Text from: http://www.chem.unl.edu/zeng/joy/mclab/mcintro.html

Introduction to Monte Carlo Methods

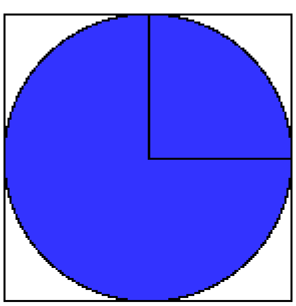
The expression "Monte Carlo method" is actually very general. Monte Carlo (MC) methods are stochastic techniques--meaning they are based on the use of random numbers and probability statistics to investigate problems. You can find MC methods used in everything from economics to nuclear physics to regulating the flow of traffic. Of course the way they are applied varies widely from field to field, and there are dozens of subsets of MC even within chemistry. But, strictly speaking, to call something a "Monte Carlo" experiment, all you need to do is use random numbers to examine some problem.

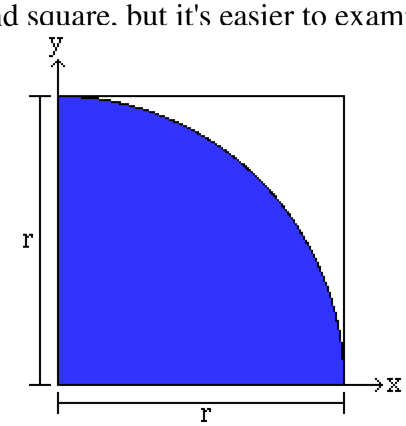
The use of MC methods to model physical problems allows us to examine more complex systems than we otherwise can. Solving equations which describe the interactions between two atoms is fairly simple; solving the same equations for hundreds or thousands of atoms is impossible. With MC methods, a large system can be sampled in a number of random configurations, and that data can be used to describe the system as a whole.

"Hit and miss" integration is the simplest type of MC method to understand, and it is the type of experiment used in this lab to determine the HCl/DCl energy level population distribution. Before discussing the lab, however, we will begin with a simple geometric MC experiment which calculates the value of pi based on a "hit and miss" integration.

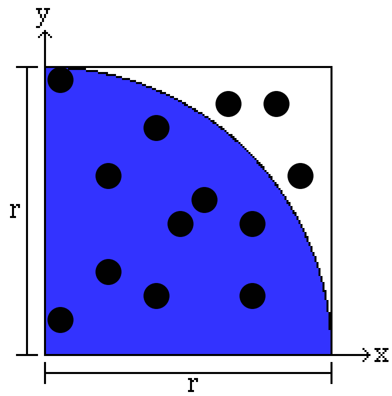
Monte Carlo Calculation of Pi

The first figure is simply a unit circle circumscribed by a square. We could examine this problem in terms of the full circle and square, but it's easier to examine just one quadrant of the circle, as in the figure below.





If you are a very poor dart player, it is easy to imagine throwing darts randomly at this figure, and it should be apparent that of the total number of darts that hit within the square, the number of darts that hit the shaded part (circle quadrant) is proportional to the area of that part. In other words, $\frac{\text{\# darts hitting shaded area}}{\text{\# darts hitting inside square}} = \frac{\text{area of shaded area}}{\text{area of square}}$



If you remember your geometry, it's easy to show that

$$\frac{\text{\# darts hitting shaded area}}{\text{\# darts hitting inside square}} = \frac{\frac{1}{4}\pi r^2}{r^2} = \frac{1}{4}\pi$$

or

$$\pi = 4\,\frac{\text{\# darts hitting shaded area}}{\text{\# darts hitting inside square}}$$

If each dart thrown lands somewhere inside the square, the ratio of "hits" (in the shaded area) to "throws" will be one-fourth the value of pi. If you actually do this experiment, you'll soon realize that it takes a very large number of throws to get a decent value of pi...well over 1,000. To make things easy on ourselves, we can have computers generate random* numbers.

Programming Assignment: write a simple monte carlo simulation to estimate the value of pi. Have the user enter the number of iterations. (Option: you can try to automatically stop the iterations by comparing the estimate to the known value.)

Save the random coordinates in text file. Load up the file in Excel and plot the values. (Make sure the file that you write is not too large…..)