

**Problem:**

This assignment builds on your solution of home assignment 03. Your task is to compute, by the Monte Carlo method, the relative change in the distance the fission neutron flies to its first collision when the atomic concentration of the material is increased by 0.01% (compared to the concentration that you selected in home assignment 03).

- First, try to compute this result by running two independent simple sampling simulations (at the two different atomic concentrations). Repeat the experiment and evaluate the standard deviation of the relative change of the distance the fission neutron flies to its first collision.
- Second, compute the result by the correlated sampling method. Evaluate the standard deviation of the result and compare it to the result you got in the first part of this assignment.

### **Nuclear Fission:**

Each uranium-235 (U-235) atom has 92 protons and 143 neutrons, for a total of 235. The particle arrangement within uranium-235 is somewhat unstable, and the nucleus can dissolve if energized by an outside source. When a U-235 nucleus absorbs an added neutron, it swiftly splits into two halves. This is known as fission. When a U-235 nucleus divides, two or three neutrons are released. As a result, the chance of starting a chain reaction exists.

The task at hand is to calculate the mean distance that the fission neutrons fly till their first collision. To carry out the said task, I took into consideration a particular system mentioned before in the problem i.e., an infinite system composed of a single fissile nuclide at a reasonable mass density.

### **Transition Kernel:**

We know that transition kernel,  $T$ , is the probability density function of the distance,  $s$ , traversed by a neutron to next collision. To perform a simple sampling simulation to evaluate the mean distance that fission neutrons fly to the first collision, I made use of the cumulative distribution function derived from transformation of the given probability density function

$$T = \sum_t (\vec{r}, E) e^{-\Sigma_t s} \text{ --- [1]}$$

where,  $\Sigma_t$  is the total macroscopic cross-section of a given nuclide. In addition to that, we assumed that the total macroscopic cross section is constant along the flight in between the two collisions.

Knowledge concerning the physics of the fission process is summarized in various nuclear data libraries such as JEFF, ENDF, or ENSDF. JEFF and ENDF list the cross sections of a wide range of nuclear reactions as well as the fission yields. ENSDF, on the other hand, is primarily concerned with nuclear structural data. We can find the distance,  $s$ , to first collision of neutrons using the microscopic cross-section values collected from ENDF B-VIII.0 including the incident neutron energies via the JANIS database. These data can be used to simulate the values of distances,  $s$ , to first collision of neutrons by the help of cumulative distribution function and inverse transform of it.

We know that

$$\Sigma_t = N\sigma_t \quad \text{--- [2]}$$

where,  $N$  is the atomic number density and  $\sigma_t$  is the microscopic cross-section.

Therefore, the cumulative distribution function of the transition kernel,  $T$ ,

$$F_s = \int_0^s \sum_t (\vec{r}, E) e^{-\Sigma_t \acute{s}} d\acute{s} = 1 - e^{-\Sigma_t s} \quad \text{--- [3]}$$

(Homogeneous material)

Let the generated random number be,  $\mathcal{U}$ , which lives in the interval  $(0, 1)$ .

From [3], we get

$$\mathcal{U} = 1 - e^{-\Sigma_t s} \quad \text{--- [4]}$$

Therefore, we can make  $s$  the subject of the equation shown above to obtain

$$s = -\frac{1}{\Sigma_t} \ln(1 - \mathcal{U}). \text{ --- [5]}$$

Since the term  $(1 - \mathcal{U})$  is also a random number from interval  $(0, 1)$ . We can rewrite [5] as

$$s = -\frac{1}{\Sigma_t} \ln(\mathcal{U}). \text{ --- [6]}$$

By generating random values of  $\mathcal{U}$ , I got different values of  $s$  using cross section values. The cross-section values are found for the nearest incident energy of the neutron by using simple mathematical tool of linear interpolation. I have used the built-in interpolation module of Python “NumPy” library to find the cross-section values for nearest incident energy values of neutrons.

**Graph:**

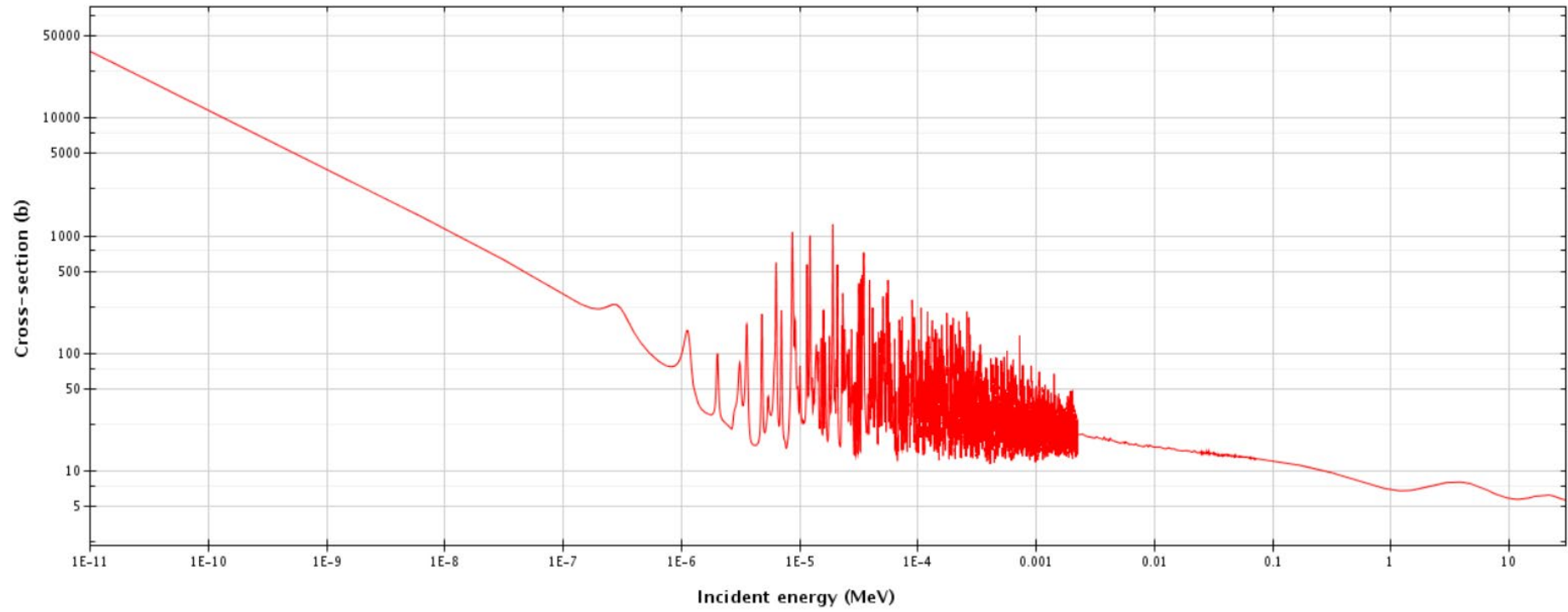


Fig. 1: NEA / Incident neutron data / ENDF/B-VIII.0 / Cross sections / U235 / MT=1: (n,total) / Cross section

### Mean and standard deviation for sampling using random variables:

After sampling  $n$  values of unknown random variable  $Y$ , the expectation value of  $Y$  can be estimated by the mean value of those generated sampling  $n$  values.

$$m_Y = \frac{1}{n} \sum_{i=1}^n y_i \text{ --- [7]}$$

According to the central limit theorem,

$$E[m_Y] = E[Y]. \text{ --- [8]}$$

In addition to that, variance of mean values of generated samples of the unknown random variable  $Y$ ,  $\sigma^2_{m_Y}$ :

$$\sigma^2_{m_Y} = \frac{\sum E[\xi_i^2]}{n^2} = \frac{\sigma^2_Y}{n} \text{ --- [9]}$$

where

$$\xi_i \equiv y_i - E[Y]. \text{ --- [10]}$$

However, the value of  $\sigma^2_Y$  is difficult to obtain but it can be estimated if a considerably substantial number of samples are taken e.g.,  $n > 10000$ .

Therefore, variance

$$\sigma^2_Y = \frac{1}{n} \sum_{i=1}^n (y_i - m_Y)^2 = \frac{1}{n} \sum_{i=1}^n y_i^2 - m_Y^2 \dots [11]$$

Hence, we just need to update the values of  $\sum y_i^2$  and  $\sum y_i$  to estimate the  $E[Y]$  and  $\sigma^2_{m_Y}$  after collecting a new sample of  $Y$ .

And the standard deviations  $\sigma$  are found by,

$$\sigma_{m_Y} = \frac{\sigma_Y}{\sqrt{n}} \dots [12]$$

### Correlated Sampling:

When calculating the difference between two extremely similar models,  $g_1$  and  $g_2$ , correlated sampling might be employed.

$$Y_1 = g_1(X) \text{ --- [13]}$$

$$Y_2 = g_2(X) \text{ --- [14]}$$

Typically,  $g_2$  is a significantly modified form of  $g_1$ . Since this difference between the expected values could be exceedingly small, the sampling would need to calculate  $E[Y_1]$  and  $E[Y_2]$  to a high degree of accuracy, which would take a significant amount of computational time.

Nevertheless, by examining the random variable, correlated sampling can easily solve this problem.

Let,

$$Z = Y_1 - Y_2 = (g_1 - g_2)(X) \text{ --- [15]}$$

Variance of  $Z$  is

$$Var[Z] = Var[Y_1] - Var[Y_2] - 2Cov[Y_1, Y_2]. \text{ --- [16]}$$



Where covariance of  $Y_1$  and  $Y_2$ ,

$$Cov[Y_1, Y_2] = E[(Y_1 - E[Y_1])(Y_2 - E[Y_2])] = E[Y_1 Y_2] - E[Y_1]E[Y_2], \dots [17]$$

is the value showing how  $Y_1$  and  $Y_2$  are related to each other.

Sampling  $Z$  is more efficient than sampling  $Y_1$  and  $Y_2$  separately using independent input random variables  $X_1$  and  $X_2$  when  $Y_1$  and  $Y_2$  are significantly positively correlated to each other. That implies that  $g_1$  and  $g_2$  are remarkably similar.

## Results:

Sampling of ten million random values of relative distance traversed by neutrons till first collision for U-235 nuclide of atomic number density,  $N = 7.98 \times 10^{21} \text{ atoms/cm}^3$  [2] and when  $N$  is increased by 0.01%:

For simple sampling:

Covariance:  $-0.238$

Mean relative distance: 3681.799

Standard deviation of relative distance: 1944157.695

Simple sampling time (in seconds): 446.469

For correlated sampling:

Covariance of relative distance: 278.719

Mean relative distance:  $9.999 \times 10^{-5}$

Standard deviation of relative distance:  $1.154 \times 10^{-16}$

Correlated sampling time (in seconds): 264.250

## Discussions:

The dataset obtained from slightly changing the value of atomic density,  $N$ , gives random values of mean distances a shift to the values. Results of mean and standard deviation of the relative distances show that simple sampling the distance individually will bring more uncertainty in the value. The standard deviation is increased by the fact that variance increased due to the covariance term being negative for simple sampling [16]. However, correlated sampling technique reduced the variance significantly as it had greater value of covariance in comparison to what we obtained from simple sampling of two variables [16]. Hence, the time to perform the simulation using correlated sampling is  $\sim 1.7$  times faster than what it took from running two simple sampling simulations ( $10^7$  samples were taken for each technique). This is because, we are only using the time to sample random number once to plug it into the two systems to get a value.

## References:

- J. R. Lamarsh, A. J. Baratta, Introduction to Nuclear Engineering, 3d ed., Prentice-Hall, 2001, ISBN: 0-201-82498-1.
- [Lessons on Monte Carlo methods and simulations in nuclear technology.](#)
- [JANIS database for cross-section values with corresponding incident neutron energies \(ENDF B-VIII.0\).](#)