Computational Physics

Lecture 8

Organisation of the course - Program

Mar 22 – Introduction to Monte-Carlo and Ising model

Mar 29 – Good Friday Bank Holiday → No class

Apr 05 – Choice of units, energy of the system

Apr 12 – Individual discussions

Second project deadline: Thursday April 25 (midnight)

Second project reports

- Deadline 25/04 - midnight.
- Submit report + code for the group on *Brightspace*.
- If you use *github*, you must also submit a code copy to *Brightspace*.
- See score sheet on *Brightspace*.
- See also the coding guidelines.

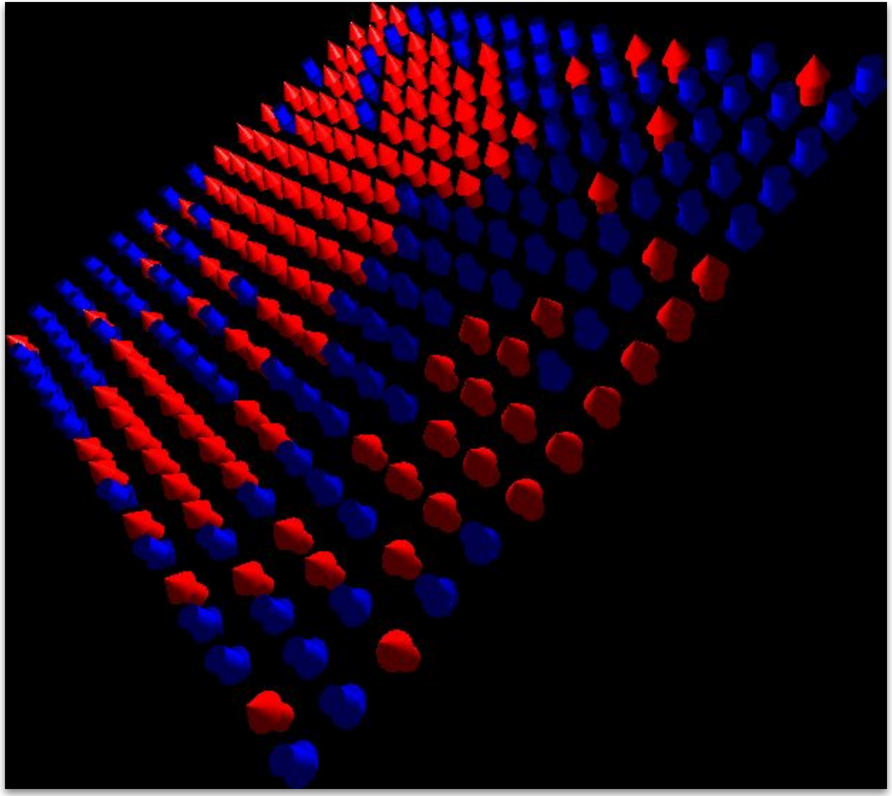
Questions?

Project 2: Monte-Carlo simulation of the Ising model

Last lecture's summary

- Considered a **2D lattice of spins** at different temperatures to study the emergence of ferromagnetism.
- Identified **very high-dimensional integrals** that can only realistically be computed via ***Monte-Carlo* integration**.
- Considered **Markov chains** as way to **sample only the important part** of the integration space.
- Derived the **Metropolis algorithm** to "go towards" and "hop around" the **equilibrium** configuration.

Goal: Ferromagnetic behaviour in a 2D material



$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i$$

The Ising model - Algorithm

1) Start with a random state x_0 (say all spin up. Or all spin random)

2) ***Try*** a different state x'
   (i.e. a different configuration by flipping just one spin!)

3) - If $E(x') < E(x)$ → Keep that new state.
   - If $E(x') > E(x)$ → Keep that state with probability $p(x')/p(x)$. Otherwise stay.

4) Go back to (2).

Recall, the energy is:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i$$

Speeding things up

We want to compute the **ratio of probabilities**.

Let's start by using exponential rules:

$p(x_1)/p(x_2) = \exp(-\beta(E_1 - E_2))$

Recall:

$$p\left(x\right) \propto e^{-\beta H(x)}$$

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$$p(x) \propto e^{-\beta H(x)}$$

$p(x_1)/p(x_2) = \exp(-\beta(E_1 - E_2))$

Also:

When flipping one spin, **no need to recompute the whole energy**. Just need the change. Only 4 terms in the grid have changed. That's cheap.

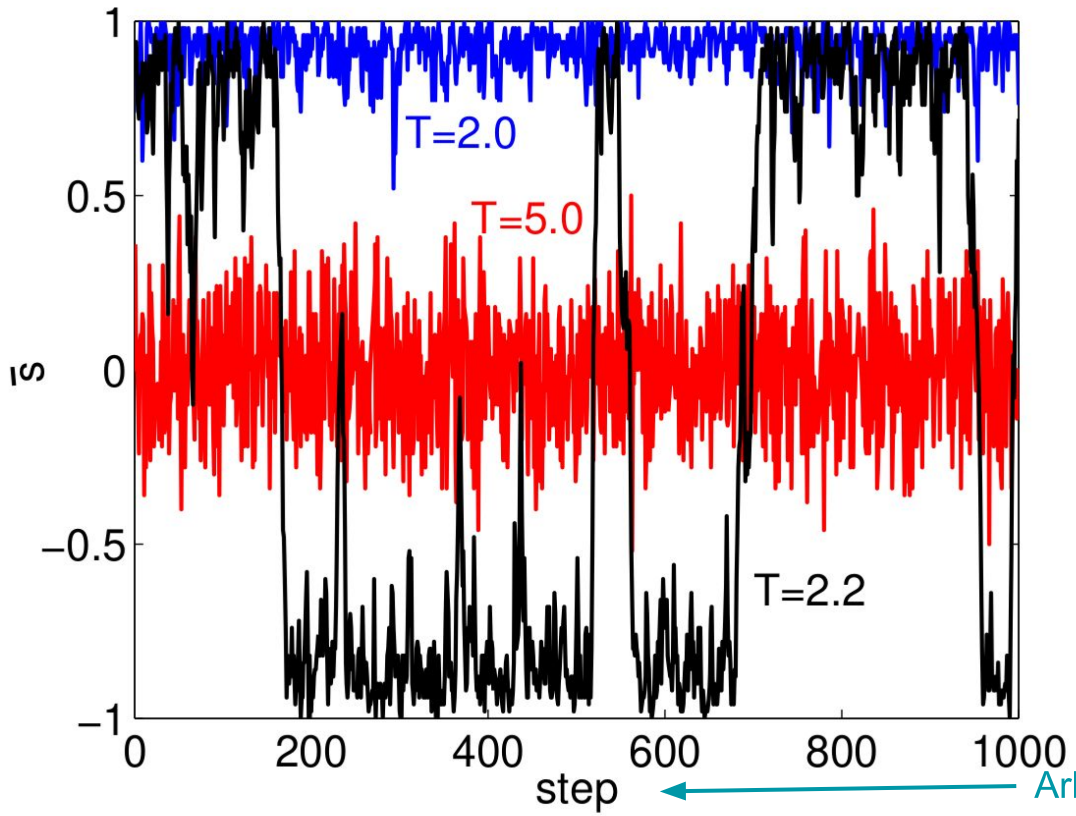
Measuring quantities

Measuring quantities

- We want to **average** out over multiple **random states** at a given T.

- How much should we wait ***in between*** separate measurements?

Example: Evolution of the mean spin



Note:
Plot made using a <u>very small</u> N

Arbitrary units

Measuring quantities

- We want to **average** out over multiple **random states** at a given T.

- How much should we wait ***in between*** separate measurements?

- We want to estimate the **correlation time $\boldsymbol{\tau}$**. The time it takes for the system to **"forget"** its previous state.

Correlation time

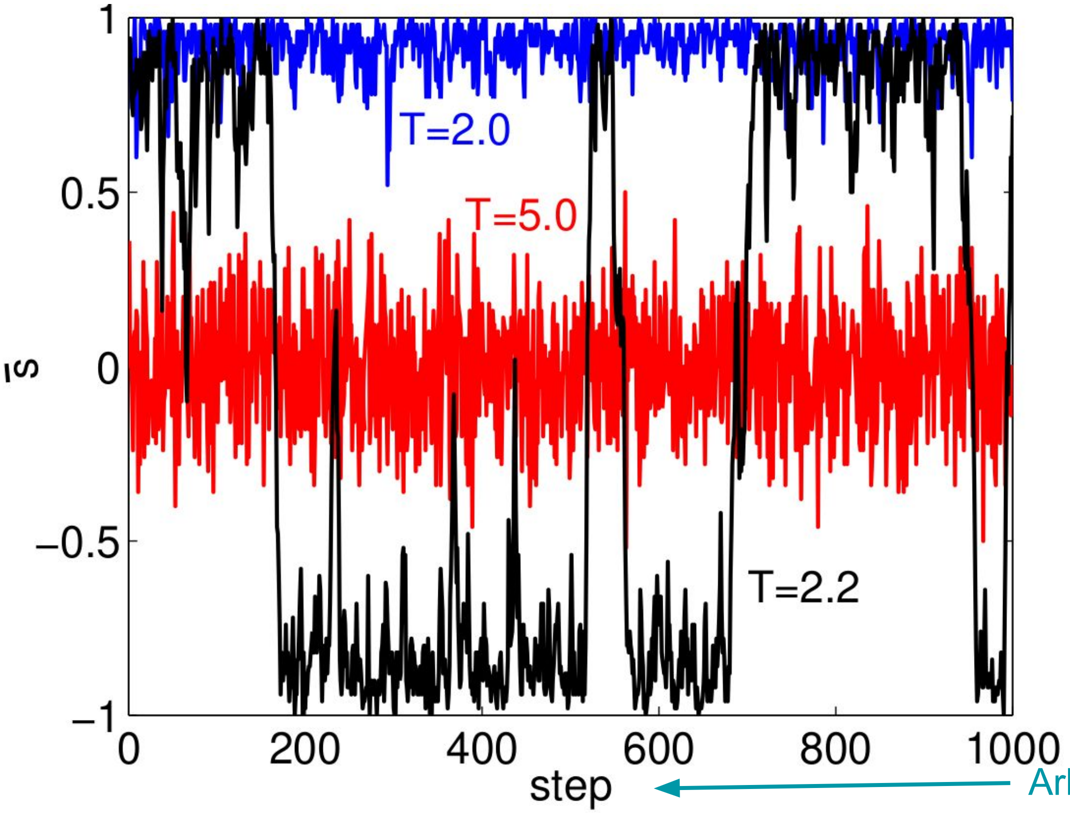
We want to measure how much a quantity m at time t' **is related to** that same quantity at time $t' + t$.

For instance:

If at t', m is larger (say) than the average.
Then at $t' + t$, it will also be above the average if t is smaller than the correlation time.

If it t is larger than the correlation time then m as that time is equally likely to be anything.

Example: Evolution of the mean spin



Arbitrary units

Autocorrelation time

We can evaluate the **autocorrelation time**:

How different from mean at time t’ + t

How different from mean at time t’

$$\begin{aligned}\chi(t) &= \int \underline{\left(m\left(t'\right) - \langle m\rangle\right)}\,\underline{\left(m\left(t'+t\right) - \langle m\rangle\right)}\,dt' \\ &= \int \left(m\left(t'\right) m\left(t'+t\right) - \langle m\rangle^2\right) dt'.\end{aligned}$$

“Average” over all t’

Discrete version

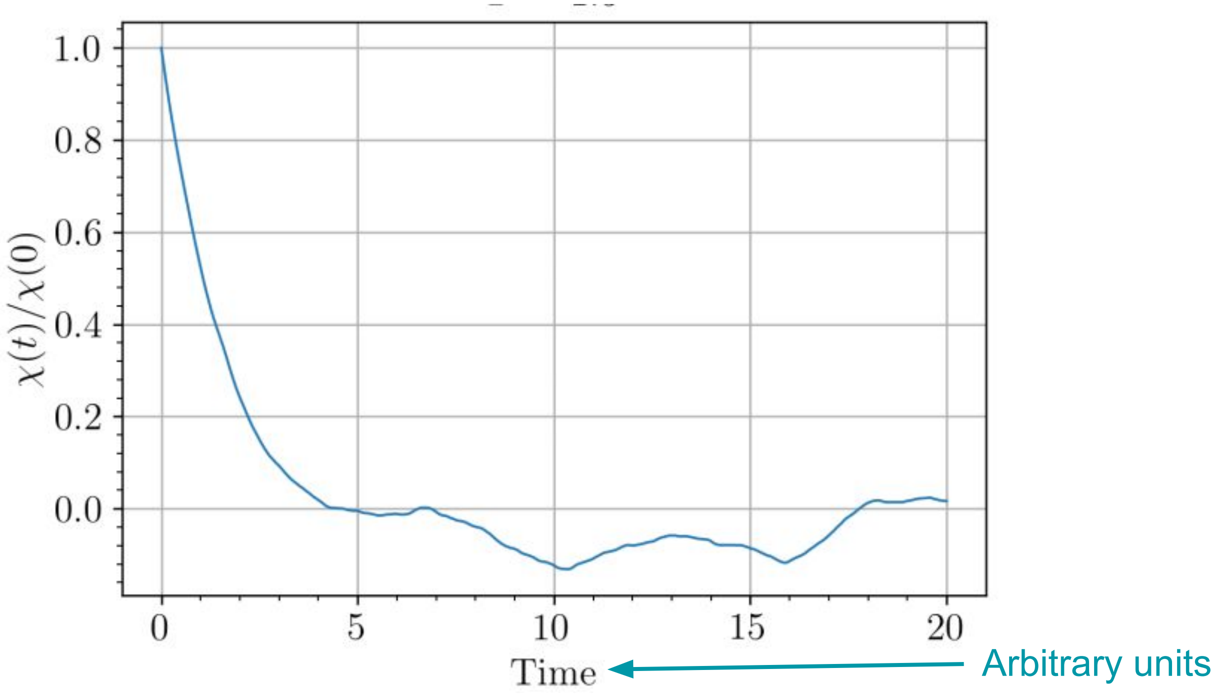
We can't integrate to infinity in the simulation and we are dealing with discrete times so we need to slightly alter the expression:

$$\begin{aligned}\chi(t) \;=\; & \frac{1}{t_{\mathrm{max}}-t}\sum_{t'=0}^{t_{\mathrm{max}}-t} m(t')\,m(t'+t) \\ & -\frac{1}{t_{\mathrm{max}}-t}\sum_{t'=0}^{t_{\mathrm{max}}-t} m(t') \times \frac{1}{t_{\mathrm{max}}-t}\sum_{t'=0}^{t_{\mathrm{max}}-t} m(t'+t)\end{aligned}$$

t_{max} is the end time (final sweep) of our simulation.

Shape of the function

Trying this on the simulations you will find that this time autocorrelation function looks like:



Shape of the function

Trying this on the simulations you will find that this time autocorrelation function looks like:

$$\chi(t) \approx \chi(0)\, e^{-t/\tau}$$

This defines the **correlation time τ**.

Computing $\boldsymbol{\tau}$

Solving for $\boldsymbol{\tau}$, we find:

$$\int_0^\infty \frac{\chi(t)}{\chi(0)} = \int_0^\infty e^{-t/\tau} dt = \tau$$

In practice, we use a **sum** instead of an integral and stop summing when $\square(t) < 0$.

Why?

Questions?

Thermal averaging

Measuring the mean of the spin (or other) is relatively **straightforward**. We can average after every sweep or **after every τ time**.

Measuring the **std. dev. is harder** because of the correlation.

One can show that $$\sigma = \sqrt{\frac{2\tau}{t_{\max}}\left(\langle m^2\rangle - \langle m\rangle^2\right)}$$ is a good choice.

This takes into account the finite number of sweeps even if $t_{max} >> \tau$.

Goals of the project

We want to measure the **mean** and **std. dev.** of the following for N^2 spins:

- Mean absolute spin: $$\langle | m | \rangle = \frac{1}{N^2} \langle | \sum_i s_i | \rangle$$
- Energy per spin: $$e = E/N^2$$
- Magnetic susceptibility: $$\chi_M = \frac{\beta}{N^2} \frac{\partial \langle M \rangle}{\partial H} = \frac{\beta}{N^2} \underline{\left(\langle M^2 \rangle - \langle M \rangle^2 \right)}$$
- Specific heat per spin: $$C = \frac{\partial E}{\partial T} = \frac{1}{N^2 k_B T^2} \frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{1}{N^2 k_B T^2} \underline{\left(\langle E^2 \rangle - \langle E \rangle^2 \right)}$$

Block Measurements

Measuring C and $\square_{\mathrm{M}}$ can be **problematic** as it is hard to get a good std. dev.

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Measuring C and $\square_{M}$ can be **problematic** as it is hard to get a good std. Dev.

This is where the **blocking method** enters.

1. Divide the measurements into (time) blocks.
2. Measure the average in each block.
3. Estimate the std. dev. in the normal way by combining the blocks.

How big should the blocks be?

Block Measurements

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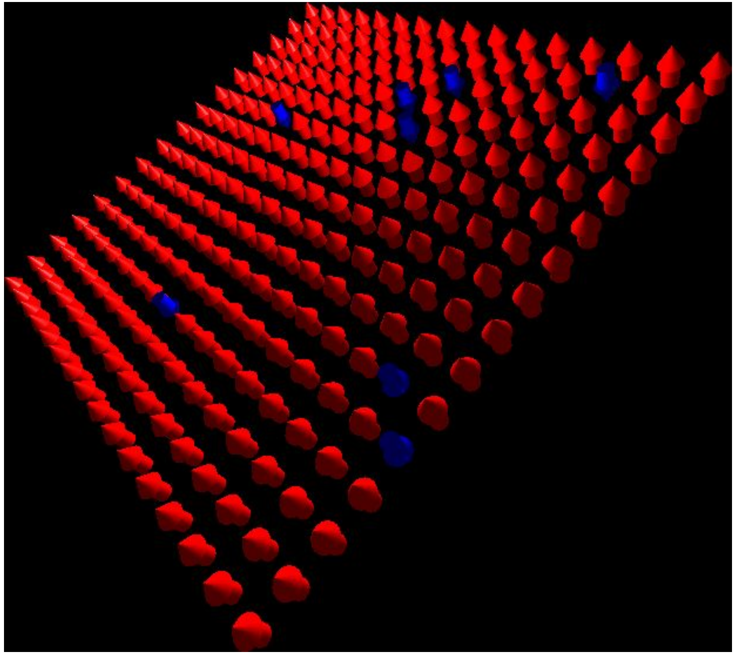
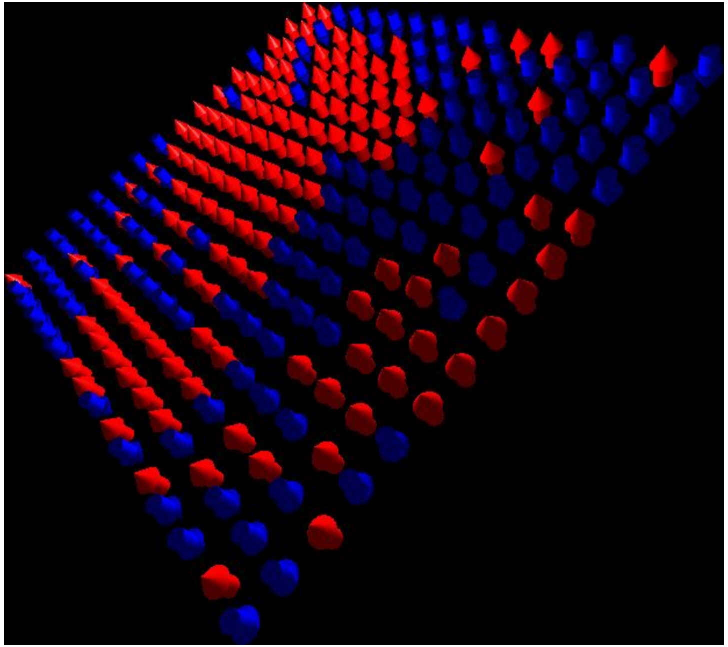
How big should the blocks be?

Clearly **longer than τ**. Otherwise the fluctuations are underestimated.

For this project a block length of **16τ** is reasonable.

Goal of the project





Final Milestones

- Study the system at **different equilibrium** temperatures from T=1 to T=4 in steps of 0.2 (in units where $J = k_B = 1$).

- **Measure τ** *after the system has reached equilibrium* and plot it as a function of *T*. **Observe what happens** around the critical temperature $T_c = 2.269$.

- Measure, **for each T**, the **average** and **standard deviation** of the magnetization per spin, energy per spin, magnetic susceptibility per spin, and specific heat per spin. **Use the block technique** for the latter two quantities.

- Comment on your findings!

Happy simulating !

Questions?

Extensions

To get the final 10% grade on the project, tackle ***one*** of the following:

1. Study the *3D* Ising model (try for instance a 25x25x25 model).
   Does it have a phase transition around a critical temperature? If so, what T_{cr}?

2. Study what happens when the second term in the Hamiltonian (the external field) is included.

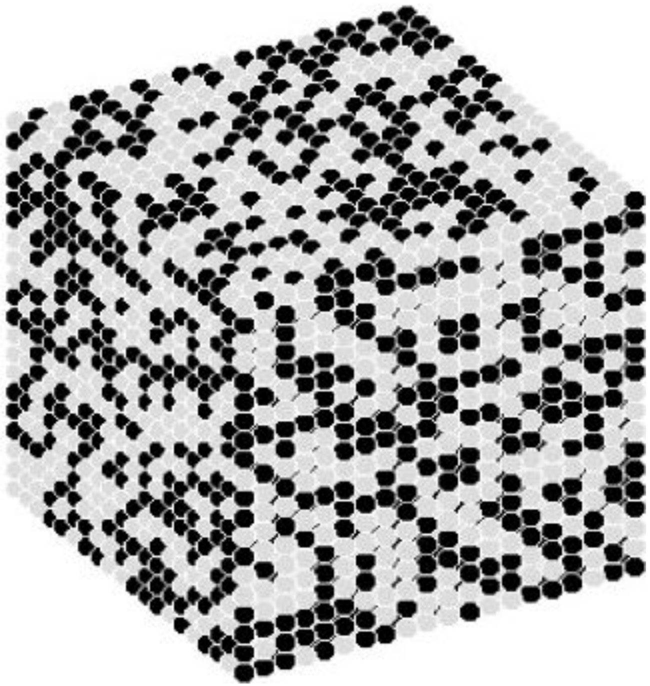
3. The Ising model only considers direct neighbours. What happens if you use more neighbours? And maybe an interaction strength depending on distance?

Extension option 1 - Three dimensions

- Is there a phase transition ?
- If so, what is its temperature?

Problem has no known analytic solution

→ let’s simulate!



Extension option 2 - External field

What happens if we switched on the external magnetic field?

Study what happens when H is increased. Is there still a phase transition?

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - \boxed{H \sum_i s_i}$$

Extension option 3 - Different neighbouring rules

The base Ising model uses direct neighbours only.

What if we consider interactions with longer range? Or with a strength that depends on distance?

Is there still a phase transition?