Exercise sheet 0

Statistical mechanics and Monte Carlo algorithm basics

PUE Advanced Computational Physics

University of Vienna - Faculty of Physics

A particle in a homogeneous gravitational field

Consider a particle in a homogeneous, one-dimensional gravitational field. Its potential energy is given by

$$U(h) = mgh \tag{1}$$

where m is the mass, g is the gravitational acceleration and $h > 0$ is the height of the particle. The particle is coupled to a heat bath at temperature T.

1 Pen and paper analysis

a. What is the Hamiltionian, $\mathscr{H}(h, v)$ of the system? (v is the velocity of the particle)

b. Calculate the classical approximation to the partition function Q.

c. Calculate the internal energy E.

d. Given an observable $A = A(h)$, write down the expectation value $\langle A \rangle$.

2 Monte Carlo simulation

Take the result from 1d. The key idea of Monte Carlo algorithms is to split the integrand into two factors $f(h)$ and $g(h)$. It can then be approximated by

$$\int \mathrm{d}h f(h) g(h) = \langle g \rangle_f \approx \frac{1}{N} \sum_{i=1}^{N} g(\xi_i), \tag{2}$$

where $\langle g \rangle_f$ is the expectation value of g under the probability distribution

$$\rho(h) = \frac{f(h)}{\int \mathrm{d}h f(h)} \tag{3}$$

and the ξ_i are a samples from ρ.

a. Set $A(h) = h$, how would you choose $f(h)$ and $g(h)$ and why?

b. Implement a simulation that uses the approximation (2) to calculate the average height and the average potential energy of the particle using the programming language of your choice. Use a random number generator to draw the sample ξ. Use the parameters $T = 300\,\mathrm{K}$, $m = 4.66 \times 10^{-26}\,\mathrm{kg}$, $k_\mathrm{B} = 1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$, and $g = 9.81\,\mathrm{m\,s^{-2}}$. Discuss your results.