



Computational Physics (PHYS6350)

Lecture 19: Problems in statistical physics

- Markov chain and Metropolis algorithm
- Ising model

Reference: Chapter 10 of *Computational Physics* by Mark Newman

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Course materials: <https://github.com/vlvovch/PHYS6350-ComputationalPhysics>

Online textbook: <https://vovchenko.net/computational-physics/>

Thermodynamic averages

For a system in statistical equilibrium at given temperature, the probability that the system is in microstate i is given by the Boltzmann formula:

$$P(E_i) = \frac{e^{-\beta E_i}}{Z}$$

$\beta = 1/(k_B T)$ is the inverse temperature

E_i is the energy in state i

$Z = \sum_i e^{-\beta E_i}$ is the partition function.

Main interest typically lies in calculating the average of various physical observables.

For an arbitrary quantity X it reads

$$\langle X \rangle = \sum_i X_i P(E_i)$$

How to calculate $\langle X \rangle$?

Thermodynamic averages and importance sampling

One possible way to estimate $\langle X \rangle$ is to sample each microstate uniformly at random, calculate X_i and accept with a weight proportional to $P(E_i)$. If we have N samples, the estimate for $\langle X \rangle$ reads

$$\langle X \rangle = \frac{\sum_{k=1}^N X_k P(E_k)}{\sum_{k=1}^N P(E_k)} = \frac{\sum_{k=1}^N X_k e^{-\beta E_k}}{\sum_{k=1}^N e^{-\beta E_k}}$$

This method does not require the evaluation of the partition function Z .

However, the method is not very efficient because it will typically sample states that do not contribute much to the result due large penalty from the Boltzmann factor $e^{-\beta E_k}$

Importance sampling: Sample the microstates directly from the Boltzmann distribution $P_i \propto e^{-\beta E_i}$

$$\langle X \rangle = \sum_i X_i P(E_i) \simeq \frac{1}{N} \sum_{k=1}^N X_k$$

Markov chain method

How to pick states from $P_i = e^{-\beta E_i} / Z$?

Markov chain method:

- Iterative procedure
- Move from state i to state $j \rightarrow$ Transition probability T_{ij}

$$\sum_j T_{ij} = 1$$

- Choose T_{ij} such that

$$\frac{T_{ij}}{T_{ji}} = \frac{P_j}{P_i} = \frac{e^{-\beta E_j} / Z}{e^{-\beta E_i} / Z} = e^{-\beta(E_j - E_i)}$$

- No need to compute the partition function Z

If state i is drawn from Boltzmann distribution $P_i = e^{-\beta E_i} / Z$ the probability to have state j in next step is

$$\sum_i T_{ij} P_i = \sum_i T_{ji} P_j = P_j \sum_i T_{ji} = P_j.$$

also follows Boltzmann distribution

Metropolis algorithm (a.k.a. Metropolis-Hastings algorithm)

Metropolis algorithm is a way to simulate the Markov chain such that $\frac{T_{ij}}{T_{ji}} = \frac{P_j}{P_i} = \frac{e^{-\beta E_j} / Z}{e^{-\beta E_i} / Z} = e^{-\beta(E_j - E_i)}$

Suppose we can make M moves from state i to a new state j – a *move set*.

- Pick a candidate next state j uniformly at random (the probability is $1/M$).
- Calculate the energy E_j of the candidate state j and compare it to the energy E_i of the current step i
 - If $E_j < E_i$, the move is unconditionally accepted.
 - If $E_j > E_i$, the move is accepted with a probability

$$P_a = e^{-\beta(E_j - E_i)}.$$

Consider the transition probabilities for the case $E_j > E_i$

- $i \rightarrow j$:
$$T_{ij} = \frac{1}{M} e^{-\beta(E_j - E_i)}$$

- $j \rightarrow i$:
$$T_{ji} = \frac{1}{M}$$

therefore
$$\frac{T_{ij}}{T_{ji}} = \frac{P_j}{P_i} = \frac{e^{-\beta E_j} / Z}{e^{-\beta E_i} / Z} = e^{-\beta(E_j - E_i)}$$

Ideal gas in a finite volume

Recall the energy states of a particle in box of length L

Solving the *Schroedinger equation* $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x)$ with boundary conditions $\psi(0) = \psi(L) = 0$

Energy levels: $E_n = \frac{\pi^2 \hbar^2}{2mL^2} n^2, \quad n = 1, 2, \dots$ **3D:** $E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2), \quad n_x, n_y, n_z = 1, 2, \dots$

Ideal gas:

$$E = \sum_{i=1}^N E_{n_x^{(i)}, n_y^{(i)}, n_z^{(i)}} \quad n_x^{(i)}, n_y^{(i)}, n_z^{(i)} \text{ enumerate the microstates}$$

The probability to have a particular state is given by the Boltzmann distribution $P \propto e^{-\beta E}$

Metropolis algorithm: pick a random particle and change one of its energy indices by ± 1

Ideal gas in a finite volume

```
# Simulates the ideal gas of N particles at temperature T
# by performing Markov chain steps using Metropolis algorithm
# Returns an array energies normalized by the number of particles times the temperature
def simulateIdealGas(T, N, steps, periodicBC):
    # Initialization
    n = np.ones([N,3],int)
    E = 0
    for i in range(N):
        E += En(n[i], periodicBC)

    # Energy per particle normalized by T
    eplot = [ E / (N * T) ]

    for k in range(steps):
        # Choose the particle
        i = np.random.randint(N)
        # Choose the component
        j = np.random.randint(3)
        tn = n[i].copy()
        # Choose the direction
        if (np.random.rand() < 0.5):
            tn[j] += 1
        else:
            tn[j] -= 1

        # If n becomes negative, by symmetry set it to positive (periodic BC)
        if (tn[j] == -1 and periodicBC):
            tn[j] = 1

        # Avoid n = 0 states if not periodic BC
        if (tn[j] == 0 and not periodicBC):
            tn[j] = 1

        # Energy difference
        dE = En(tn, periodicBC) - En(n[i], periodicBC)

        if (np.random.rand() < np.exp(-dE/T)):
            n[i,j] = tn[j]
            E += dE

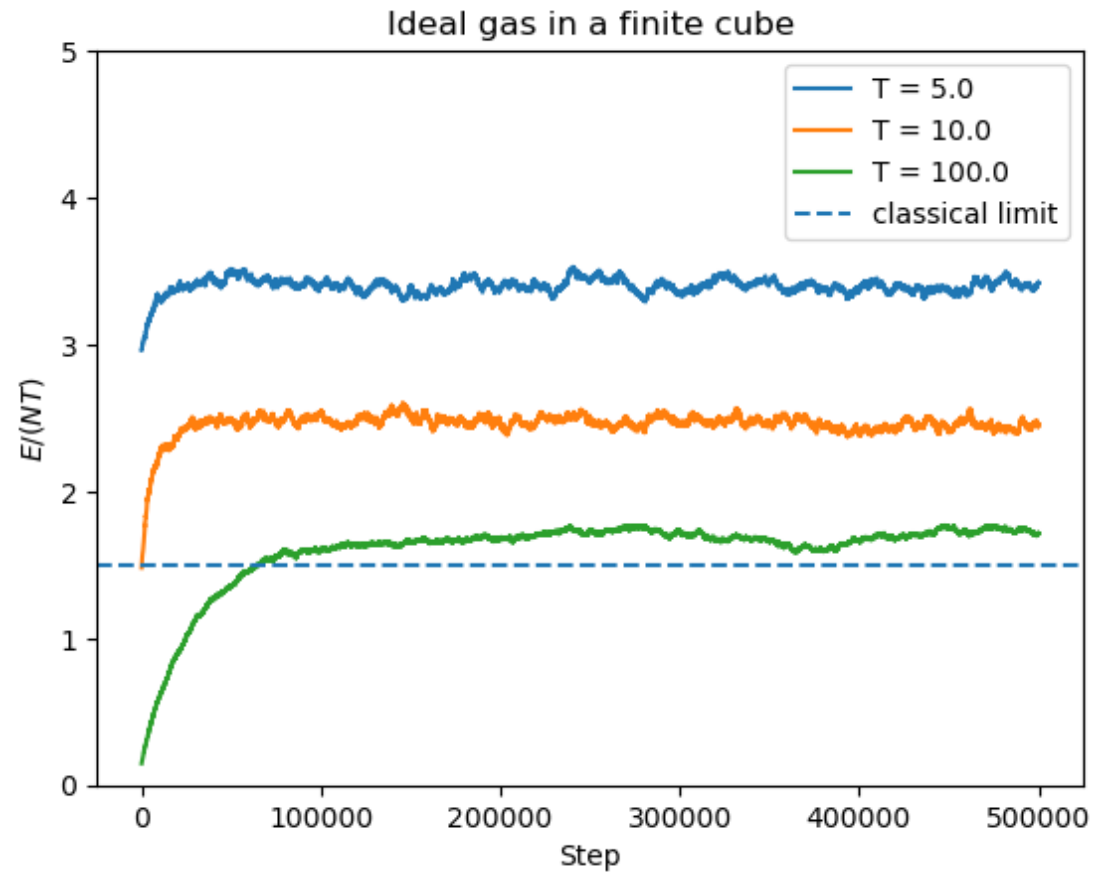
    eplot.append(E / (N * T))

    return eplot
```

```
# Calculate energy of a particle in a state n = (nx,ny,nz)
# periodicBC: apply periodic BC
def En(n, periodicBC):
    nx = n[0]
    ny = n[1]
    nz = n[2]
    factor = 0.5
    if (periodicBC):
        factor = 2.
    return factor * np.pi**2 * (nx**2 + ny**2 + nz**2)
```

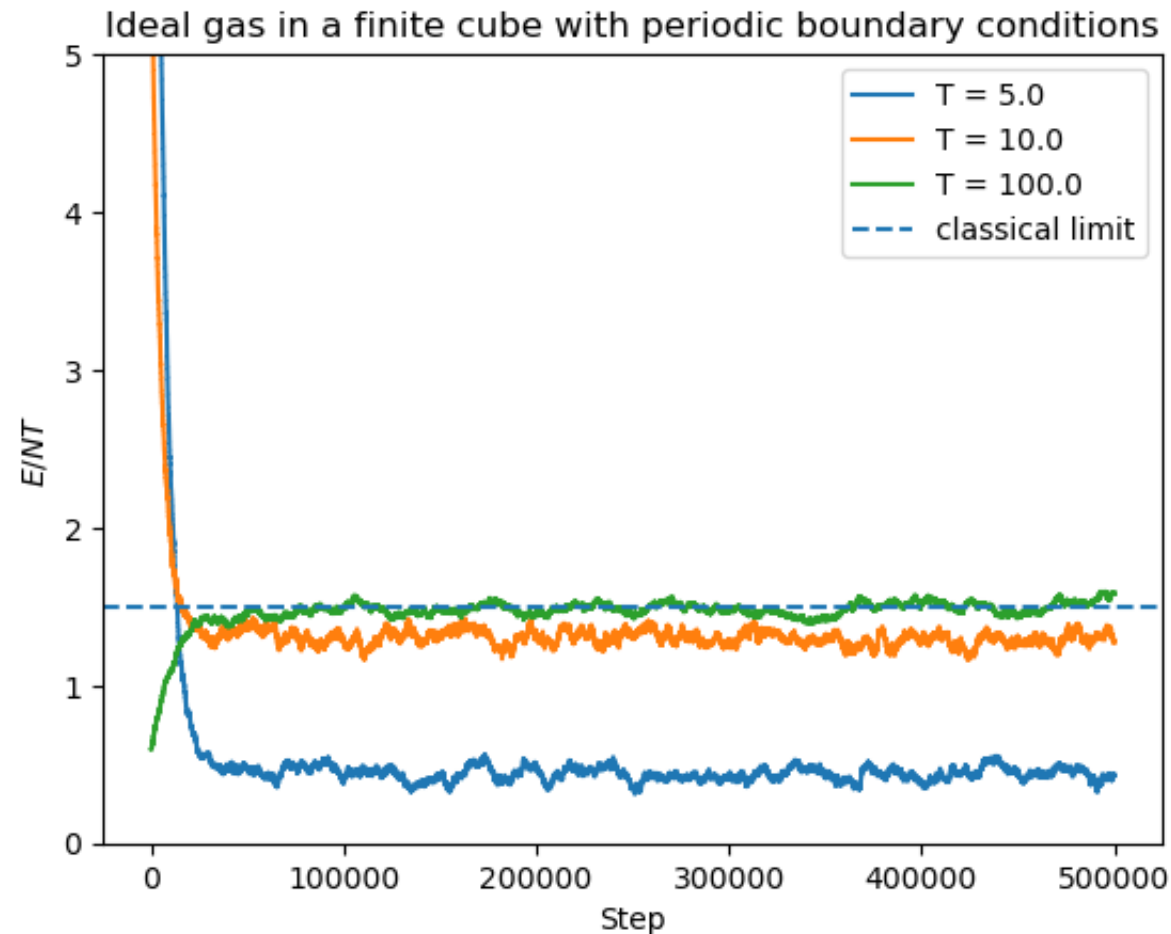
Ideal gas in a finite volume

```
N = 1000  
steps = 500000  
periodicBC = False  
Ts = [5., 10., 100.]
```



Ideal gas in a finite volume with periodic boundary conditions

Periodic boundary conditions: $\psi(x) = \psi(x + L)$ \longrightarrow $E_{n_x, n_y, n_z} = \frac{2\pi^2 \hbar^2}{mL^2} (n_x^2 + n_y^2 + n_z^2), \quad n_x, n_y, n_z = 0, 1, \dots$



2D Ising model

Ising model represents a system of spins (magnetic dipoles) on a lattice.

Without external magnetic field, the energy reads

$$E = -J \sum_{\langle ij \rangle} s_i s_j$$

$J > 0$: ferromagnetic, sum over neighbors only

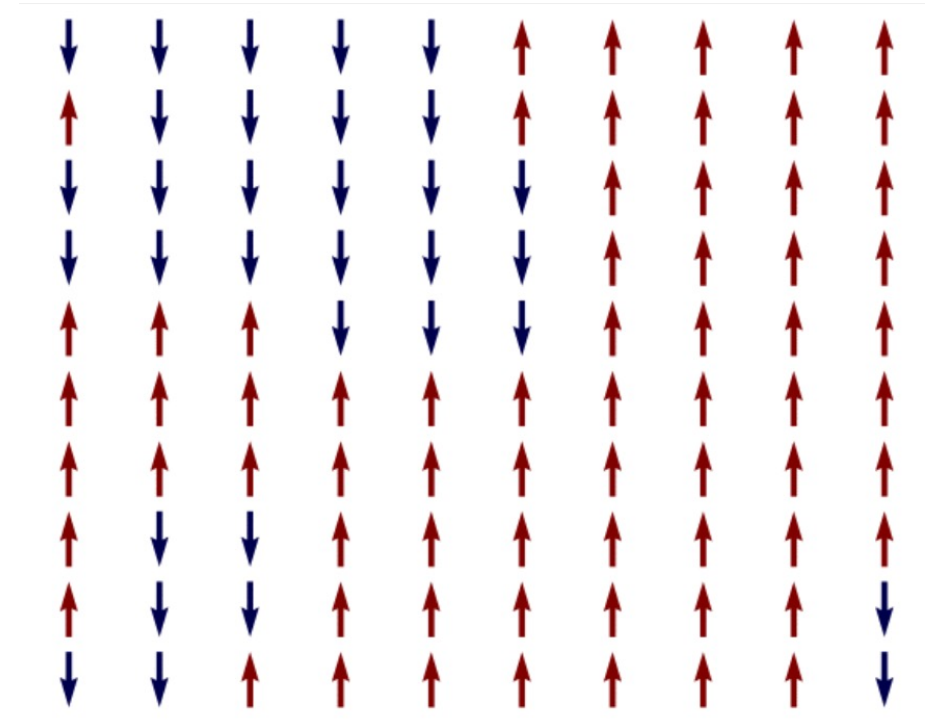
Magnetisation:

$$M = \sum_i s_i$$

Below the Curie temperature

$$\frac{k_B T_C}{J} = \frac{2}{\ln(1 + \sqrt{2})} = 2.27$$

exhibits spontaneous magnetization $|M| > 0$



2D Ising model

Metropolis algorithm for 2D Ising model:

- At each step have spin configuration s_i
- Randomly pick a spin i and flip its orientation, $s_i \rightarrow -s_i$
- Calculate the energy difference

$$\Delta E = 2J \sum_j s_i s_j$$

- Accept the new state with probability

$$P_a = e^{-\Delta E/T}$$

2D Ising model

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- Accept the new state with probability

$$P_a = e^{-\Delta E/T}$$

```
# Simulates the 2D Ising system of NxN spins at temperature T
# by performing Markov chain steps using Metropolis algorithm
# Returns arrays energies and magnetizations at each step
def simulateIsing(T, N, steps):
    spins = -1 + 2 * np.random.randint(0, high = 2, size=(N,N))

    E = IsingE(spins)
    M = IsingM(spins)

    # Energy
    eplot = [ E ]
    # Magnetisation
    Mplot = [ M ]

    for k in range(steps):
        # Pick the lattice site randomly
        i = np.random.randint(N)
        j = np.random.randint(N)

        # Energy change from flipping the site
        dE = IsingdEflip(spins, i, j)

        # Flip the spin with some probability
        if (np.random.rand() < np.exp(-dE/T)):
            spins[i,j] = -spins[i,j]
            E += dE
            M += 2 * spins[i,j]

        eplot.append(E)
        Mplot.append(M)

    return eplot, Mplot
```

2D Ising model

Simulate $T = 1 < T_C$ several times

20x20 system

```
N = 20
steps = 500000
periodicBC = True
Temperature = 1.
Ts = np.empty(5)
Ts.fill(Temperature)
eplots = []
Mplots = []

for T in Ts:
    resE, resM = simulateIsing(T, N, steps)
    eplots.append(resE)
    Mplots.append(resM)
```

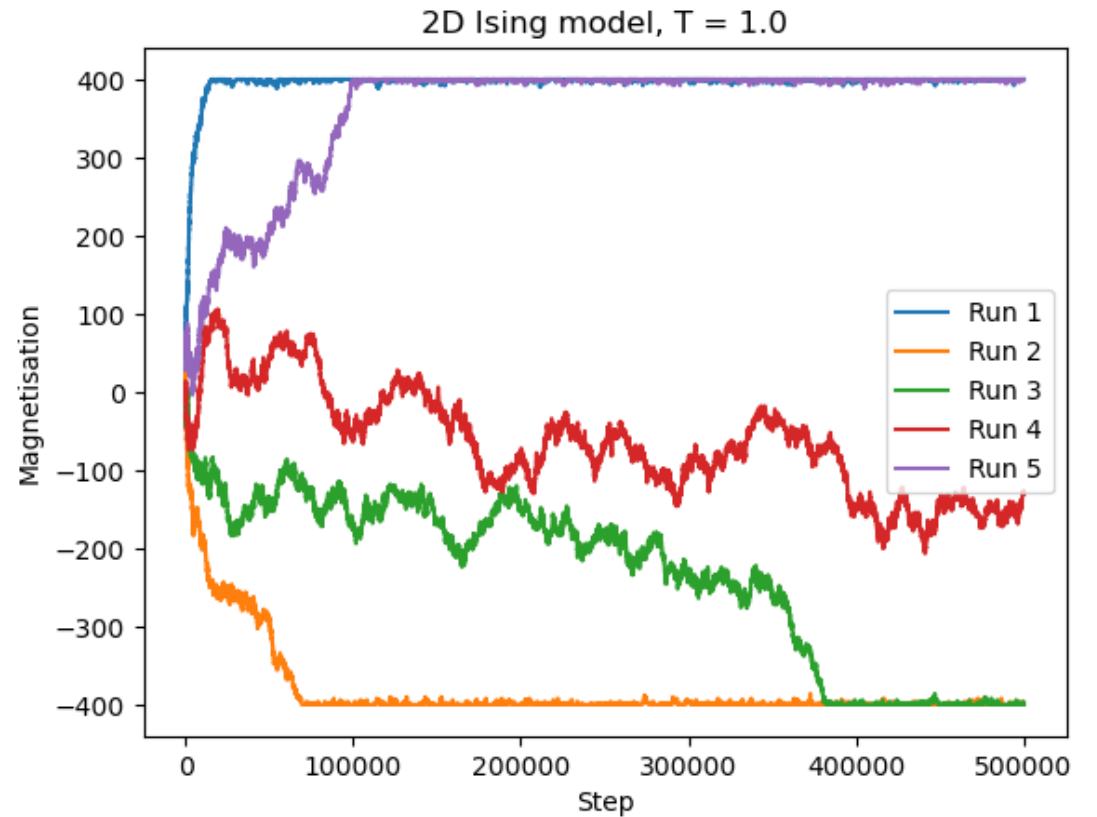
2D Ising model

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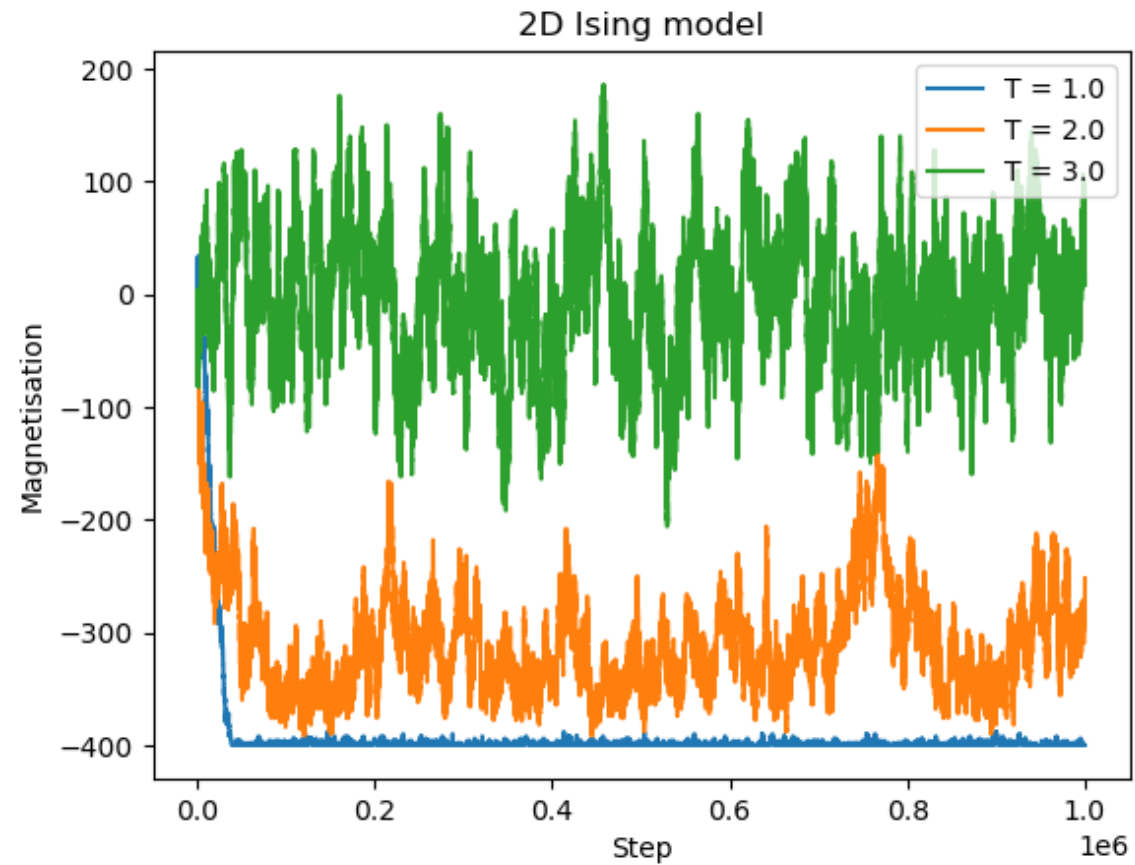
for T in Ts:
    resE, resM = simulateIsing(T, N, steps)
    eplots.append(resE)
    Mplots.append(resM)
```



Spontaneous magnetization!

2D Ising model

Try different temperatures



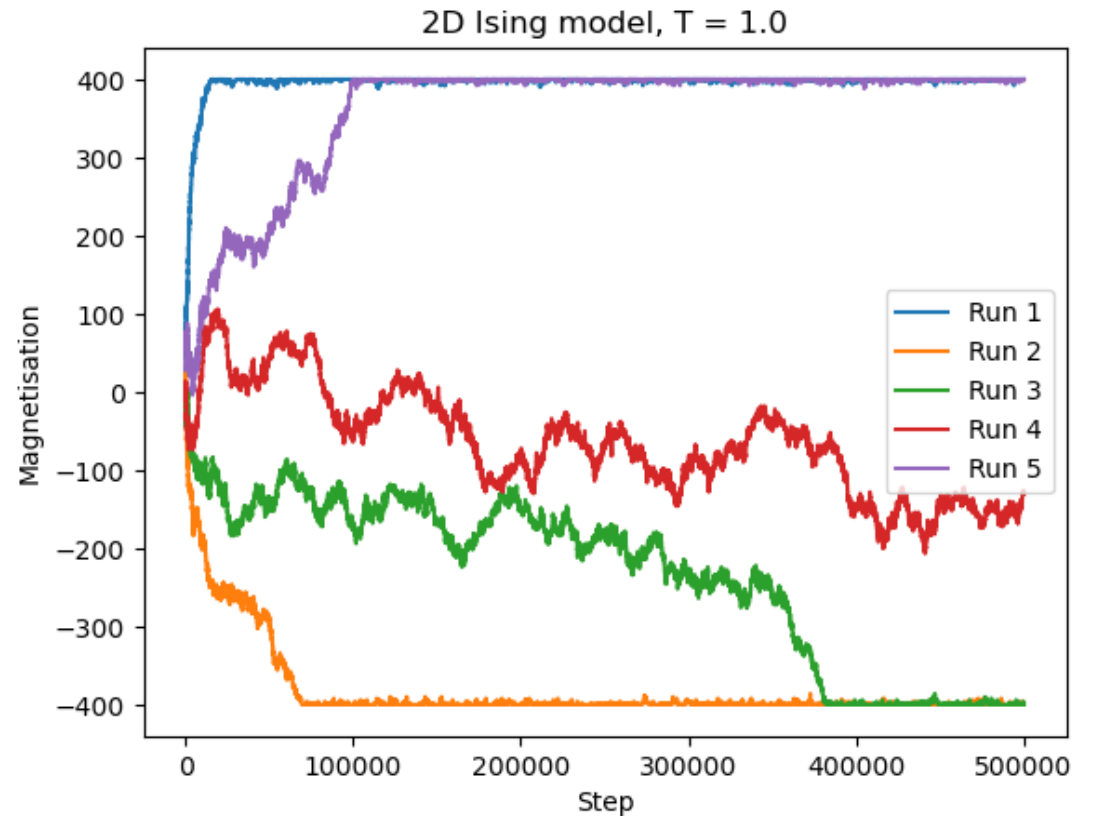
2D Ising model

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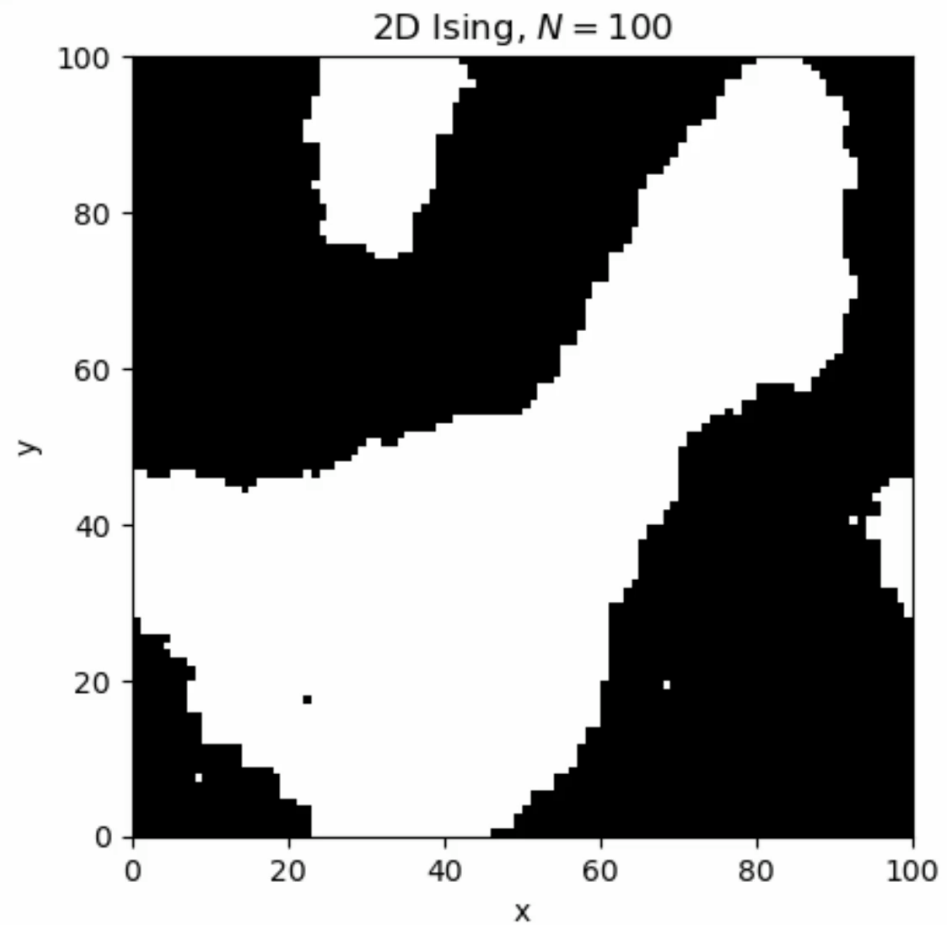
for T in Ts:
    resE, resM = simulateIsing(T, N, steps)
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```



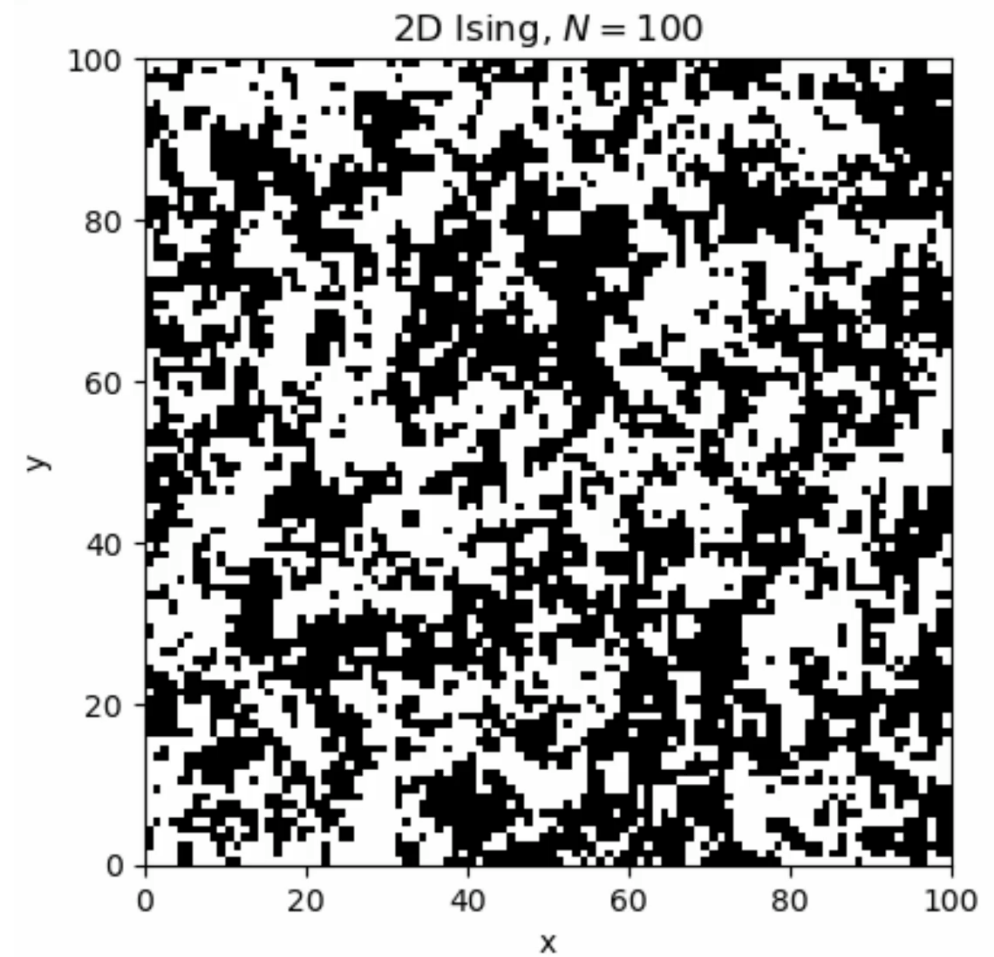
Spontaneous magnetization!

2D Ising model

$$T < T_c$$

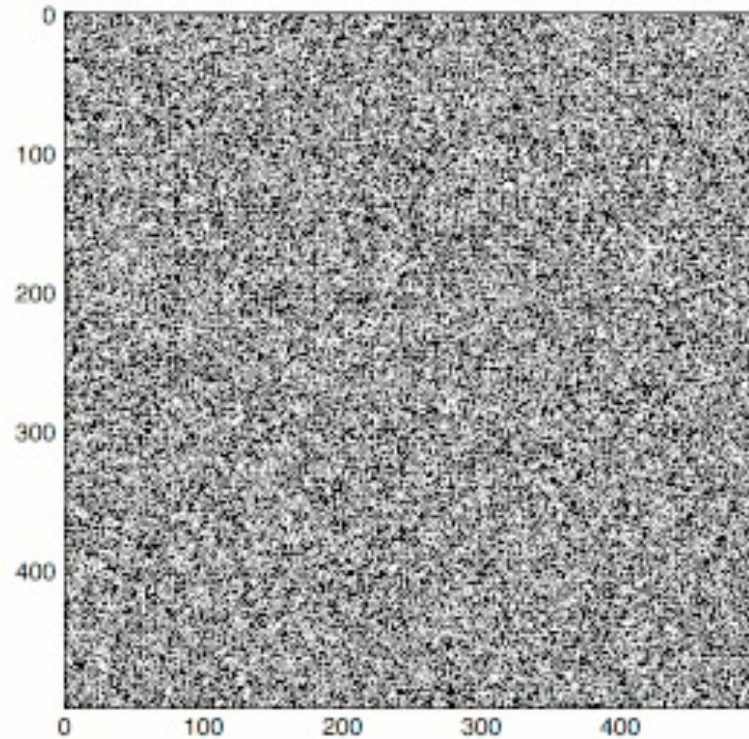


$$T > T_c$$



2D Ising model

Large system (500x500)



Credit: Wikipedia