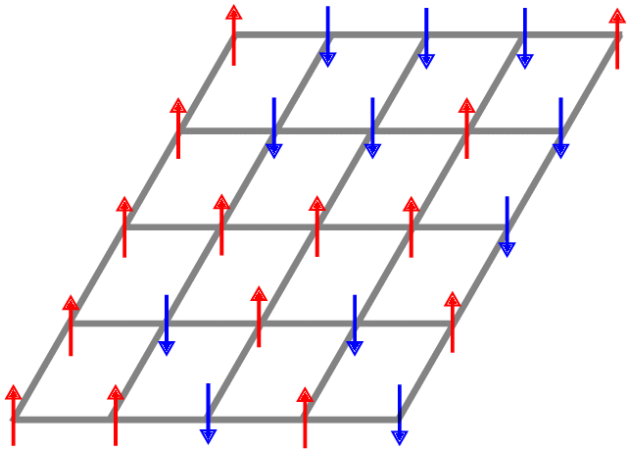
# The Ising Model of a magnetic material



$$E = -J \sum_{<ij>} S_i S_j$$

- The spins $S_i$ can take two possible values +1 or -1
- Interaction only between pairs of nearest-neighbours <ij>
- $J > 0$ is the strength of exchange interaction (units of energy)

This is a model of a permanent magnet (ferromagnetism) **with a phase transition.**

Think about the following:

- How is the minimum energy state? (T= 0K)
- How is going to be the system at $T \rightarrow \infty$ ?
- What ***happens at a finite temperature*** T ?

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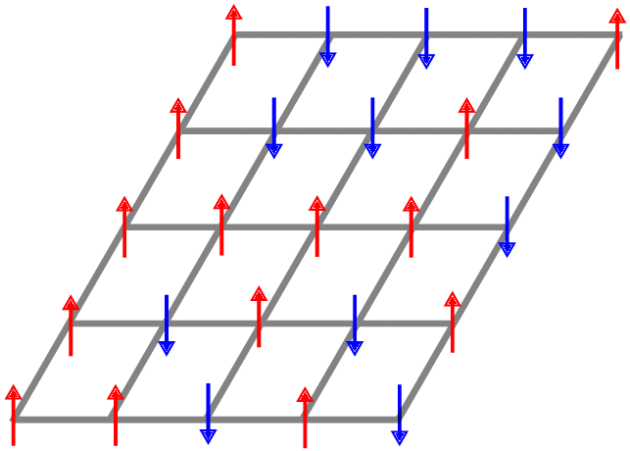

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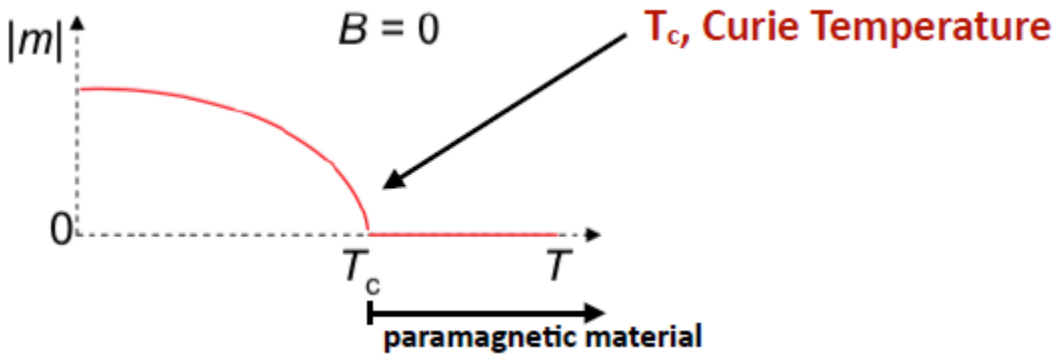
The goal is to determine the equilibrium state at a given T:

- At which temperatures the system is at an ordered (magnetized) phase with $m \neq 0$?
- At which ones in a disordered (non magnetic) phase $m = 0$?

$$m = \frac{\langle S \rangle}{N},$$



# The Ising Model of a magnetic material

How to solve the model? Monte Carlo?

**"Direct" Monte Carlo (as in the first example calculation of Pi) involves uniform random exploration of all states compatible with the constraints**

$2^{NxN}$ states

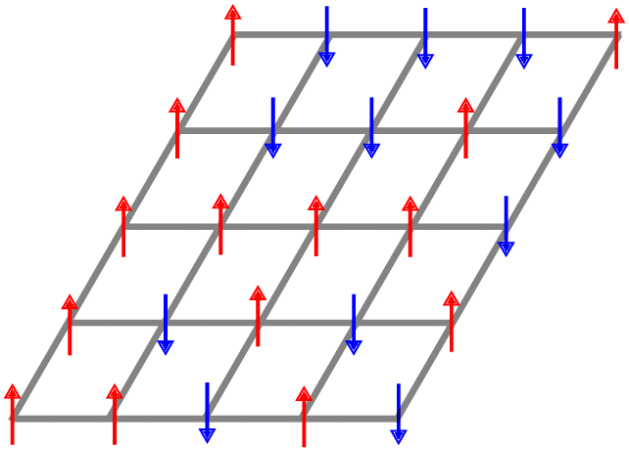
=> for N=16 we have $\approx 10^{77}$ states
=> for N=64 we have $\approx 10^{8000}$ states

- Recall that the Universe age is $5 \times 10^{17}$ s

**Direct MC impossible at any conceivable computer speed !! => Metropolis (Markov chain)**

# The Ising Model of a magnetic material

## Monte Carlo – Markov Chain Algorithm for the Ising Model



- Consider an initial state (*o*) with energy U(o) (arbitrary initial condition)
- Try a new state (n) with energy U(n) **by flipping a randomly selected spin**
- **Decide to accept or reject the move** from *o* to *n*

*If* $U(n)-U(o) < 0$ => accept the move from *o* to *n*

*If* $U(n)-U(o) > 0$ => accept the move from *o* to *n* with a probability given by the Boltzmann factor:

$$p(o \to n) = \exp\left[-\frac{U(n) - U(o)}{k_B T}\right]$$

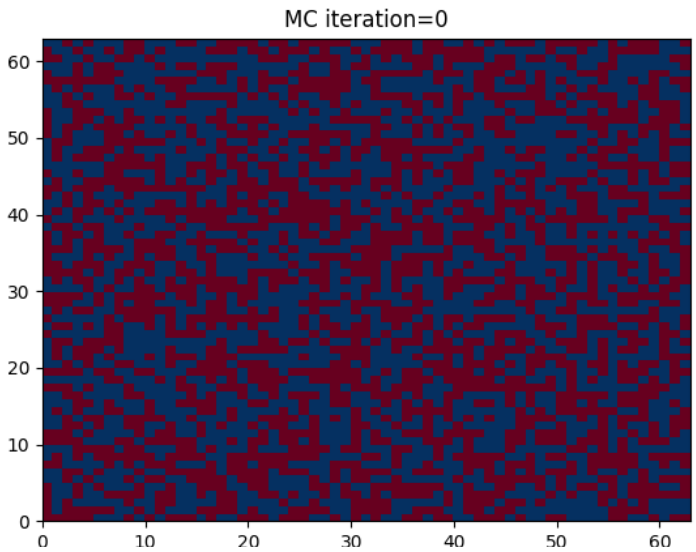
- Repeat over and over again until some convergence criterion is achieved

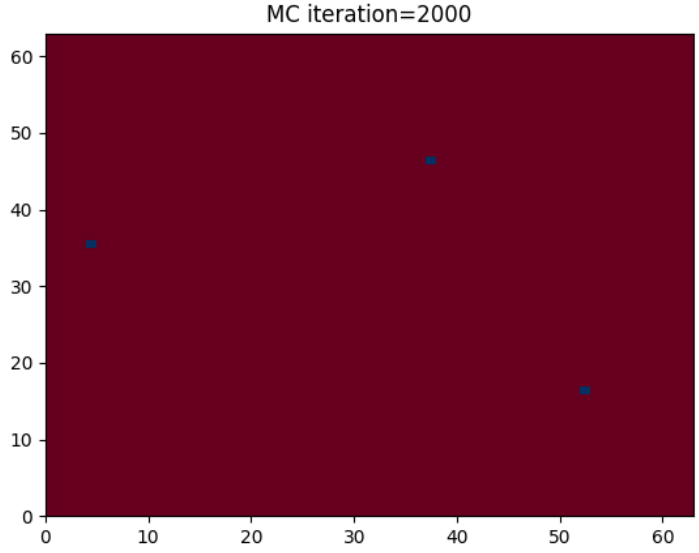
https://github.com/jfaraudo/Monte_Carlo_Metropolis_Examples

# The Ising Model of a magnetic material

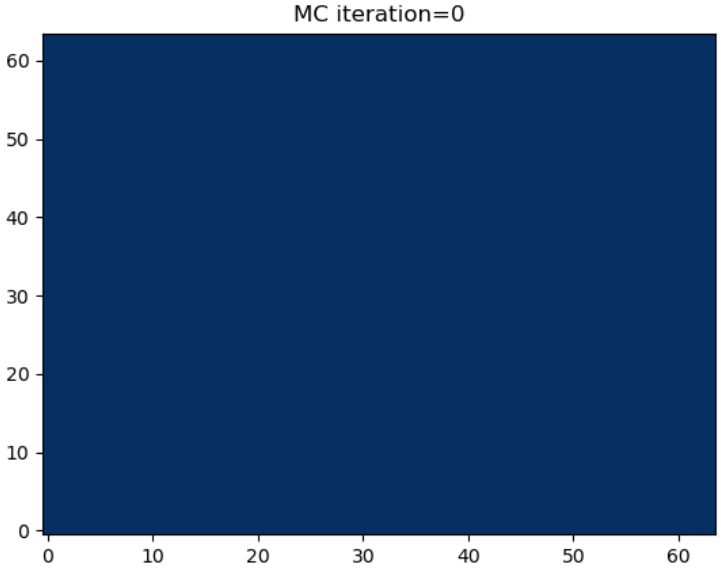
Typical Simulation results:

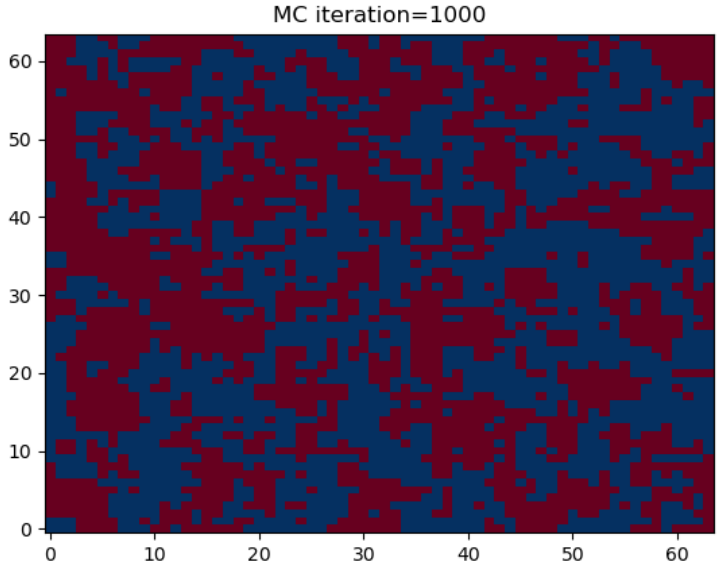
Simulation at Low Temperature
$K_B T = 1.2\ J$




Simulation at high Temperature
$K_B T = 2.5\ J$

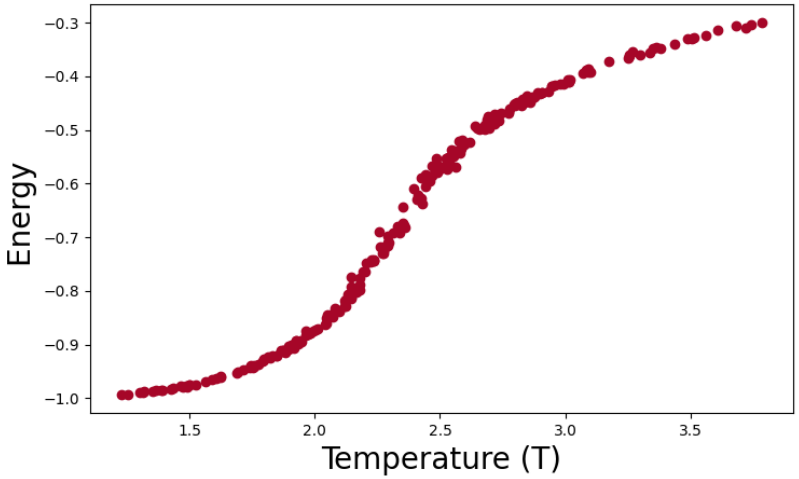


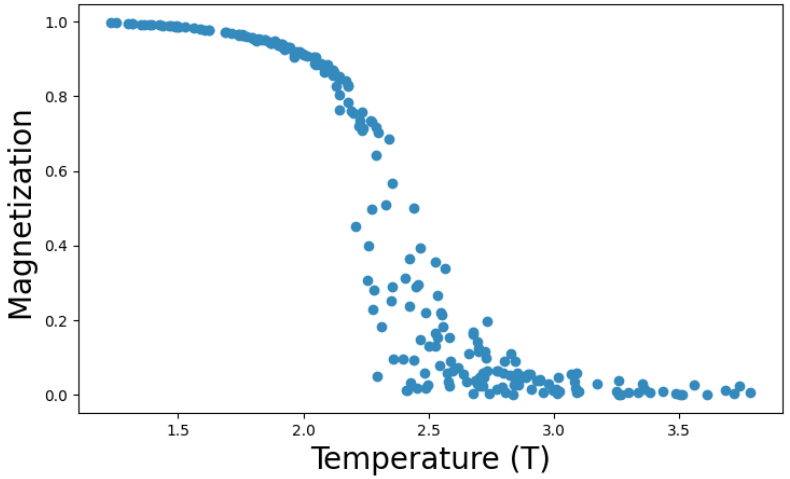



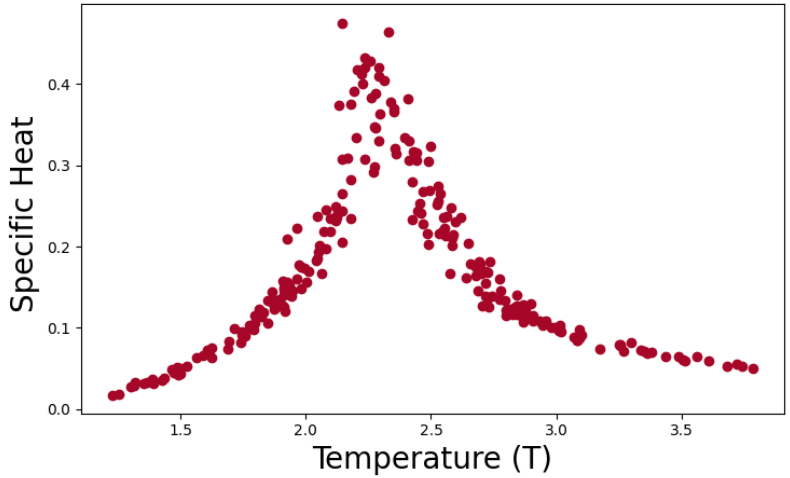

https://github.com/jfaraudo/Ising-model

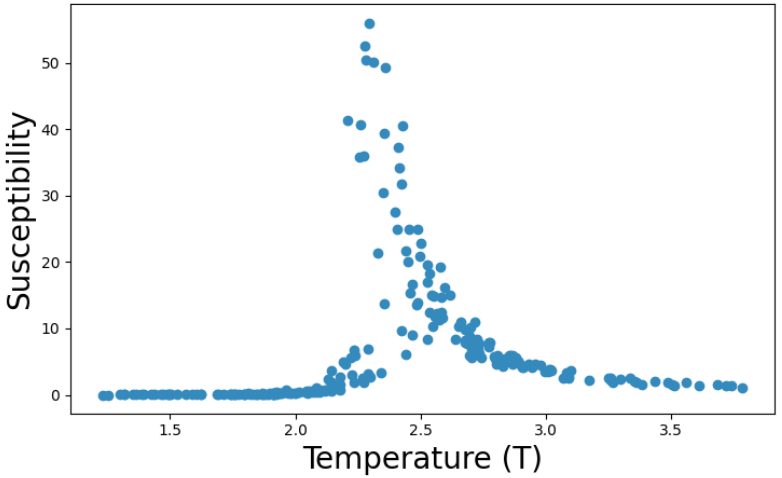
# The Ising Model of a magnetic material

Collecting the results for different temperatures




Dimensionless (reduced) Temperature

$T^* = K_B T / J$

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