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Subject: NPRE 555 – Computer Project 1 Report

1. Problem Statement

The purpose of this exercise is to write a Monte Carlo code to calculate the multiplication factor and simulate the flux distribution for one-speed neutrons in a slab reactor of thickness, a = 1 m with isotropic scattering. The properties of the slab are given as:

$$\Sigma_a = 0.12cm^{-1},\ \Sigma_s = 0.05cm^{-1},\ \nu\Sigma_f = 0.15cm^{-1} \text{ for } 0 < x < 50cm$$
$$\Sigma_a = 0.10cm^{-1},\ \Sigma_s = 0.05cm^{-1},\ \nu\Sigma_f = 0.12cm^{-1} \text{ for } 50cm < x < 100cm$$

2. Methodology

2.1. Monte Carlo Neutron Tracking Procedure

Generally, the first step of the Monte Carlo method is assuming a neutron source distribution in the domain. However, due to the simplicity of this problem, instead of assuming an initial source distribution, a threshold is set according to the macroscopic fission cross sections of both regions of the slab. The left region has a $\nu\Sigma_f$ of 0.15cm^{-1} while the right region has a $\nu\Sigma_f$ of 0.12cm^{-1}. The threshold is determined as,

$$\text{Threshold} = \frac{\nu\Sigma_{f,1}}{\nu\Sigma_{f,1} + \nu\Sigma_{f,2}} = \frac{0.15\,cm^{-1}}{0.15\,cm^{-1} + 0.12\,cm^{-1}} = \frac{5}{9}. \tag{1}$$

With the threshold set, a random number between 0 and 1 is generated using the built-in pseudo random number generator. If the number is less than the threshold, the neutron is born in the left region, and if the number is greater than the threshold, the neutron is born in the right region.

Once the birth location of the neutron is determined, the neutron will travel for a distance at a direction. The probability that the neutron has a collision at a distance s is described by the probability distribution function as,

$$T(s) = \Sigma_t(s)\exp\left[-\int_0^s \Sigma_t(s')ds'\right], \tag{2}$$

where Σ_t is the total macroscopic cross section. A random number, ξ is generated and corresponded to the cumulative distribution function, in the form of,

$$-\ln\xi = \int_0^s \Sigma_t(s')ds', \tag{3}$$

where

$$s = -\frac{\ln(1-\xi)}{\Sigma_t}\ . \tag{4}$$

The direction of the path of the neutron is determined by generating two random numbers, one for the elevation angle, θ, and the other one for the azimuthal angle, ϕ as,

$$\begin{aligned}\theta &= \pi \cdot \xi_1 \\ \phi &= 2\pi \cdot \xi_2\end{aligned} \tag{5}$$

where $\xi_{1,2}$ are random numbers. With the distance and angles determined, the distance traveled by the neutron in the Cartesian coordinates is determined using a built-in function known as 'sphr2cat'. Since this is a 1-D problem, only the distance in the *x*-direction is considered.

With the knowledge of the travel distance, the new location of the neutron is determined. If the new location is less than zero or greater than one, the neutron is considered to have leaked from the slab and the procedures described above are restarted for the next neutron. If the neutron crosses the boundary into the other region, its distance to the next regional boundary is determined and the distance to the next collision is determined. On the other hand, if the neutron remains in the region, the neutron is considered to have undergone collision. The type of collision is determined by first setting a threshold according to the absorption and scattering cross section of the region,

$$\text{Threshold} = \frac{\Sigma_a}{\Sigma_s + \Sigma_a}. \tag{6}$$

A random number is generated and if it is less than the threshold, the neutron is considered to have been absorbed, the neutron history is terminated, the location is recorded, and a new neutron history is restarted. Conversely, if the random number is greater than the threshold the neutron is considered to have been scattered. A random number is generated to determine the scattered angle of the neutron and another random number is generated and sampled using the CDF described in Eq. 4 to determine the new location of the neutron. The procedures are repeated until the neutron either leaks from the slab or is absorbed, after which its history is terminated, locations are recorded, and the history of another neutron is restarted.

Once the history of the last neutron is terminated and recorded, the scalar flux, ϕ and the effective multiplication factor, k_{eff} are determined. The scalar flux is calculated as,

$$\phi = \frac{\text{Collision Rate}}{\Sigma_t V}, \tag{7}$$

where V is an arbitrary volume for this work. The collision rate is described as the number of collisions in a given amount of time, which is arbitrary as this is a steady-state problem. Lastly, the effective multiplication factor is defined as,

$$k_{eff} = \frac{N_f}{N_a + N_l}, \tag{8}$$

where N_f is the number of neutrons fissioned, N_a is the number of neutrons absorbed, and N_l is the number of neutrons leaked from the medium.

3. Results and Discussions

3.1. Scalar Flux and Effective Multiplication Factor

The normalized scalar flux with 1,000,000 neutrons is presented in Fig. 1. In general, the flux profile has a rather uniform bell shape, with the maximum flux located at the center of the slab and a decaying trend near both external surfaces. However, it is observed that the flux profile is slightly higher on the left region than the right region. This is likely due to the fact that the macroscopic fission cross section is higher in the left region than the right region.

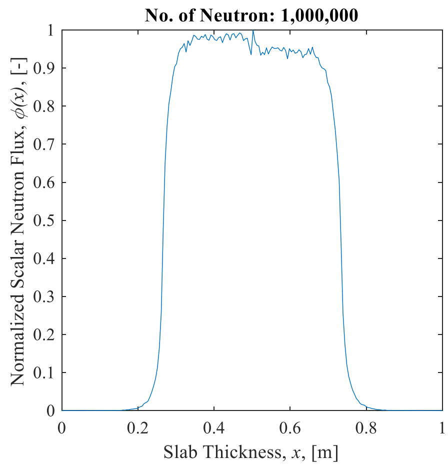

Fig. 1: Normalized scalar flux profile in the slab with an initial number of neutrons of 1,000,000.

Besides, the scalar flux has a smooth profile between $0 < x < 0.3$m and $0.7\text{m} < x < 1$ m, and a rough profile between approximately $0.3\text{m} < x < 0.7$m. It is postulated that the rough profile is due to the high collision rates near the middle of the slab. The profile can be smoothened by increasing the number of neutrons at the cost of computational time, as shown by the flux profiles in Fig. 2, where the flux profiles with 1000, 10000, and 100000 neutrons are plotted.

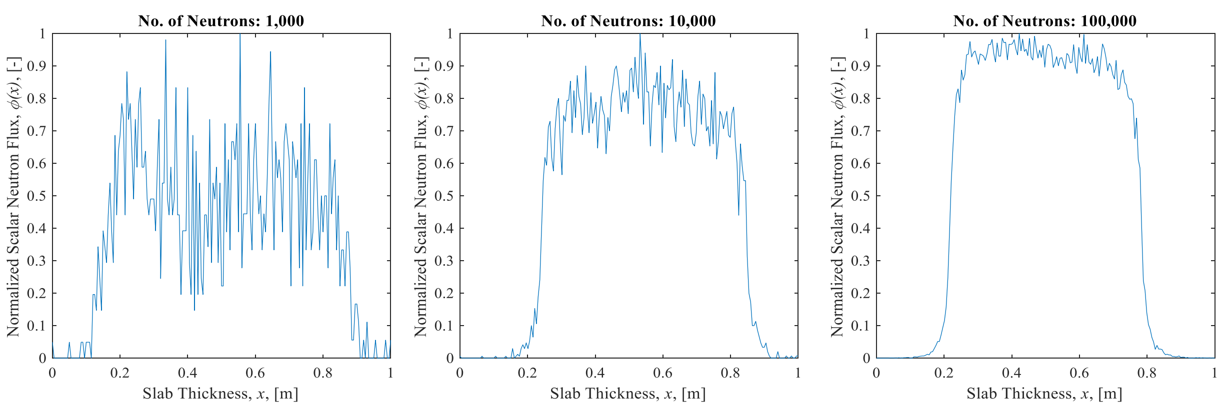

Fig. 2: Scalar flux profiles with 1000, 10000, and 100000 neutrons.

For the case with 1,000,000 initial neutrons, the effective multiplication factor is determined to be 1.189, as tabulated in Table 1. The effective multiplication factors for cases for different number of initial neutrons are compared where the values are observed to converge at approximately 1.189.

Table 1: Effective multiplication factor for cases with different number of initial neutrons.

Number of Initial Neutrons	1,000	10,000	100,000	1,000,000
Number of Neutrons Born	1,251	12,433	124,263	1,247,419
Number of Absorbed Neutron	1,020	10,127	101,105	1,015,137
Number of Leaked Neutrons	33	365	3401	34033
K_{eff}	1.1881	1.185	1.189	1.189

3.2. Possible Issues with Monte Carlo Code

It is postulated that the Monte Carlo code presented in this work might have some unresolved issues regarding its accuracy. A sharp discontinuity is observed in the flux profile at approximately x = 0.5m for cases with 5,000,000 and 10,000,000 initial neutrons, as shown in Fig. 3. The discontinuity is not observed in the previous cases likely due the rough profile caused by the comparatively low number of neutrons. The definitive cause behind the discontinuity has not been determined. However, it is hypothesized that the discontinuity is likely due to the definition of scalar flux used in this work, which only accounts for collisions that take place within the volume. As the boundary between the two regions is not considered as a part of the volume, collisions that take place at this location are thus accounted wrongly.

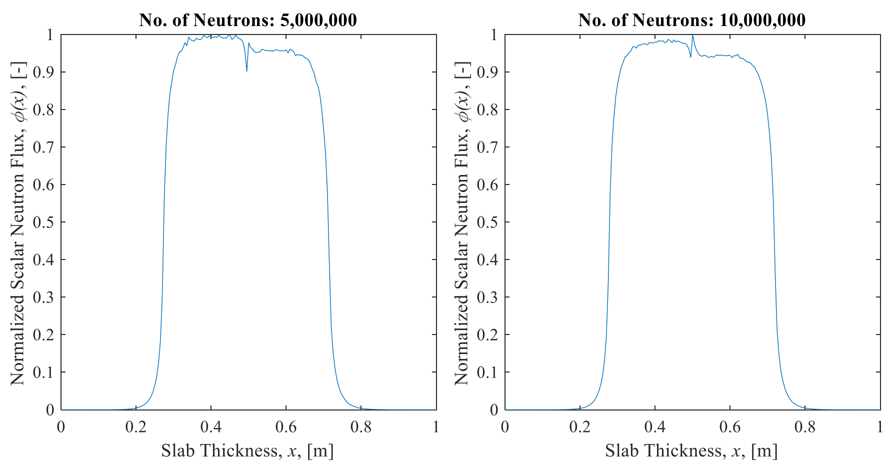

Fig. 3: Scalar flux profiles with 5,000,000 and 10,000,000 initial neutrons, with sharp discontinuity at the center.

4. Conclusions

A Monte Carlo code is written to simulate neutron transport in two-region 1-D slab. The flux profile has a uniform bell-like shape. The effective multiplication factor is calculated to be 1.189. It is determined that increasing the number of initial neutrons produces a smoother flux profile. However, it is observed that with a high neutron numbers, the flux profile has a discontinuity at the center of the slab. The definitive cause of the discontinuity has yet to be determined but it is postulated to be the consequence of the definition of scalar flux used in this work, which miscounts the number of collisions that occur at the boundary between the two regions.