Monte Carlo - Background

Computational Physics

4. október 2010

Overview

In this chapter we shall use phase transitions and a simple model that shows a phase transition, the Ising model, to give a physical approach to “Monte Carlo” methods.

Later on, we shall introduce further fields where Monte Carlo methods are heavily used.

1 Phase transitions

All around we have material in different phases

- Blood plasma in a liquid phase
- Stones in a solid state
- Oxygen in the air in a gas phase

Under different conditions all these systems can be in different phases

The phase can be governed by, temperature, pressure, volume, and magnetic field

In our environment we have some materials, like water, coexisting in all phases

1.1 The melting of ice

In an ice cube, just below freezing, the H_2O molecules are are strongly correlated due to the

$$\boxed{\text{van der Waals forces}}$$

The molecules move slightly around the equilibrium position and most of the energy is stored in vibrations linearly proportional to the temperature T

$$E_{\text{vib.}} \sim k_B T$$

with k_B the Boltzmann constant

- $\boxed{T < 0°C}$

  Molecules stick together, strong correlation (ice).

$$E_{\text{vib.}} < E_{\text{Binding energy of ice}}$$

- $\boxed{0°C < T < 100°C.}$

  Moderate correlation, molecules slip and flow (water).

$$E_{\text{Binding energy of ice}} < E_{\text{vib.}} < E_{\text{Binding energy of water}}$$

- $\boxed{T > 100°C}$

  Almost no correlation, "free" motion of molecules (vapor).

$$E_{\text{vib.}} > E_{\text{Binding energy of water}}$$

1.2 Cooperation

All around us we have particles, atoms, molecules, electrons, and ions interacting with various strength.

Phase transitions, and other processes in nature, are caused by collective motion of the entities in the system. The properties of individual entities are lost and phenomena occur that are not expected for single-entities.

Examples:

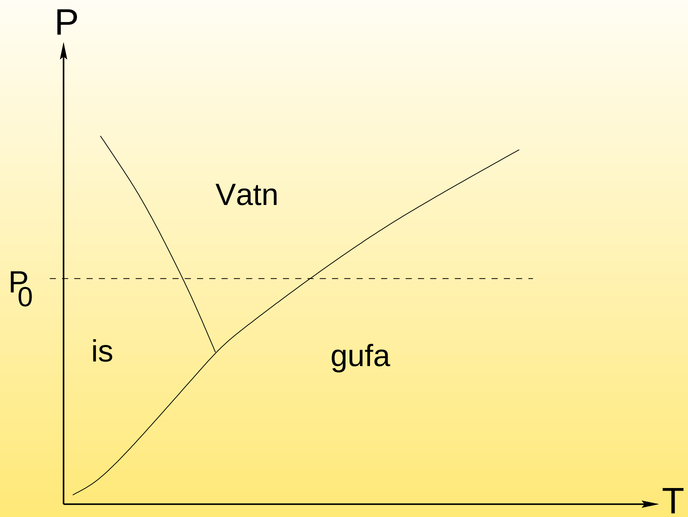
- Superconduction in some metals at low T.
- Macroscopic magnetic phenomena.

  $\rightarrow$: **Emergent behavior**.

1.3 Phase diagrams

More variables than temperature can control phase transitions. Examples are pressure (P), volume (V), and magnetic field (H).

If there is more than one relevant variable it is convenient to use phase diagrams to determine the phase as a function of T of P...



From the phase diagram we see:

- How the boiling point changes with P.
- How the melting point decreases with increasing P.

2 Monte Carlo methods

- Name used for many computational methods that in one way or another rely on random numbers.
- One might think these methods are only used for processes that are inherently random, this is not true.

Examples of application:

- Calculation of high-dimensional integrals.
- Ground state energy of molecules.
- Motion and energy loss of neutrons in solid state.

2.1 How does MC work?

Often we need an average value of **very** many terms. It can be the original problem we are interested in or a problem has been transformed into that form.

The average (or the mean value) is a sum over all terms multiplied by the probability of each term P.

$$\boxed{\overline{E} = \sum_i P(E_i) E_i}$$

Often the number of terms is so large that we can never calculate all of them.

Here MC helps by selecting the most probable terms and find their mean value.

Similar ideas are behind polls, where a small ensemble is focused on, in order to find out the properties of a much larger ensemble.

(Of course there are many approximation schemes that do not rely on Monte Carlo methods).

2.2 MC and integration

Often algorithms for numerical integration use equally spaced points in the interval to estimate the integral

$$\boxed{I = \int_a^b dx\, f(x) \simeq \sum_{i=1}^{N} \alpha_i f(x_i)}$$

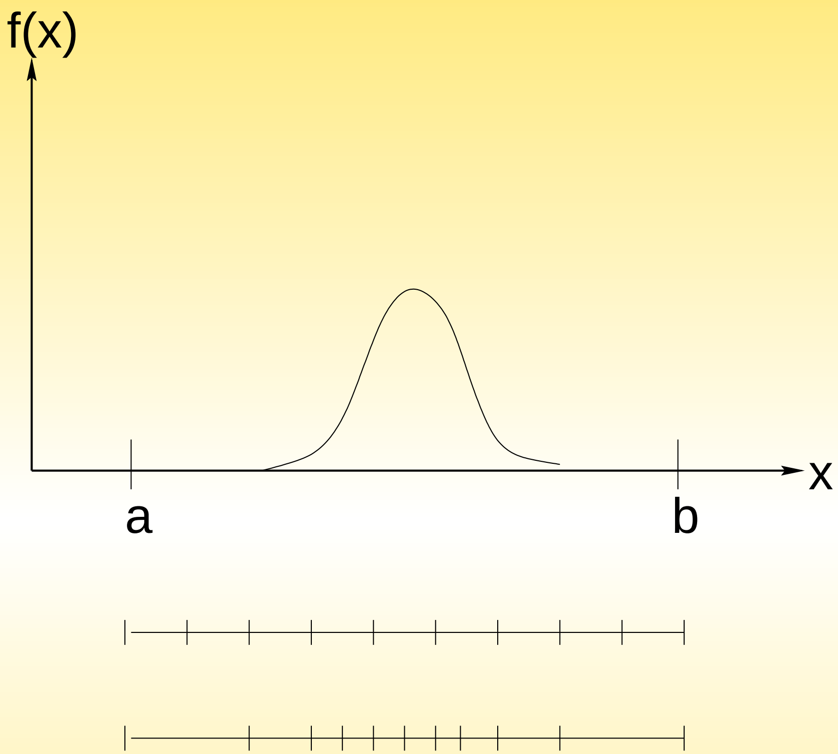
where x_i are equally spaced in (a, b).

The sum can be tracked as a mean value, and MC methods can be used for the integral

$$\boxed{I = \int_a^b dx\, f(x) \simeq \frac{1}{N}\sum_{i=1}^{N} f(x_i)}$$

where x_i are randomly selected in (a, b).

MC methods make it possible to select most of the points where the integrand is large.



→ Better estimate of an integral for the same number of points!

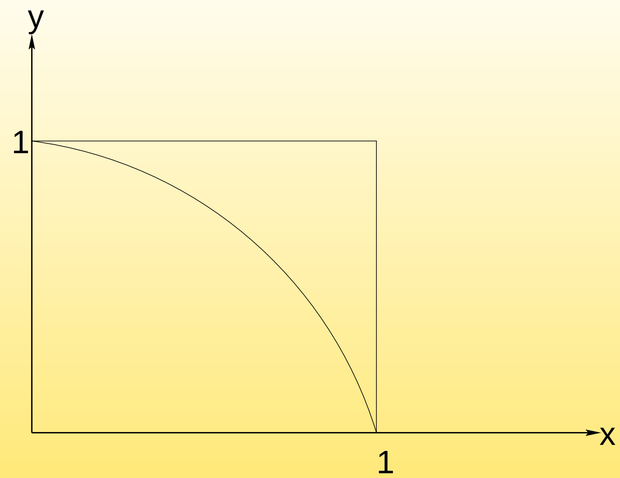
How are the points distributed in the interval?

2.3 Another MC example

The number π calculated by random numbers. π can be defined by the integral

$$\pi = 4 \int_0^1 dx \int_0^1 dy \; \theta(1 - x^2 - y^2)$$

where θ is the Heaviside step function.



We make many random number pairs (x_i, y_i), $i = 1, \ldots, N$. Then

$$\pi = 4\frac{1}{N}\sum_{i=1}^{N}\theta(1 - x_i^2 - y_i^2).$$

This sum is simply the number of random number pairs inside the quarter circle.

This can simply be extended to higher dimensions, for example 3

$$\pi = \frac{3}{4}\,8\,\frac{1}{N}\sum_{i=1}^{N}\theta(1 - x_i^2 - y_i^2 - z_i^2).$$

2.4 Error estimate in MC

Consider the integral

$$I = \int_a^b dx f(x) \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f(x(y_i))}{w(x(y_i))} = \frac{1}{N} \sum_{i=1}^{N} f_i.$$

The laws of statistics give

$$\sigma_I^2 = \frac{\sigma_f^2}{N} = \frac{1}{N} \left(\frac{1}{N} \sum_{i=1}^{N} f_i^2 - \left(\frac{1}{N} \sum_{i=1}^{N} f_i \right)^2 \right)$$

where σ_f is the width of the distribution of the $f_i' s$ (independent of N for very large N) and σ_I is the error in the integral.

Important is that $\boxed{\sigma_I = \frac{\sigma_f}{\sqrt{N}}}$

3 Simplistic approach to statistical physics

- Is the branch of physics describing large ensembles of interacting particles using either classical or quantum physics in conjunction with statistics.
- Consider a system in one of many states $\alpha = 1, 2, \ldots$ with energy E_α. We assume the system is in equilibrium with a thermal bath at temperature T.

  The probability that the system is in state α is given by

  $$P(E) = \frac{1}{Z} e^{-\beta E_\alpha}$$

  where $\beta = 1/k_B T$ and $Z = \sum_\alpha e^{-\beta E_\alpha}$.
- This probability distribution is the canonical distribution and is valid for systems in equilibrium with a heat bath at T.

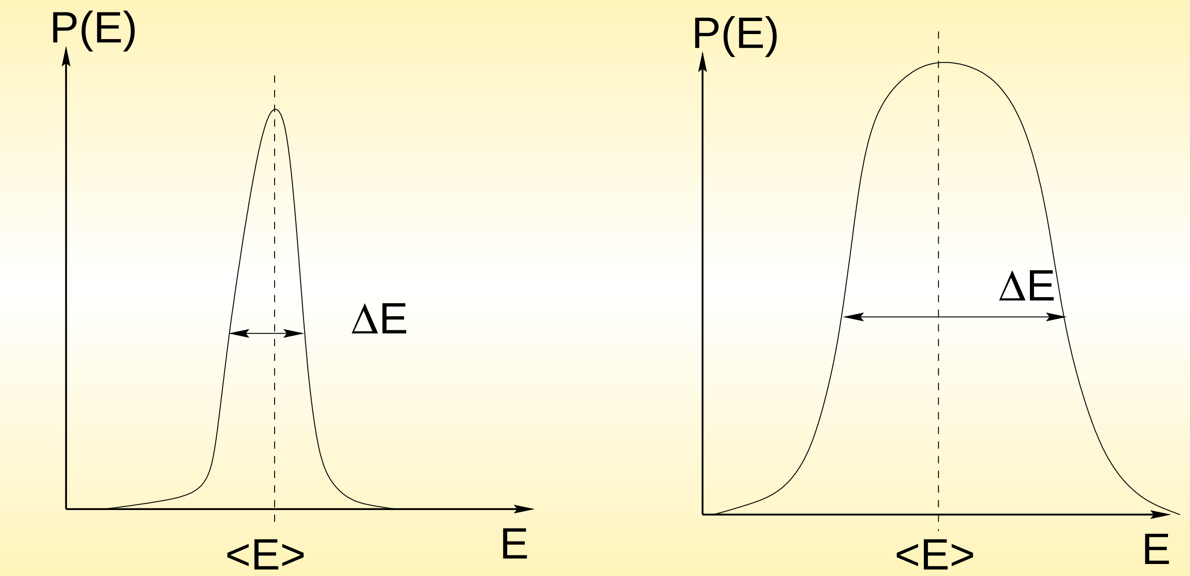
- On basis of this distribution we can calculate many quantities
  - Mean energy, (written as $\overline{E}$ or $\langle E \rangle$)

$$\overline{E^n(T)} = \sum_\alpha E_\alpha^n \, P(E_\alpha).$$

  - Fluctuation of the energy (distribution width)

$$\Delta E(T) = \left(\overline{E^2(T)} - \left(\overline{E(T)} \right)^2 \right)^{1/2}.$$

  - And much more.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