Monte Carlo Simulation of Gamma Rays

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Abstract:

This project aims to utilize Monte Carlo simulation as a tool to study the transport of gamma radiation in complex media. Gamma photon behavior as it travels through a medium and interacts with its atomic and molecular components, including scattering and absorption, will be modelled by the simulation. The Monte Carlo approach will give a thorough knowledge of the intricate physical processes involved in gamma radiation transport by randomly selecting a large number of particle trajectories.

1. Introduction

Designing radiation shielding, imaging, and treatment systems that are safe and effective requires the use of radiation transport modeling. A potent method for modelling the movement of radiation through materials is Monte Carlo simulation. It entails producing a sizable number of random particle histories and seeing how they interact with the substance. The simulation can produce statistically reliable forecasts of the radiation dispersion, energy deposition, and other important characteristics by repeatedly performing this procedure.

Given the intrinsic randomness of gamma rays, Monte Carlo simulation is a suitable approach for simulating their behavior. Gamma rays may interact with materials in a variety of ways, such as pair creation, Compton scattering, and photoelectric absorption. Each sort of contact has a different likelihood of happening depending on variables such the gamma ray's energy, the substance it is travelling through, and the angle of incidence. All of these elements are by nature probabilistic.

Gamma ray activity is not completely unexpected since scientists have created mathematical models that describe the likelihood of certain sorts of interactions taking place. However, due to the gamma rays' intrinsic unpredictability, Monte Carlo simulation is a useful tool for simulating their behavior in a variety of real-world applications.

We can better comprehend radiation interactions with matter using the simulation data. By generating random paths for gamma rays through a material, it is possible to simulate the probability of various outcomes, such as absorption or scattering, as well as the energy deposited in the material. This information is crucial for designing safe and effective radiation shielding, imaging, and therapy systems, which are widely used in science, engineering, and medicine. This project seeks to utilize Monte Carlo simulation for modeling the transport of gamma rays through a specific material or geometry. Moreover, Analyzing the effects of various input parameters on the simulation results, such as the number of particles, the material composition, and the scoring method.

2. Overview of the existing research

Several studies have investigated the behavior of gamma rays as they interact with different materials. It has been observed that gamma rays deposit most of their energy slightly after they hit the medium[1], a phenomenon known as the skin sparing effect. This effect has been observed not only in human tissue but also in other materials. The exact magnitude of this effect varies depending on the energy of the gamma rays and the properties of the medium. Moreover, studies have demonstrated that the number of gamma rays passing through various materials, including aluminum, lead, water, and others, decreases with depth[2]. Higher-density materials such as lead result in a steeper decrease in the number of gamma rays as they penetrate deeper into the material. Therefore, degree of attenuation depends on the energy of the gamma rays, the density and composition of the material, and the distance traveled. These observations are important for understanding how gamma rays interact with different materials and for designing effective radiation shielding and therapy systems.

3. Different Types of Interactions for Gamma Rays with Matter

3.1. Photoelectric Absorption

When a gamma photon transmits all of its energy to an atomic electron, the electron escapes from its orbit around the nucleus and undergoes a form of interaction known as photoelectric absorption. The photon disappears, and the electron is then referred to as a photoelectron. For this interaction to take place, the gamma photon's energy must be higher than or equal to the electron's binding energy. The probability of this interaction is proportional to the third power of the atomic number Z of the material and to the fourth power of the photon energy. This means that materials with higher Z values and lower photon energies have a higher probability of undergoing photoelectric absorption. Photoelectric absorption is an important process in the interaction of gamma rays with matter because it results in the complete absorption of the photon and contributes to the total attenuation of the gamma beam.

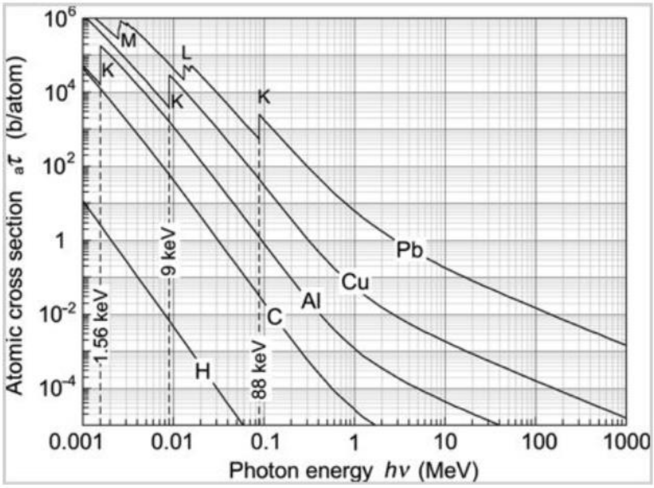

Figure 1 - Atomic Cross Section for Photoelectric effect with respect to Photon Energy [4]

3.2. Compton Scattering(Incoherent)

Compton scattering is a type of interaction that occurs when a photon interacts with matter. In Compton scattering, the photon transfers some of its energy and momentum to a loosely bound electron in the material, causing the photon to scatter in a different direction and lose energy. The scattered photon has a longer wavelength and lower energy than the original photon. The energy transferred to the electron depends on the angle at which the new photon is emitted, with larger energy transfers occurring at smaller angles. The Compton formula, which links the change in the scattered photon's wavelength to the scattering angle and the gamma ray's original wavelength by, may be used to describe the Compton scattering process.

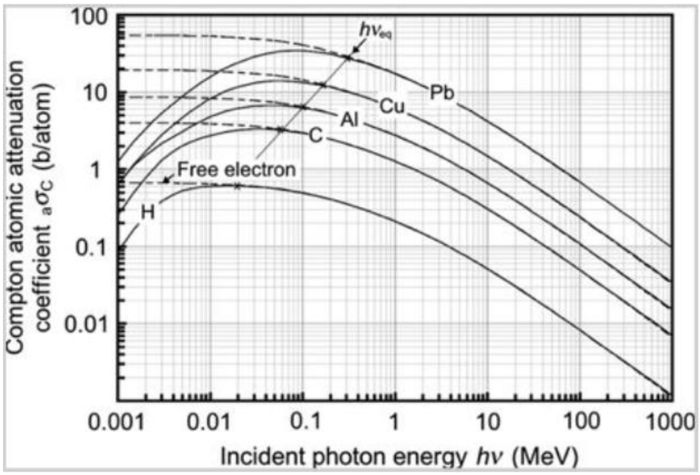

Figure 2 - Compton scattering atomic cross section with respect to incident photon energy [4]

$$\Delta\lambda = \lambda' - \lambda = \lambda_C(1 - \cos\theta) \quad (1)$$

Where $\lambda' \equiv$ wavelength of scattered photon, $\lambda_C \equiv$ Compton wavelgnth $= \frac{h}{m_e c}$. According to this formula, the wavelength of a scattered photon grows as the scattering angle shrinks, expanding the scattered photons' energy spectrum. The energy of the gamma ray and the atomic number of the substance it is interacting with affect the likelihood of Compton scattering.

3.3. Rayleigh Scattering(Coherent)

When photons scatter off atoms or molecules in a substance, a sort of interaction known as "Rayleigh scattering" takes place. It bears Lord Rayleigh's name since he was the one who initially explained the phenomena in the late 19th century. In contrast to Compton scattering, the incoming photon's energy is not taken up by the atom or molecule. Instead, the photon interacts with the entire atom or molecule, causing it to vibrate and scatter the photon with the same energy and frequency in a new direction. The blue tint of the sky is a result of Rayleigh scattering., since the shorter wavelength of blue light makes it easier to disperse than other hues. The atomic or molecular density of the material and the frequency of the incoming photon both affect how likely Rayleigh scattering is to occur.

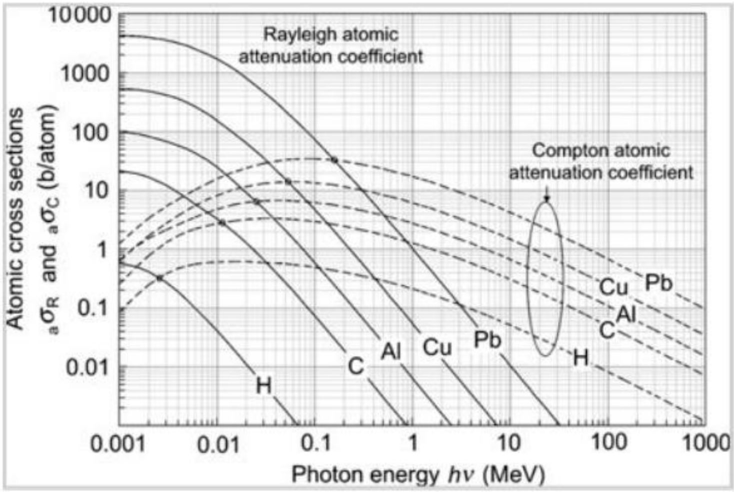

Figure 3 - Rayleigh scattering atomic cross section with respect to incident photon energy compared with Compton scattering atomic cross section[4]

3.4. Pair Production

An electron-positron pair is created when a gamma photon interacts with the nucleus of an atom, a process known as nuclear pair formation. The rest mass energy of an electron-positron pair, 1.02 MeV, is the minimum threshold energy required for this operation. The gamma photon must interact with the nucleus' electric field, which supplies the pair with the requisite energy. In the end, the positron created in this process will annihilate with an electron, emitting two gamma rays.

On the other hand, electronic pair formation happens when a gamma photon combines with an atomic electron to create an electron-positron pair. The rest mass energy of an electron-positron pair, 1.02 MeV, is the minimum threshold energy required for this operation. The gamma photon must interact with an atomic electron's electric field, which supplies the pair with the required energy. In the end, the positron created in this process will annihilate with an electron, emitting two gamma rays. Higher atomic numbers and lower photon energy are the conditions where electronic pair formation is most likely to take place.

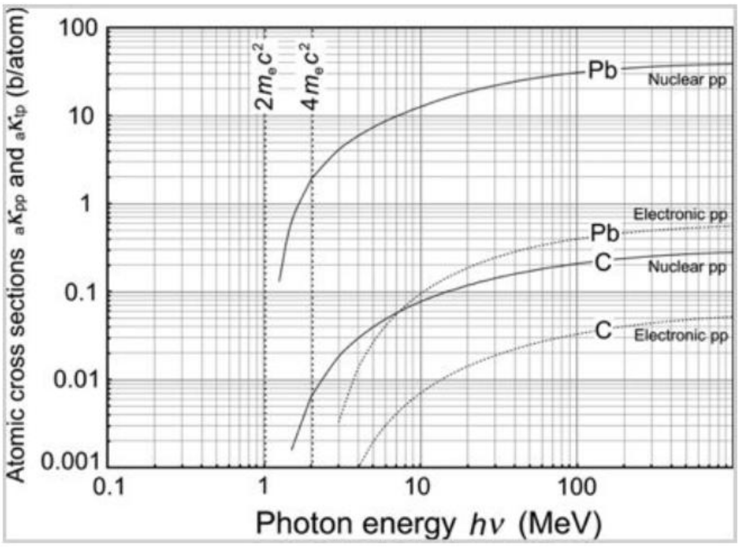

Figure 4 – Atomic Cross Section for Pair Production[4]

4. Attenuation of photon beams

4.1. Linear Attenuation Coefficient

The Beer-Lambert rule, which states that the intensity of the beam diminishes exponentially with distance traversed through the medium, may be used to quantitatively model the linear attenuation of gamma rays as they pass through a material

$$\mathrm{I}(x) = \mathrm{I}_0\, e^{-\mu \cdot x} \quad (2)$$

Where $\mathrm{I}(x)$ is the intensity of the beam at a distance x inside the medium, and μ is the linear attenuation coefficient of the medium. The gamma ray energy and the material's characteristics, such as its density and atomic make-up, affect the linear attenuation coefficient.

The attenuation coefficient gauges how much a substance lessens a radiation beam's intensity as it passes through it. It relies on a number of variables, including as the material's density and thickness as well as the energy and kind of incoming radiation. The atomic cross section, on the other hand, is a measure of the probability of a particular type of interaction between a photon and an atom or molecule in the material. The relationship between these two quantities can be described using the identity of the total linear attenuation coefficient

$$\mu = \tau + \sigma_R + \sigma_C + \kappa \quad (3)$$

Where $\tau \equiv$ Photoelectric effect, $\kappa \equiv$ pair production, $\sigma_R \equiv$ Rayleigh, $\sigma_C \equiv$ Compton Cross sections

4.2. Mass Attenuation Coefficient.

The linear attenuation coefficient is the easiest absorption coefficient to determine experimentally, but because it depends on the density of the absorbing substance, it is not frequently tabulated. For example, the linear attenuation coefficients of water, ice, and steam are different at a given energy, even though they are the same material. Rather, mass attenuation Considering that it measures the likelihood that a certain element would interact with gamma rays, coefficient is more frequently tabulated than the linear attenuation coefficient

$$\frac{\mu}{\rho} = \frac{\tau}{\rho} + \frac{\sigma_R}{\rho} + \frac{\sigma_C}{\rho} + \frac{\kappa}{\rho} \quad (4)$$

Where $\frac{\mu}{\rho} \equiv Total\ mass\ attenuation\ coefficient$. As the cross section increases, the probability of an interaction occurring increases as well, leading to a greater attenuation of the radiation. Therefore, the attenuation coefficient will also increase proportionally to the cross section. This is why the plot of the attenuation coefficient often has the same behavior as the plot of the atomic cross section(Figure.5).

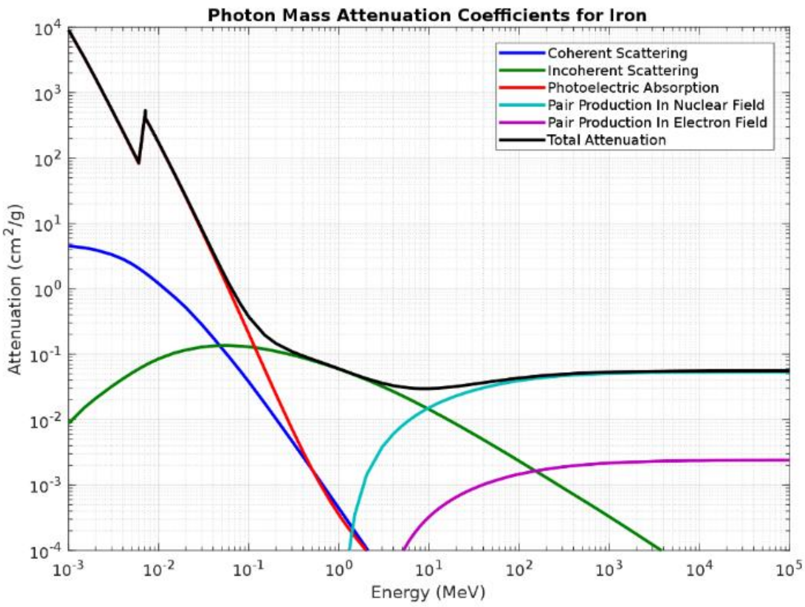

Figure 5 - Coherent scattering, Compton(incoherent) scattering, photoelectric absorption, and two different pair creation processes all contribute to the mass attenuation coefficient of iron.[5]

5. Monte Carlo for Random Sampling

As we discussed in section 1, the gamma radiation interactions are inherently random, in the sense that the mechanism of which the photon is undergoing is subject to different distributions. For example, the distance to the next interaction, s, is subject to this distribution:

$$p(s)ds = \frac{1}{\lambda} 2e^{-s/\lambda} ds$$

And the scattering angle, θ, follows this complicated distribution:

$$p(\theta)d\theta = \frac{d\sigma_{KN}}{d\Omega} 2\pi \sin\theta\, d$$

Where σ_{KN} is the Klein-Nishina cross section, which has the following form:

$$\sigma_C = Z2\pi r_e^2 \left(\frac{1+k}{k^2} \left[\frac{2(1+k)}{1+2k} - \frac{\ln(1+2k)}{k} \right] + \frac{\ln(1+2k)}{2k} - \frac{1+3k}{(1+2k)^2} \right)$$

The problem is that we do now know how to randomly sample random points for θ, so in order to do that, we will rely on Acceptance / Rejection method in Monte Carlo.

Suppose we want to randomly sample points according to the distribution $p(x)$ which we do not know how to sample from. We will use a distribution which we know how to sample from, $U(x)$, which is typically a uniform distribution scaled to the maximum of $p(x)$. We will randomly sample a point, (x_i, y_i), we will check whether y_i falls inside the distribution, i.e., we will compute $y_i \leq p(x_i)$, if it is true, then we will accept the point in our random sampling, if not, we will reject it and sample a new point (x_{i+1}, y_{i+1}). An illustration is shown in the next figure:

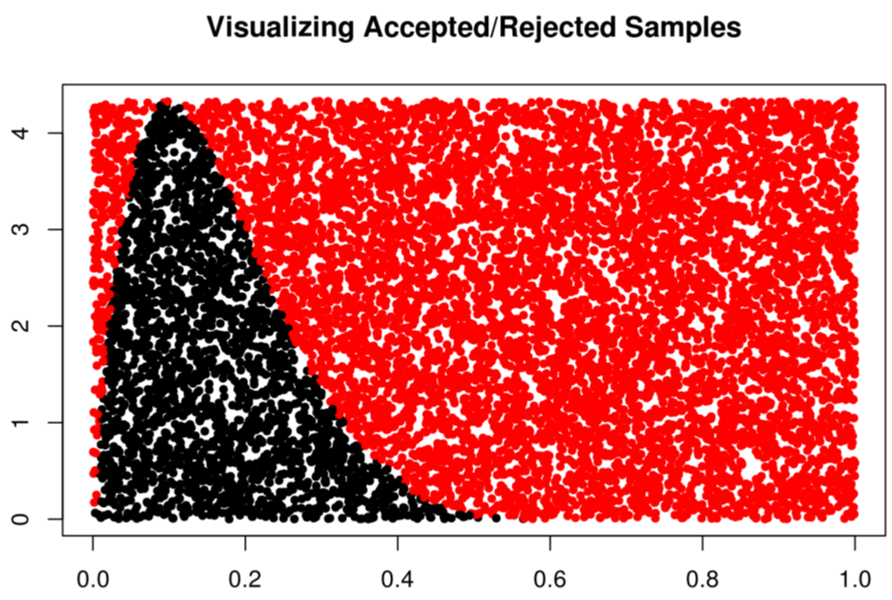

Figure 6 - Visualization of the Acceptance/Rejection sampling

Now, we will discuss the procedure to apply this method to radiation transport.

i. Define the experiment setup: Specify the dimensions of the target's geometry, material composition, and the position and energy of the gamma source.
ii. Obtain cross sections: From the material composition and the energy of the gamma ray, obtain Compton and photoelectric cross sections. This can be obtained by approximating formulas or from experiments.
iii. Randomly sample the distance to the next interaction: Sample the distance to next interaction according to $p(s)$. See Figure 12.
iv. Determine the interaction: Randomly choose the interaction by uniformly sampling a point between (0,1) where the intervals are split in two subintervals with a length proportional to the corresponding cross sections.
v. If photoelectric: The photon will deposit all of its energy and disappear. Go back to (iii).
vi. If Compton: randomly sample the scattering angle according to $p(\theta)$. See Figure 12.
vii. Update the energy: By conservation of energy and momentum, compute the new energy of the photon. Go back to (iii).

viii. Repeat the process: Repeat the simulation for a large number of photons to obtain statistically significant results. By simulating a sufficient number of gamma ray photons, we can obtain reliable statistical data on the overall behavior of gamma rays interactions.

6. Our Simulation Setup

6.1. Geometry to model

The Geometry of the medium that the gamma rays will originate from the axis of a cylinder made out of water(border and within) with Constituents (Atomic Number : Fraction by Weight)

$$Z = 1: 0.111898$$

$$Z = 8: 0.888102$$

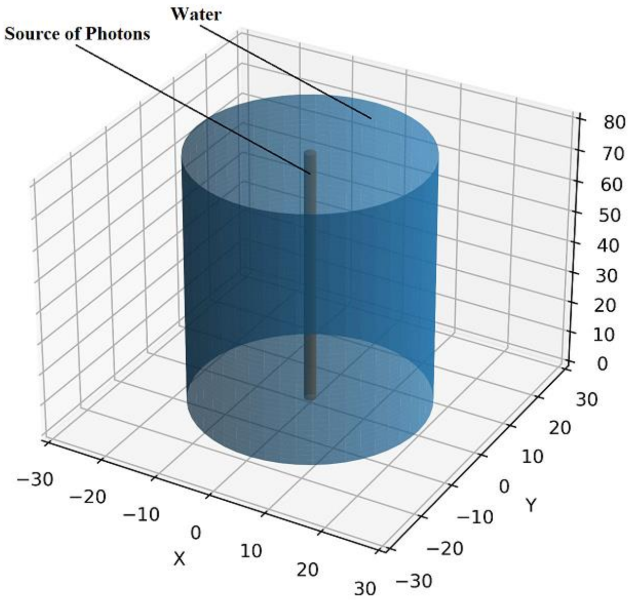

Figure 7 –Overview of the cylindrical medium which the photons will travel in

Photon trajectories inside the cylinder are to be visualized.

6.2. Code and Input Parameters

Our simulation code for modeling gamma rays inside a medium is implemented in Python (see Appendix). Python is a well-liked programming language with a reputation for clarity and simplicity, making it the perfect option for scientific simulations. We have access to robust tools for data analysis, visualization, and mathematical computations thanks to its broad library ecosystem. By leveraging Python's flexibility, we can efficiently handle the simulation processes, particle tracking, energy deposition calculations, and analyzing the results. The use of Python allows us to develop a robust and user-friendly codebase for our gamma ray simulation project.

The photoelectric effect and Compton scattering are the dominant interactions for most practical applications involving gamma rays. The photoelectric effect is especially significant at lower energies (Figure.5). Thus, in the Python code that was used for the simulation, we have chosen to focus on the two primary interactions: photoelectric effect and Compton scattering. By focusing on these two primary interactions, our simulation can provide valuable insights into the behavior of gamma rays in the medium while keeping the computational demands manageable. While other interactions may occur in specific scenarios or at higher energies, their inclusion would introduce additional complexity that is beyond the scope of our current simulation.

The cross sections for photoelectric effect and Compton scattering at various photon energies were obtained from tables provided by the X-Ray Cross Sections Database (XCOM) website. The website offers detailed tabulated data on the cross sections of various interaction processes, including photoelectric effect and Compton scattering, for different photon energies and target materials. These cross sections are crucial for accurately simulating the interactions of gamma rays with matter in our

Monte Carlo simulation. By utilizing the reliable and validated cross section data from the XCOM database, we ensure the fidelity and accuracy of our simulation results. Some tabulated values of the cross sections of both interactions at different photon energies are plotted below (Figure.6)

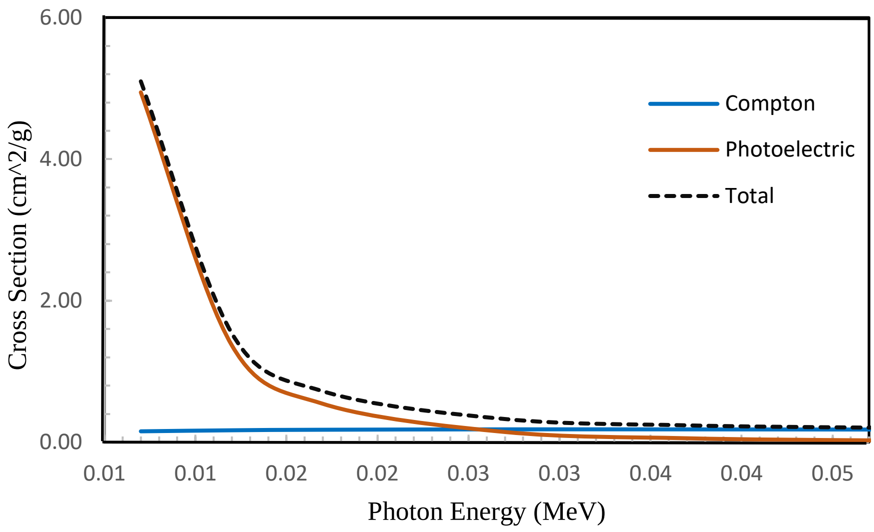

Figure 8 - Cross Section of Photoelectric Effect and Compton Scattering for different Photon Energies ($0.01 - 0.05\ MeV$) from a Table Provided by XCOM[5]

7. Results and Analysis

In this section, the obtained results and their analysis are presented. The analysis includes various visualizations, such as histograms with depth-dose curves, to examine the energy deposition characteristics. Additionally, the trajectories of the gamma rays inside the cylinder will be shown in three different views: a top view to observe the deviations of gamma rays from the center, a side view to visualize the lateral scattering, and a three-dimensional view for a comprehensive understanding of the simulation results. Furthermore, the probability distributions of the straight distance traveled without photoelectric/Compton interaction $p(s)$ and the scattering angle distribution $p(\theta)$ from Compton scattering will be analyzed (see the appendix for more visualizations that examines different parameters).

7.1. Energy Deposition

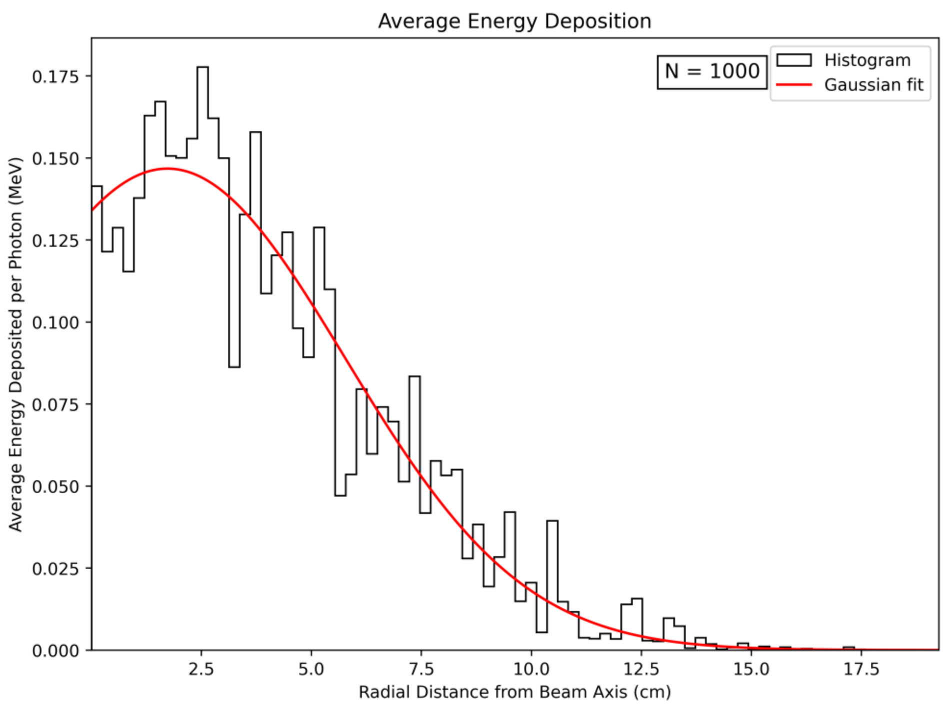

Figure 9 - Energy Deposition as a function of radial distance from the cylinder axis(1000 Photon)

The simulation results exhibit a characteristic pattern of energy deposition within the cylindrical medium. This behavior is in line with our expectations and aligns with the physical processes involved. One notable observation is the presence of the "skin sparing effect" in the energy deposition profile. This phenomenon refers to a reduced energy deposition in the outer layers of the medium, particularly near the surface. The skin sparing effect holds significance in radiation therapy applications, and this effect allows for more precise targeting of deeper tissues while preserving the health of the surrounding skin.

7.2. Top View

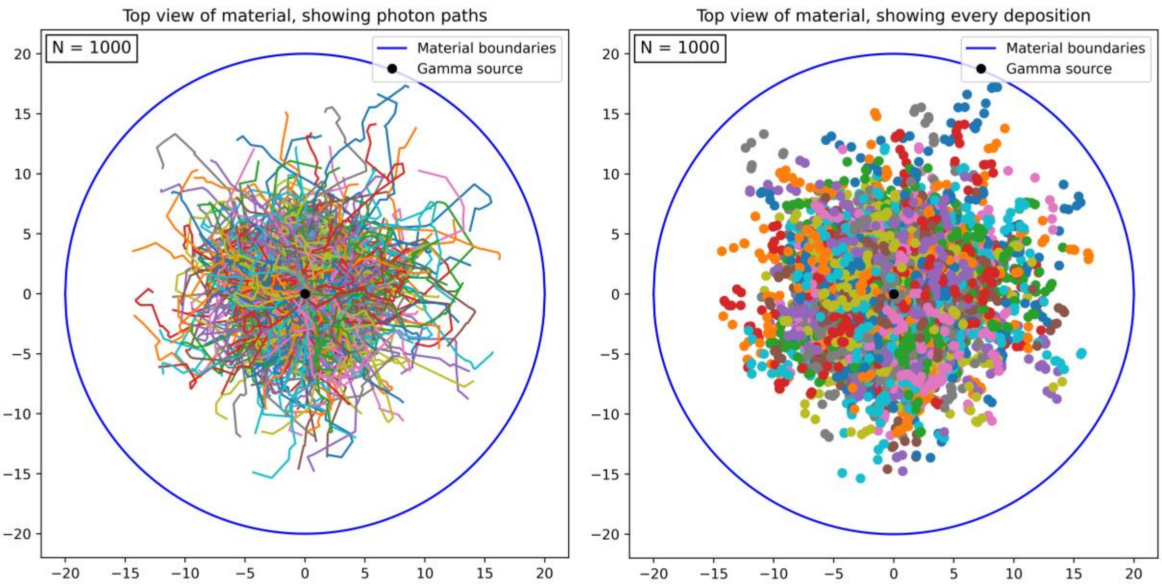

Figure 9 - Top view of the Cylinder showing the paths of 1000 photon(left), and positions at which photons exchanged energy with the medium(right)

This observation suggests that the majority of gamma rays undergo interactions and scatter within the medium before reaching the surface. As a result, only a limited fraction of the initial gamma rays effectively penetrates through the entire depth of the cylinder and interact with the surface.

7.3. Side View

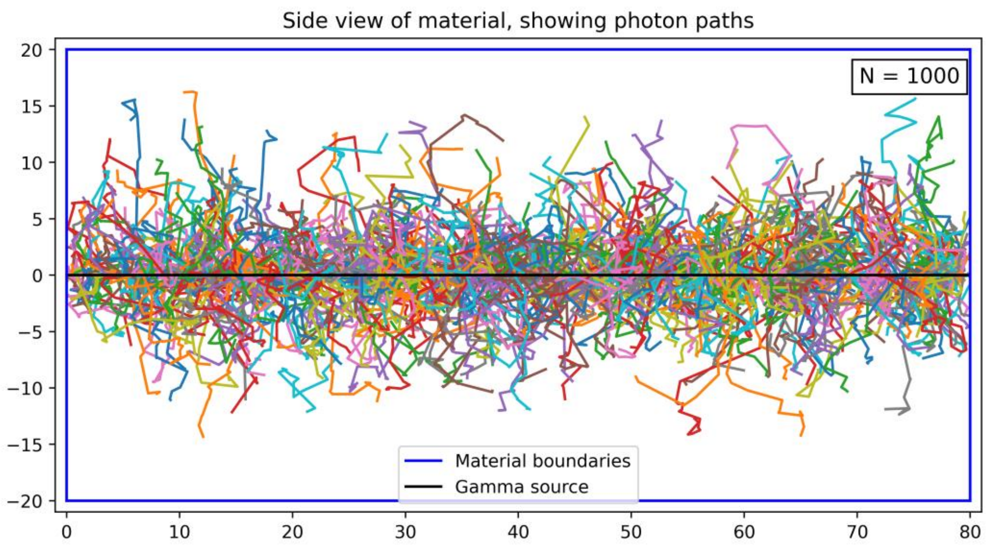

Figure 10 - Side view of the cylinder showing the paths of 1000 photon.

Similarly, the side view reinforces the understanding that gamma rays undergo significant attenuation and scattering as they travel through the medium.

7.4. Three-Dimensional View

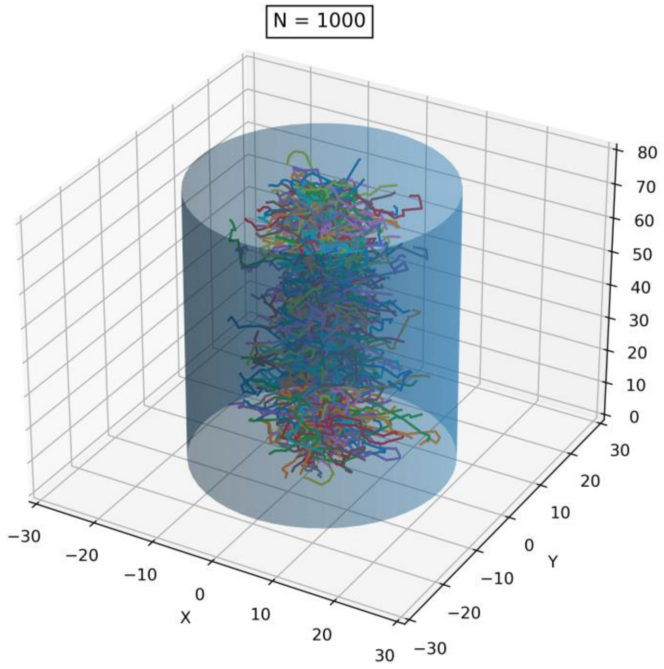

Figure 10 - Three-Dimensional view of the cylinder showing the path of 1000 photon.

7.5. $p(s)$ and $p(\theta)$ Distributions

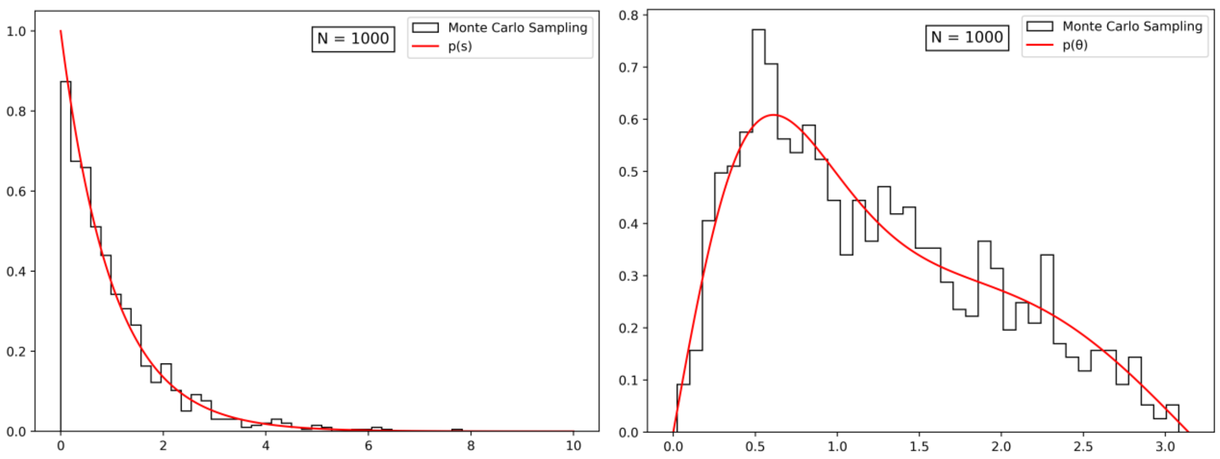

Figure 12 – Straight distance traveled(left) and Compton scattering angle(right) distributions.

The $p(s)$ distribution reveals that a significant number of gamma rays traveled very short distances, typically less than 1 cm, in a straight path without undergoing significant scattering or interaction. On the other hand, the $p(\theta)$ distribution represents the probability of scattering angles resulting from Compton scattering. The distribution shows a fair probability throughout the range of scattering angles, indicating that gamma rays interact with the atoms or electrons of the medium at various angles.

8. Discussion and Conclusion

8.1. strengths and limitations of the Monte Carlo simulation method for radiation transport

One of the strengths of Monte Carlo simulation is its ability to accurately model complex radiation interactions and transport processes. This level of detail allows for a comprehensive analysis of radiation transport phenomena.

Monte Carlo simulation is computationally costly and will not work if the cross sections cannot be obtained. We did not include the pair production process, as it will drastically increase the computational cost.

8.2. recommendations for future research in this area

The expulsion of pair production may not be ideal since there ought to be this kind of interaction since the photon needs at least 1.02 MeV in order to trigger pair production. Considering pair production in this simulation can lead to an increase in the overall energy deposition due to the additional energy contributed by the created electron-positron pairs. This means that the total energy deposited per photon may increase. For higher energy photons, pair production becomes more significant, and the energy deposition curve may exhibit sharper peaks due to the additional energy contributed by the created electron-positron pairs.

As a final thought, including more interactions into the calculations may have a significant effect on the results. Considering the influence of additional interactions, such as pair production, could lead to a better understanding of the energy deposition pattern and provide more realistic simulations. This can give deeper insights into the behavior of gamma rays and their effects on various materials and environments, ultimately advancing scientific knowledge and practical applications in fields such as radiation therapy, nuclear engineering, and radiation detection.

9. References

[1] F. Arqueros and G. D. Montesinos. A simple algorithm for the transport of gamma rays in a medium

[2] S Sukara and S Rimjeam. Simulation of Gamma Rays Attenuation Through Matters Using the Monte Carlo Program

[3] G. Nelson and D. Reilly. Gamma-Ray Interactions with Matter

[4] Podgorsak E. B., Radiation Physics for Medical Physicists, Springer, 2nd ed., 2010.

[5] Graph data came from The National Institute of Standards and Technology's (NIST) XCOM database.

Appendix

Code:
https://github.com/ibralyousef/UnderGrad/blob/main/00_Python/01_For%20Physics/Monte%20Carlo%20for%20Gamma%20Ray%20Transport.ipynb

In this section, we will examine the paths of photons as they traverse through different materials and explore the implications of material density on photon transport. Dense materials play a critical role in determining the behavior of photons, particularly in terms of their ability to penetrate and interact with matter. Due to the higher probability of photoelectric absorption, dense materials present a major obstacle for photons to pass through. In contrast, photons may travel farther on their routes before substantial interactions happen when they contact with less dense substances like air or water. The same amount of photons and energy will be used to evaluate six different materials.: H, Li, Os, W, Pb, Ti.

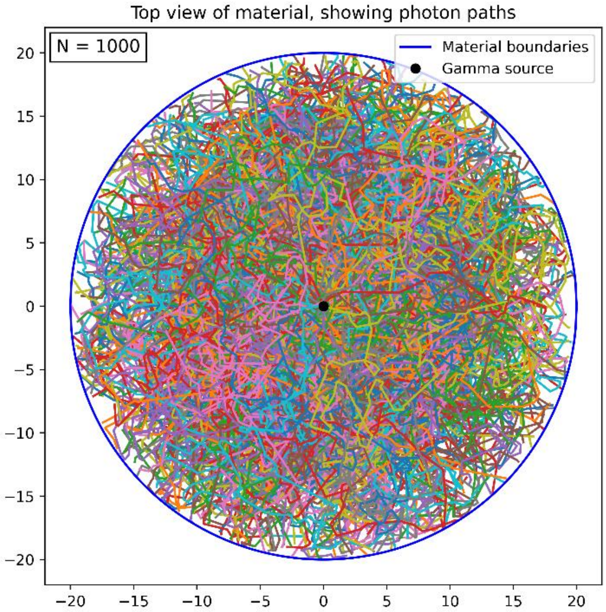

Figure I - H

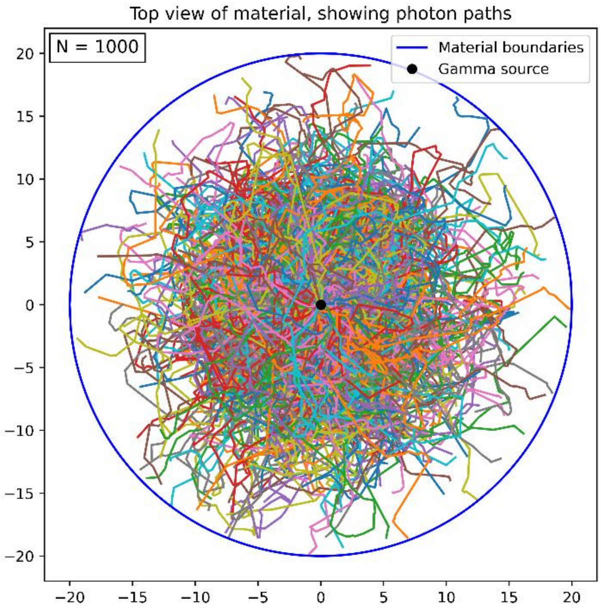

Figure II Li

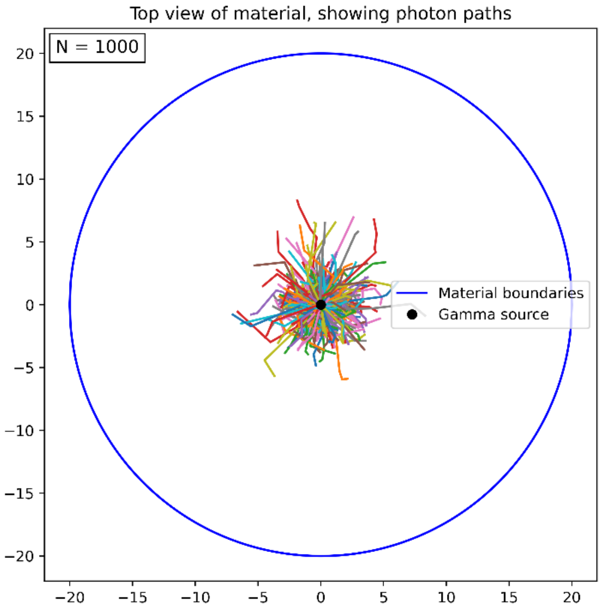

Figure III - Os

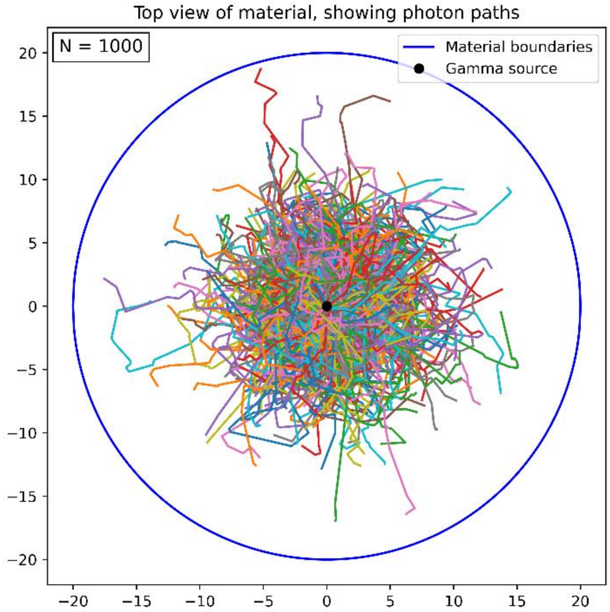

Figure IV - W

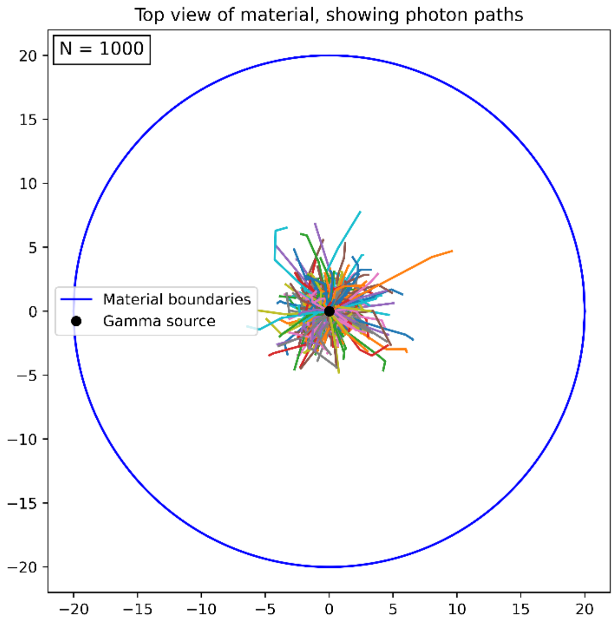

Figure V - Pb

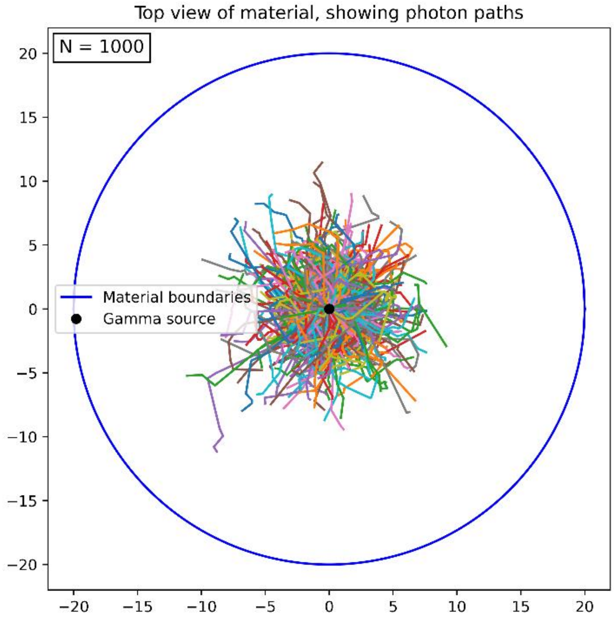

Figure VI - Ti

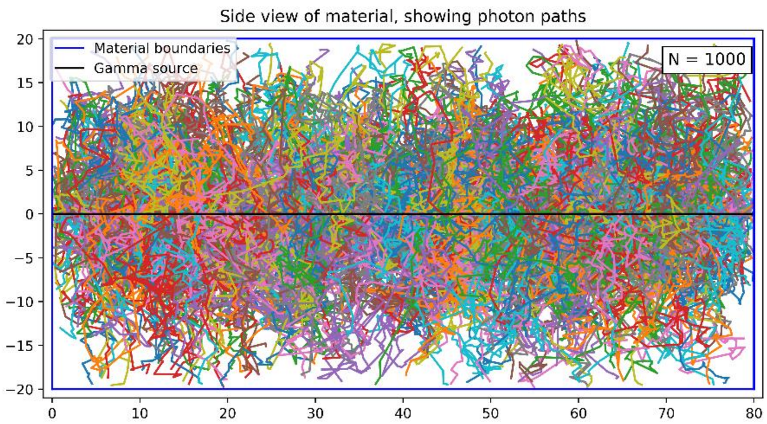

Figure VII - H

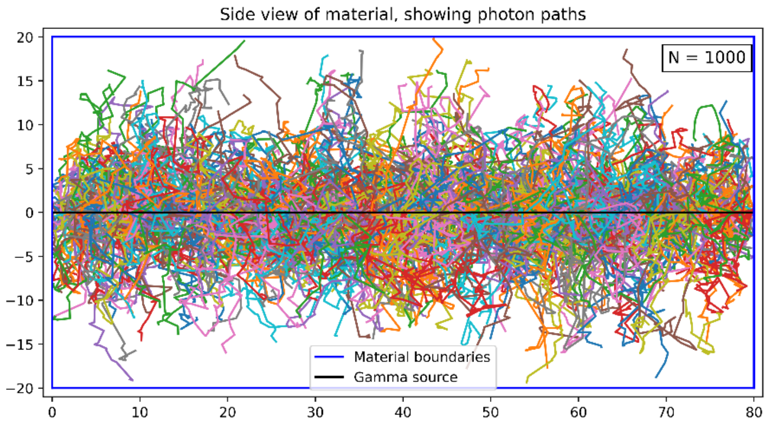

Figure VIII - Li

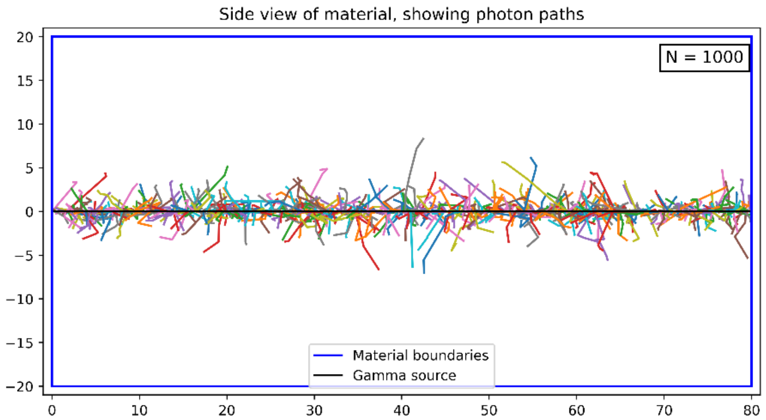

Figure IX - Os

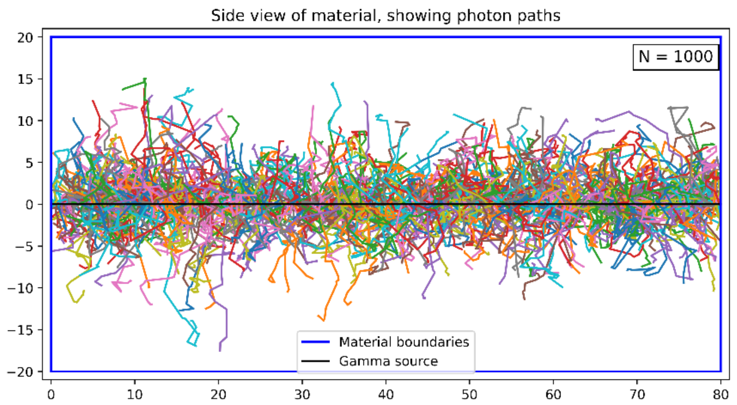

Figure X - W

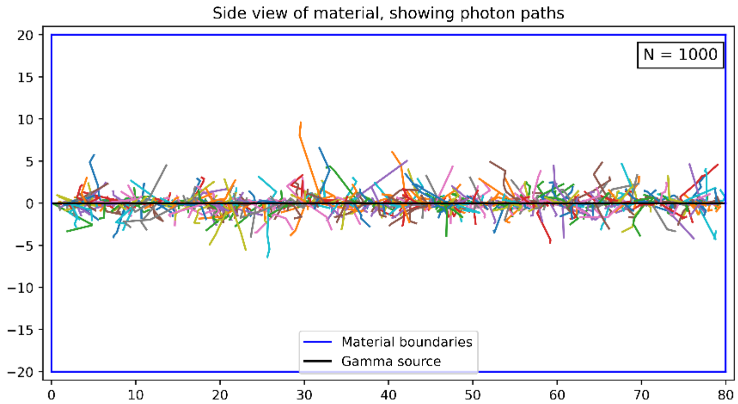

Figure XI - Pb

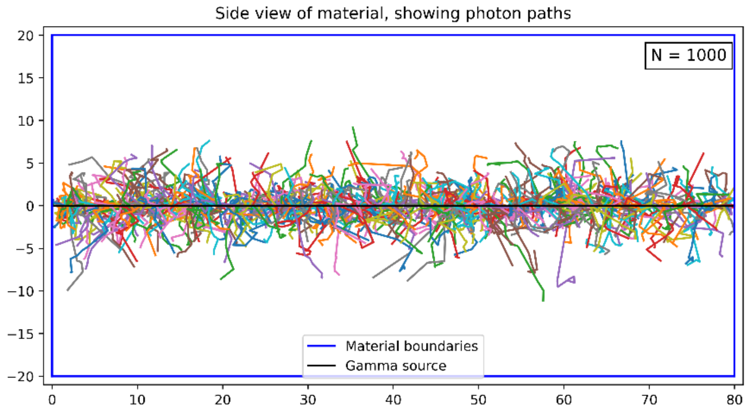

Figure XII - Ti

The results of our simulation align with our expectations, demonstrating the influence of material density on photon interactions. As anticipated, denser materials exhibited a higher cross section for photoelectric absorption, particularly at higher photon energies. This leads to a rapid loss of energy and a reduced penetration depth. Conversely, our simulation revealed a contrasting pattern for materials with lower density, such as H gas. In H gas, photons exhibited longer paths and traveled more freely through the material before experiencing significant interactions. This behavior is attributed to the reduced probability of photon-electron interactions due to the sparse arrangement of atoms in less dense materials.