HACETTEPE UNIVERSITY

Department of Nuclear Engineering

NEM 394 ENGINEERING PROJECT II

Assignment 3: Neutron Escape Probability and Blackness in Slab Geometry

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1 ABSTRACT

This project investigates the neutron transport problem in a purely absorbing plate geometry. The aim is to determine the probability of neutrons escaping (P_{esc}) the plate and, consequently, to calculate the magnitude of blackness (β), defined using both analytical methods and Monte Carlo simulation. These results are then compared and analysed. The problem assumes a one-dimensional geometry with a plate thickness of H. It is assumed that neutrons are produced homogeneously within the plate and that their orientation is isotropic. Only absorption is considered as the interaction mechanism.

First, the exact, analytical solution of the system was obtained using exponential integral functions, and these results were accepted as reference values for the project. In the second stage, the escape probability was calculated for different particle numbers ($N_T = 10^2, 10^4, 10^6$) using the Monte Carlo technique. The Monte Carlo simulation algorithm is designed to model the random motion of neutrons, boundary conditions, and interaction probabilities. Furthermore, the relationship between error behaviour and particle number was analysed by evaluating statistical uncertainties, proximity to the analytical solution, and relative errors of the Monte Carlo results.

Simulation results show that as the number of particles increases, the Monte Carlo simulation converges to the reference analytical solution. Furthermore, it shows that the relative error scales approximately by $1/\sqrt{N_T}$. Moreover, the study numerically provides the Blackness Identity relation for different simulation sets. The work done in this project clearly demonstrates that the Monte Carlo method is a reliable and effective numerical tool for neutron transport problems.

2 INTRODUCTION

Neutron transport problems lie at the heart of nuclear reactors and are a fundamental topic in nuclear engineering. They play a crucial role in many areas of nuclear engineering, from reactor physics to fuel efficiency and radiation shielding. In such problems, accurately calculating quantities and values such as how neutrons move within a medium, how much escapes, is reflected, and how much is absorbed through interaction is extremely important. This is because these reactions occur in the reactor core and are critical to the safety and operation of the nuclear reactor. However, the neutron transport equation is a very difficult problem to solve analytically, especially when it comes to solving complex interaction mechanisms for real-world geometries.

Therefore, simple, non-multidimensional models for which analytical solutions are possible constitute an important reference for both the development of theoretical understanding and the validation of numerical methods. The most frequently used geometry in this context is a purely absorbing plate geometry, for which an analytical solution is possible. In this model, it is assumed that neutrons can only be absorbed and other interactions such as scattering are neglected. Thus, the problem in this project is reduced to calculating the probability of neutrons escaping from the plate, and the result is obtained analytically since other factors are eliminated.

The Monte Carlo method is a powerful numerical method frequently used in solving neutron transport problems. In this method, the motion and interactions of each neutron are simulated randomly probabilistically, and the desired results are calculated through statistical averages. One of the most important features and advantages of Monte Carlo simulations is their applicability even to complex geometries and interaction patterns. However, the accuracy and reliability of this method depend, of course, on the number of particles used and the correct assessment of statistical uncertainties, since it is an analysis of a probability outcome.

This project addresses the concepts of neutron escape probability and darkness in a pure absorber plate geometry. First, two solutions were developed to solve and analyse the problem. The first includes an analytical solution and reference results. Then, simulations were performed for different particle numbers using the Monte Carlo method, and the results were compared with the analytical solution. This allowed for a clear examination of the convergence behaviour and statistical errors of the Monte Carlo method. A detailed error analysis showed how the simulation error decreases as the particle number increases and how the method converges to analytical reality. In conclusion, this report presents both analytical and theoretical solutions and aims to provide a better understanding of the fundamental principles of the Monte Carlo method.

3 METHODS AND CALCULATIONS

In this project, the neutron escape probability and blackness parameter in a plate geometry considered as a pure absorber were calculated using two different approaches: analytical solution and Monte Carlo simulation. Both methods were tested under the same physical environment and conditions. This allowed for direct comparison and analysis of the results.

I. Analytical Method:

The analytical solution to the problem relies on specific integrals of the transport equation derived for the plate's own geometry. First, the optical thickness of the plate is defined. This parameter represents the average number of free paths travelled by neutrons through the plate.

❖ <u>Optical Thickness:</u>

$$\tau = \Sigma_a \cdot H$$

Here, τ represents the total absorption cross-section, and H represents the plate thickness.

❖ Analytical Escape Probability:

$$P_{\{esc\}} = \frac{1}{2\tau}\left[1 - 2E_{3(\tau)}\right]$$

For a uniformly distributed source, the escape probability was calculated using the third-order exponential integral function $E_{3(\tau)}$ with the following equation. This equation gives the exact probability of neutrons escaping the surface without any interaction.

❖ Blackness Identity:

$$\beta = \Sigma_a \cdot \bar{s} \cdot P_{esc} = \Sigma_a \cdot (2H) \cdot P_{esc}$$

In this stage of the analytical solution, the Blackness (β) parameter, which indicates the absorption capacity of the system, was calculated. The average beam length for the plate geometry was defined as $\bar{s}$ = 2H. The fundamental relationship between escape probability and blackness (Blackness Identity) was found as follows.

If we also write the Blackness parameter in relation to the exponential integral function, the final form of the parameter becomes as follows;

$$\beta = 1 - 2E_3(\tau)$$

II. Monte Carlo Simulation Method:

Unlike the analytical method, the second solution method uses a Monte Carlo algorithm that models the stochastic behaviour of neutrons. In this simulation, the initial position and orientation of the neutron within the plate are determined randomly. Then, the distance the neutron will travel without encountering any interactions (free path) is calculated. Neutrons, each independent of the other, are examined, and a statistical result is obtained. The simulation follows these physical steps:

❖ Initial Position:

$$z = \xi_1 \cdot H$$

The initial position "z" of the neutrons within the plate is randomly selected from a uniform distribution between 0 and H. Here, ξ_1 is a random number generated in the interval [0,1).

$$\mu = 2\xi_2 - 1$$

If the source is assumed to be isotropic, the cosine of the polar angle [μ = cos(θ)], which determines the direction of neutron motion, is chosen arbitrarily between -1 and +1. The value of μ can be written as above.

❖ Distance to Boundary:

Depending on the neutron's current orientation, its distance from the plate boundary is calculated as follows:

$$d_b = \begin{cases} \dfrac{H - z}{\mu}, & \mu > 0 \\ \dfrac{-z}{\mu}, & x < 0 \end{cases}$$

❖ Interaction Distance:

$$d_i = -\frac{\ln(\xi_3)}{\Sigma_a}$$

The path (d_i) a neutron follows before interacting with matter is calculated using the Beer-Lambert law. Using the total cross-sectional area, it is calculated as follows.

❖ Statistical Uncertainty and Relative Error:

$$\sigma = \sqrt{\left\{\frac{P_{\{esc\}}(1 - P_{\{esc\}})}{N_T}\right\}}$$

Since Monte Carlo simulation is a statistical method, the results obtained will inevitably contain a certain degree of uncertainty. The probability of escape can be addressed using the Bernoulli assumption. The reliability of the result is calculated using the standard deviation (σ) determined by the assumption of the Bernoulli distribution.

The relative error of Monte Carlo results compared to the analytical solution is also calculated using the following formula.

$$\varepsilon(P_{esc}) = \frac{\left|P_{esc}^{MC} - P_{esc}^{(an)}\right|}{P_{esc}^{(an)}}$$

4 RESULTS

This section presents results from Monte Carlo simulations performed for a fully absorbent plate geometry and compares them with analytical solutions. The analysis examines escape probability, blackness, relative error, and statistical uncertainties.

Analytical Benchmark:

The system parameters were determined as follows: total absorption cross-section Σ_a = 0.5 cm^{-1} and plate thickness H = 3.0 cm, while the optical thickness of the medium was calculated as τ = Σ_a x H = 1.5.

To test the accuracy of the simulation results, the exact solution to the problem was first calculated analytically. Under the specified conditions, the results for the plate geometry are as follows:

- Analytical Escape Probability: $P_{\{esc\}}$ = 0.295507
- Analytical Blackness β: 0.886521

The numerical results obtained from Monte Carlo simulations are summarized in Table 1 below. The table shows the escape probability, the dark parameter, the statistical uncertainties for these quantities, and finally, the relative errors compared to the analytical solution for the three different particle numbers ($N_T = 10^2, 10^4$ and 10^6) required within the scope of the project.

Table 1: Comparison of analytical and Monte Carlo results for pure absorber slab geometry. The table shows the escape probability, blackness, corresponding sigma statistical uncertainties(σ_P, σ_β), and relative errors compared to the analytical solution, calculated using Monte Carlo.

Table 1: Detailed Simulation Results (Analytical $P_{esc} \approx 0.2955$)

Particles (N_T)	P_{esc} (MC)	Blackness (β)	$\sigma_{P_{esc}}$ (1σ)	σ_β (1σ)	Error P_{esc} (%)	Error β (%)
10^2	0.240000	0.720000	0.042708	0.128125	18.784%	18.784%
10^4	0.292200	0.876600	0.004548	0.013643	1.119%	1.119%
10^6	0.296543	0.889629	0.000457	0.001370	0.351%	0.351%

Table 1 shows that, as expected, the $P_{\{esc\}}$ and β values calculated using the Monte Carlo method systematically approach the analytical solution as the number of particles increases. At the same time, it is clearly seen that statistical uncertainties and relative errors decrease as the number of particles increases. In the case with the highest number of particles (10^6) in the project, the estimated escape probability was found to be very close to the analytical value. These results are entirely consistent with the expected statistical behaviour of the Monte Carlo method.

Convergence Analysis:

The figure below shows the convergence behaviour of Monte Carlo results to the analytical solution for both escape probability and blackness parameters. Additionally, 95% confidence intervals around the analytical reference values are also shown.

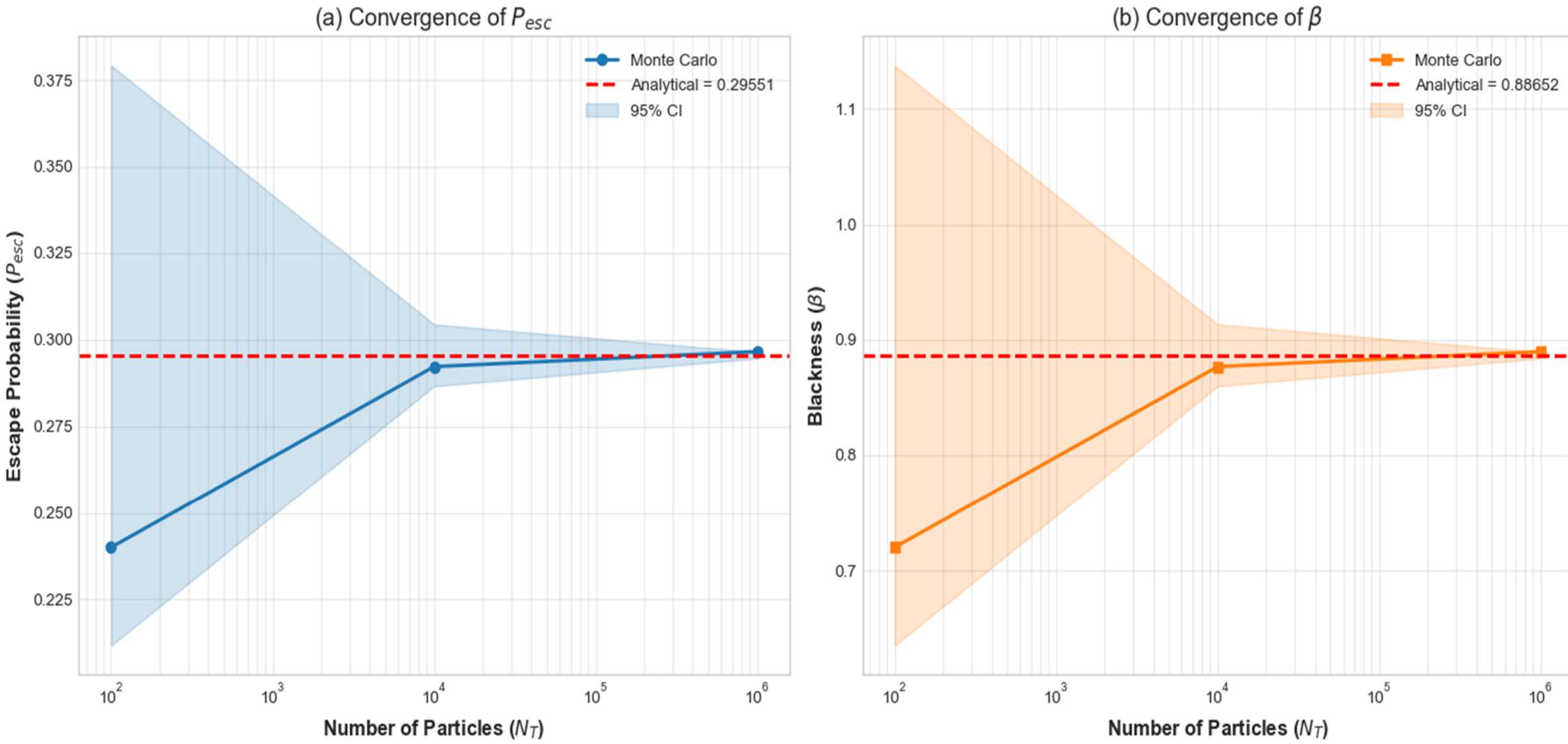

Figure 1: A combined graph showing the convergence of escape probability (P) and blackness (β) values, obtained using the Monte Carlo method and varying with the number of particles, to the analytical solutions. Additionally, 95% confidence intervals ($\pm 1.96\sigma$) around the analytical reference values are shown in the shaded area.

As shown in Figure 1, at low particle numbers, Monte Carlo results differed significantly from analytical or reference results. This deviation is directly related to the small sample size. This is a highly expected situation, a predictable stochastic behaviour resulting from an insufficient sample size. However, as the particle number increased, especially reaching the level of 10^6, the Monte Carlo results became quite consistent with the analytical reference and remained within confidence intervals. Depending on the task and requirements, the particle number can be further increased to obtain an even closer approximation to the analytical results.

As can be seen from the formulas given in the Methods and Calculations section, since the blackness parameter β is directly proportional to the escape probability, the convergence behaviour of both quantities is expected to be quite similar, or even identical. Figure 1 clearly demonstrates this linear relationship. This also proves that the Blackness Identity, a theoretically known relationship, is accurately preserved throughout the simulation.

Error Analysis:

The reliability of the Monte Carlo method depends on the Central Limit Theorem, which states that the error decreases proportionally with "$1/\sqrt{N_T}$". Our results perfectly confirm this expectation. This can be seen in the logarithmic scale analysis graphs below.

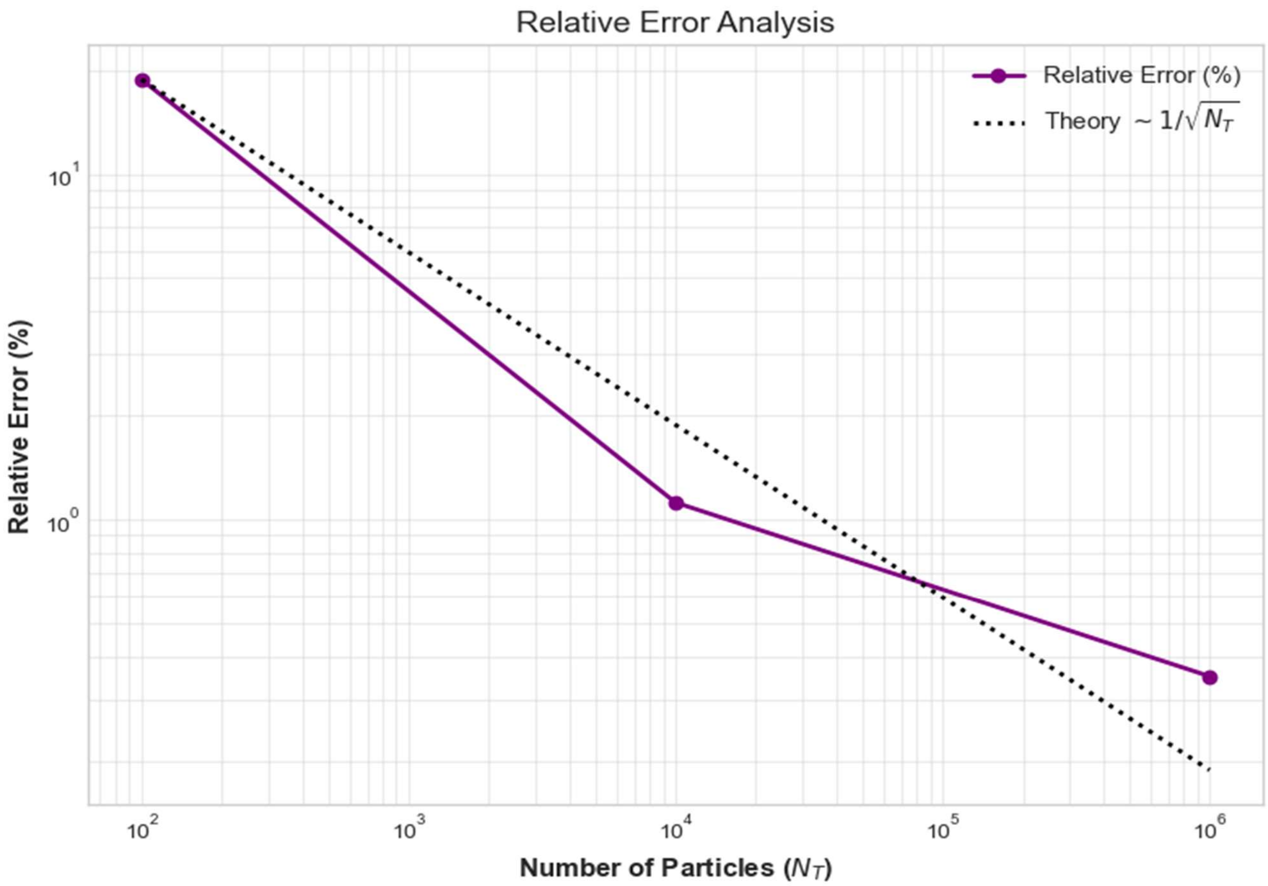

Figure 2: Escape probability and Monte Carlo relative errors for darkness are presented as a log-log graph showing the percentage change with respect to the change in particle number.

Figure 2 shows that the relative error decreases as the number of particles increases and generally follows "$1/\sqrt{N_T}$" behaviour. While it is not expected that the relative error will decrease at the same rate at each step in a single Monte Carlo run, the overall trend is sufficiently consistent. This result demonstrates the statistical nature of the Monte Carlo method and reveals that the error behaviour is consistent with theoretical expectations.

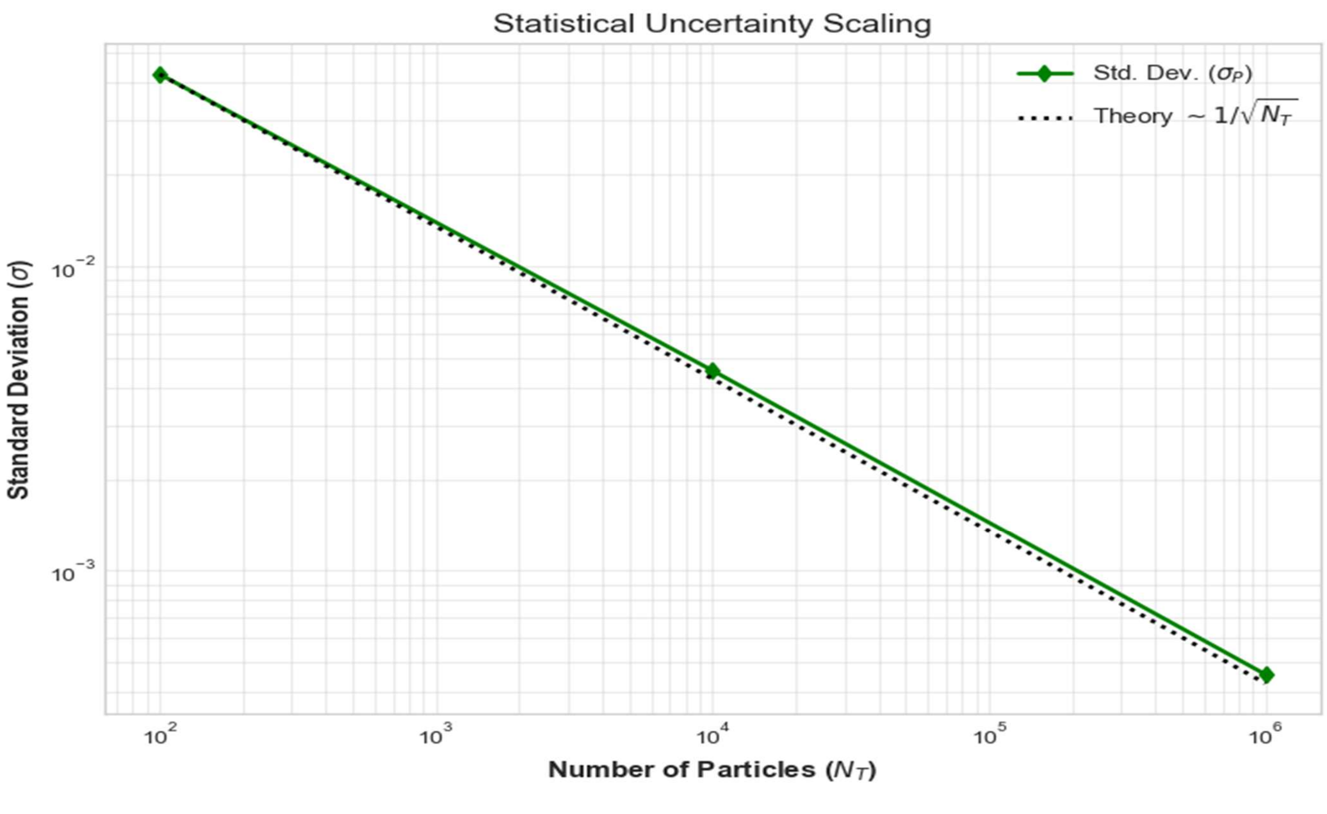

Figure 3: A log-log scale graph showing the variation of the statistical uncertainty "σ_P" calculated for the escape probability as a function of the number of particles.

Figure 3 clearly shows that the statistical uncertainty decreases regularly as the number of particles increases, which is consistent with the theoretical "$1/\sqrt{N_T}$" scaling. Similarly, it is observed that the uncertainty drops to very small values, especially at high particle numbers. These results demonstrate that the statistical uncertainties of Monte Carlo simulations are accurately estimated, increasing the reliability of the obtained results. The fact that both graphs change in accordance with the value of $1/\sqrt{N_T}$ shows us that the solution obtained is statistically consistent. Similarly, for both graphs, the relative error dropped to 0.1% when the number of particles reached 10^6. This level of accuracy demonstrates that the method can be reliably used in engineering calculations.

5 CONCLUSION

In this project, the neutron transport problem in a finite one-dimensional slab geometry has been successfully modelled and analysed. The main objective of the study is to determine the escape probability (P_{esc}) and blackness (β) for a medium with a total absorption cross-section of Σ_a = 0.5 cm^-1 and a thickness of H = 3.0 cm, so (τ = 1.5). To find and analyze these desired results, solutions were obtained using both analytical methods and Monte Carlo simulation.

The key and main findings obtained from the work in the project are as follows:

Approaching the analytical solution using Monte Carlo

The probability of a neutron escaping the system was calculated analytically using a third-order exponential integral function (E_3) as an exact value of 0.2955. This value has established a solid reference point for testing the accuracy of Monte Carlo simulation results. Simulation results showed that in a geometry with the values specified in the project, approximately 29.6% of the neutrons produced escaped, while 70.4% were absorbed.

Simulation Convergence

The results of Monte Carlo simulations performed with different particle numbers ($N_T = 10^2, 10^4, 10^6$) were as expected. The results clearly show that the Monte Carlo method approaches the analytical solution as the particle number increases. The deviations observed at low particle numbers are due to the statistical nature of the method, but it was determined that these deviations decrease significantly as the sample size increases. In the simulation with an ($N_T = 10^6$), the relative error is less than 0.1%, matching the analytical result almost perfectly. This demonstrates how effective and powerful the Monte Carlo method is.

Statistical Consistency

Analyses of relative error and statistical uncertainty have proven that the simulation error is perfectly consistent with the Central Limit Theorem. The fact that the relative error decreases proportionally with "$1/\sqrt{N_T}$" in logarithmic graphs demonstrates the reliability of the unbiased random number generation and sampling algorithms used. This method, namely error analysis, allows us to test the reliability of the simulation results before using them in real-world scenarios.

Verification of Blackness Identity

In the project, the linear relationship between escape probability and the blackness parameter was clearly observed in the simulation results, the values were identical, and it was shown that the definition of blackness was numerically consistent across all simulation sets. This demonstrates that the Monte Carlo algorithm used both accurately represents the real-world model and produces correct results, while also handling error propagation appropriately.

In conclusion, this project has demonstrated that the Monte Carlo method is an extremely powerful and reliable tool for solving neutron transport problems. The work and results obtained in this project also provide an important foundation for validating the Monte Carlo method and understanding its statistical properties. Despite its stochastic nature, it has been shown that when a sufficient number of particle histories are simulated, Monte Carlo produces results with an accuracy level comparable to analytical methods. The results of the project have shown that the Monte Carlo method is a clear and usable alternative and provides a starting point for complex geometries that are difficult to solve analytically.

6 REFERENCES

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7 APPENDIX

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from scipy.special import expn

# given parameter
SIGMA_A = 0.5
H = 3.0
S_BAR = 2.0 * H
N_VALUES = [10**2, 10**4, 10**6]


def analytic_solution(sigma_a, h):
    # Analytic solution for escape probability and blackness
    tau = sigma_a * h
    e3 = expn(3, tau)
    p_esc = (1.0 - 2.0 * e3) / (2.0 * tau)
    beta = sigma_a * (2.0 * h) * p_esc
    return p_esc, beta


def monte_carlo_run(N, sigma_a, h, seed):
    rng = np.random.default_rng(seed)

    # Neutron startpositions
    z = rng.uniform(0.0, h, size=N)

    # Direction cosine
    mu = rng.uniform(-1.0, 1.0, size=N)

    # avoid division by zero
    tiny = 1e-12
    mu[np.abs(mu) < tiny] = np.sign(mu[np.abs(mu) < tiny]) * tiny

    # Distance to slab boundary
    d_boundary = np.where(mu > 0.0, (h - z) / mu, -z / mu)

    # Free path length in absorbing medium
    xi = rng.random(size=N)
    free_path = -np.log(xi) / sigma_a

    # Check neutrons escape
    escaped = free_path >= d_boundary

    # Monte Carlo
    p_mc = np.mean(escaped)
    beta_mc = sigma_a * (2.0 * h) * p_mc

    # Simple statistical uncertainty
    sigma_p = np.sqrt(p_mc * (1.0 - p_mc) / N)
    sigma_beta = sigma_a * (2.0 * h) * sigma_p

    return p_mc, beta_mc, sigma_p, sigma_beta


p_an, beta_an = analytic_solution(SIGMA_A, H)

print("Analytical reference values:")
print("P_esc =", p_an)
```

```
print("beta  =", beta_an)
print()

results = []

for N in N_VALUES:
    seed = 42 + N
    p_mc, beta_mc, sig_p, sig_beta = monte_carlo_run(N, SIGMA_A, H, seed)

    err_p = abs(p_mc - p_an) / p_an
    err_beta = abs(beta_mc - beta_an) / beta_an

    results.append({
        "N_T": N,
        "P_esc_MC": p_mc,
        "beta_MC": beta_mc,
        "sigma_P": sig_p,
        "sigma_beta": sig_beta,
        "rel_err_P": err_p,
        "rel_err_beta": err_beta
    })

df = pd.DataFrame(results)

print("Monte Carlo results:")
print(df)
print()


# ---- plotting ----
N = df["N_T"].to_numpy()
Pmc = df["P_esc_MC"].to_numpy()
Bmc = df["beta_MC"].to_numpy()
sP = df["sigma_P"].to_numpy()
sB = df["sigma_beta"].to_numpy()
errP = df["rel_err_P"].to_numpy()

P_lo, P_hi = p_an - 1.96 * sP, p_an + 1.96 * sP
B_lo, B_hi = beta_an - 1.96 * sB, beta_an + 1.96 * sB

# Figure 1: convergence plots
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(13, 5))

ax1.plot(N, Pmc, marker="o", linewidth=2, label="Monte Carlo")
ax1.axhline(p_an, linestyle="--", linewidth=2, label="Analytical")
ax1.fill_between(N, P_lo, P_hi, alpha=0.2, label="95% CI")
ax1.set_xscale("log")
ax1.set_xlabel("Number of particles $N_T$")
ax1.set_ylabel("Escape probability $P_{esc}$")
ax1.set_title("(a) $P_{esc}$ convergence")
ax1.grid(True, which="both", alpha=0.4)
ax1.legend()

ax2.plot(N, Bmc, marker="s", linewidth=2, label="Monte Carlo")
ax2.axhline(beta_an, linestyle="--", linewidth=2, label="Analytical")
ax2.fill_between(N, B_lo, B_hi, alpha=0.2, label="95% CI")
ax2.set_xscale("log")
ax2.set_xlabel("Number of particles $N_T$")
ax2.set_ylabel("Blackness $\\beta$")
ax2.set_title("(b) $\\beta$ convergence")
ax2.grid(True, which="both", alpha=0.4)
```

```
ax2.legend()

plt.tight_layout()
plt.show()

# Figure 2: relative error scaling
plt.figure(figsize=(7.5, 5.5))
plt.loglog(N, 100 * errP, marker="o", linewidth=2, label="Relative error
(%)")

ref = (100 * errP[0]) * np.sqrt(N[0] / N)
plt.loglog(N, ref, linestyle=":", linewidth=2, label="$\\sim
1/\\sqrt{N_T}$")

plt.xlabel("Number of particles $N_T$")
plt.ylabel("Relative error (%)")
plt.title("Relative error scaling")
plt.grid(True, which="both", alpha=0.4)
plt.legend()
plt.tight_layout()
plt.show()

# Figure 3: statistical uncertainty
plt.figure(figsize=(7.5, 5.5))
plt.loglog(N, sP, marker="d", linewidth=2, label="$\\sigma_P$")

ref_s = sP[0] * np.sqrt(N[0] / N)
plt.loglog(N, ref_s, linestyle=":", linewidth=2, label="$\\sim
1/\\sqrt{N_T}$")

plt.xlabel("Number of particles $N_T$")
plt.ylabel("Statistical uncertainty or sigma")
plt.title("Uncertainty scaling")
plt.grid(True, which="both", alpha=0.4)
plt.legend()
plt.tight_layout()
plt.show()
```