6 Checkpoint 6

Aim of Checkpoint

This checkpoint is an alternative to *Checkpoints 1 to 3* for people who have had previous JAVA experience, and/or found these checkpoints trivial. This checkpoint is also an initial introduction to *computer simulation* and is strongly recommended for Computational Physics students.

Submission Dates

It is expected that this checkpoint is completed during the **sixth** laboratory session if you have started at checkpoint 4.

Final submission date for this checkpoint is: **5.00 pm, Thursday 3rd November**

Monte Carlo Integration

When analytic integration is impractical, either due to complicated expressions or difficult boundary conditions, then we have to resort to numerical integration. This checkpoint investigates the very flexible technique of *Monte Carlo* integration which obtains a statistical estimate for the integral and is especially applicable where there are geometrically complicated boundary conditions.

If we have a function two-dimensional $f(x,y)$ defined over at area V and we uniformly sample this area, then the probability density function at position (x,y) is simply given by,

$$\rho(x,y) = \frac{1}{V}$$

The expectation value for $f(x,y)$ over this area is,

$$\langle f(x,y)\rangle = \int f(x,y)\,\rho(x,y)\,dx\,dy$$

which by substitution for $\rho(x,y)$ gives

$$\int f(x,y)\,dx\,dx = V\,\langle f(x,y)\rangle$$

allowing us to obtain the value of the integral from the expectation value.

We can yow obtain an *estimate* for the expectation value by taking N sample point $(x_i,y_i)i = 1 \rightarrow N$ by:

$$\langle f(x,y)\rangle \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i,y_i)$$

so giving us an *estimate* for the integral.

Estimate of on Area

Take the simple example of estimating an area W enclosed by a known area V as shown in figure 1. If we choose a point at random within area V then the probability p that this point is

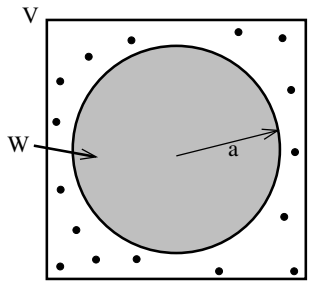

Figure 1: Area to be estimated

within area W is given by

$$p = W/V$$

so if we know, or can estimate p then the unknown area W is simply given by

$$W = V\,p$$

More formally, if the area W is defined by the two-dimensional function $f(x,y)$ such that

$$\begin{aligned} f(x,y) &= 1 \quad \text{if } (x,y) \text{ is within area } W \\ &= 0 \quad \text{else} \end{aligned}$$

then we have that,

$$\iint f(x,y)\,dx\,dy = W$$

To estimate p we randomly choose a points uniformly in V and count the number that are also in W. So if we randomly select N points of which N_W are within W then we obtain an estimate

$$p \approx \frac{N_W}{N}$$

which will improve as $1/\sqrt{N}$. So provided we can easily determine if a point is "inside" or "outside" W we have a very simple integration scheme that works for complicated boundary conditions.

This technique is very general and can be very easily extended to higher dimensions where most other numerical techniques tend to converge rather slowly or suffer from numerical error problems.

Computing Tasks

Task 1: Calculate of π

Use the Monte Carlo integration technique to estimate the value of π as a function of number of points N and plot out the magnitude of the error between the estimate and the accepted value against the number of points considered with the error being display with the `SimpleGraph` class.

Use your program to estimate how many point you must take to obtain a value for π to 4 significant figures.

Hint: The area of a circle of unit radius is π !

Task 2: Volume of Water Molecule

The simplest model for a molecule is *spherical* atoms with fixed bond-lengths and angles. In all cases the bond-lengths (distance between the atom centres) are smaller than the atomic diameters so the molecule consists of a series of overlapping spheres. The volume of such a structure is difficult, usually impossible, to calculate analytically and has to be numerical estimated. The aim of this computing task is to calculate the volume of a water molecule by Monte Carlo integration.

The water molecule consists of two hydrogen and one oxygen atom arranged as shown in figure 2 with parameters:

Radius of Oxygen	r_O	1.4 Å
Radius of Hydrogen	r_H	1.1 Å
$O-H$ Bond length	d_{O-H}	0.95 Å
Bond Angle	θ	104.5°

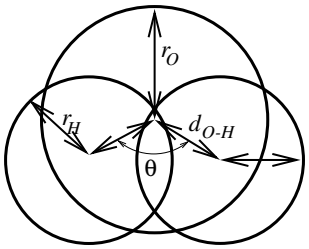

Figure 2: Plan of water molecule

Write a program to use Monte Carlo integration to calculate the volume of the water molecule (in $\mathring{A}^3$) to a given precision. In writing your program you should consider,

1. enclosing the molecule in an appropriate sized "box" (smallest possible) to minimise the computational cost,
2. how to estimate the precision of the calculation,
3. how the program is written so that it can easily used for other (more complex) molecules with more than three atoms, (think about how to hold the position and radii of the spheres).

This program is "non-trivial", especially if your try and write it all as a `main` program. Think how you can alter the `Point` class from the last section to an `Atom` class, (an `Atom` is a sphere of given radius about a `Point`!), and what *methods* you should use. Remember the main bit of your program will be asking if a `Point` is "inside" an `Atom`!

Checking for correctness

This is the first program you have written that you do not easily "know" in advance what you will get. To check that you code works you need an estimate. Suggest how you can obtain an analytical *estimate*, for the above values and compare these with the obtained results.

End of Checkpoint

When you have completed both your program call a demonstrator and show them the code, and the numerical results the comparison with the analytical estimate and discuss the results you have obtained. This is the end of **checkpoint 6**. Ensure that the demonstrator checks off your name.

Material Needed

It is *strongly* advised that you use *objects* for the second checkpoint here, so you will need the final optional section.