

# PHYS 420: Computational Physics

## Homework 2

Due Tuesday, Sep 19, 2017

Here are some comments on coding and presenting your work.

PLEASE READ THEM CAREFULLY.

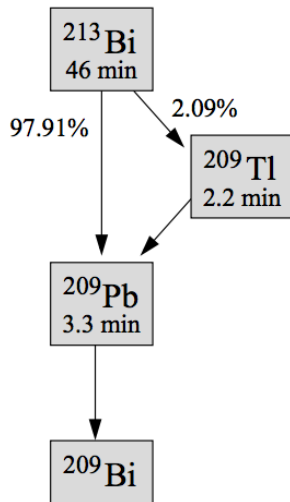
1. The answers to the questions may include the computer code and output, in addition to any writing that might be needed. If you are not sure what is required please ask me, preferably before the last evening before the homework is due.
2. Please assemble all parts of a question together. I don't want to have the code for all the questions together, followed by all the output, followed by all the explanations. Rather, I require all parts of question 1, followed by all parts of question 2, etc.
3. In some problems, there will be many lines of output only a few of which are relevant. To save paper just print the relevant lines. You could indicate the missing lines by a line with something like .....
4. In problems where you have to show that the error goes as a certain power of a small parameter  $h$ , choose values for  $h$  which decrease in a geometric (rather than arithmetic) sequence (i.e. divide by 2 or 10, whichever is most appropriate, each time).
5. Keep things simple.
6. Make sure that constants are defined with the desired precision.

Now we start the questions.

### 1. Generating Random Numbers

- a. Generate Samples of (x,y) coordinates that fill a square uniformly such that x & y values fall in a range between -1 and +1. Be able to specify the number of xy-pairs to be generated,  $N_{total}$ .
- b. Count the number of points in your sample that happen to fall inside the inscribed circle centered at the origin with a radius =1,  $N_{circle}$ . Calculate the ratio:  $Ratio = 4N_{circle}/N_{total}$ .
- c. Plot the sampled data over the entire range of the square. Please inscribe the circle used in part b. Points outside of the circle color Red and points inside the circle color Blue for  $N_{total}=10000$ .
- d. Plot the Ratio you calculated as a function of  $N_{tot}$ . Vary  $N_{tot}$  from 10 to  $10^6$ . Does this ratio converge to a finite value? What should this value be? Does this make sense? Draw a dashed horizontal line denoting the expected ratio value.

## 2. Radioactive decay chain



The isotope  $^{213}\text{Bi}$  decays to stable  $^{209}\text{Bi}$  via one of two different routes, with probabilities and half-lives thus:

$$\lambda = \frac{1}{\tau} = \frac{\ln(2)}{t_{1/2}}$$

(Technically,  $^{209}\text{Bi}$  isn't really stable, but it has a half-life of more than  $10^{19}$  years, a billion times the age of the universe, so it might as well be.)

Starting with a sample consisting of 10000 atoms of  $^{213}\text{Bi}$ , simulate the decay of the atoms by dividing time into slices of length  $\Delta t = 1$  s each and on each step doing the following:

- For each atom of  $^{209}\text{Pb}$  in turn, decide at random, with the appropriate probability, whether it decays or not. Count the total number that decay, subtract it from the number of  $^{209}\text{Pb}$  atoms, and add it to the number of  $^{209}\text{Bi}$  atoms.
- Now do the same for  $^{209}\text{Tl}$ , except that decaying atoms are subtracted from the total for  $^{209}\text{Tl}$  and added to the total for  $^{209}\text{Pb}$ .
- For  $^{213}\text{Bi}$  the situation is more complicated: when a  $^{213}\text{Bi}$  atom decays you have to decide at random with the appropriate probability the route by which it decays. Count the numbers that decay by each route and add and subtract accordingly.

Note that you have to work up the chain from the bottom like this, not down from the top, to avoid inadvertently making the same atom decay twice on a single step.

Keep track of the number of atoms of each of the four isotopes at all times for 20000 seconds and make a single graph showing the four numbers as a function of time on the same axes.

For full credit turn in a printout of your program and a copy of the graph it produces.

3. Monte Carlo integration: Calculate a value for the integral

$$I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx,$$

using the importance sampling technique we discussed in class.

$$I = \int_a^b f(x)p(x) \approx \frac{1}{N} \sum_{i=1}^N f(x_i)$$

- Calculate a value for the integral using a uniform probability distribution,  $p(x) = 1$ , for an arbitrary number of samplings,  $N$ .
- Show that the probability distribution  $p(x)$  from which the sample points should be drawn is given by

$$p(x) = \frac{1}{2\sqrt{x}}$$

and derive a transformation formula for generating random numbers between zero and one from this distribution. Be careful what you define as  $f(x)$  in the integrand.

- Make a plot of the integral values as calculated from a. and b. as a function of  $N$ , ranging from 10 to 1000000. A log scale for the x-axis may be useful. Look up the true value for this integral and show it as a dashed horizontal line. Use 3 different colors for each line and label them.

4. Simpson's rule:

- Using Simpson's 1/3 rule, write a program to calculate an approximation for the integral  $\int_0^1 (1 + 2x + 3x^2 + 4x^3 + \alpha x^4) dx$ , where  $\alpha$  is a variable number for this problem. Be able to input the number of integrand intervals,  $N$ .
- For  $\alpha=0$ , run your program for  $N=1, 10, 100, 1000, 10000$ , and  $100000$ . What is the difference between these values for the integral and the actual value for the integral? Can you write down an expression describing this difference?
- For  $\alpha=5$ , run your program for  $N=1, 10, 100, 1000, 10000$ , and  $100000$ . What is the difference between these values for the integral and the actual value for the integral? Can you write down an expression describing this difference?
- For  $N=100000$ , run your program for  $\alpha= 0.01, 0.05, 0.1, 0.5, 1.0, 5.0$  and  $10.0$ . What is the difference between these values for the integral and the actual value for the integral? Can you write down an expression describing this difference?

## 5. Brownian Motion

Brownian motion is the motion of a particle, such as a smoke or dust particle, in a gas, as it is buffeted by random collisions with gas molecules. Make a simple computer simulation of such a particle (in two dimensions) as follows. The particle is confined to a square grid or lattice  $L \times L$  squares on a side, so that its position can be represented by two integers  $i, j = 0 \dots L - 1$ . It starts in the middle of the grid. On each step of the simulation, choose a random direction—up, down, left, or right—and move the particle one step in that direction. The particle is doing a “random walk.” The particle is not allowed to move outside the square of the lattice—if it tries to do so, choose a new random direction to move in.

Write a program to do this calculation for a million steps of the random walk with  $L = 101$  and make an animation on the screen of the position of the particle. (We choose an odd length for the side of the square so that there is one lattice site exactly in the center.)

## 6. Gauss Quadrature

Evaluate the integral using Gauss-Legendre Quadrature:

$$I = \int_0^1 \frac{\tan^{-1} \sqrt{x^2+2}}{\sqrt{x^2+2}(x^2+1)} dx,$$

at various orders, from  $N=2, 4, 8, 16, 32$ . Calculate the absolute difference between the integral estimate for each  $N$  with the true answer,  $I = 5\pi^2/96$ . You can find the nodes and weights of many Gauss-Quadratures here:

<http://keisan.casio.com/exec/system/1329114617>.