Exercise: Monte Carlo Methods in Action

Dr Benjamin J. Morgan[1] and Dr Andrew R. McCluskey[1,2]

[1] *Department of Chemistry, University of Bath, email: b.j.morgan@bath.ac.uk*
[2] *Diamond Light Source, email: andrew.mccluskey@diamond.ac.uk*

September 17, 2019

Aim

In this exercise, you will develop Monte Carlo code for sampling the potential energy landscape of bonds stretchs and angle bends in a H_2O molecule.

1 Monte-Carlo sampling

Monte-Carlo is a method for the sampling of some probability distribution. We will introduce this sampling method by considering a group of children playing a game where they first draw a large circle and then a square around it, where the diameter of the circle (d) is equal to the length of the side of the square (a) on a beach (similar to that shown in Figure 1). The children then take turns randomly throwing pebbles into the square (with obviously some landing in the circle), with each throw counting as a *trial* and each that lands inside the circle as a *hit*.

The trials are technically sampling the area of the square (A_s), while the hits sample the area of the circle (A_c). Therefore, the ratio of the number of hits (N_{hits}) to the number of trails (N_{trials}) is equal to the ratio of the area of the circle to the square,

$$\frac{N_{hits}}{N_{trials}} = \frac{A_c}{A_s} = \frac{\pi(d/2)^2}{a^2} = \frac{\pi}{4}, \text{ where } d = a. \tag{1}$$

2 Classical modelling

3 Potential energy landspace

References

Figure 1: The pattern drawn on the beach.