Laboratório de Computação e Visualização Científica

Visualizing Monte-Carlo sampling of the Ising model phase space

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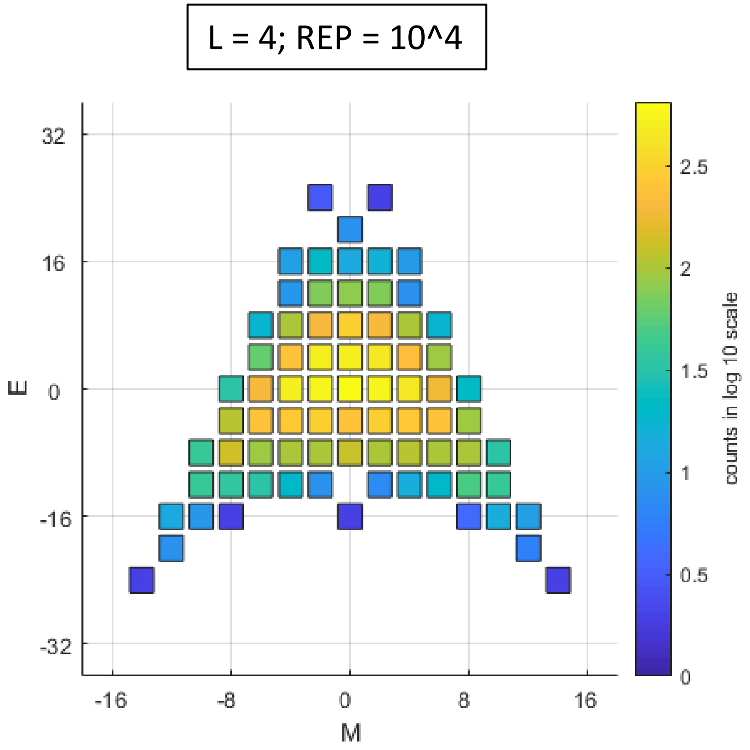
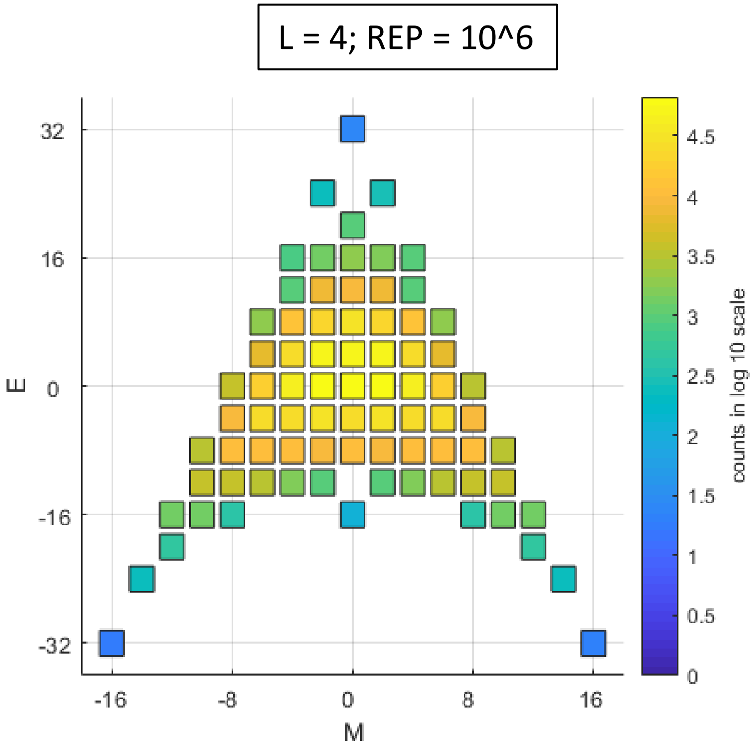
From the last class:

- The Ising model is a simple description of a magnetic material, and can be used to estimate the thermodynamic properties of ferromagnets.
- These thermodynamic properties can be easily calculated if we have an estimate of the Joint Density of States (JDOS), which is a table of all possible magnetization M and energy E values, together with the degeneracy (number of possible configurations with a given M,E pair).
- We have explored a simple Monte-Carlo approach of generating random spin configurations to visualize the phase space of the Ising model. It works, but not in an efficient way. It is worse than making a sequential list of possible states.

Phase space sampling with random spin configuration sampling

- Phase space sampling is denser near M=0 and E=0
- Only with large sampling it is possible to get data for the following states/configurations
    - All spins up (M=16,E=-32)
    - All spins down (M=-16, E=-32)
    - Checkerboard (M=0, E=32)
- This system has 65536 possible configurations, and 10^6 samples were needed to see the full phase space





More efficient Monte-Carlo methods:

- These are more advanced methods to better sample the phase space, and so obtain better JDOS estimates:
  - Wang-Landau
  - Hüller-Pleimling
  - Random Path Sampling
  - and more…

- They are naturally more complex than sampling random spin configurations
- Visualization helps to better understand their strengths and weaknesses

Wang-Landau method [2001]

VOLUME 86, NUMBER 10 PHYSICAL REVIEW LETTERS 5 MARCH 2001

Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States

Fugao Wang and D. P. Landau
Center for Simulational Physics, The University of Georgia, Athens, Georgia 30602
(Received 25 October 2000)

Our algorithm is based on the observation that if we perform a random walk in energy space with a probability proportional to the reciprocal of the density of states $\frac{1}{g(E)}$, then a flat histogram is generated for the energy distribution. This is accomplished by modifying the estimated density of states in a systematic way to produce a "flat" histogram over the allowed range of energy and simultaneously making the density of states converge to the true value. At the very beginning of the random walk, the den-

Hüller-Behringer method [2002]

International Journal of Modern Physics C, Vol. 13, No. 7 (2002) 947–956

MICROCANONICAL DETERMINATION OF THE ORDER PARAMETER CRITICAL EXPONENT

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A highly efficient Monte Carlo method for the calculation of the density of states of classical spin systems is presented. As an application, we investigate the density of states $\Omega_N(E, M)$ of two- and three-dimensional Ising models with N spins as a function of energy E and magnetization M. For a fixed energy lower than a critical value $E_{c,N}$ the density of states exhibits two sharp maxima at $M = \pm M_{sp}(E)$ which define the microcanonical spontaneous magnetization. An analysis of the form $M_{sp}(E) \propto (E_{c,\infty} - E)^{\beta_\varepsilon}$ yields very good results for the critical exponent β_ε, thus demonstrating that critical exponents can be determined by analyzing directly the density of states of finite systems.

Random Path Sampling [2014]

IEEE TRANSACTIONS ON MAGNETICS, VOL. 50, NO. 11, NOVEMBER 2014 1002204

Thermodynamics of the 2-D Ising Model From a Random Path Sampling Method

J. S. Amaral[1,2], J. N. Gonçalves[1], and V. S. Amaral[1]

[1]Departamento de Física and CICECO, Universidade de Aveiro, 3810-193 Aveiro, Portugal
[2]IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Rua do Campo Alegre, 678, 4169-007 Porto, Portugal

We then consider summing over states obtained from random path sampling from the fully ordered +1 to -1 magnetization states. At each step, a random spin in the +1 state is flipped, with a probability of 1.

With a sufficient number of sweeps, an estimate of individual energy and magnetization states is obtained, together with their degeneracy.

Flat Scan Sampling [2022]

Accurate Estimate of the Joint Density of States via Flat Scan Sampling

J. C. Inácio,[1] A. L. Ferreira,[2] and J. S. Amaral[1,*]

[1]*Departamento de Física and CICECO - Aveiro Institute of Materials, 3810-193 Aveiro, Portugal*
[2]*Departamento de Física and i3N, 3810-193 Aveiro, Portugal*
(Dated: March 8, 2022)

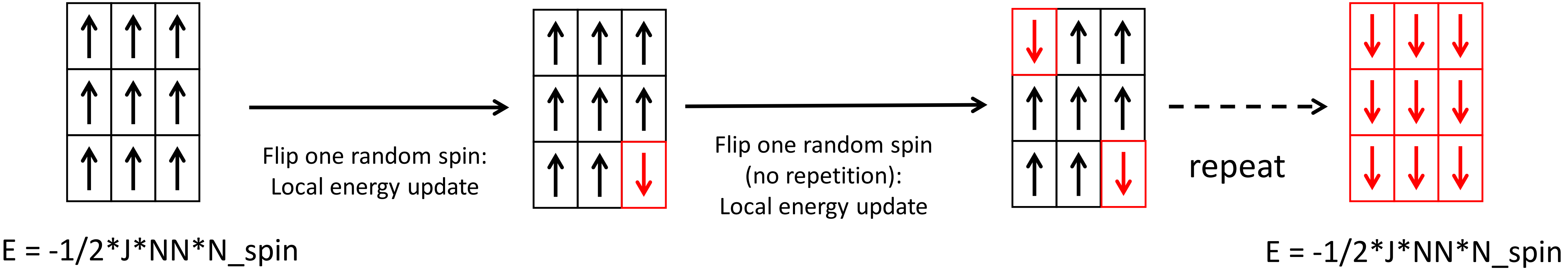
A Monte Carlo method to estimate the Joint Density of States $g(E,M)$ of the Ising and Ising-like models is presented. The method is applied to the well-known 2D Ising model, and is shown to be accurate, efficient, and embarrassingly parallel. The method presented offers major improvements over existing approaches. Furthermore, we obtain $g(E,M)$ estimates for the spin S Ising model, with the spin number $S = \{1/2, 1, 3/2, 2\}$, thus showing that the algorithm can handle larger and more complex (E,M) phase spaces.

https://arxiv.org/pdf/2203.02718v1.pdf

Random Path Sampling

- The method [1] forces a flat-magnetization sampling histogram by sweeping magnetization states from total +1 to -1

One full RPS sweep (Ising model)



- Energy calculations are local (fast)
- Embarrassingly parallel (each sweep is independent) – not a random walk!
- Easy implementation, generalization and parallelization

[1] J. S. Amaral et al., IEEE Trans. Magn. 50 1002204 (2014)

Random Path Sampling: Validation [1]

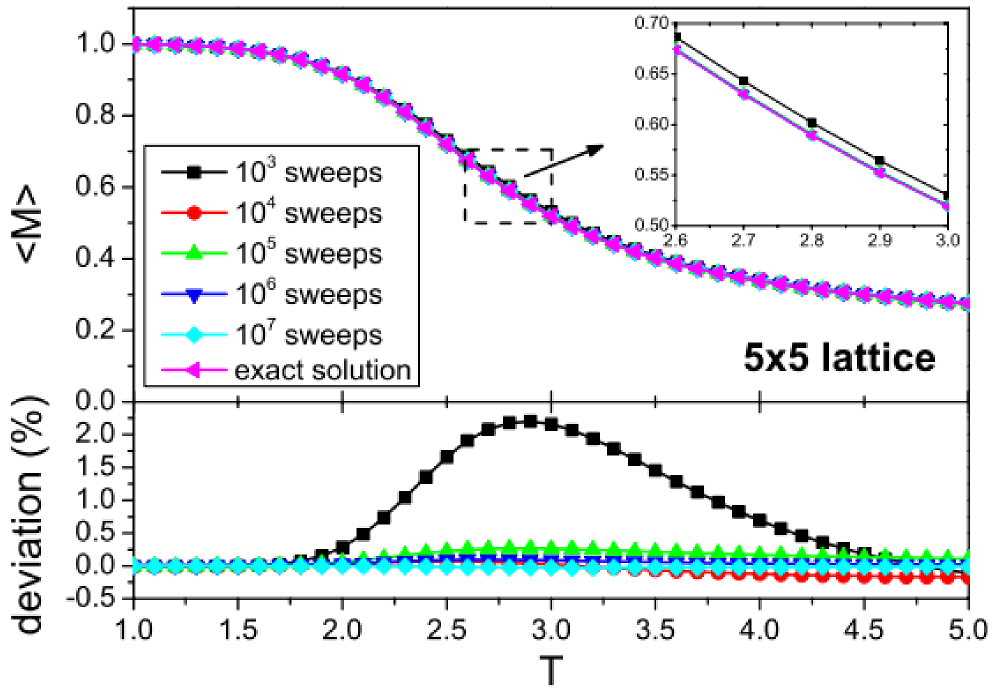


Fig. 1. T dependence of average absolute value of magnetization $\langle|M|\rangle$, of the 2-D Ising model with periodic boundary conditions, as described in text, for a square 5×5 lattice. Full symbols indicate results with varying numbers of sweeps, and the full symbols with dashed line the exact result. Bottom plot shows relative deviation to the exact result. Lines are eye-guides.

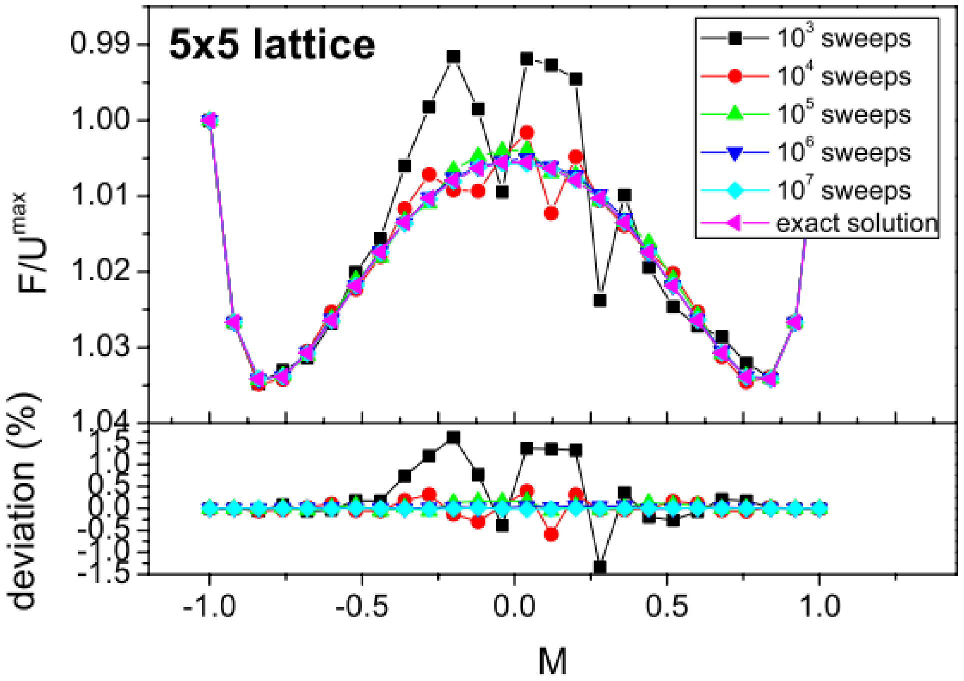


Fig. 2. Normalized free energy dependence on magnetization, of the 2-D Ising model with periodic boundary conditions, as described in text, for a square 5×5 lattice. Full symbols indicate results with varying numbers of sweeps, and the full symbols with dashed line the exact result. Bottom plot shows relative deviation to the exact result. Lines are eye-guides.

[1] J. S. Amaral et al., IEEE Trans. Magn. 50 1002204 (2014)

Random Path Sampling: Implementation (I)

The previous random configuration method:

```
for k = 1:REP
    %
    S_vector(:,1) = randsample([-1, 1],N_atm,true,[0.5,0.5]);
    M(k,1) = sum(S_vector(:,1));
    E(k,1) = function_Energy_Ising_2D_SS(L, S_vector);
    %
end
```

The RPS method:

```
for k = 1:REP % loop through all requested RPS loops
    %
    S_vector = ones(N_atm, 1); % vector with up spins
    SFV(:,1) = randperm(N_atm); % spin flip vector (sequence of spins to flip)
    %
    for q = 2:N_atm % loop through magnetization values
        %
        S_vector(SFV(q-1)) = -1; % flip the spin
        %
        E_new = - S_vector(SFV(q-1)) .* ( ...
            S_vector(nnxpos((SFV(q-1)))) + ...
            S_vector(nnxneg((SFV(q-1)))) + ...
            S_vector(nnypos((SFV(q-1)))) + ...
            S_vector(nnyneg((SFV(q-1))))); % energy of bonds to NN
        %
        E_all(k, q) = E_all(k, q-1) + 2*E_new; % build the energy matrix
        %
    end
    %
end
```

Random Path Sampling: Implementation (II)

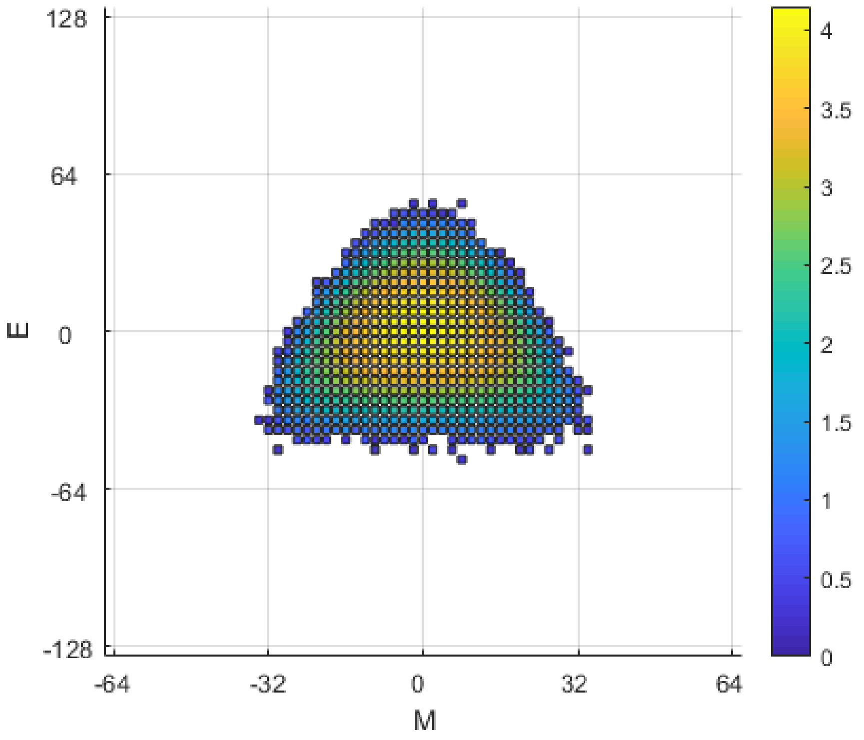
- For each RPS sweep, there are N_atm+1 (the number of possible magnetization values) configurations sampled
- We can easily benchmark both methods, taking this in mind:
  - RPS: L = 8, REP = 1E6 (65*1E6 sampled configurations)
    - RPS time 12.8726 seconds
    - (E,M) histogram time 43.3236 seconds
    - RPS + histogram time 56.1962 seconds
  - MC: L = 8, REP = 1E6 (1E6 sampled configurations)
    - MC time 35.4572 seconds
    - (E,M) histogram time 12.5676 seconds
    - MC + histogram time 48.0247 seconds
  - The RPS method is ~ 50 times faster, per sampled configuration

Random Path Sampling: Implementation (III)

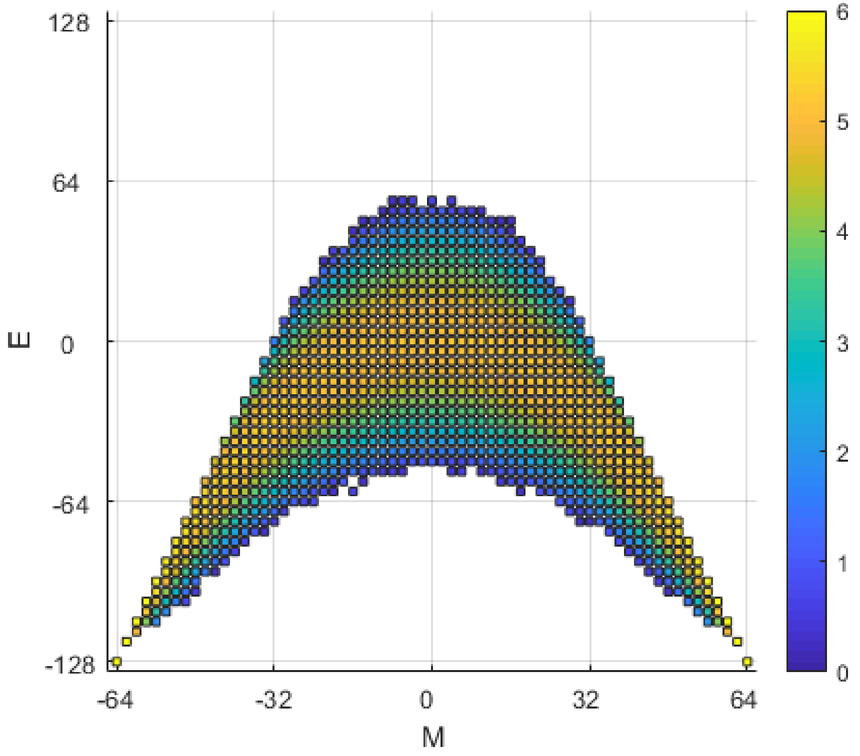
- The differences between both methods are simple in terms of outputs and building the histograms
  - The main RPS cycle builds an "E_all" matrix, which lists all observed energy values. Each column represents magnetization values between all spins up and all spins down
  - The magnetization histogram is flat, due to the method itself (by construction)
  - The sampling of the energy-magnetization phase space should be very different compared to the previous MC method
  - We should also be able to show how the JDOS estimate converges, and also that it converges to the exact value.
- The method itself has a simple concept and implementation, but still has difficulties coping with "large" systems like 8x8 and larger

Random Path Sampling: Phase space sampling performance comparison

- We can compare the (E,M) sampling histograms for both the simple MC and RPS methods, for the 8x8 system and REP=1E6



The MC method, as expected, samples the region near E=0,M=0



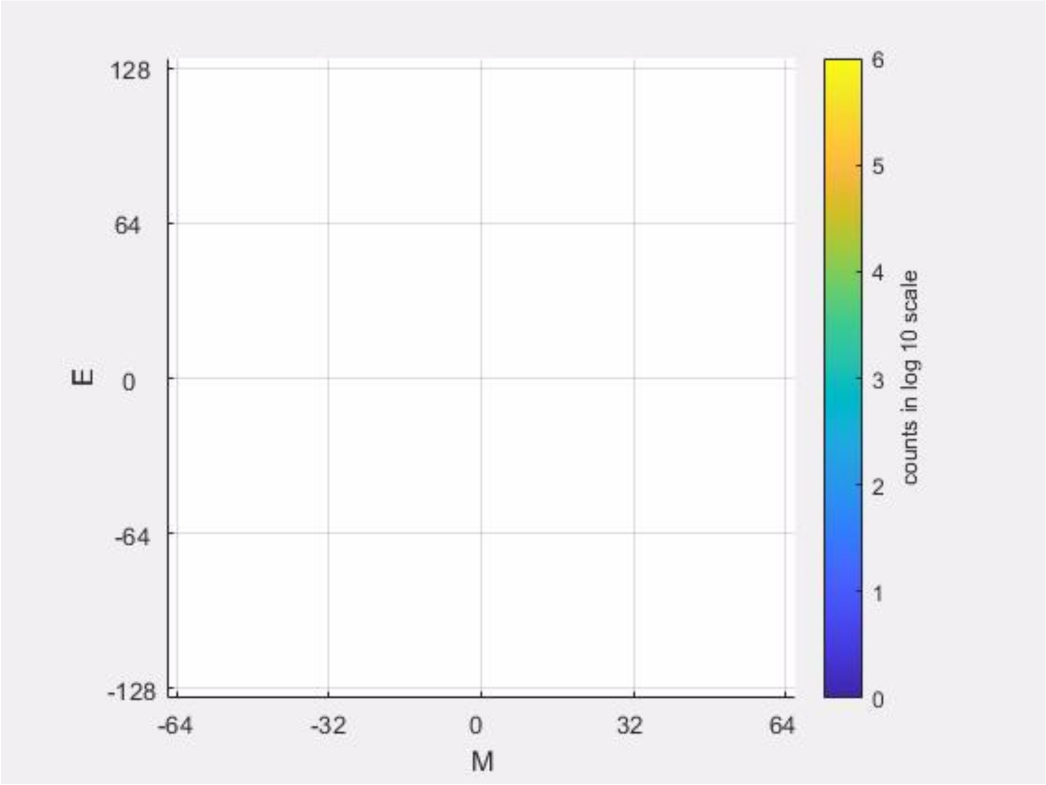
The RPS method extends the phase space sampling, but does not sample all possible states

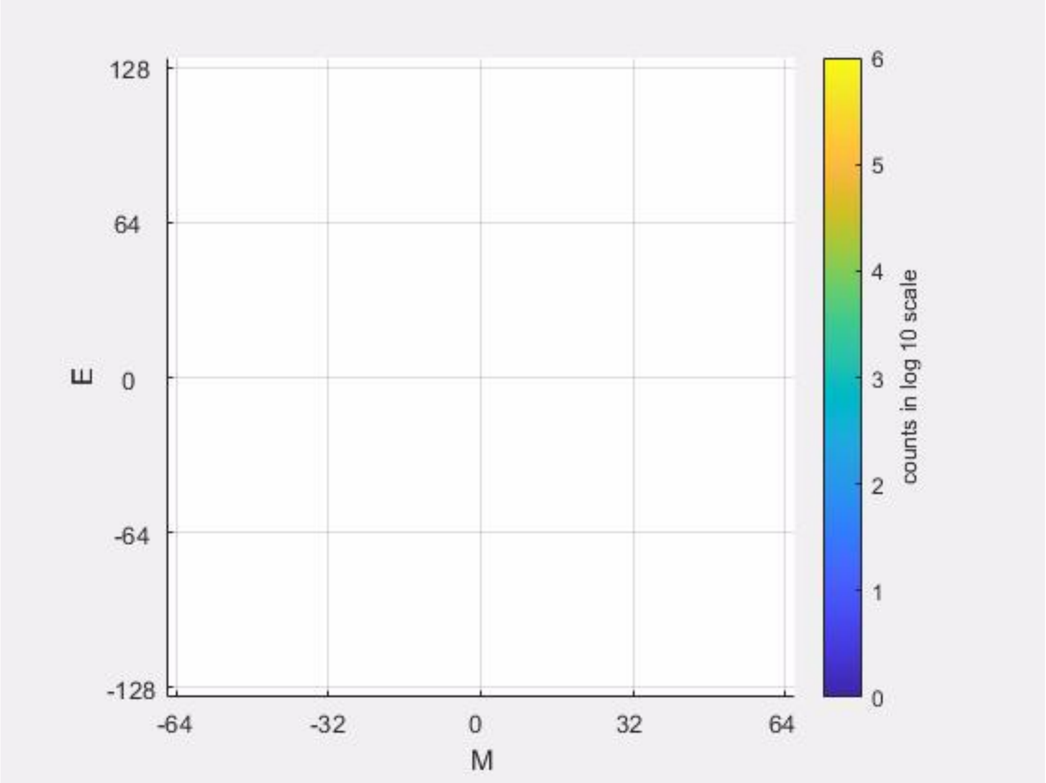
Random Path Sampling: Phase space sampling performance comparison (videos)

- The previous result becomes clearer if we compare the phase space sampling throughout

RPS method, L = 8; REP = 10^6

MC method, L = 8; REP = 10^6





Making videos from plots in Matlab

- One quick way to make videos in Matlab is by saving plots as video frames, easily done by using getframe:

```
plot(…)
drawnow()
F(framenumber) = getframe(gcf);
```

- The F variable is then a set of frames that can be easily visualized using matlab

```
fig = figure;
movie(fig,F,1)
```

- To save this variable to an .avi file, you can use the VideoWriter function in a for cycle:

```
fig = figure;
v = VideoWriter('video.avi');
open(v);
%
for k = 1:length(F(:))
   %
   movie(fig,F(k),1)
   frame = getframe(gcf);
   writeVideo(v,frame);
   %
end
%
close(v);
```

Overview

- You have two main Matlab scripts that estimate the JDOS of the 2D Ising model in a square lattice of a linear size L, with periodic boundary conditions. Each script uses a different Monte-Carlo method, one for a simple approach of generating random configurations, and the other for the RPS method
- Using the provided scripts and code for making videos, can you reproduce the videos shown in slide 15?

WORK!

The Wang-Landau method

- The Wang-Landau method is another MC method that allows to estimate the JDOS of the 2D Ising model. It has its advantages and disadvantages. It is considerably more complex than the two previous approaches, so we will focus on its main points

Wang-Landau method [2001]

VOLUME 86, NUMBER 10 PHYSICAL REVIEW LETTERS 5 MARCH 2001

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Our algorithm is based on the observation that if we perform a random walk in energy space with a probability proportional to the reciprocal of the density of states $\frac{1}{g(E)}$, then a flat histogram is generated for the energy distribution. This is accomplished by modifying the estimated density of states in a systematic way to produce a "flat" histogram over the allowed range of energy and simultaneously making the density of states converge to the true value. At the very beginning of the random walk, the den-

The Wang-Landau method in practice

- A random walk in phase space, starting in a random configuration
- The success ratio of each random walk step is the ratio between the JDOS of the current and target point in E,M phase space.
- The JDOS itself starts as a constant number (e.g. 1), which is updated throughout the random walk steps by multiplying its value by the JDOS update weight factor, f
- A histogram is built counting both accepted and rejected steps, until it is considered “flat”. When that happens f is updated (ex: starting with value f=2, and when the histogram is flat, f = sqrt(f); the histogram is cleared
- The main parameters are the flatness criteria (e.g. p = 0.95), and the lowest limit weight number of the JDOS update (e.g. f = 1 + 10^-8)

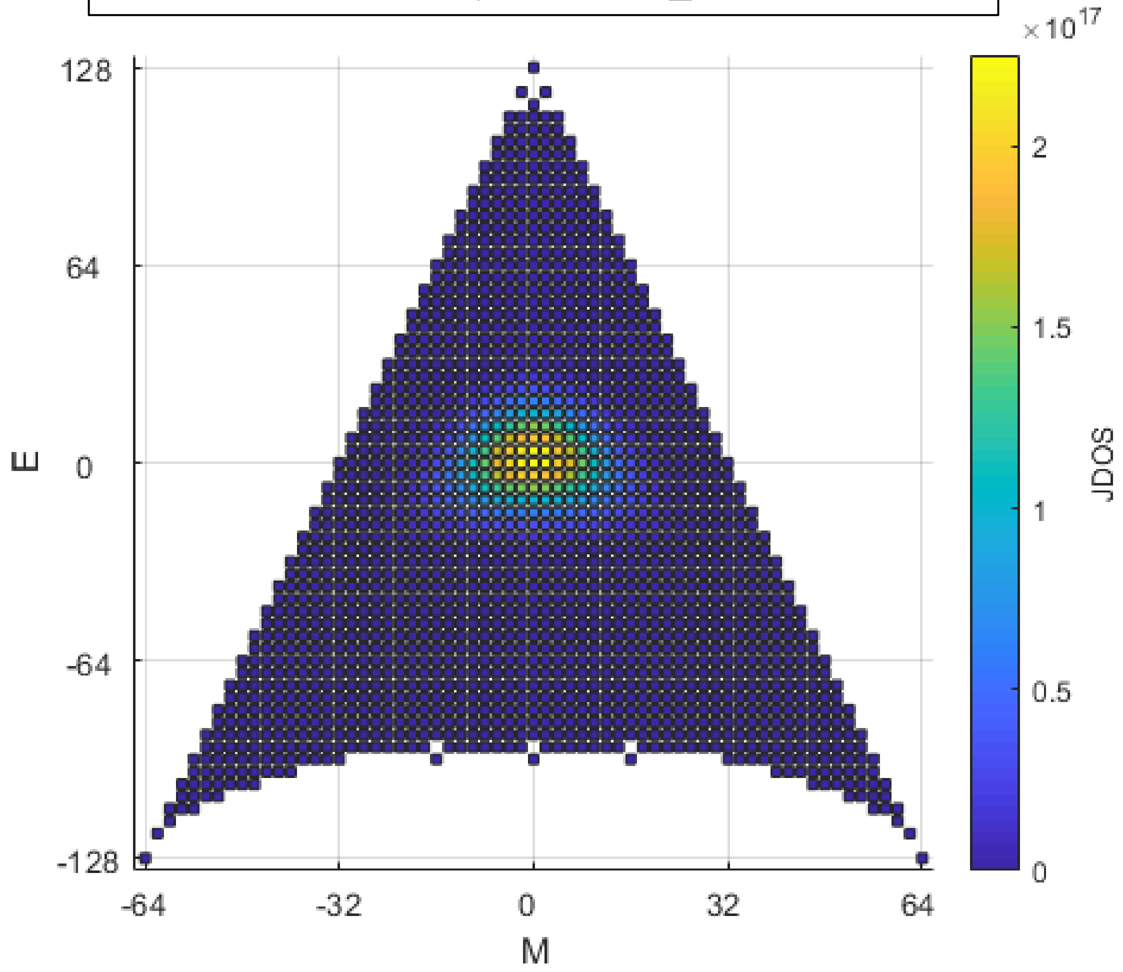
D. P. Landau, Shan-Ho Tsai, and M. Exler, "A new approach to Monte Carlo simulations in statistical physics: Wang-Landau sampling," Am. J. Phys. **72**, 1294–1302 (2004)

http://stp.clarku.edu/simulations/ising/wanglandau/index.html

Wang-Landau JDOS estimate for 8x8

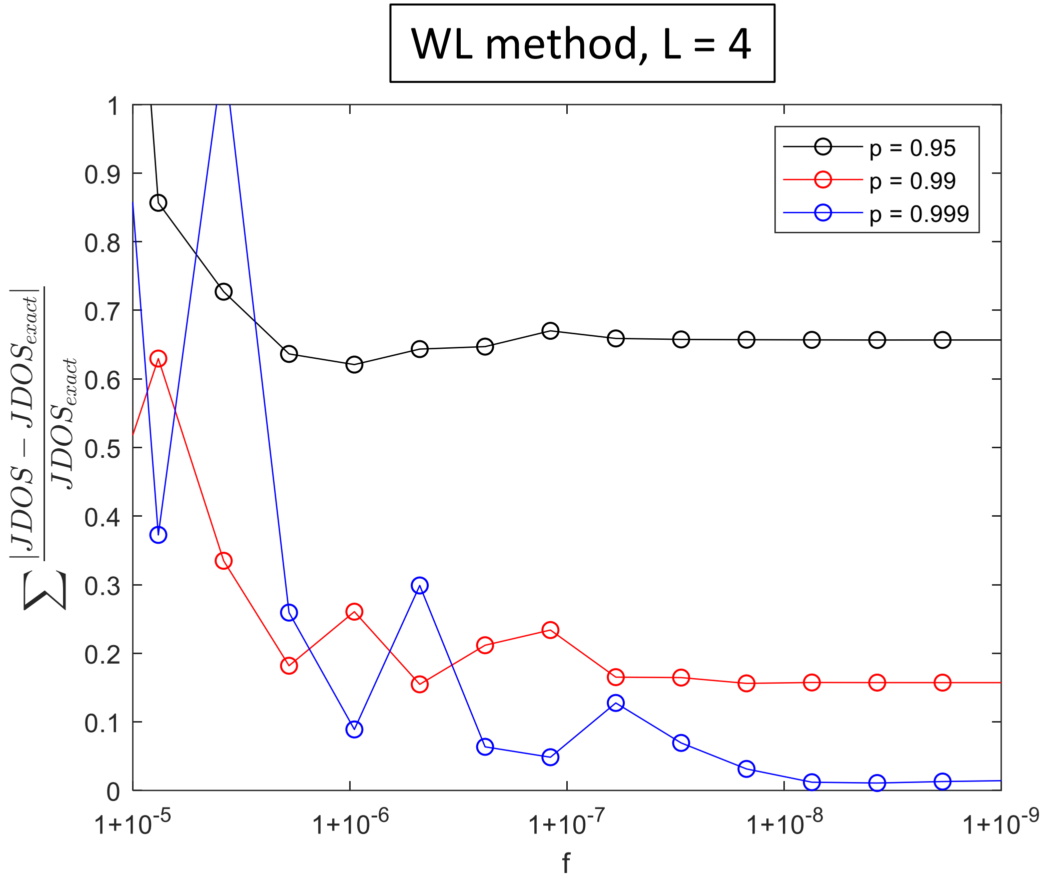
- As the histogram is cleared throughout the method, the way to visualize the phase space sampling is to look at the JDOS result
- This WL run had very rough parameters, and took about 5 hours to run
- The phase space is completely sampled, but this does not tell us about the convergence or accuracy of the method
- By construction of the method, the phase space should be completely explored when the JDOS is first updated

WL method, L = 8; p = 0.75; f_min = 1 + 1E-4



Convergence and accuracy of the WL method

- For the 4x4 lattice we can compare the deviation from the exact result, and see that while the JDOS estimate converges, there will always be a deviation
- The WL method (by construction) will sample the full phase space efficiently, but the final JDOS accuracy will depend on the parameters used [1].



[1] C. Zhou and R. N. Bhatt, Understanding and improving the Wang-Landau algorithm, PHYSICAL REVIEW E 72, 025701 (2005)

Conclusions

- While simple in construction, the Ising model is rich in physics, together with practical use in the computational materials design of ferromagnets
- The thermodynamics of the model can be obtained from the joint density of states (JDOS), which is a list of all possible spin configurations with a given energy and magnetization pair of values, together with their degeneracy
- For large system sizes the number of possible configurations is too large to list, so Monte-Carlo (MC) methods can be employed
- We have covered three different MC methods to estimate the JDOS of the Ising model: the simple generation of random configurations, the RPS method and Wang-Landau methods
- These methods explore the phase space in different ways, and visualization helps to clearly and efficiently show their strengths and weaknesses

What I expect

- That you can adequately show via plots and videos how these three Monte-Carlo methods work, and behave differently in terms of
  - Phase space exploration
  - Convergence and accuracy

- In the process, I hope some of the Matlab plot/video tricks you have learned will be useful for you in the future

- The required report for your module 1 evaluation will focus on phase space exploration and convergence/accuracy of the 4x4 Ising lattice with periodic boundary conditions. The exact JDOS solution for that system has been made available.

END