Homework Due Feb 10

1.) Use Monte Carlo Integration to evaluate the integral of e^{-x} dx over the interval from 0 to 1 using n = 10, 20, 50, 100, 200, 500, 10000, 10000, and 50000. Calculate the error with respect to the exact answer. Plot the results using a logarithmic scale to show the rate of growth. Determine a how the error changes as a function of n.

2.) Shielding calculations of alphas, betas, x-rays and neutrons are often carried out utilizing a random walk calculations. Assume you have a wall 5 m thick and 5 m high. Let a neutron beam hit the wall, 4 m off the floor. The mean free path of neutrons in the wall is 1 m. After a collision, let the probability of scattering in any direction be equal. Neutrons can escape from top, bottom, or side of the wall. The scattering events are inelastic and the neutron loses 10% of its energy with each collision. When the kinetic energy of the neutron is 0, it is absorbed by the wall. Calculate the percentage of neutrons that will escape from the wall. How does this change if we build the wall out of something that absorbs 15% of the energy per collision? Include plots of a few representative paths.

3.) The development of Quantum Mechanics has allowed us to far better understand our physical world. Unfortunately, this has greatly complicated the calculations that we have to perform to get this understanding. One of the more important integrals that we have to calculate is the overlap integral between two orbitals involved in the bonding of molecules and solids. In the case of H_2, the overlap integral between two 1s orbitals is given by:

$$S = \int \Psi_a^*(\mathbf{r})\Psi_b(\mathbf{r}-\mathbf{R})\,dV$$

The H 1s orbital has the form:

$$\Psi_a = \frac{1}{\sqrt{\pi}} a_0^{\frac{-3}{2}} e^{\frac{-r}{a_0}}$$

Remember that this is a 3D orbital.
Evaluate the overlap integral for two 1s orbitals as a function of interatomic spacing, R.

Compare your computational result to the analytic result for this integral:

$$\int \Psi_a^*(\mathbf{r})\Psi_b(\mathbf{r}-\mathbf{R})\,dV = \left(1+\frac{R}{a_0}+\frac{1}{3}\left(\frac{R}{a_0}\right)^2\right)e^{-\frac{R}{a_0}}$$

Explore the effect of both the number of guesses and the size of the bounding box as the extent of the orbital goes out to infinity. Evaluation of this integral is often helped by utilizing a weighting function.

4.) Repeat 3 with the overlap between a H 1s orbital on one site and a H $2p_x$ orbital on the second site.

The H $2p_x$ orbital has the form:

5.) Draw a fractal Koch Snowflake. Make the choice of iterations user selectable.