Monte Carlo simulations 2004. Exercise 3

To be handed in Tue Mar 2, solutions given Thu Mar 4 10:15.

1. (6 p) Write a program which evaluates the volume of an N-dimensional hypersphere using Monte Carlo simulation, with the hit-and-miss approach. N should be a parameter in the code. The code should also calculate the statistical uncertainty. Hand in the code and results.

2. (6 p) Write a program which evaluates the volume of an N-dimensional hyperspheres using Monte Carlo simulation, with the sampling approach. N should be a parameter in the code. It should also calculate the statistical uncertainty. Hand in the code and results.

3. (18 p) In our research group we have recently examined the sticking of CH_3 radicals on single dangling bonds on diamond (111) surfaces [Träskelin et al, J. Appl. Phys. 93, 1826 (2003)]. The MD simulations which really do this are very slow, so we needed to find a good stratified sampling scheme to obtain statistics as efficiently as possible. After the initial simulations were done, we found that the sticking probability f can be approximated in the following form:

$$d = 3.0/\sqrt{2} + 0.5\cos^2(3\theta) \tag{1}$$

$$f = \begin{cases} 1, & \text{if } r \leq d - 0.5; \\ 0.5 - 0.5\sin(\pi(r-d)), & \text{if } d - 0.5 < r < d + 0.5; \\ 0, & \text{if } r \geq d + 0.5; \end{cases} \tag{2}$$

$$\tag{3}$$

Here (r, θ) gives the distance from the dangling bond (located at $r = 0$) in polar coordinates. The length unit is Å. When the function $f(r, \theta)$ is integrated over the plane (r, θ) or (x, y) it gives the sticking cross section in units of Å^2. Use this approximative function to examine which way to MC integrate the plane gives the best answer. Assume that the MD simulations are limited to a statistics of 900 events. a) obtain an accurate reference value for the integral using numerical or analytical integration. Then MC integrate the function using b) direct integration in cartesian coordinates, c) direct integration in polar coordinates, d) fully stratified MC integration in cartesian coordinates, and e) partially stratified MC integration in polar coordinates using 20 intervals of width 0.15 Å in r.

For comparison with the lecturers results, use the integration interval between -3 Å and 3 Å in x and y in cartesian coordinates, and between 0 and 3 Å in r in polar coordinates.

You do not need to calculate the error of each MC integration separately. Instead you can simply repeat each case 10 times and then calculate the average and its error of the 10 results obtained. Comment on how accurate the four different schemes are compared to each other. Which one seems the best?

Do not return the code (if you get the wrong answer in some part, you get no points from it).

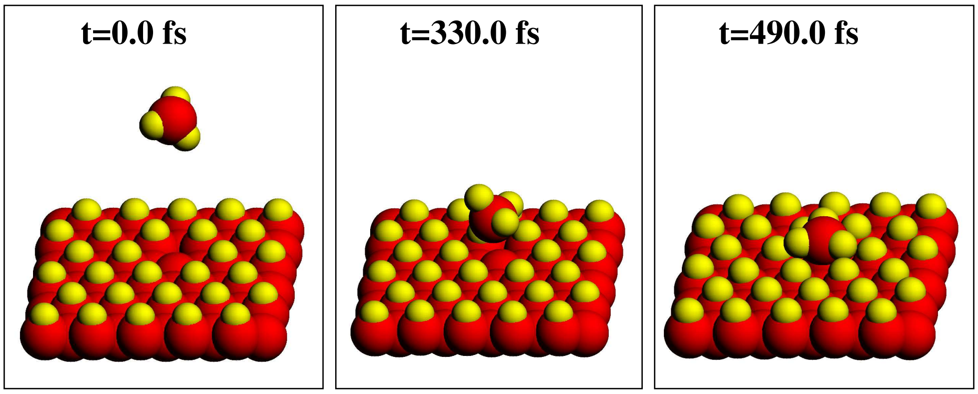

Figure 1: Illustration of the sticking process. The carbon atoms are shown in red and the H atoms in yellow. The dangling bond is the C atom with no H on top in the middle.

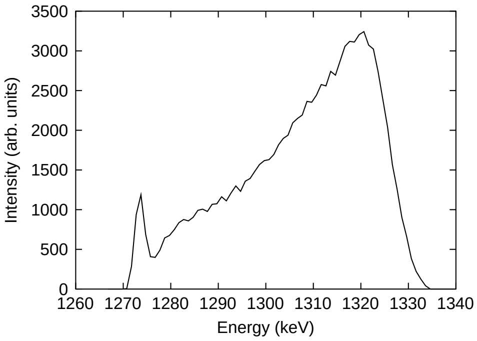

Figure 2: The DSA lineshape used in exc. 4.

4. (12p) Consider the distribution `dsa_nonegative.dat` given on the course web page and Fig. 2. This is a γ-ray distribution from a Doppler-broadened nuclear lifetime state measured in the Accelerator laboratory [K. Arstila et al, Nucl. Instr. and Meth. in Phys. Res. B 101 (1995) 321-326] Assume you will repeat this measurement, but can generate only 300 counts of statistics in the repeated measurements. Using the procedure outlined in lecture notes section 6.1, generate enough synthetic data sets to determine the statistical uncertainty of the mean for such 300-count distributions. Note that the uncertainty may be unsymmetric. Also compare with the uncertainty of the mean calculated using Gaussian statistics for the individual distributions. Report the obtained synthetic data uncertainties and the Gaussian ones. If you are certain your answer is right, you do not need to return the code.

You may freely use your (or the lecturers) solution to exercise 2.3 as a starting point.