

Day 1. Ising Model – Numerical Demonstrations

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1. Download and Compile MD++

Direct your browser to <http://micro.stanford.edu/~caiwei/Forum/2004-12-12-MD++/>
Download the latest MD++ source file, e.g. md++-2011-03-11.tar.gz, to your home directory.
You can also download the package using the `wget` command.

On your Unix/Linux workstation, do

```
$ cd ~  
$ wget http://micro.stanford.edu/~caiwei/Forum/2004-12-12-MD++/md++-2011-03-11.tar.gz  
$ mkdir Codes  
$ cd Codes  
$ tar zxvf ~/md++-2011-03-11.tar.gz
```

MD++ will be unzipped in the `~/Codes/MD++` directory.

To compile the code, do

```
$ cd MD++  
$ make ising build=R
```

This will create the executable `ising_gpp` in the `~/Codes/MD++/bin` directory. If you have intel compiler, you can use

```
$ make ising build=R SYS=intel
```

This will create the executable `ising_intel`, which may run faster than `ising_gpp`.

More information about how to use MD++ can be found at:

http://micro.stanford.edu/wiki/MD%2B%2B_Manuals

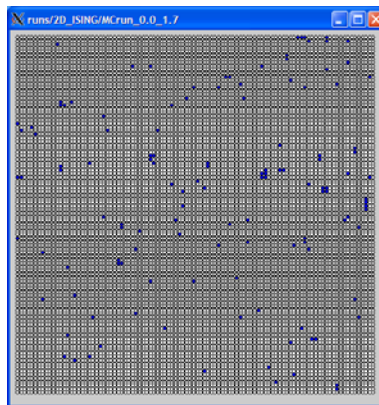
2. Monte Carlo (MC) Simulation of the Ising Model

2.1. Run MC simulation

Execute the following commands.

```
$ cd ~/Codes/MD++  
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_Mcrun.tcl 0.0 1.7 10000
```

The first argument (0.0) specifies **h**, the magnetic field. The second argument (1.7) specifies **kBT**, the temperature. The third argument (10000) specifies **totalsteps**, the simulation time in unit of Monte Carlo steps per site (MCSS).



The simulation will open a window (see above) displaying the flipping of the spins during the MC simulation. White squares are -1 spins and blue squares are +1 spins. In this example, the Ising model is a 100 x 100 square lattice with $J = 1$. At each MC step, the algorithm choose a spin randomly and attempts to flip it.

2.2. Process MC simulation results

At the end of this simulation, the following lines will be printed on the terminal.

```
Magnetization from Monte Carlo Simulation =-0.9701 +- 0.00341467421579  
Magnetization from Analytic Onsager Solution=0.970077811602  
Average Largest Cluster Size = 7
```

The first line is the average magnetization (i.e. average value of the spins). We can see that most of the spins are pointing downward (-1) in this simulation. The second line prints the analytic solution predicted by Onsager. The third line prints the average value of the largest cluster (islands of +1 spins) during the simulation.

More data are saved in the `~/Codes/MD++/runs/2D_Ising/MCrun_0.0_1.7` directory. The `prop.out` file contains statistical information taken periodically during the simulation. To see the content of this file, do

```
$ tail -3 runs/2D_ISING/MCrun_0.00_1.7/prop.out
9997 -9628 186 10000 25 1
9998 -9638 181 10000 15 1
9999 -9682 159 10000 8 1
```

There are six columns in the `prop.out` file. Their meaning is explained below.

Column 1 : time in MCSS

Column 2 : $Stot = N_{up} - N_{down}$ (Magnetization is defined as $Stot/N_{tot}$)

Column 3 : N_{up} , number of up (+1) spins

Column 4 : $N_{tot} = N_{up} + N_{down}$, total number of spins

Column 5 : N_c , size of largest cluster

Column 6 : for debug purposes in FFS simulation. You can ignore this.

3. Forward Flux Sampling (FFS) Simulation of the Ising Model

3.1. Run FFS simulation

The syntax for FFS simulation command is the following.

```
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_FFS1cpu.tcl m1 m2 h kBT
```

where

`m1` : the starting interface id

`m2` : the stopping interface id

`h` : magnetic field

`kBT` : temperature

First, execute the following commands.

```
$ cd ~/Codes/MD++
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_FFS1cpu.tcl 0 4 0.06 1.7
```

This performs various parts of the FFS simulation. First, it performs brute force MC simulations to compute the nucleation rate I_0 (of reaching interface λ_0). Then it computes the transition probabilities of successfully reaching the next interface from the previous one, i.e., $P(\lambda_1 | \lambda_0)$, $P(\lambda_2 | \lambda_1)$, $P(\lambda_3 | \lambda_2)$, $P(\lambda_4 | \lambda_3)$.

Next, execute the following command.

```
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_FFS1cpu.tcl 5 100 0.06 1.7
```

This computes transition probabilities, $P(\lambda_5 | \lambda_4)$, $P(\lambda_6 | \lambda_5)$, ..., until a cut-off interface determined automatically by MD++ (usually less than 100).

3.2. Process FFS simulation results

The data is stored in the `prop.out` file in the directory named
`~/Codes/MD++/runs/2D_Ising/FFS_0.06_1.7/CPUno_1`

After the FFS simulation is completed (to the last λ interface), the data are processed and the following files will be created in the directory named
`~/Codes/MD++/runs/2D_Ising/FFS_0.06_1.7`

The content and their meaning are given beneath the filenames.

```
total0.txt
29999          13          13
Simulation time in MCSS      # of times reaching interface  $\lambda_0$ 
The (nucleation) rate of reaching interface  $\lambda_0$  is  $I_0 = 13/29999$ 
```

```
total1.txt
449           51          51
# of trial from  $\lambda_0$       # of trajectories reaching  $\lambda_1$ 
By default, the code moves to the next interface once 51 successful trajectories have
been sampled. The transition probability is  $P(\lambda_1 | \lambda_0) = 51/449$ .
```

Similarly, `total[m].txt` contains data from interface $\lambda_{[m-1]}$ to $\lambda_{[m]}$.

The spin configurations saved at each FFS step (from $\lambda_{[n-1]}$ to $\lambda_{[n]}$) can be found in directory `~/Codes/MD++/runs/2D_Ising/FFS_0.06_1.7/run_[n]`.

4. Umbrella Sampling (US) Simulation of the Ising Model

4.1. Run US simulation

The US simulations can be started only after the FFS simulations have successfully finished. This is because the FFS simulations prepare the initial conditions for US simulations. The syntax for US simulation command is the following.

```
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_US.tcl N n_c h_w h kBT
```

where

`N` : the index number of the umbrella sampling window

`n_c` : the center of the bias potential

`h_w` : the half width of the histogram

`h` : magnetic field

`kBT` : temperature

As an example, execute the following commands.

```
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_US.tcl 0 6 8 0.06 1.7
```

After the simulation finishes, folder `~/Codes/MD++/runs/2D_Ising/FFS_0.06_1.7/UMB_0` contains the following three data files.

`Narray.txt` : the n-axis of the histogram, where n is the size of largest nucleus

`Freq.txt` : raw data of histogram, number of times a given nucleus size is sampled

`Prob.txt` : raw histogram multiplied by $\exp(W/kBT)$ where W is the bias function

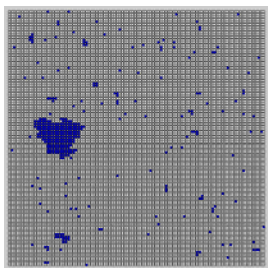
Note that the bias function is only apply when `n_c` < 0.7 λ_0 . When the bias function is not applied, `Freq.txt` should be identical to `Prob.txt`.

5. Visualization of Saved Spin Configurations

The spin configurations saved from MC, FFS and US simulations can be visualized using the `Day1_ising_show.tcl` script file, followed by the file name you wish to view. For example, execute the following command.

```
$ bin/ising_gpp scripts/LLNL2010/Day1_ising_show.tcl \
    runs/2D_ISING/FFS_0.06_1.7/run_6/FFS_6_0001.cn.gz
```

You should see something like the following, in which an island (nucleus) is clearly visible.



References:

[1] S. Ryu and W. Cai, "The Validity of Classical Nucleation Theory for Ising Models", *Phys. Rev. E*, 81, 030601 (R) (2010).

[2] S. Ryu and W. Cai, "Numerical Tests of Nucleation Theories for the Ising Models", *Physical Review E*, 82, 011603 (2010).

Appendix A. Numerical Homework

1. Run MC simulations of 2D (100x100) Ising model at $h = 0$ and $J = 1$ at several temperatures. Plot averaged magnetization as a function of temperature on top of Onsager's analytic solution

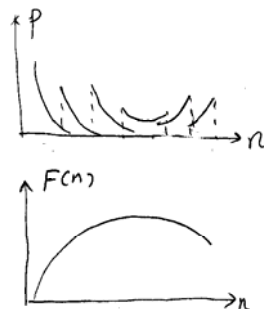
$$M = [1 - (\sinh 2\beta)^{-4}]^{1/8}, \text{ where } \beta = 1/kBT.$$

2. Run FFS simulations of 2D (100x100) Ising model at $h = 0.06$, $J = 1$ and $kBT = 1.7$. Obtain nucleation rate:

$$I = I_0 * P(\lambda_N | \lambda_0).$$

Plot one spin configuration at each interface λ_i .

3. Run US simulations of 2D (100x100) Ising model at $h = 0.06$, $J = 1$ and $kBT = 1.7$, using 20 windows of half width $n_w = 8$, centered at $n_c = 6 + 12i$, where $i = 0, 1, 2, \dots, 19$. Convert the probability data (in `prob.txt` files) into a single continuous curve for the free energy $F(n)$.



Appendix B. Homework Solutions

1. MC simulations

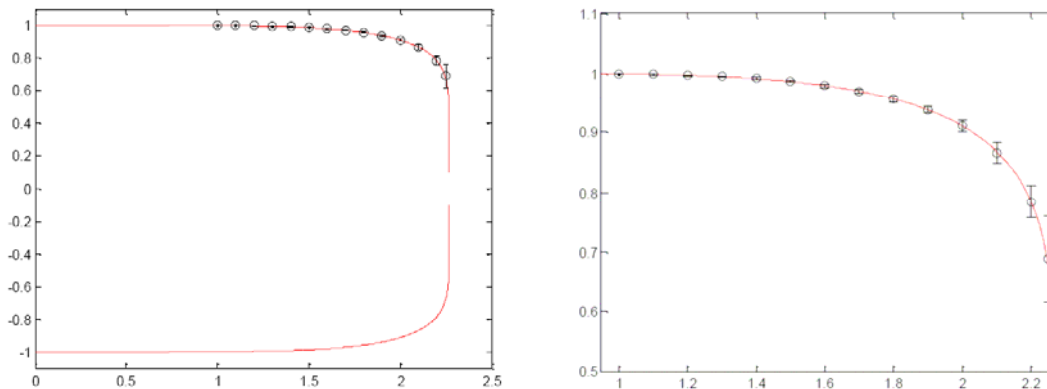
```
%% Matlab code for plotting the result
clear;

%% Onsager's analytic formula
kBT1=[0.0:0.001:2.268 2.269:0.00000001:2/log(1+sqrt(2))];
M1=(1-(sinh(2./kBT1)).^(-4)).^(1/8);

%% Numerical results
kBT=[ 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 ...
      1.8 1.9 2.0 2.1 2.2 2.25];
M =[ 0.9993 0.9985 0.9971 0.9949 0.9914 0.9866 0.9797 0.9699 ...
     0.9570 0.9380 0.9111 0.8656 0.7837 0.6893];
dM =[ 0.0004 0.00058 0.00082 0.0011 0.0016 0.0020 0.0026 0.0034 ...
     0.0044 0.0062 0.0099 0.0171 0.0273 0.0721];

%% Plot data
figure(1)
plot(kBT1,M1,'r--',kBT1,-M1,'r--')
hold on
errorbar(kBT,M,dM,'ko')
ylim([-1.1 +1.1])

figure(2)
plot(kBT1,M1,'r--',kBT1,-M1,'r--')
hold on
errorbar(kBT,M,dM,'ko')
xlim([0.95 max(kBT1)])
ylim([0.5 1.1])
```



Red curve: analytic formula. Black symbols: numerical data. Right: a close-up view.

2. FFS simulations

Here are the results obtained from running a longer FFS simulation than in the example.

For the following λ array (`Narray.txt`),

44 66 88 115 142 169 196 228 260 292 324 ...

we get

$$I_0 = 0.00039 \text{ MCSS}^{-1}$$

$$P(\lambda_N | \lambda_0) = P(\lambda_1 | \lambda_0) \times P(\lambda_2 | \lambda_1) \times \dots \times P(\lambda_N | \lambda_{N-1}) = 2.3 \times 10^{-4}$$

with a relative error of $dP/P \sim 0.22$

Hence

$$I = I_0 \times P(\lambda_N | \lambda_0) = 9.0 \times 10^{-8} \text{ MCSS}^{-1}$$

The following are the raw data from the simulation.

```
==> total0.txt <==
99999 39 39          →  $I_0 = 39/99999 \text{ MCSS}^{-1}$ 

==> total1.txt <==
842 101 101          →  $P(\lambda_1 | \lambda_0) = 101/842$ 

==> total2.txt <==
423 101 101          →  $P(\lambda_2 | \lambda_1) = 101/423$ 

==> total3.txt <==
407 101 101

==> total4.txt <==
289 101 101

==> total5.txt <==
192 101 101

==> total6.txt <==
173 101 101

==> total7.txt <==
156 101 101

==> total8.txt <==
142 101 101

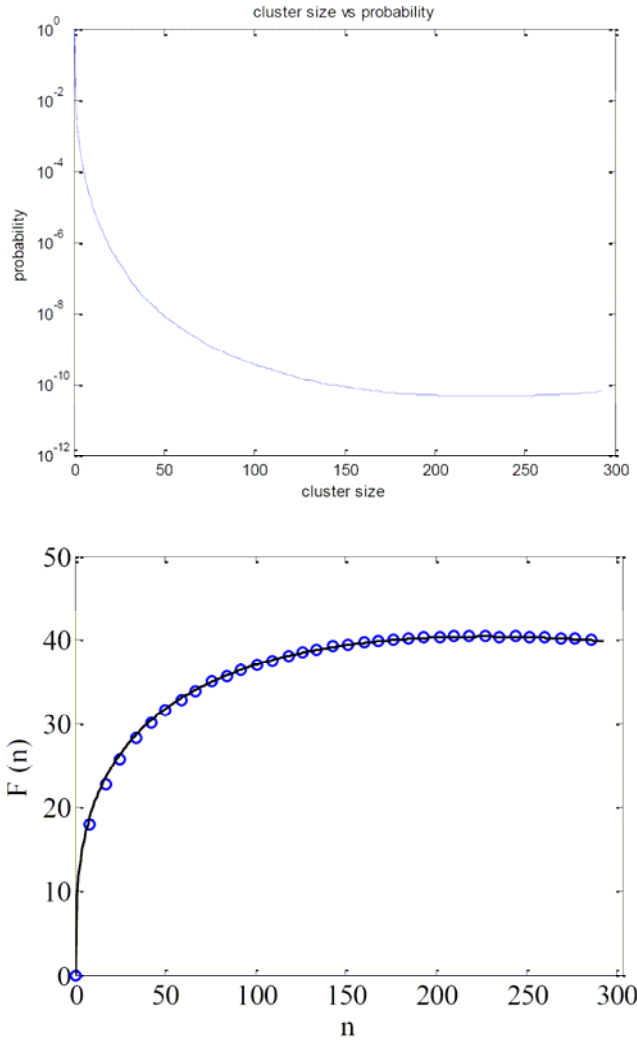
==> total9.txt <==
130 101 101

==> total10.txt <==
106 101 101

==> total11.txt <==
114 101 101
```


3. US simulations

The overlapping histogram method (Ref. Frenkel and Smit, Understanding Molecular Simulations, Academic Press, 2002) is used to piece together the histogram from different sampling windows.



Circles: US data. Black solid line: analytic predictions. The analytic expressions can be found in Ryu and Cai 2010 (see References).

The data above allows us to **compare the nucleation rates** predicted by **FFS** and that from classical nucleation theory (**CNT**). From MC simulation using the configurations containing the critical nucleus (see References), the attachment rate to the nucleus is found to be $f_c^+ = 34.25 \text{ MCSS}^{-1}$. The rate predicted by CNT is

$$I^{\text{CNT}} = N_{\text{tot}} f_c^+ \Gamma \exp(-F_c/kBT) = 10^4 \times 34.25 \text{ MCSS}^{-1} \times 0.0052 \times \exp(-40.4/1.7) = 8.3 \times 10^{-8} \text{ MCSS}^{-1}$$

This is in good agreement with the prediction from the FFS simulation,

$$I^{\text{FFS}} = I_0 \times P(\lambda_N | \lambda_0) = 9.0 \times 10^{-8} \text{ MCSS}^{-1}$$