Monte Carlo Simulation of a NaI Scintillation Detector

Final Project Documentation

December 14, 2025

1 Introduction

The objective of this project is to simulate the transport of photons from a monoenergetic gamma point source into a Sodium Iodide (NaI) scintillation detector using Monte Carlo methods. The simulation accounts for the source geometry, the detector resolution (modelled by Gaussian noise), and the stochastic nature of photon interactions (Photoelectric effect, Compton scattering, and Pair production).

The primary goal of this documentation is to present the resulting gamma spectra and analyze the detector's efficiency under various geometric and energetic configurations.

2 Code Description

The program is written in Python, utilizing `NumPy` for vector operations and `SciPy` for data interpolation. The code is designed to be readable, with detailed comments explaining the specific logic within the source file itself.

2.1 Physical Model

The simulation models a cylindrical NaI crystal in a vacuum. Cross-sections are obtained from the NIST XCOM database and interpolated linearly for continuous energy values. The particle tracking relies on standard Monte Carlo techniques:

- **Path Length:** Sampled from the exponential attenuation distribution.
- **Interactions:** Chosen probabilistically based on the relative cross-sections at the current photon energy.
- **Scattering:** New directions and energies (e.g., for Compton scattering) are sampled using rejection methods (Kahn's method) to match physical differential cross-sections.

2.2 Key Functions

The program is modularized into the following key functions:

Function/Class	Description
`XCOMDataFromFile`	Loads cross-section data from text files and creates linear interpolation functions for energy-dependent lookup.
`intersection`	Calculates the entry and exit points of a photon ray with the cylindrical detector volume. Returns the distance to the boundary.
`isotropic_dir`	Generates a random normalized direction vector uniformly sampled over the unit sphere.
`track_photon`	Recursive core function. Simulates the photon's path, sampling distance to interaction, determining interaction type, and calculating energy deposition. Handles pair production via recursion.
`run_simulation`	Wrapper function that initializes the geometry, runs the particle loop for N particles, applies Gaussian broadening to the deposited energy, and calculates efficiencies.

Table 1: Overview of the primary program functions.

3 Simulation Results and Analysis

3.1 Gamma Spectrometry (Task i)

The simulation recorded gamma spectra for two distinct radioisotope configurations: Cesium-137 ($E_\gamma =$ 661.7 keV) and Cobalt-60 ($E_\gamma = 1332.5$ keV).

3.1.1 Spectrum A: Cesium-137

The spectrum recorded for the 661.7 keV source is shown in Figure 1.

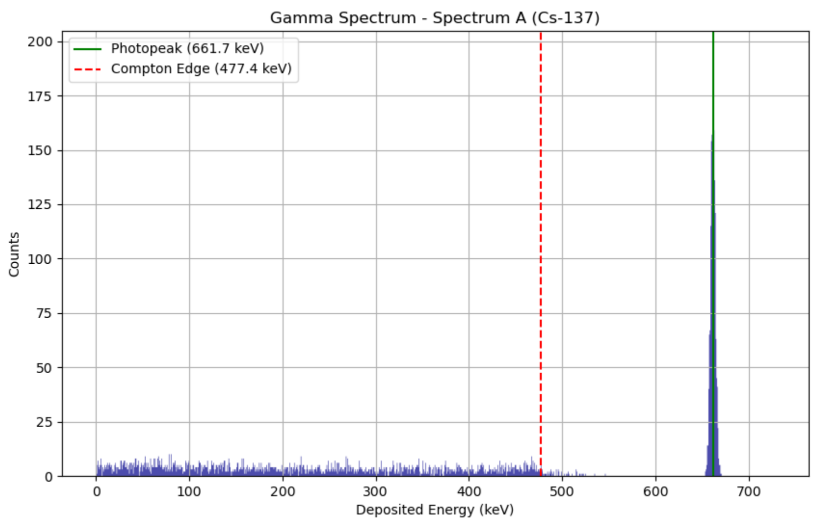

Figure 1: Gamma spectrum for Cs-137 (Spectrum A). The green line marks the photopeak, and the red dashed line marks the theoretical Compton edge.

Analysis:

- **Photopeak:** A clear, Gaussian-shaped peak is visible at 661.7 keV. This feature corresponds to photoelectric absorption events where the photon's entire energy is deposited within the crystal.
- **Compton Continuum:** To the left of the photopeak, a continuum of counts is observed. This is caused by Compton scattering events where the scattered photon escapes the detector, leaving only a fraction of the initial energy.

- **Compton Edge:** The theoretical maximum energy transfer to an electron in a single Compton scatter is given by:

$$E_{edge} = \frac{E_\gamma}{1 + \frac{m_e c^2}{2E_\gamma}} \tag{1}$$

  For $E_\gamma = 661.7$ keV, the calculated edge is approx 477.4 keV. The simulation results (red dashed line) align perfectly with the sharp drop-off in the continuum, validating the physics implementation.

3.1.2 Spectrum B: Cobalt-60

The spectrum for the higher energy 1332.5 keV source is shown in Figure 2.

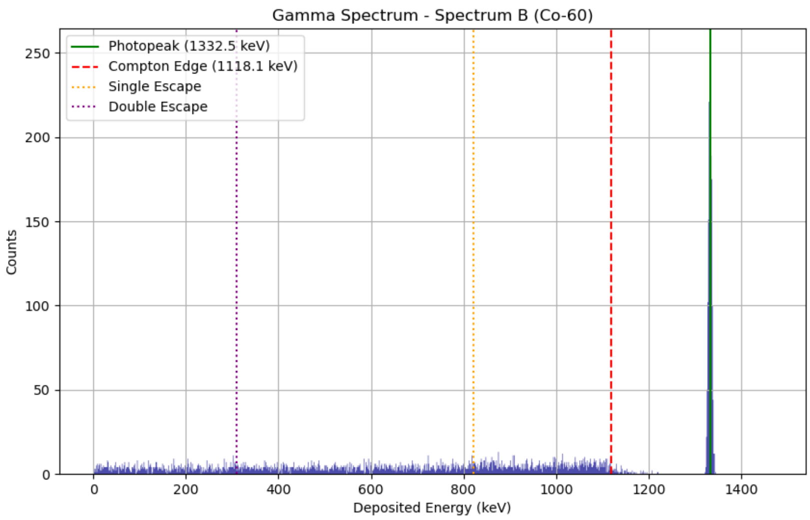

Figure 2: Gamma spectrum for Co-60 (Spectrum B). Dotted lines indicate single (orange) and double (purple) escape peaks.

Analysis:

- **Pair Production Artifacts:** Since the source energy (1.33 MeV) exceeds the pair production threshold (1.022 MeV), distinct escape peaks are visible:
  - **Single Escape Peak (SEP):** At 821.5 keV ($E_\gamma - 511$ keV). This occurs when one annihilation photon escapes the detector.
  - **Double Escape Peak (DEP):** At 310.5 keV ($E_\gamma - 1022$ keV). This occurs when both annihilation photons escape.
- **Valley Region:** The region between the Compton edge and the photopeak is populated by multiple scattering events. The counts here are due to photons that scattered multiple times, depositing most—but not all—of their energy before escaping.

3.2 Efficiency vs. Source Position (Task ii)

The variation of detector efficiency was analyzed by moving the source linearly from $\mathbf{r}_{start} = (1.0, 3.5, 2.0)$ to $\mathbf{r}_{end} = (-4.0, -1.5, 2.0)$.

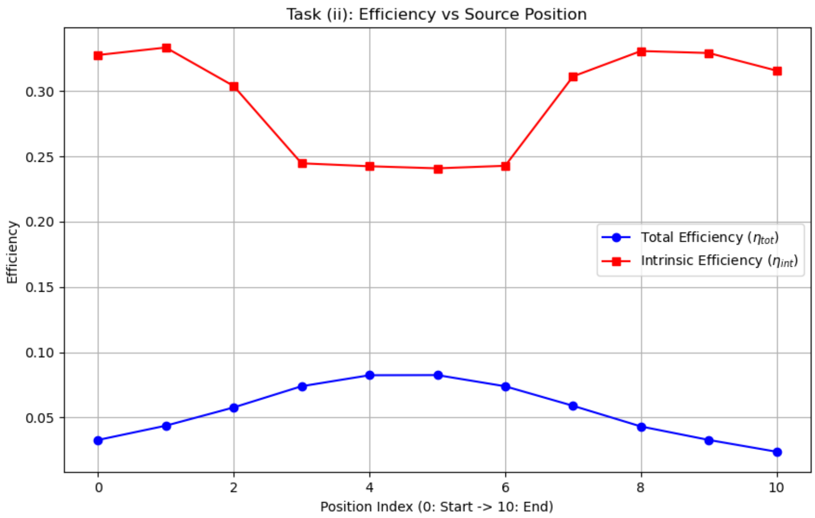

Figure 3: Total and Intrinsic efficiency as a function of source position index.

Discussion:

- **Total Efficiency (η_{tot}):** The blue curve shows a distinct peak around indices 4–5. Geometrically, these positions correspond to the point of closest approach between the source path and the detector. As the distance decreases, the solid angle subtended by the detector increases, maximizing the number of photons hitting the crystal.
- **Intrinsic Efficiency (η_{int}):** The red curve exhibits a dip in the central region where η_{tot} peaks. This inverse relationship can be explained by path length geometry. When the source is close to the detector (central indices), a higher fraction of rays enter at oblique angles near the edges or corners of the cylinder. These rays have a shorter average path length through the active volume compared to rays entering the flat face from a distance, leading to a higher probability of escape without interaction.

3.3 Efficiency vs. Source Energy (Task iii)

The dependency of efficiency on photon energy was simulated from 0.4 MeV to 4.0 MeV.

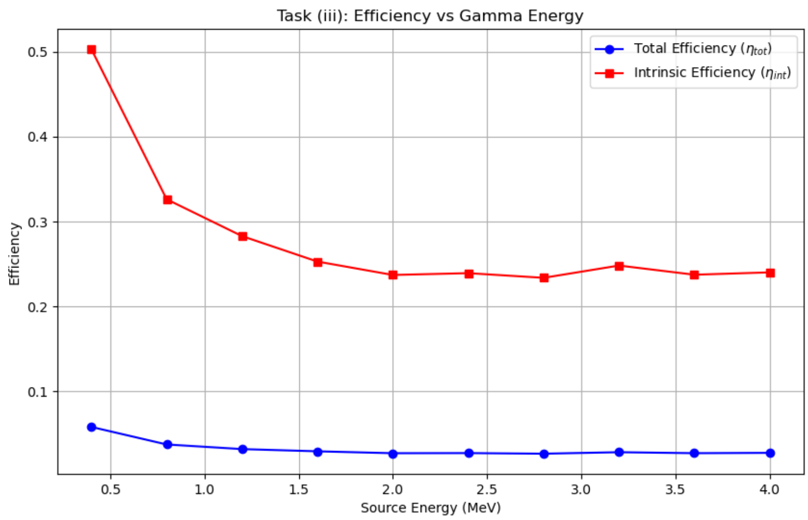

Figure 4: Total and Intrinsic efficiency as a function of incident photon energy.

Discussion:

- **Total Efficiency (η_{tot}):** There is a monotonic decrease in total efficiency as energy increases. This is a direct consequence of the attenuation coefficient $\mu(E)$ decreasing at higher energies. High-energy photons are more penetrating, reducing the probability of interaction within the fixed volume of the detector.
- **Intrinsic Efficiency (η_{int}):**
  - **Low Energy Regime ($<$ 1 MeV):** The efficiency drops sharply. This dominates because the photoelectric cross-section decreases rapidly ($\propto E^{-3.5}$) and Compton scattering favors forward emission with higher probability of escape.
  - **High Energy Regime ($>$ 2 MeV):** The curve flattens out. While scattering interactions decrease, the cross-section for pair production begins to rise (proportional to $\ln E$ and Z^2). This new interaction channel compensates for the loss in Compton/Photoelectric probability, stabilizing the fraction of energy deposited per incident photon.

4 Conclusion

This project successfully implemented a Monte Carlo simulation to model the response of a NaI scintillation detector to gamma radiation. By tracking individual photon histories and accounting for stochastic interactions—photoelectric absorption, Compton scattering, and pair production—the program generated realistic gamma spectra for Cesium-137 and Cobalt-60 sources.

The validation of the model was confirmed by the accurate reproduction of spectral features:

- The simulated Compton edge for Cs-137 aligned closely with the theoretical value of 477.4 keV.
- Distinct single and double escape peaks were observed for Co-60, consistent with pair production mechanics above the 1.022 MeV threshold.