

# 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. The simulation will model the behaviour of gamma photons as they propagate through a medium and interact with its atomic and molecular constituents, considering only Compton scattering and photoelectric effect of 1 MeV gamma photons. 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. Monte Carlo for Random Sampling

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,  $\theta$ , follows this complicated distribution:

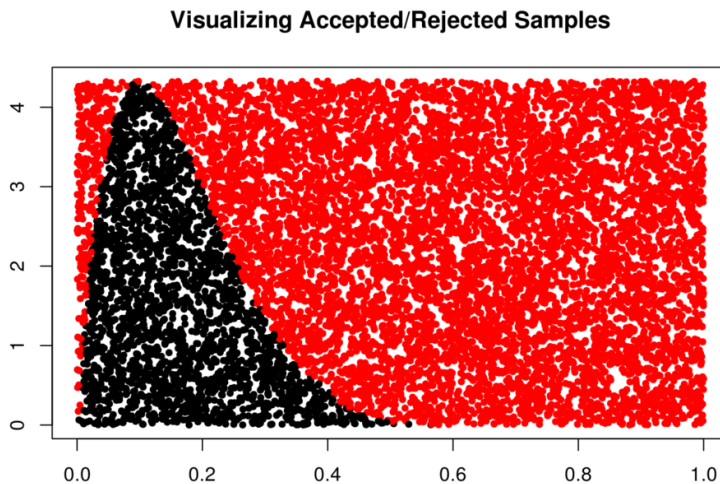
$$p(\theta)d\theta = \frac{d\sigma_{KN}}{d\Omega} 2\pi \sin \theta d$$

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

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

The problem is that we do now know how to randomly sample random points for  $\theta$ , 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:



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.

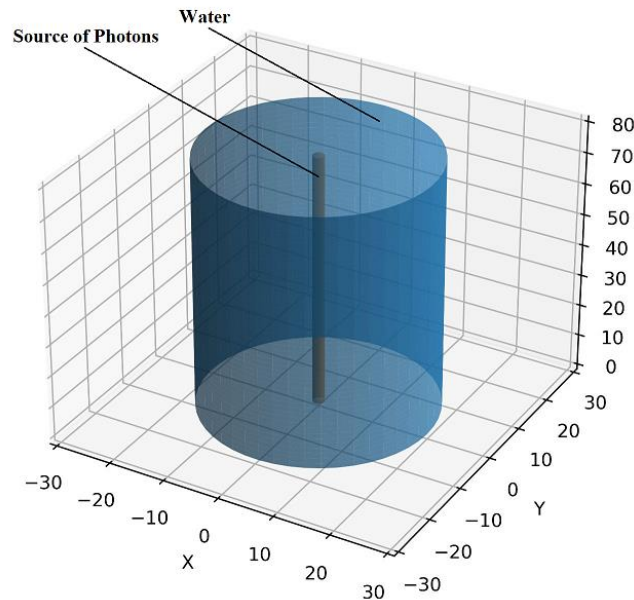
## 2. Our Simulation Setup

### 2.1. 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



Overview of the cylindrical medium which the photons will travel in

Photon trajectories inside the cylinder are to be visualized.

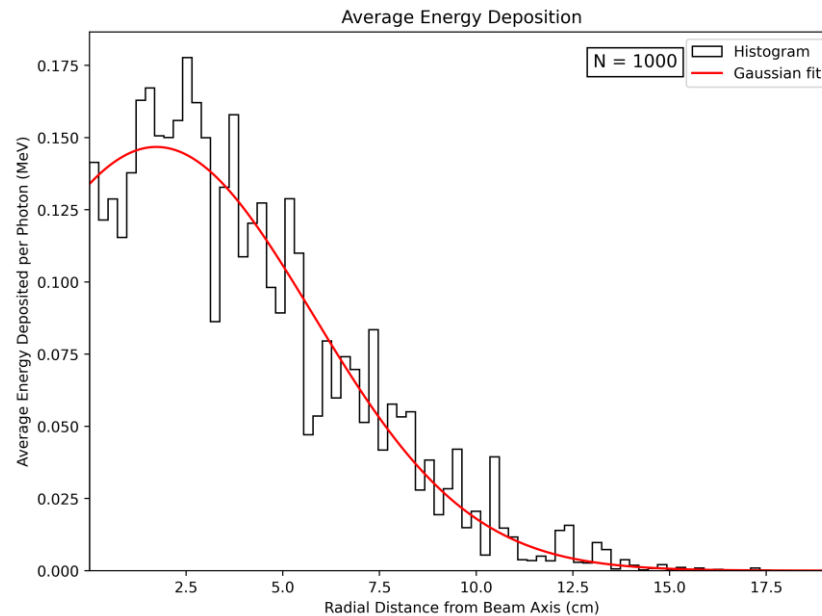
### 2.2. Code and Input Parameters

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. 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.

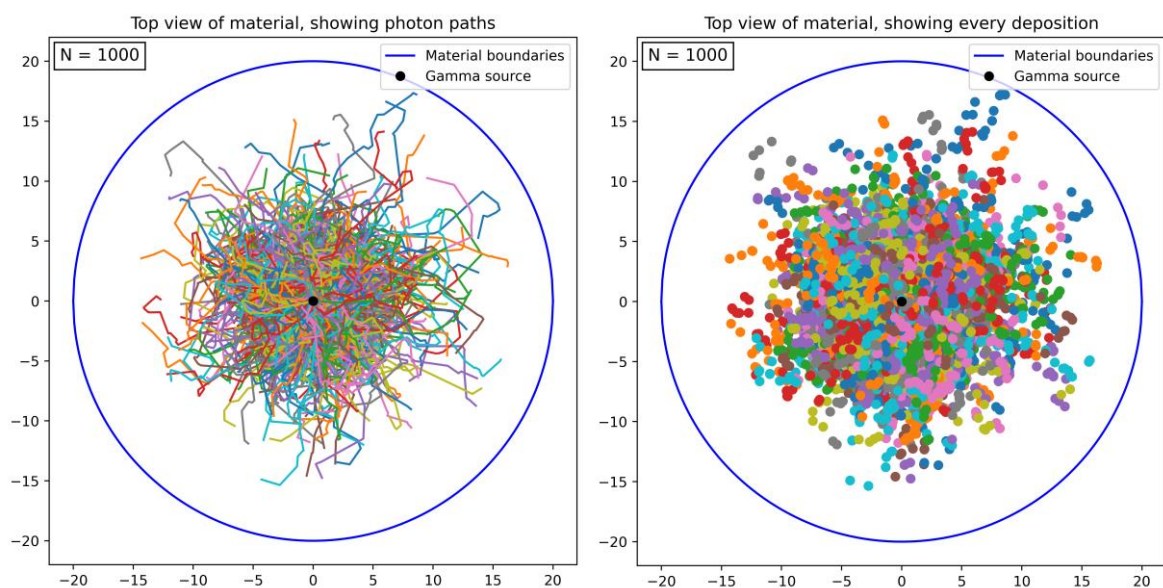
The cross sections for photoelectric effect and Compton scattering at various photon energies were obtained from tables provided by the X-Ray Cross Sections Database (XCOM) website, and linearly interpolated them.



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.

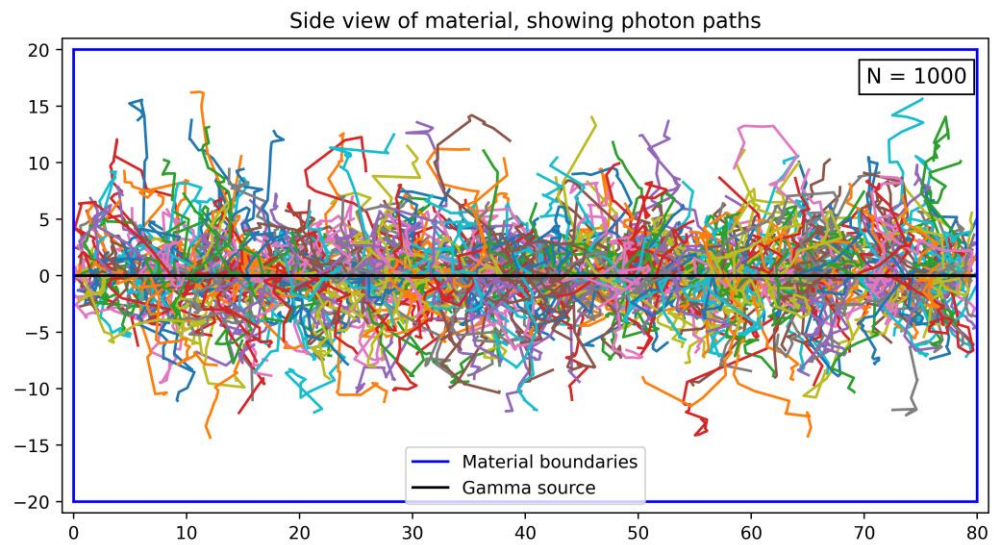
### 2.3. Top View



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

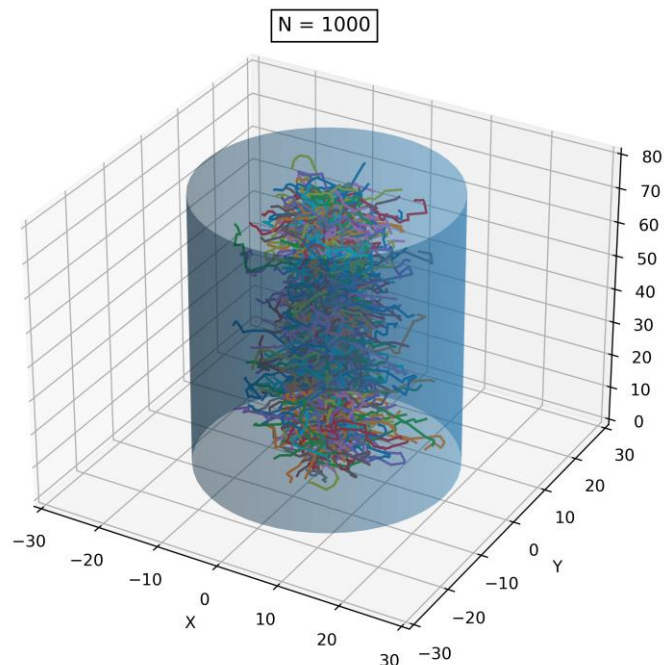
This observation suggests that the majority of gamma rays undergo interactions and scatter within the medium before reaching the surface. As a result, only a limited fraction of the initial gamma rays effectively penetrates through the entire depth of the cylinder and interact with the surface.

#### 2.4. Side View



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

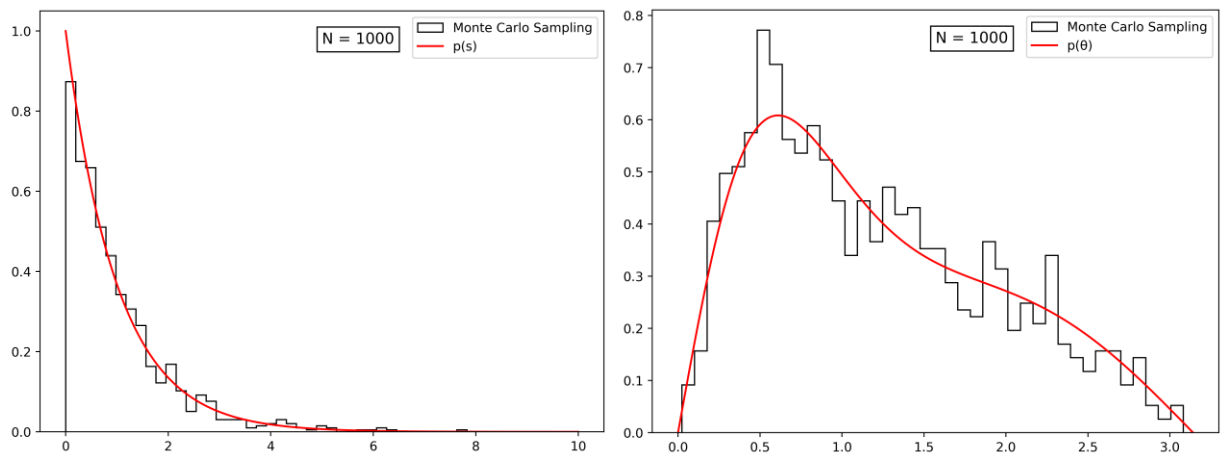
#### 2.5. Three-Dimensional View



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

#### 2.6. $p(s)$ and $p(\theta)$ Distributions





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.

### 3. Verification

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.

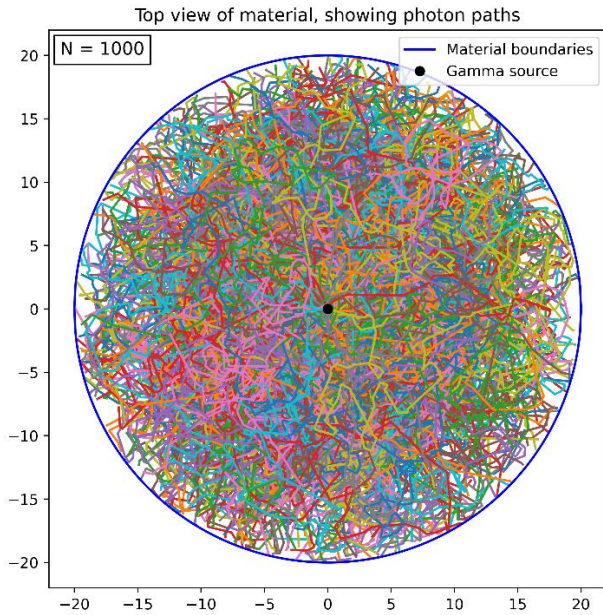


Figure I - H

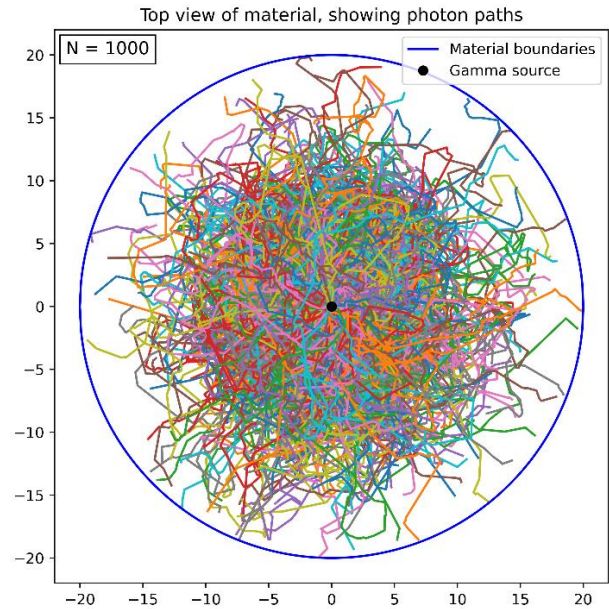


Figure II Li

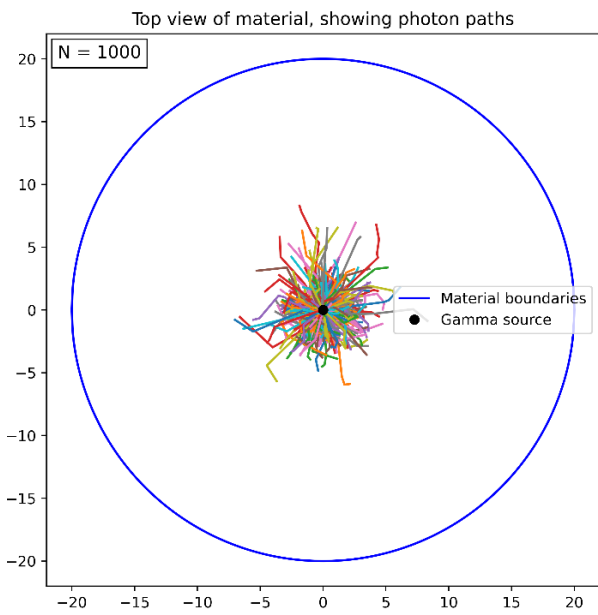


Figure III - Os

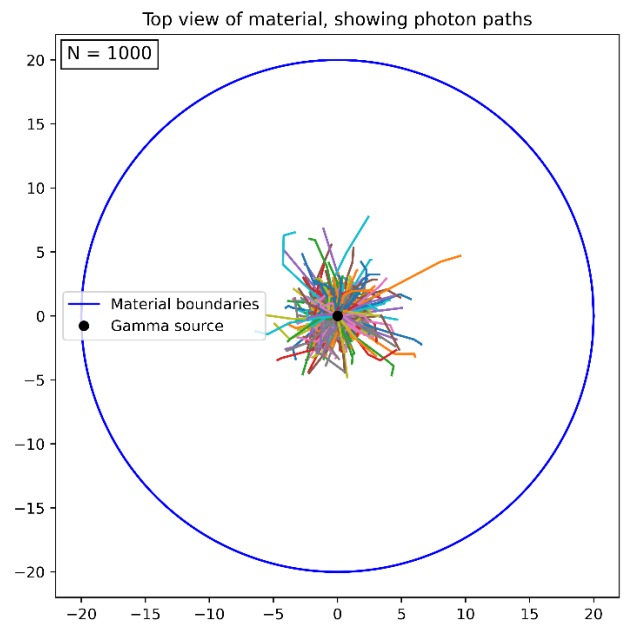


Figure V - Pb

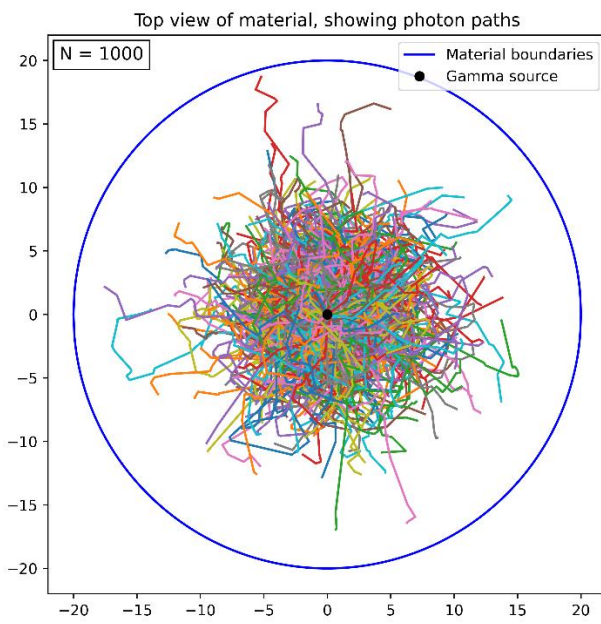


Figure IV - W

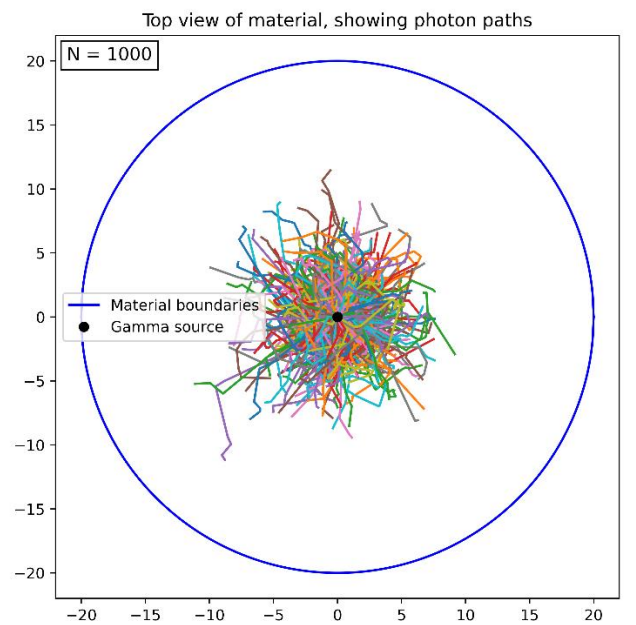


Figure VI - Ti

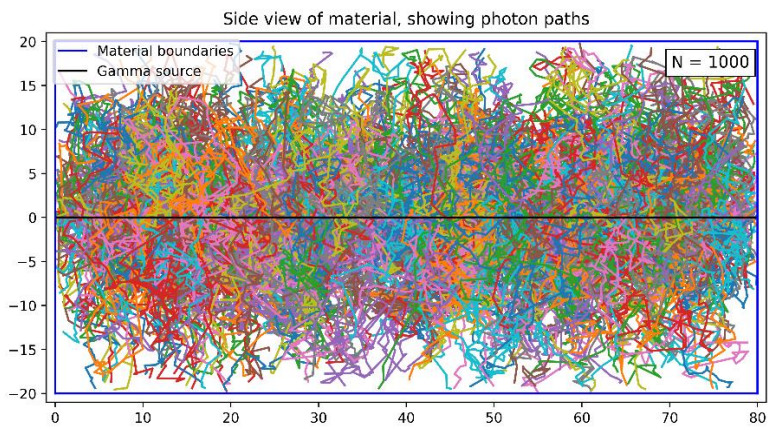


Figure VII - H

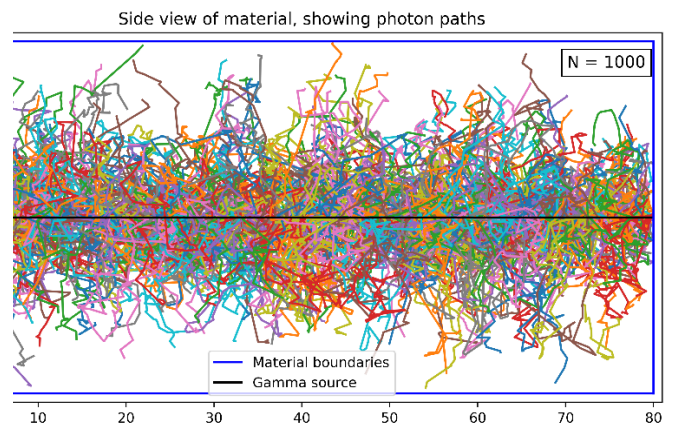


Figure VIII - Li

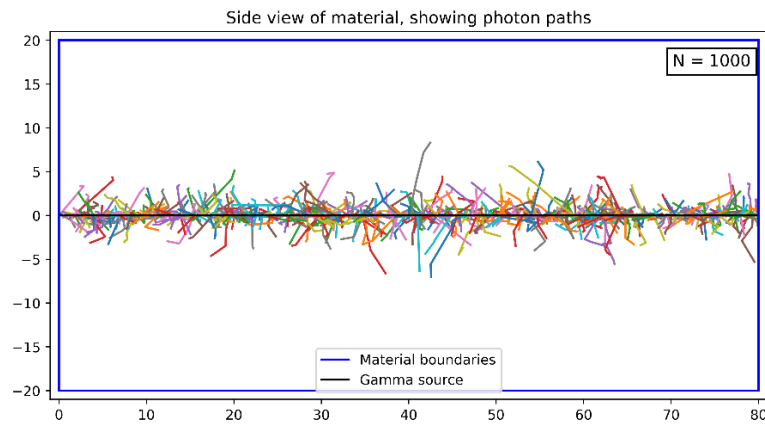


Figure IX - Os

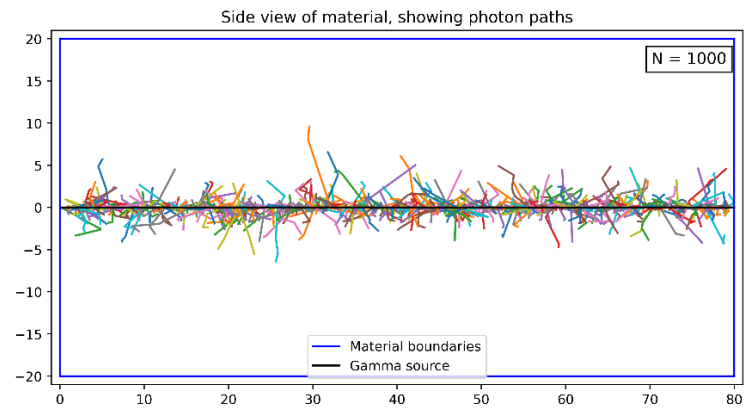


Figure XI - Pb

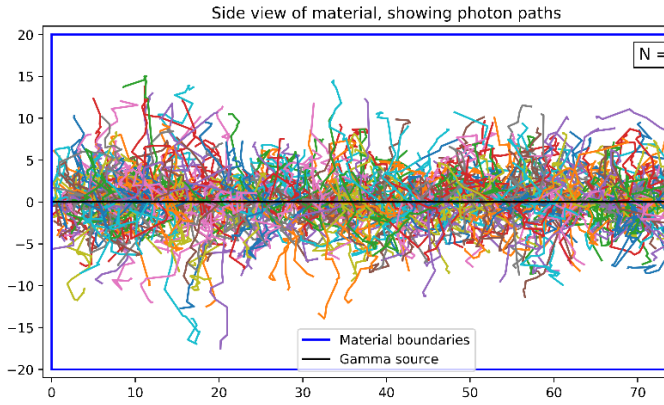


Figure X - W

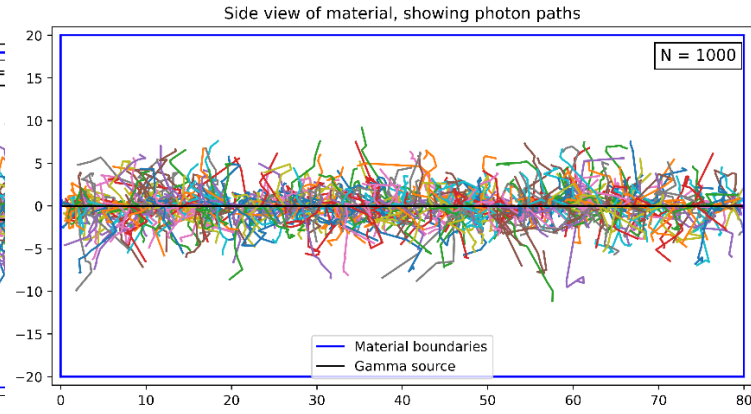


Figure XII - Ti

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.

#### 4. 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:

```
import numpy as np, matplotlib.pyplot as plt
from functools import partial
from scipy.optimize import curve_fit
from scipy.special import factorial

# Cross-sections for water (better collapsed)
Photon_Energy = []
Incoher_Scatter = []
Photoel_Absorb = []
Tot_wo_Coherent = []
data = '''1.000E-03 1.319E-02 4.076E+03 4.076E+03
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3.000E-03 7.075E-02 1.919E+02 1.919E+02
4.000E-03 9.430E-02 8.197E+01 8.207E+01
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6.400E-01 8.690E-02 9.926E-06 8.691E-02
6.490E-01 8.636E-02 9.576E-06 8.637E-02
6.580E-01 8.584E-02 9.246E-06 8.585E-02
6.670E-01 8.532E-02 8.933E-06 8.533E-02
6.760E-01 8.481E-02 8.637E-06 8.482E-02
6.850E-01 8.431E-02 8.358E-06 8.432E-02
6.940E-01 8.382E-02 8.094E-06 8.383E-02
7.030E-01 8.334E-02 7.845E-06 8.334E-02
7.120E-01 8.286E-02 7.610E-06 8.287E-02
7.210E-01 8.239E-02 7.389E-06 8.240E-02
7.300E-01 8.193E-02 7.180E-06 8.194E-02
7.390E-01 8.147E-02 6.983E-06 8.148E-02
7.480E-01 8.103E-02 6.797E-06 8.103E-02
7.570E-01 8.058E-02 6.622E-06 8.059E-02
7.660E-01 8.015E-02 6.458E-06 8.016E-02
7.750E-01 7.972E-02 6.303E-06 7.973E-02
7.840E-01 7.930E-02 6.158E-06 7.930E-02
7.930E-01 7.888E-02 6.021E-06 7.889E-02
8.020E-01 7.847E-02 5.892E-06 7.848E-02
8.110E-01 7.807E-02 5.772E-06 7.807E-02
8.200E-01 7.767E-02 5.658E-06 7.767E-02
8.290E-01 7.727E-02 5.549E-06 7.728E-02
8.380E-01 7.688E-02 5.444E-06 7.689E-02
8.470E-01 7.650E-02 5.343E-06 7.651E-02
8.560E-01 7.612E-02 5.245E-06 7.613E-02
8.650E-01 7.575E-02 5.149E-06 7.575E-02
8.740E-01 7.538E-02 5.054E-06 7.538E-02
8.830E-01 7.501E-02 4.959E-06 7.502E-02
8.920E-01 7.466E-02 4.866E-06 7.466E-02
9.010E-01 7.430E-02 4.772E-06 7.430E-02
9.100E-01 7.395E-02 4.678E-06 7.395E-02
9.190E-01 7.360E-02 4.583E-06 7.361E-02
9.280E-01 7.326E-02 4.488E-06 7.326E-02
9.370E-01 7.292E-02 4.391E-06 7.293E-02
9.460E-01 7.259E-02 4.293E-06 7.259E-02
9.550E-01 7.226E-02 4.194E-06 7.226E-02
9.640E-01 7.193E-02 4.094E-06 7.193E-02
9.730E-01 7.161E-02 3.993E-06 7.161E-02
9.820E-01 7.129E-02 3.890E-06 7.129E-02
9.910E-01 7.097E-02 3.786E-06 7.098E-02
1.000E+00 7.066E-02 3.681E-06 7.066E-02 '''
Photon_Energy = np.array([item.split()[0] for item in data.splitlines()]).astype('float64')
Incoher_Scatter = np.array([item.split()[1] for item in data.splitlines()]).astype('float64')
Photoel_Absorb = np.array([item.split()[2] for item in data.splitlines()]).astype('float64')
Tot_wo_Coherent = np.array([item.split()[3] for item in data.splitlines()]).astype('float64')

sigma_pe = lambda x: np.interp(x, Photon_Energy, Photoel_Absorb)
sigma_c = lambda x: np.interp(x, Photon_Energy, Incoher_Scatter)

# Simulation parameters
params={
    'E':1/.51, # initial energy of photon per electron rest energy
    'z':80, # depth cm
    's':20, # radius cm
    'N':2000, # number of photons
}

```

```

# Monte Carlo simulation (acceptance-rejection method)
def monte_carlos(p,x_min=0,x_max=1,p_max=1):
    trial=(np.random.uniform(x_min,x_max),np.random.uniform(0,p_max))
    while trial[1]>p(trial[0]):trial=(np.random.uniform(x_min,x_max),np.random.uniform(0,p_max))
    return trial[0]

# p(s) and p(theta) for acceptance-rejection method
p_s=lambda s: np.exp(-s)/(1-np.exp(-s_max))
p_theta=lambda q,g=1:(np.sin(q)/2/(1+g*(1-np.cos(q)))**2*(1+np.cos(q)**2+g**2*(1-np.cos(q))**2/(1+g*(1-np.cos(q)))))\
    /((1+g)/g**2*(2*(1+g)/(1+2*g)-np.log(1+2*g)/g)+np.log(1+2*g)/2/g-(1+3*g)/(1+2*g)**2)
s_max=np.sqrt(params['z']**2+params['s']**2/4) # for cylinder

# Conditions for photon in or out of medium
def in_cylinder(v,s,h):
    """
    Checks if a point is in a cylinder of radius s and height h.
    v: vector
    s: radius
    h: height
    """
    x,y,z=v
    r=np.sqrt(x**2+y**2)
    boolean=True
    if z>h or z<0: boolean=False
    if r>s: boolean=False
    return boolean

# Generate a sample of 1000 values using the Monte Carlo method
sample_s = [monte_carlos(p_s, 0, 10) for _ in range(1000)]

# Define a grid of x-values for plotting p(s)
x = np.linspace(0, 10, 10000)

# Plot the histogram and p(s) on the same plot
plt.hist(sample_s, bins=40, density=True, label='Monte Carlo Sampling', histtype='step', color='k')
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.plot(x, p_s(x), label='p(s)',c='r')
plt.legend()
plt.show()

# Generate a sample of 1000 values using the Monte Carlo method
sample_theta = [monte_carlos(p_theta, 0, np.pi) for _ in range(10000)]

# Define a grid of x-values for plotting p(s)
x = np.linspace(0 , np.pi, 10000)

# Plot the histogram and p(s) on the same plot
plt.hist(sample_theta, bins=40, density=True, label='Monte Carlo Sampling', histtype='step', color='k')
plt.plot(x, p_theta(x), label='p(theta)',c='r')
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.legend()
plt.show()

# Main algorithm
def path():
    depositions=[]
    E = [params['E']]
    theta,phi=[np.random.uniform(0,np.pi)], [np.random.uniform(0,2*np.pi)]
    # x=[np.array([0.2*params['s']*np.cos(np.random.uniform(0, 2*np.pi)),0.2*params['s']*np.sin(np.random.uniform(0, 2*np.pi)),0])]
    x=[np.array([0,0,np.random.uniform(0,params['z'])])]
    s=[monte_carlos(p_s,x_max=params['z'],p_max=p_s(0))]
    x.append(x[-1]+s[-1]*np.array([np.sin(theta[-1])*np.cos(phi[-1]),np.sin(theta[-1])*np.sin(phi[-1]),np.cos(theta[-1])]))
    while in_cylinder(x[-1],params['s'],params['z']):
        choice=np.random.choice(['compton','photoelectric'],p=[sigma_c(E[-1]*0.51)/(sigma_c(E[-1]*0.51)+sigma_pe(E[-1]*0.51)),sigma_pe(E[-1]*0.51)/(sigma_c(E[-1]*0.51)+sigma_pe(E[-1]*0.51))])
        if choice=='compton':

```

```

        # Scattering direction
        sc_phi=np.random.uniform(0,2*np.pi)
        sc_theta=monte_carlos(partial(p_theta,g=E[-1]),0,np.pi,p_max=np.max(p_theta(np.linspace(0,np.pi,10000),E[-1])))
        # Compton scattering
        E.append(E[-1]/(1+E[-1]*(1-np.cos(sc_theta))))
        # New interaction point
        s.append(monte_carlos(p_s,x_max=params['z'],p_max=p_s(0)))
        theta.append(np.arccos(np.cos(theta[-1])*np.cos(sc_theta)+np.sin(theta[-1])*np.sin(sc_theta)*np.cos(sc_phi)))
        phi.append(phi[-1]+np.arcsin(np.sin(sc_theta)*np.sin(sc_phi)/np.sin(theta[-1])))
        x.append(x[-1]+s[-1]*np.array([np.sin(theta[-1])*np.cos(phi[-1]),np.sin(theta[-1])*np.sin(phi[-1]),np.cos(theta[-1])]))
        depositions.append(E[-2]-E[-1])
    else:
        E.append(0)
        depositions.append(E[-2]-E[-1])
        return {
            'E':E,
            'depositions':depositions,
            's':s,
            'x':x
        }
    x.pop(-1)
    return {
        'E':E,
        'depositions':depositions,
        's':s,
        'x':x
    }

# Run simulation
gammas=[path() for _ in range(params['N'])]

# Show 3D setup

# Define the larger cylinder coordinates
z = np.linspace(0, 80, 50)
theta = np.linspace(0, 2*np.pi, 50)
z, theta = np.meshgrid(z, theta)
r = 20
x = r*np.cos(theta)
y = r*np.sin(theta)

# Define the smaller cylinder coordinates
z_small = np.linspace(0, 80, 50)
theta_small = np.linspace(0, 2*np.pi, 50)
z_small, theta_small = np.meshgrid(z_small, theta_small)
r_small = 1
x_small = r_small*np.cos(theta_small)
y_small = r_small*np.sin(theta_small)

paths=[(np.array(gamma['x'][:,0]),np.array(gamma['x'][:,1]),np.array(gamma['x'][:,2])) for gamma in gammas]
fig=plt.figure(figsize=(8,6),tight_layout=True)
ax=fig.add_subplot(1,1,1,projection='3d')

# Create the 3D plot
ax.plot_surface(x, y, z, alpha=0.45)
# ax.plot_surface(x_small, y_small, z_small, alpha=0.7)
for path in paths: ax.plot3D(path[0],path[1],path[2])
# Set the axis labels and limits
ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel('Z')
ax.set_xlim(-30, 30)
ax.set_ylim(-30, 30)
ax.set_zlim(0, 80)

# Show the plot
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.title('3D plot of the setup')
plt.show()

# Plot top view of material
paths=[(np.array(gamma['x'][:,0]),np.array(gamma['x'][:,1])) for gamma in gammas]

```



```

fig=plt.figure(figsize=(8,6),tight_layout=True,facecolor='w')
ax=fig.add_subplot(1,1,1,aspect='equal')
for path in paths: ax.plot(path[0],path[1])
x=np.linspace(-params['s'],params['s'],500)
y=np.sqrt(params['s']**2-x**2)
ax.plot(x,y,'b', label='Material boundaries')
ax.plot(x,-y,'b')
ax.plot(0,0,'ko', label='Gamma source')
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.legend()
plt.title('Top view of material, showing photon paths')
plt.show()

points=[(np.array(gamma['x'])[-1,0],np.array(gamma['x'])[-1,1]) for gamma in gammas]
fig=plt.figure(figsize=(8,6),tight_layout=True,facecolor='w')
ax=fig.add_subplot(1,1,1,aspect='equal')
for point in points: ax.plot(point[0],point[1], 'o')
x=np.linspace(-params['s'],params['s'],500)
y=np.sqrt(params['s']**2-x**2)
ax.plot(x,y,'b', label='Material boundaries')
ax.plot(x,-y,'b')
ax.plot(0,0,'ko', label='Gamma source')
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.title('Top view of material, where the photon were fully absorbed')
plt.legend()
plt.show()

# Plot side view of material
paths=[(np.array(gamma['x'])[:,0],np.array(gamma['x'])[:,2]) for gamma in gammas]
fig=plt.figure(figsize=(8,6),tight_layout=True,facecolor='w')
ax=fig.add_subplot(1,1,1,aspect='equal')
for path in paths: ax.plot(path[1],path[0])
ax.set_xlim(-1,params['z']+1)
ax.set_ylim(-params['s']-1,params['s']+1)
ax.plot([0,params['z']], [params['s'],params['s']], 'b', label='Material boundaries')
ax.plot([0,params['z']], [-params['s'],-params['s']], 'b')
ax.plot([0,params['z']], [0,0], 'k', label='Gamma source')

ax.plot([params['z'],params['z']], [-params['s'],params['s']], 'b')
ax.plot([0,0], [-params['s'],params['s']], 'b')
plt.title('Side view of material, showing photon paths')
plt.legend()
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.show()

# Create a plot of the histogram with the fitted curves
def gaussian(x, mean, amplitude, standard_deviation):
    return amplitude * np.exp( - (x - mean)**2 / (2*standard_deviation ** 2))
def poisson(x, mean, amplitude):
    return amplitude * np.exp(-mean) * mean**x / factorial(x, exact=False)
# Define the z range for the histogram
# Extracting Energy deposition
# Initialize the arrays for energy depositions and x, y, z coordinates
E, x, y, z = [], [], [], []

# Populate the arrays by looping over the gammas
for gamma in gammas:
    E.extend(np.array(gamma['depositions']))
    x.extend(np.array(gamma['x'])[1:, 0])
    y.extend(np.array(gamma['x'])[1:, 1])
    z.extend(np.array(gamma['x'])[1:, 2])

# Convert the arrays to numpy arrays
E = np.array(E)
x = np.array(x)
y = np.array(y)
z = np.array(z)
pt = np.sqrt(x**2 + y**2)
pt_min = 0
pt_max = params['s']
pt_bins = np.linspace(pt_min, pt_max + 1,len(pt)+1)
bins= 80
# Calculate the total energy deposition for each z bin

```

```

E_avg = []
for i in range(len(pt_bins) - 1):
    mask = (pt >= pt_bins[i]) & (pt < pt_bins[i+1])
    E_bin = E[mask]
    E_bin_avg = np.mean(E_bin) if len(E_bin) > 0 else 0
    E_avg.append(E_bin_avg)
E_avg = np.array(E_avg)/params['N']

bin_heights, bin_borders = np.histogram(pt, weights=E_avg, bins=bins,density=True)
bin_widths = np.diff(bin_borders)
bin_centers = bin_borders[:-1] + bin_widths / 2
popt_gaussian, _ = curve_fit(gaussian, bin_centers, bin_heights)
x_interval_for_fit = np.linspace(bin_borders[0], bin_borders[-1], 10000)
fig = plt.figure(facecolor='w', figsize=(8,6), tight_layout=True)
plt.hist(pt, weights=E_avg, histtype='step', color='k', bins=bins, label='Histogram',density=True)
plt.xlabel('Radial Distance from Beam Axis (cm)')
plt.ylabel('Average Energy Deposited per Photon (MeV)')
plt.title('Average Energy Deposition')
plt.plot(x_interval_for_fit, gaussian(x_interval_for_fit, *popt_gaussian),label='Gaussian fit',
c='red')
plt.legend()
plt.xlim(pt.min(), pt.max())
plt.gcf().set_size_inches(8, 6)
plt.gcf().dpi = 500
plt.show()

```