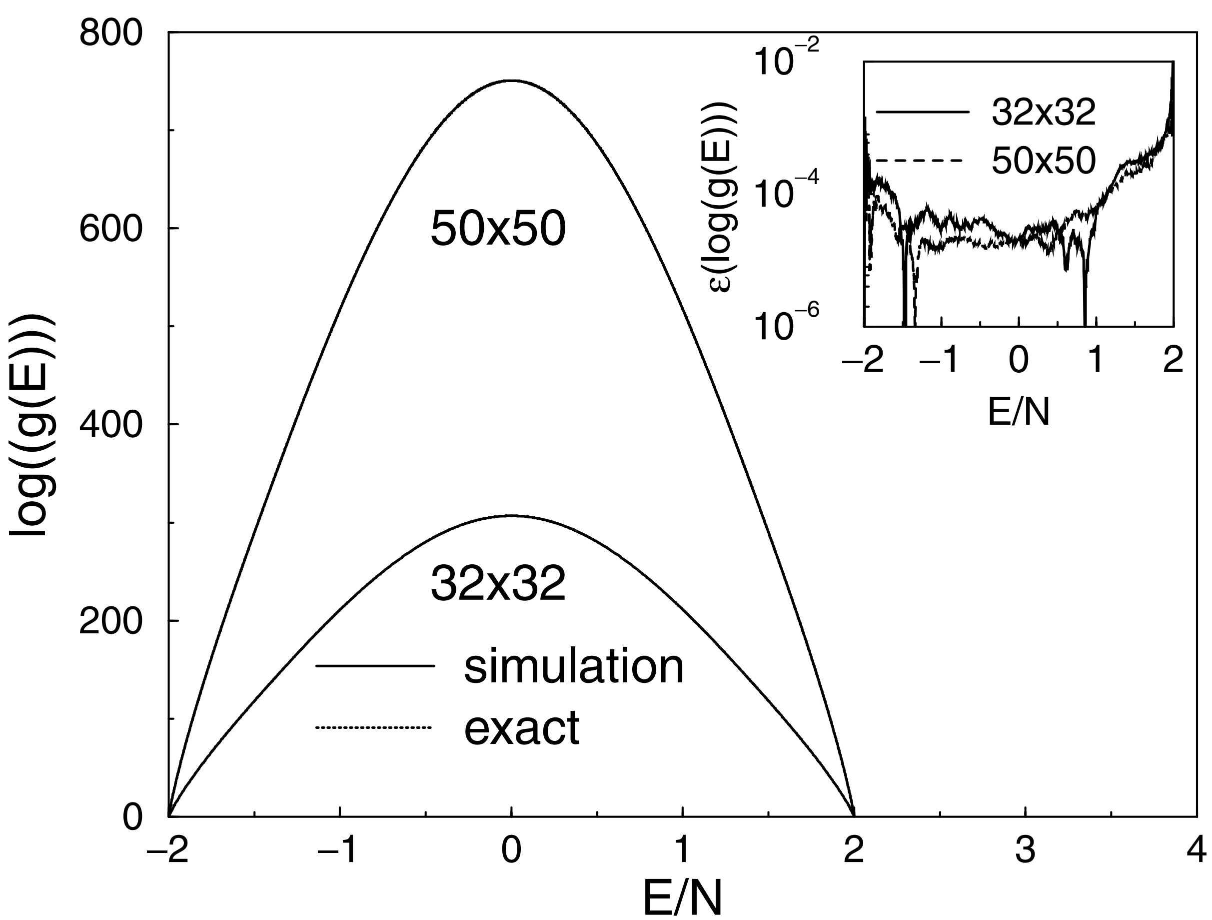
"gradual" change of f

1. Initially $f=f_0$ (*e.g.* $f_0 = e^1$)
2. Loop i
   - If (the histogram *h(E)* becomes "flat"?)
     - Then, we decrease f_i as
       $f_{i+1} = (f_i)^x$ (*e.g.* $x = 1/2$),
       and reset the histogram.
3. Repeat until f_i becomes enough small (e.g. $f \sim \exp(10^{-8})$)

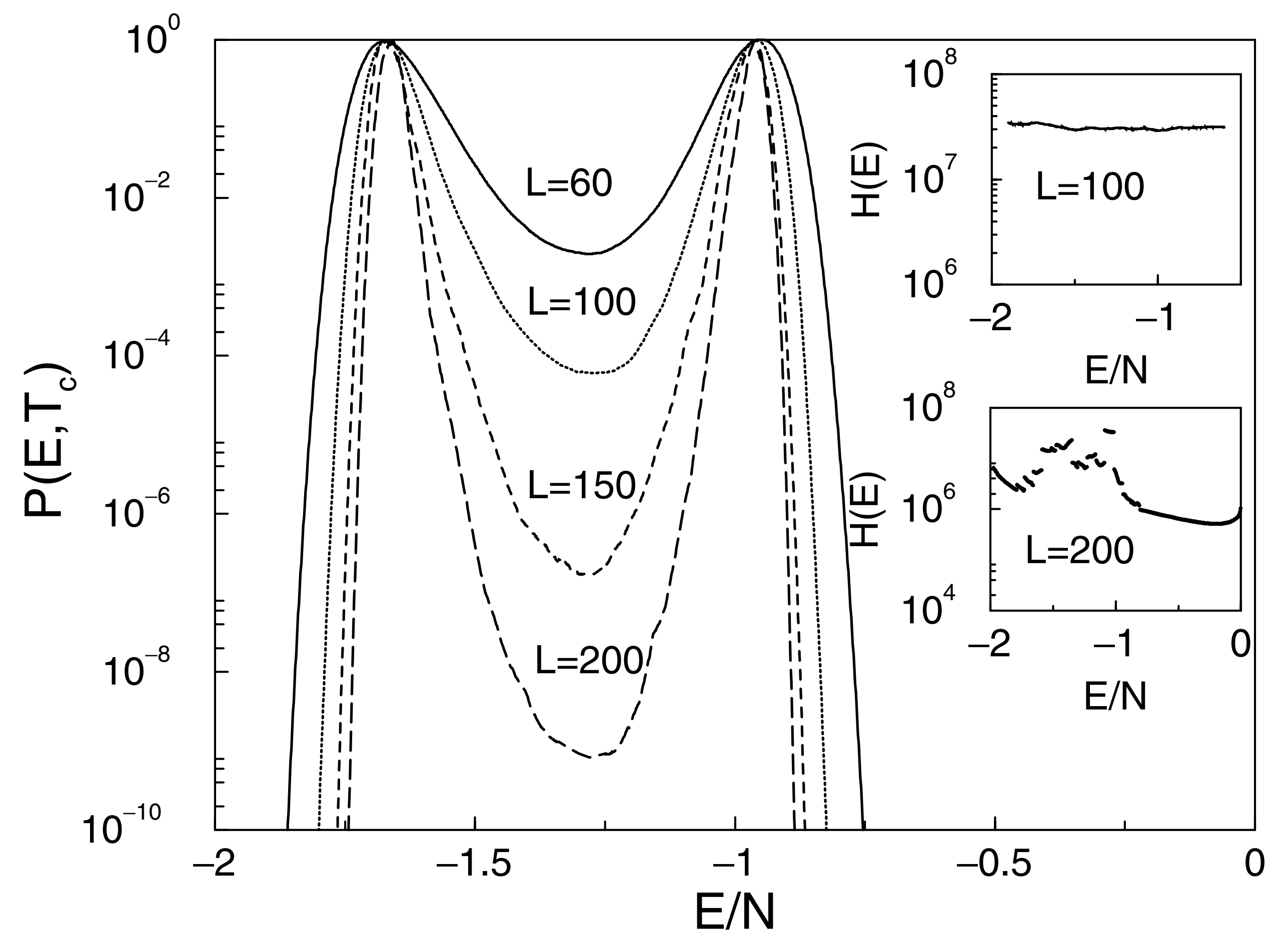
Power of Wang-Landau method

F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001)

Density of state of 2D-Ising model



Density of state of q=10 Potts model



We can obtain very accurate density of state by Wang-Landau method!

Replica Exchange method

Replica exchange (parallel tempering)

A different types of extended ensemble:

Usual MC or MD considers one parameter and one realization:

$$\boxed{T,\ \Gamma = \{S_i\}, \{\boldsymbol{q}_i, \boldsymbol{p}_i\}}$$

Replica exchange method considers
multiple parameter sets together with multiple realizations:

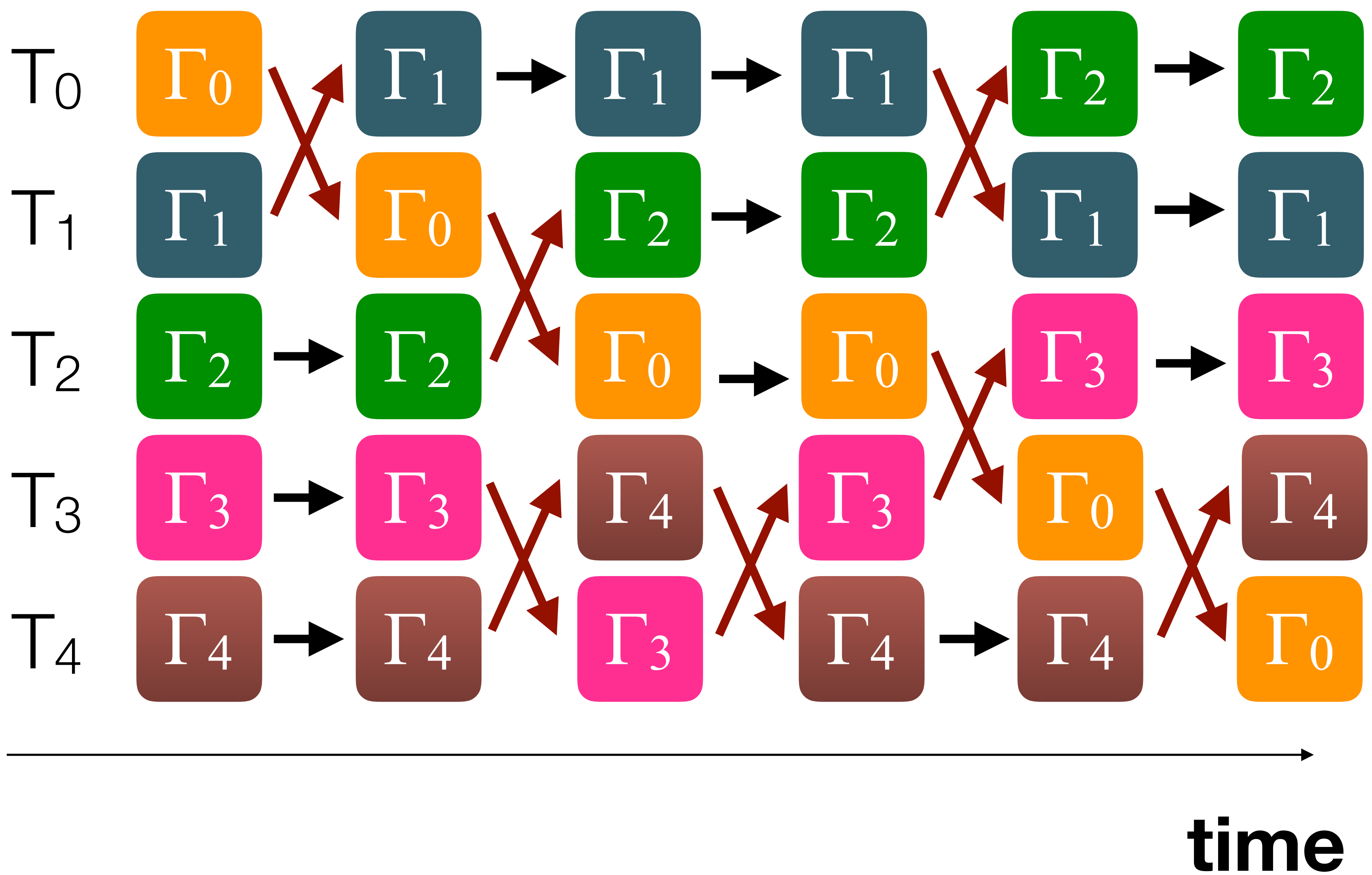
$$\{T_0, T_1, \cdots, T_M\},\ \{\Gamma_0, \Gamma_1, \cdots, \Gamma_M\},$$

Try to sample "(M+1)-dimensional" joint-distribution

$$\boxed{P(\Gamma_0, \Gamma_1, \cdots, \Gamma_M; T_0, T_1, \cdots, T_M)}$$

“Replica exchange”

Along simulation, we “exchange” the relationship between parameter and realization

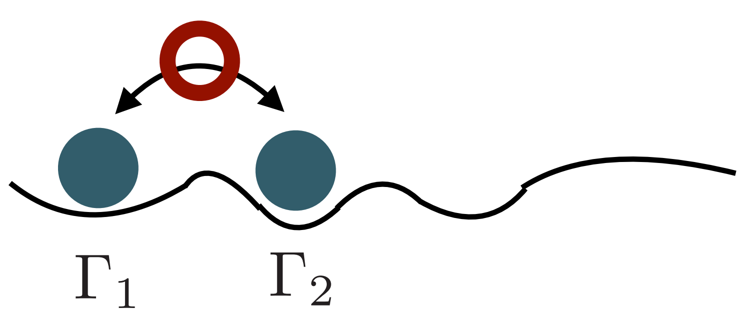


Purpose of replica exchange

Free energy landscape depends on the parameter

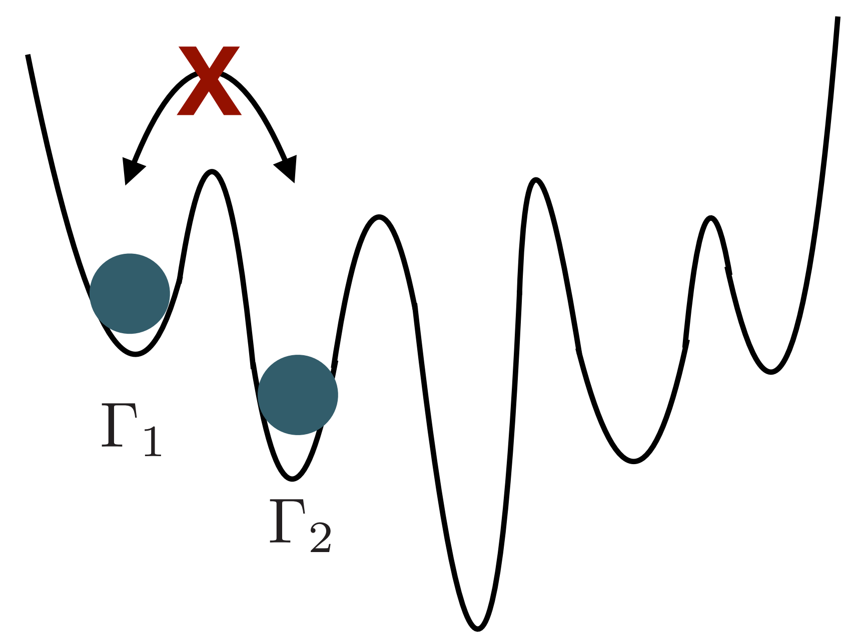
High temperature:T_h

Γ easily moves to other points!



Low temperature:T_l

Γ hardly moves to other minima!



Make a pass like:

$$\{\Gamma_1, T_l\} \rightarrow \{\Gamma_1, T_h\} \rightarrow \{\Gamma_2, T_h\} \rightarrow \{\Gamma_2, T_l\}$$

low **high** **high** **low**

* Parameter is not necessary a temperature.

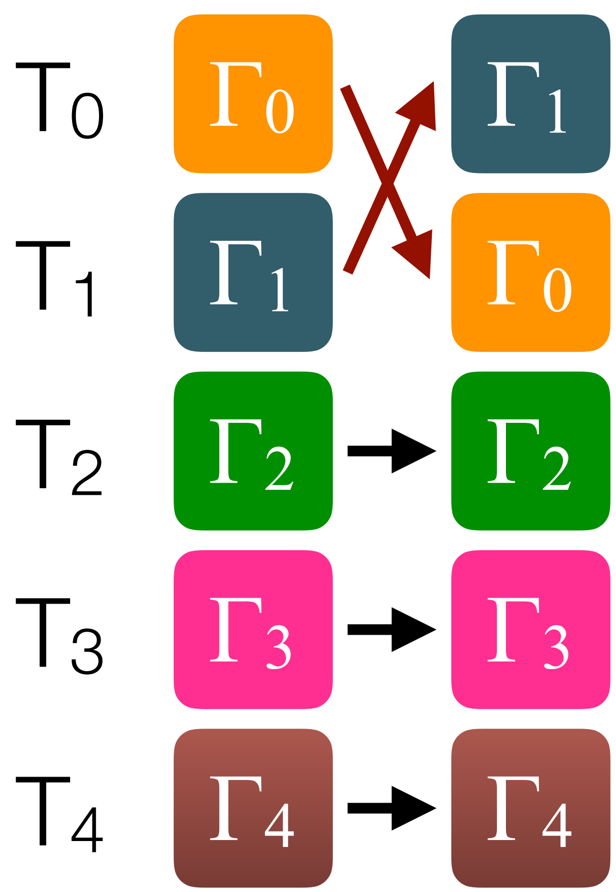
Markov Chain Monte Carlo for Replica Exchange

Target steady state distribution:

$$P(\Gamma_0, \Gamma_1, \cdots, \Gamma_M; T_0, T_1, \cdots, T_M) \propto e^{-\sum_i^M \beta_i E_i}$$

$$E_i \equiv \mathcal{H}(\Gamma_i)$$

Metropolis method:



$\mathcal{T}$ **:sequence of temperatures**

$$\mathcal{T} = \{T_1, T_0, T_2, \cdots\}$$

$$\underbrace{\{T_0, \Gamma_0\}, \{T_1, \Gamma_1\}}_{\mathcal{T}_{01}} \to \underbrace{\{T_1, \Gamma_0\}, \{T_0, \Gamma_1\}}_{\mathcal{T}_{10}}$$

Transition probability

$$W_{\mathcal{T}_{01} \to \mathcal{T}_{10}} = \min\left(1, \frac{P(\{\Gamma_i\}; \mathcal{T}_{10})}{P(\{\Gamma_i\}; \mathcal{T}_{01})}\right)$$

$$\frac{P(\{\Gamma_i\}; \mathcal{T}_{10})}{P(\{\Gamma_i\}; \mathcal{T}_{01})} = \frac{e^{-\beta_1 E_0 - \beta_0 E_1}}{e^{-\beta_0 E_0 - \beta_1 E_1}}$$

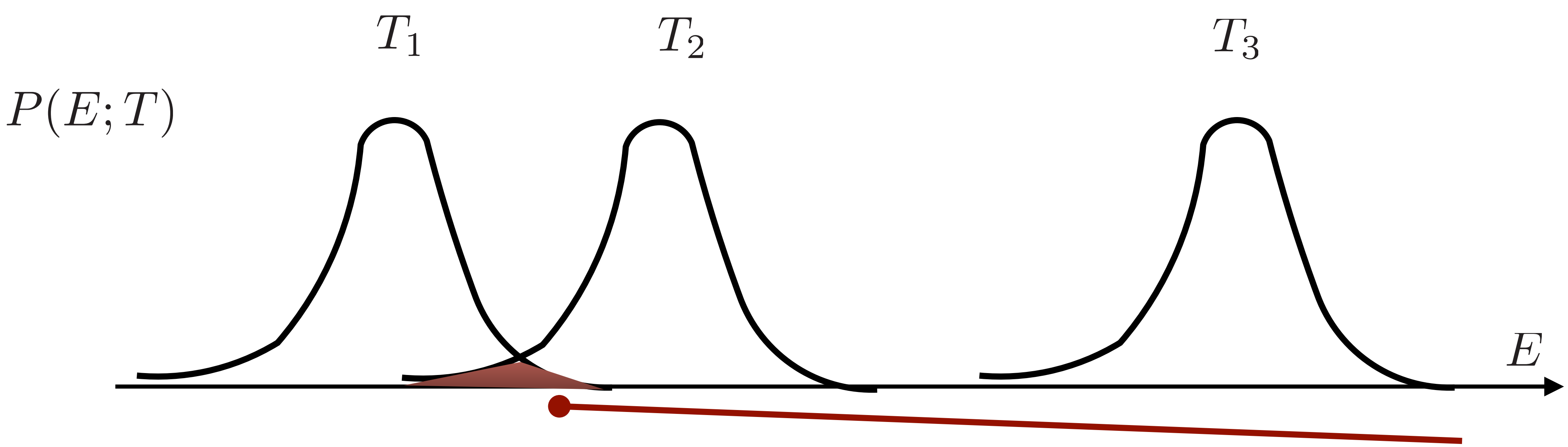
$$= e^{(\beta_0 - \beta_1)(E_0 - E_1)}$$

Select of temperature sequence

$$\boxed{\frac{P(\{\Gamma_i\};\mathcal{T}_{10})}{P(\{\Gamma_i\};\mathcal{T}_{01})} = e^{(\beta_0-\beta_1)(E_0-E_1)} = \frac{P(E_1;T_0)P(E_0;T_1)}{P(E_0;T_0)P(E_1;T_1)}}$$

Energy distribution at $\boldsymbol{T}$

$$P(E;T)$$



Almost all exchange occurs the energy region of “overwrap”.

$$\{\Gamma_1,T_1\},\{\Gamma_2,T_2\} \to \{\Gamma_1,T_2\},\{\Gamma_2,T_1\}$$:acceptable!

$$\{\Gamma_2,T_2\},\{\Gamma_3,T_3\} \to \{\Gamma_2,T_3\},\{\Gamma_3,T_2\}$$:almost rejected!

For efficient exchange, we have to choose a sequence of temperatures so that the energy distributions have finite overwrap!

Usually we only exchange the nearest neighbor pairs of temperatures

Select of temperature sequence: Example

Suppose $C = \frac{dE}{dT} = \text{const.}$

$$\boxed{\frac{P(\{\Gamma_i\};\mathcal{T}_{10})}{P(\{\Gamma_i\};\mathcal{T}_{01})} = e^{(\beta_0-\beta_1)(E_0-E_1)}}$$

Temperature sequence satisfying almost "flat" transition probability

$$(\beta_i - \beta_{i+1})(E_i - E_{i+1}) = \text{const.}$$

$$\Leftrightarrow \quad C\frac{(T_{i+1}-T_i)^2}{T_{i+1}T_i} = \text{const.}$$

$T_{i+1}T_i \simeq T_i^2$ $\Rightarrow$ $T_{i+1} = \alpha T_i$ **:Temperatures are geometric sequence!**

Important notice:

Heat capacity C is an extensive quantity: $C \sim O(N)$

In order to keep finite overwrap, we need to increase temperature point M as

$$M \propto \sqrt{N}$$

Relaxation time of the replica exchange

In order to confirm the equilibration of the whole system,
usually we need two criterions

1. The correlation time at the highest temperature is sufficiently short,
   e.g. τ=O(1)

   ➡ If a replica visits the highest temperature, it can easily change its state Γ.

2. All replicas make several (~O(10)) round trips between
   the lowest and the highest temperatures

   ➡ The ensemble at the lower temperature is in the equilibrium.

The second part determines the relaxation time of the method.

$$\boxed{\tau_{\mathrm{RE}} \sim \text{round trip time}}$$

* If the replica exchange is an random walk:

$$\text{round trip time} \propto M^2$$

Summary of replica exchange

Algorithm:

1. Make a temperature set $\{T_1, T_2, \ldots, T_M\}$
2. Loop n

   (1) Do MC or MD for M replicas: $\{\Gamma_1, \Gamma_2, \ldots \Gamma_M; T_1, T_2, \ldots, T_M\}$

   (2) Calculate the energies of replicas

   (3) Try replica exchange based on, e.g. Metropolis method

   - Usually we alternatively try replica exchange such as
     even n; $\{1 \leftrightarrow 2\}, \{3 \leftrightarrow 4\}, \{5 \leftrightarrow 6\}, \ldots$
     odd n; $\{2 \leftrightarrow 3\}, \{4 \leftrightarrow 5\}, \{6 \leftrightarrow 7\}, \ldots$
     Note: each exchange trial is independent

   (4) Observe the quantities for $\{\Gamma_1, \Gamma_2, \ldots \Gamma_M; T_1, T_2, \ldots, T_M\}$

If we already have a MC or MD programs,
it is very easy to introduce the replica exchange method!

Introduction of ALPS for the report

ALPS（Applications and Libraries for Physical Simulation)

- Set of libraries and applications for a variety of lattice models.
- Support for spin models, Hubburd model, Kondo lattice model, …
- A lot of solvers for models:
    - Classical/Quantum Monte Carlo, Exact Diagonalization, Density Matrix Renormalization Group (DMRG), Dynamical Mean Field Theory (DMFT), Time Evolving Block Decimation (TEBD), …
    - We can select efficient solver for your problems.
    - It can be applicable to the frontier research.

ALPS Wiki http://alps.comp-phys.org/mediawiki/index.php/Main_Page

Research topics using ALPS

(since 2015)

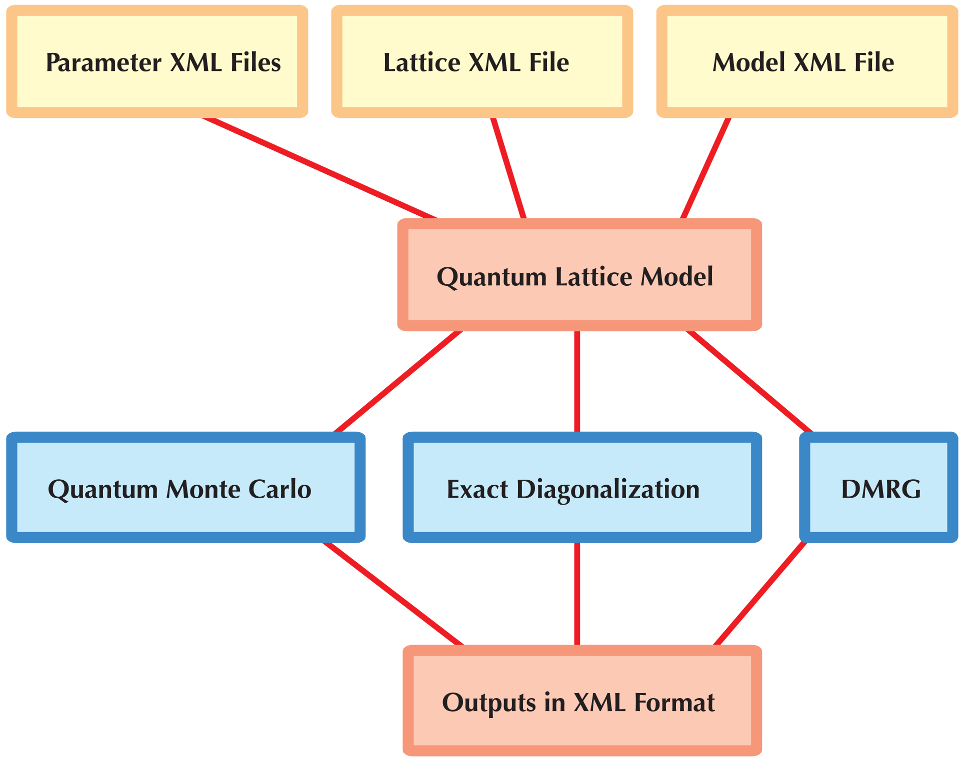
- Phase transition of ultracold atoms immersed in a BEC vortex lattice
- Entanglement entropy and topological order in resonating valence-bond quantum spin liquids
- First-order topological phase transition of the Haldane-Hubbard model
- DMFT Study for Valence Fluctuations in the Extended Periodic Anderson Model
- Static and dynamical spin correlations of the $S = 1/2$ random-bond antiferromagnetic Heisenberg model on the triangular and kagome lattices
- Transport properties for a quantum dot coupled to normal leads with a pseudogap
- Magnetic structure and Dzyaloshinskii-Moriya interaction in the $S = 1/2$ helical-honeycomb antiferromagnet α-$Cu_2V_2O_7$
- Mott transition in the triangular lattice Hubbard model: A dynamical cluster approximation study
- SU (N) Heisenberg model with multicolumn representations
- Superconductivity in the two-band Hubbard model
- Local Electron Correlations in a Two-Dimensional Hubbard Model on the Penrose Lattice

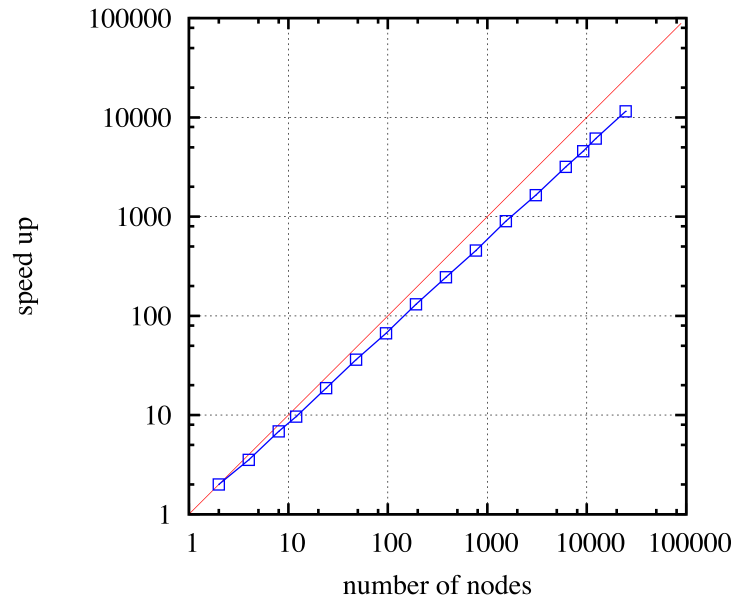
Details：http://alps.comp-phys.org/mediawiki/index.php/PapersTalks

ALPS の機能

＊MateriApps のハンズオン資料から借用

- 入出力支援
  - 格子構造, 模型は XML を用いて柔軟に指定
  - 全てのソルバーに共通した入出力形式
  - Python インターフェースを用意
    - Python から直接実行、グラフを作成
- 並列化
  - パラメータ並列のための並列化スケジューラ
  - 量子モンテカルロソルバ (looper)
    - 京で20,000ノードまで良好なスケーリング
- 競合するアプリケーション：「なし」？





Preparation of ALPS (If you use it at ECCS)

- Login to iMac and open “Terminal” application.
- Download ALPS binaries for ECCS from
  https://dl.dropboxusercontent.com/u/484163/alps-for-eccs/alps-20160816.zip
  - Probably, it will be automatically decompressed.
    (If not, double click the zip file)
  - Move the folder to home (or your preferable place)
    cd
    mv Downloads/alps-20160816 .
  - Run configure file
    . alps-20160816/bin/alpsvars.sh
  - Check spinmc and simplemc
    spinmc --help
    simplemc --help

Download of example (tutorial) files

- From ITC-LMS: https://itc-lms.ecc.u-tokyo.ac.jp/portal/login
  or
  github: https://github.com/compsci-alliance/many-body-problems

  Download and decompress the example files "ALPS_examples.zip"

- Move the folder ALPS_examples to home (or your preferable place) . In the case of ECCS iMac,
  cd
  mv Downloads/ALPS_examples .

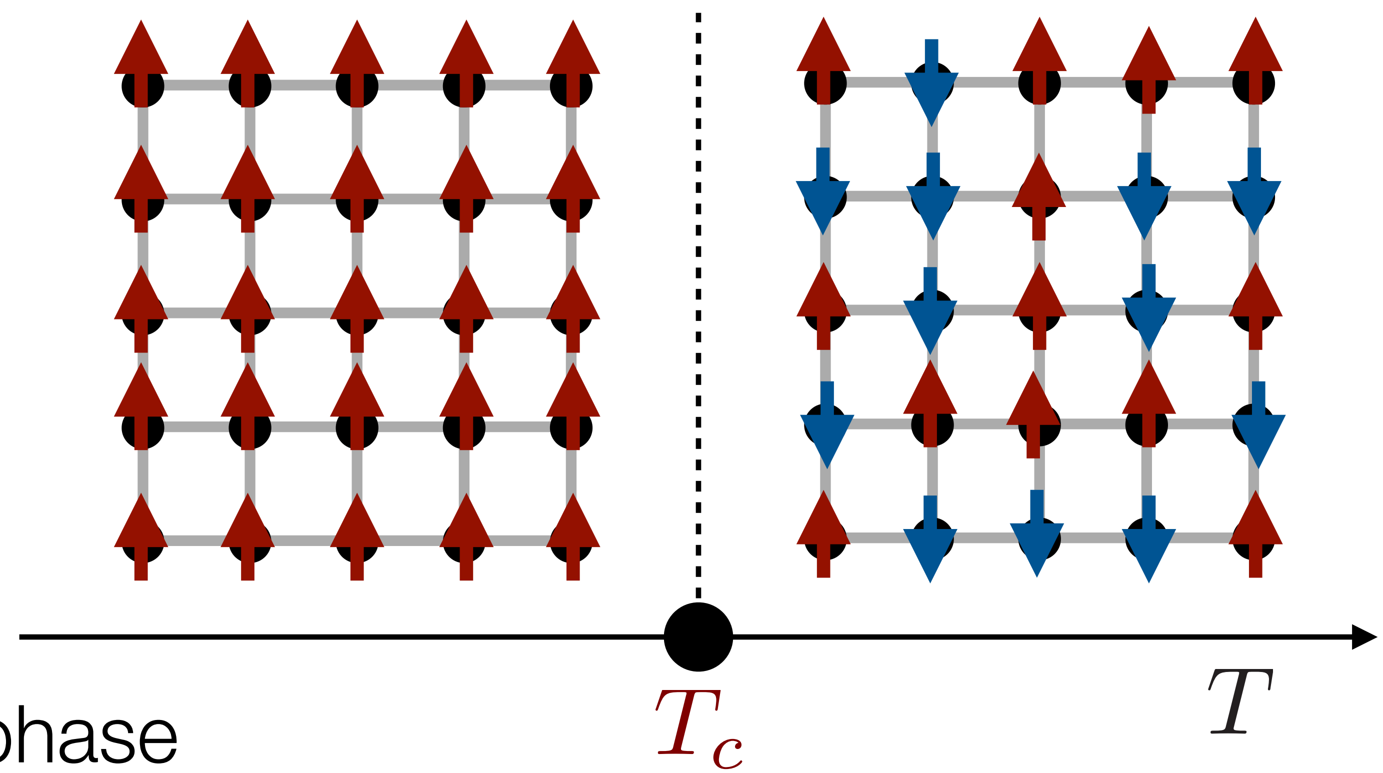
Exercise (not a report)

- Square lattice Ising model

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

  - Continuous transition at $T=T_c$,

$$T_c/J = \frac{2}{\ln(1+\sqrt{2})} = 2.26918531\ldots$$



    - $T>T_c$: Para magnetic phase
    - $T<T_c$: Ferro magnetic phase

  - By Monte Carlo simulation (Metropolis algorithm), see the phase transition!

Simulation by simplemc

- **simplemc**: classical Monte Carlo simulator using Metropolis Algorithm
- Move to ALPS_examples
  - *cd*
  - *cd ALPS_examples*
- *Transform parameter file to XML format*
  - *parameter2xml parm9a*
- Run simulation（It takes approximately five minites）
  - *simplemc parm9a.in.xml*
- Plot the results（Specific heat, Energy, square of the Magnetization）
  - *python plot9a.py*
  - （If you close three windows (graphs), python script will stop)

Explanation of parameter file: parm9a

```
LATTICE="square lattice"
J=1
ALGORITHM="ising"
SWEEPS=65536
L=8
{ T=5.0 }
{ T=4.5 }
{ T=4.0 }
{ T=3.5 }
{ T=3.0 }
{ T=2.9 }
{ T=2.8 }
{ T=2.7 }
...
```

Define lattice: if you write “simple cubic lattice” here, you can simulate 3D

Define interaction: $J > 0$ ferromagnetic

Define model: Ising , XY, Heisenberg

Define Monte Carlo steps:

1 MC step = trial of flips for all spin

＊THERMALIZATION

In order to reduce the effect of initial condition we do THERMALIZATION step MC calculation without observation.

If you don’t explicitly write it, it is automatically set to 1/8 of SWEEPS

Lattice size：$L \times L$

List of temperatures:

- Parameters in {}: parameter for 1 simulation
  - MC simulation is repeated for # of {}.
- Parameters outside of {}: common parameter for all calculation after them.

Explanation of plotting file: plot9a.py

Python script

Extract the result from the data files: **pyalps.loadMeasurements**

Setting for the X and the Y axes: **pyalps.collectXY**

Plotting: **matplotlib**

```
data = pyalps.loadMeasurements(pyalps.getResultFiles(prefix='parm9a'),
    ['Specific Heat', 'Magnetization Density^2', 'Energy Density'])
for item in pyalps.flatten(data):
    item.props['L'] = int(item.props['L'])

magnetization2 = pyalps.collectXY(data, x='T', y='Magnetization Density^2', foreach=['L'])
magnetization2.sort(key=lambda item: item.props['L'])

pyplot.figure()
alpsplot.plot(magnetization2)
pyplot.xlabel('Temperture $T$')
pyplot.ylabel('Magnetization Density Squared $m^2$')
pyplot.legend(loc='best')
```

Report problem 1:

- By editing the parameter file parm9a, try to simulate the following systems
  1. Square lattice Ising model of larger system sizes than L=32 (e.g. L=64, 128, …)
     - Discuss that the relationship among SWEEP, L, and error bar of physical quantities
     - Plot the "binder ration of magnetization" and compare the crossing point of them to the true critical point.
       - It can be done by adding "Binder Ratio of Magnetization" to **pyalps.loadMeasurements** in **plot9a.py** and edit properly **pyalps.collectXY**
     - Try anything you can do
     - (Advanced) Try finite size scaling of the binder ratio, and specific heat.
  2. Cubic lattice Ising model of larger system sizes
     - Do the same tasks with the case of the above square lattice model.
       - Note: In the case of 3D you may need longer time to simulate the model. Thus, the largest size becomes smaller than that of 2D.
     - (Advanced): Try XY or Heisenberg models and determine transition temperature from *e.g.* the crossing point of binder ratio.

Report problem 1: Tips

- If you change the name of parameter file, you also need to edit the corresponding part of the plotting script.
- If you want to see the number directly, you can use python script **textout9a.py .**

  If you output the number to a file:

  python textout9a.py > filename.txt

  (If you use the script for the binder ratio or other quantities, you need to edit it.)
- Note: if SWEEP is too small, MCMC can not correctly sample the equilibrium ensemble!. If you change the parameter, you should check the SWEEP dependence of the results.

Report problem 2:

- Suppose that you have a (sub) program **MC(*Γ*,*T*,*E*)** which perform MC update for input *Γ* at a temperature *T* and returns new *Γ* and its energy *E.*

    1. Make a (pseudo) program to perform a replica exchange Monte Carlo.

        1. Define the maximum and the minimum temperatures.
        2. Determine sequence of *M* temperatures.
           (You may use geometric sequence explained in today's lecture. In this case, the common ratio *α* is determined by T_{max}, T_{min} and *M*.)
        3. Implement the replica exchange Monte Carlo by using e.g. Metropolis method.

        - You can use c, c++, fortran, python, …, or a pseudo code.
        - You can assume that you have a random number generator **make_random(r)** which return uniformly distributed random number $r \in [0, 1)$

    2. (Advanced) If you have a MC or MD program for single run (or if you can write it), try to run the above program and observe the dynamics of replicas, such as turn around time, acceptance ratio of replica exchange, … for a model you like.

Report problem 3 (optional)

- Write a comment to the lecture of classical many body systems, e.g.,
  - How do you feel the contents of the lecture?
    - Too easy, Boring, Too difficult, Too biased to the interest of the lecturer, …
  - What topics do you want to learn if you have the next chance?
  - Do you have any idea to improve the quality of the lecture?
    - Tutorial using computers, Use black board, …

Deadline

- Submit your report through the system of ITC-LMS
  - The deadline is July. 31st.
- If you have any troubles or questions, please freely ask me
  - at the future lectures,
  - by e-mail: t-okubo@phys.s.u-tokyo.ac.jp
  - or come to my office **Sci. Bldg. #1 940.**
    (It is better to get an appointment by e-mail.)

References (books)

- “A Guild to Simulations in Statistical Physics” D.P. Landau and D. Binder, Cambridge University Press.
- “Computational Physics”, J. Thijssen，Cambridge University Press.
（「計算物理学」J.M.ティッセン著、松田和典他訳、シュプリンガー・フェアラーク東京.
- 「分子シミュレーション」上田顯著、裳華房.

PCOMS workshop

期日：6月7日

場所：柏の葉キャンパス

駅前サテライト

対象：

M2（博士進学予定），
博士課程の学生,
研究員、若手教員

参加申し込み・情報

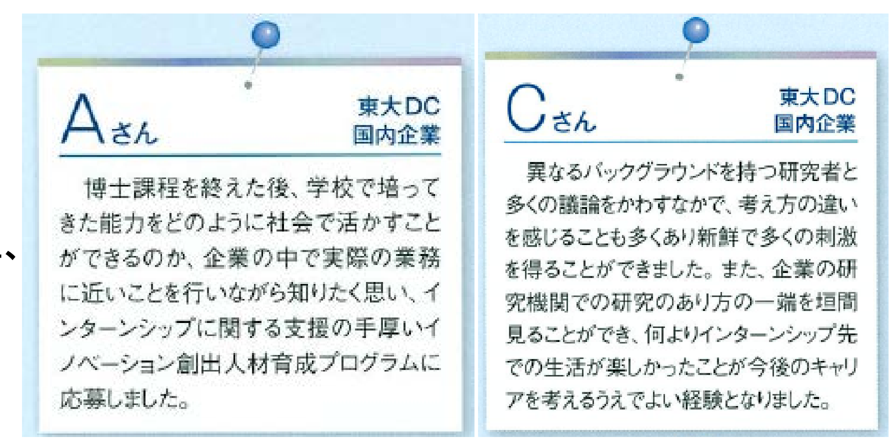
5月26日（金）まで

http://pcoms.issp.u-tokyo.ac.jp/events

企業人材ニーズ vs 博士人材シーズ マッチングワークショップ

キャリアパス、広げてみませんか！

企業の人材ニーズと、博士人材の技術シーズをぶつけ合い、マッチングを図って、博士人材を参画企業への研究インターン実施(別紙参照)や企業連携研究に導くことを目的としています。午前中は、企業における計算機科学・計算科学の最近の活用事例も紹介いただきます。是非ご参加ください。


Aさん 東大DC 国内企業

博士課程を終えた後、学校で培ってきた能力をどのように社会で活かすことができるのか、企業の中で実際の業務に近いことを行いながら知りたく思い、インターンシップに関する支援の手厚いイノベーション創出人材育成プログラムに応募しました。

Cさん 東大DC 国内企業

異なるバックグラウンドを持つ研究者と多くの議論をかわすなかで、考え方の違いを感じることも多くあり新鮮で多くの刺激を得ることができました。また、企業の研究機関での研究のあり方の一端を垣間見ることができ、何よりインターンシップ先での生活が楽しかったことが今後のキャリアを考えるうえでよい経験となりました。

開催: 平成 29 年 6 月 7 日(水)10:00–19:30

場所: 東京大学フューチャーセンター2F
(柏の葉キャンパス駅前徒歩 1 分)

対象: 修士課程 2 年で博士課程進学予定の院生、博士後期課程の院生、研究員、若手教員など。教職員の聴講も OK。

参画: 出光興産㈱、NEC、新日鐵住金㈱、トヨタ㈱、㈱日産アーク、日本ゼオン㈱、富士通研究所㈱

進行:
10:00～10:50 「全固体電池における材料インフォマティクス手法を用いた新材料探索」
「トヨタ自動車における計算材料科学への取り組み」」(トヨタ自動車)
10:50～11:40 「社会課題解決のための高性能データ分析技術」(NEC)
13:00～13:10 ガイダンス(PCoMS、イノベーション創出人材育成事業・インターン実施に関して)
13:10～15:10 企業人材ニーズ説明(20 分／1社 予定)
15:30～17:30 博士人材シーズ説明(参加者よりショートプレゼン＆ポスター発表を予定)
17:30～19:30 企業説明ブース巡回・情報交換会

申込: http://pcoms.issp.u-tokyo.ac.jp/events (締切:平成 29 年 5 月 26 日(金)正午)