UNIVERSITY OF LUXEMBOURG
Physics and Materials Science
Research Unit (PHYMS)

09 – Monte Carlo Methods

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History

The term **Monte Carlo** refers to a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results.

Historically, Monte Carlo methods were first developed for the needs of the *Manhattan project*.

They were developed by two prominent mathematicians, J. von Neumann and S. Ulam. Their work was secret and therefore a code name was required.

Their colleague, N. Metropolis, suggested using the name *Monte Carlo* which refers to the famous casino where Ulam's uncle would borrow money from relatives to gamble.

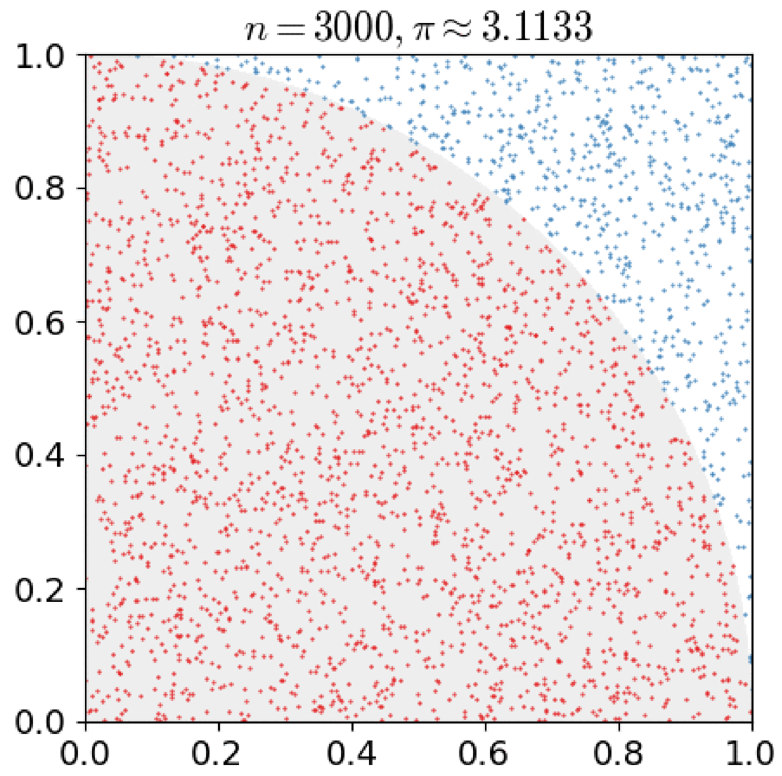
Applications

- Numerical computation of integrals in multidimensional spaces
- Quantum Monte Carlo methods solve the many-body Schroedinger equation
    - Variational Monte Carlo (VMC)
    - Diffusion Monte Carlo (DMC)
- Simulation and optimization problems in general:
    - Computer chess program
    - Traveling salesman problem

Monte Carlo Integration: Area of a Circle

The procedure:

1. Draw a unit square, then inscribe a circular sector (quadrant) within it
2. Uniformly scatter a given number of points over the square
3. Count the number of points inside the quadrant, i.e. having a distance from the origin of less than 1: $\sqrt{x^2 + y^2} \leq 1$
4. The ratio of the inside-count and the total-sample-count is an estimate of the ratio of the two areas, $\pi/4$. Multiply the result by 4 to estimate π



Monte Carlo Integration: Area of a Circle

This is equivalent to the evaluation of the following double integral:

$$I = \iint_{square} f(x,y)\,dxdy = 4r^2 \cdot \underbrace{\iint_{square} f(x,y)\frac{1}{4r^2}dxdy}$$

uniform probability

where: $f(x,y) = \begin{cases} 1, & x^2+y^2 \leq r^2 \\ 0, & x^2+y^2 > r^2 \end{cases}$

The average value $\bar{f}$ of $f(x,y)$ over the square $[-1,1] \times [-1,1]$

Monte Carlo estimate:

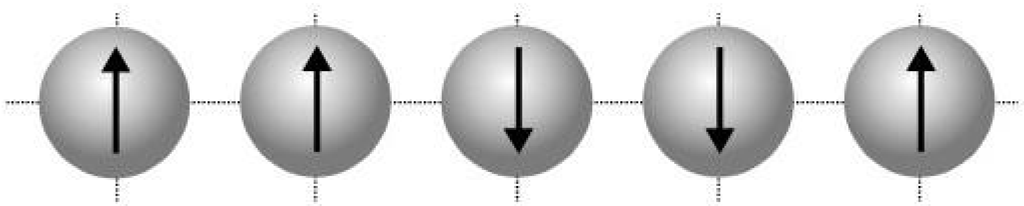
$$I = \iint_{square} f(x,y)\,dxdy \approx 4r^2\bar{f} \pm \frac{4r^2}{\sqrt{N}}\sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(f(x_i,y_i)-\bar{f}\right)^2}$$

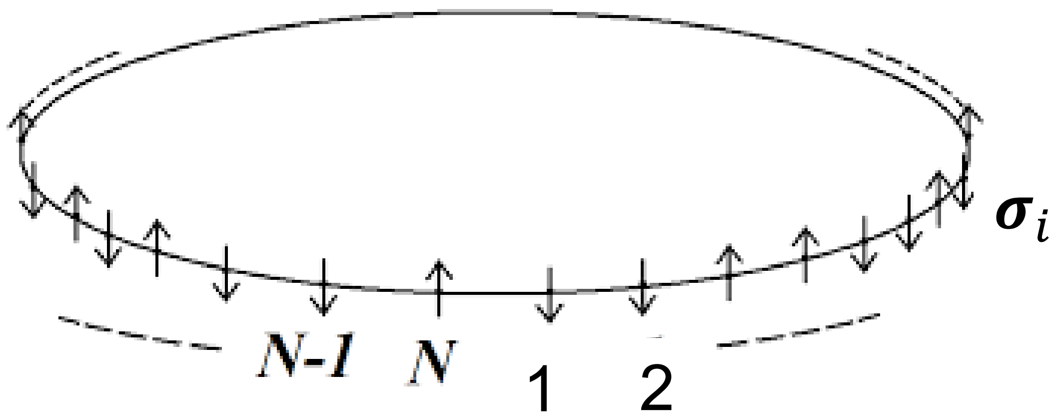
$$\bar{f} = \frac{1}{N}\sum_{i=1}^{N} f(x,y) = \frac{N_{in}}{N_{in}+N_{out}} \approx \frac{\pi}{4}$$

The error of Monte Carlo calculations scales as $1/\sqrt{N}$

Ising Model of Ferromagnetism

The chain of spins (+1 or -1)





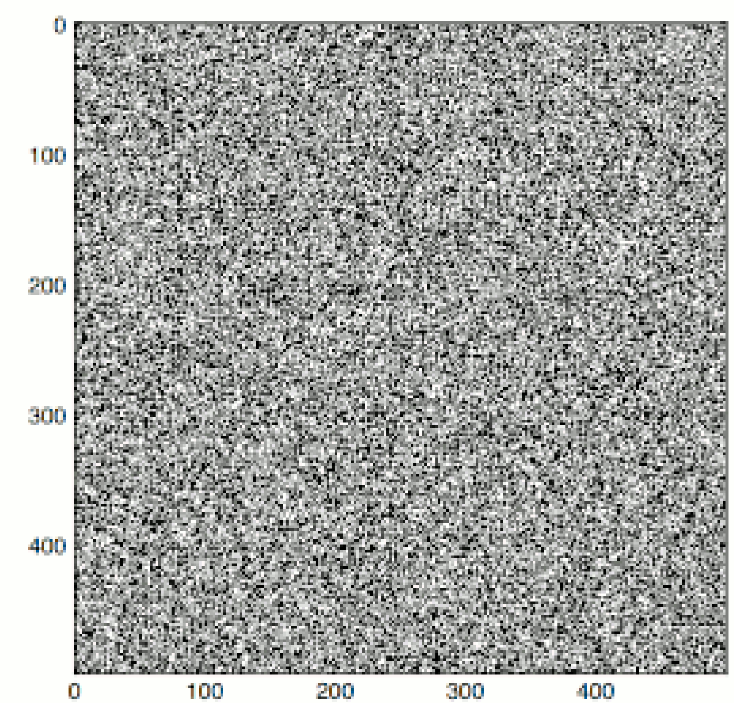
The 1D Ising Hamiltonian:

$$H(\{\boldsymbol{\sigma}\}) = -J \sum_{i=1}^{N} \boldsymbol{\sigma}_i \boldsymbol{\sigma}_{i+1}$$

Periodic boundary conditions:

$$\boldsymbol{\sigma}_{N+1} = \boldsymbol{\sigma}_1$$

Quench of 2D Ising system (500 × 500) starting from a random configuration

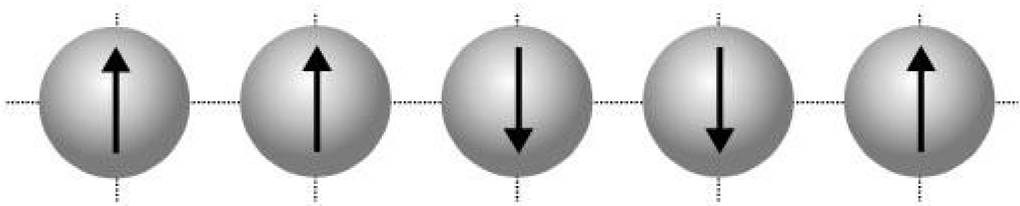


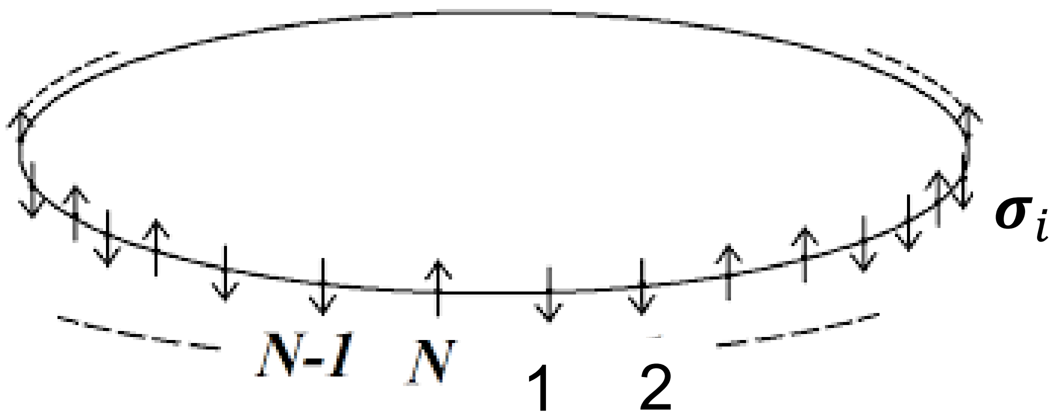
The significance: the first model in statistical physics predicting the phase transition to the ferromagnetic state at low T

Note: this is not the simulation of dynamics of the system, but rather the optimization (relaxation)

Analytical Solution

The chain of spins (+1 or -1)





The 1D Ising Hamiltonian:

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Periodic boundary conditions:

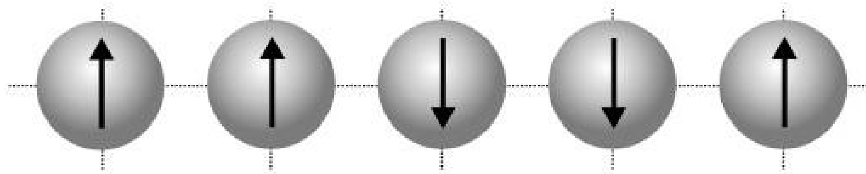
$$\boldsymbol{\sigma}_{N+1} = \boldsymbol{\sigma}_1$$

$$E = NJ \cdot \tanh(-J/T)$$

$$M = \sum_{i=1}^{N} \boldsymbol{\sigma}_i = 0$$

Within the 1D Ising model, the phase transition to the ferromagnetic state is not possible at any temperature $T > 0$

Metropolis Algorithm



1. Generate a random initial spin configuration $\{\sigma_i\}_{i=1}^{N}$ with the energy E_0
2. Flip a random spin and calculate the energy E_t of this trial state;
3. Calculate the difference in energy generated by the spin flip, $\Delta E = E_t - E_0$ and the associated transition probability $p = \exp(-\Delta E/T)$:
   - If $\Delta E \leq 0$, then we accept the spin flip because the trial spin configuration is energetically favoured over the initial state;
   - If $\Delta E > 0$, then we compare the transition probability p to a random number $r \in [0,1)$. We accept the new configuration if $r \leq p$. Otherwise, we keep the spin unflipped.
4. Update the average energy, magnetization, etc.
5. Repeat steps (2) to (4) with the chosen spin configuration until thermal equilibrium has been reached.