Module 2: Monte Carlo Integration **Due: January 29, 2026, 5:00 PM**

Testing of a random number generator:

Q1. Use the provided random number generator (bad_rnd.f90). Generate 1000 random numbers and plot the scatter plot to observe whether they are correlated. What do you conclude about the quality of the generator?

Q2. Use a random number generator which generates uniform random numbers between 0 and 1.

a. Plot probability distribution data to prove that you have random numbers with uniform deviate.

b. Do a scatter plot to show that the random numbers are uncorrelated.

c. Calculate the correlation function to convince yourself that random numbers have no correlation.

d. Calculate the standard deviation (SD) of the random numbers about the mean.

Changing distribution:

Q3. Generate random numbers with (a) exponential (e^{-2x}) and (b) Gaussian (with SD=2) distributions.

Evaluation of π:

Q4. Using the trapezoidal method calculate $\int_0^1 \frac{4}{1+x^2}\,dx$ to determine the value of π (pi). Compare the computed value with the "actual" value. You can determine the "actual" value using $\pi = \tan^{-1} 1$. Do not use $\pi = 22/7$. Why?

Choose n=100, 1000,……,10^9, where n is the number of grid points (use both single and double precision) and evaluate the integral. Do a log-log plot of the absolute value of the error versus n. Do you obtain the plot as per your expectation? Explain. Fit the appropriate region to a straight line. What is the value of the slope? Is it according to your expectation?

Q5. Now we will estimate π using random numbers (Buffon's needle experiment).

Suppose you have a grid of lines separated by distance d. We throw needles of length l ($l<d$) on this grid. The probability P that the needle intersects any one of the lines is $P = \frac{2l}{\pi d}$. Write a code using a random number generator to perform the experiment. The ratio of the number of times the needle hit a line (n_{hit}) and the number of throws (n_{throw}) will give you the probability P. Using this estimate the value of π. Vary n_{throw}. Plot the absolute error vs. n_{throw}. Does the error (as a function of n_{throw}) vary as you expect?

Which of the two methods (used in Q4 and Q5) is more efficient?

Multidimensional integration using importance sampling:

Q6. We will compute the electron-electron interaction energy of the He atom. Assume that each electron can be modelled like that of an electron of H atom in 1s state, i.e., $\psi_{1s}(\boldsymbol{r}_i) = e^{-\alpha r_i}$, where $\alpha = 2$ is a parameter and $r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}$. Let us assume that the wave function for two electrons is given as:

$$\psi(r_1, r_2) = e^{-\alpha(r_1+r_2)}.$$

The correlation energy is given by:

$$\langle\frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\rangle = \int_{-\infty}^{\infty} d\boldsymbol{r}_1 d\boldsymbol{r}_2 e^{-2\alpha(r_1+r_2)} \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

Write a program that computes the following multi-dimensional integral using the (a) brute force (uniform distribution) and (b) importance sampling Monte Carlo integration methods. If you do not know the exact value of the integral, how do you compute the error? Compare the efficiency of the two methods.

Hint: Switch to spherical coordinates:

$$d\boldsymbol{r}_1 d\boldsymbol{r}_2 = r_1^2 dr_1 r_2^2 dr_2 d\cos\theta_1 \; d\cos\theta_2 \, d\phi_1 d\phi_2$$

with $\frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \equiv \frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_1^2 - 2r_1 r_2 \cos\beta}}$,

where $\cos\beta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)$