Computational Modeling of Gamma Spectra from Standard Radioactive Sources

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Introducción a la Investigación Teórica
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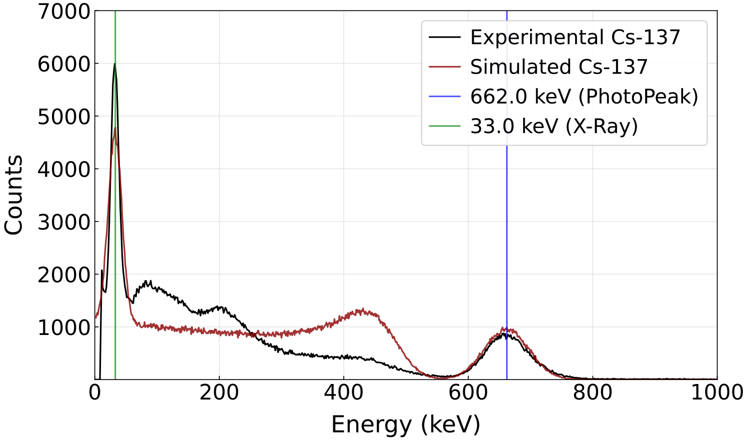
Outline

1. (Some interesting) preliminary comments
2. Code description
3. Results

Continuing from where we left off

We were going to **simulate the experimental gamma spectra** of the sources ^{137}Cs, ^{22}Na, ^{88}Y, ^{133}Ba, ^{54}Mn, and ^{57}Co under two distinct experimental scenarios.



Latest state of the project

The remaining tasks to be addressed were:

Multiple Source Decays

Some radioactive sources emit photons at several energies and all corresponding photopeaks must be properly taken into account.

Multiple Compton Scattering

In realistic photon–matter interactions, photons may undergo successive Compton scattering events, remaining energetic enough to interact multiple times.

Backscattering Environment

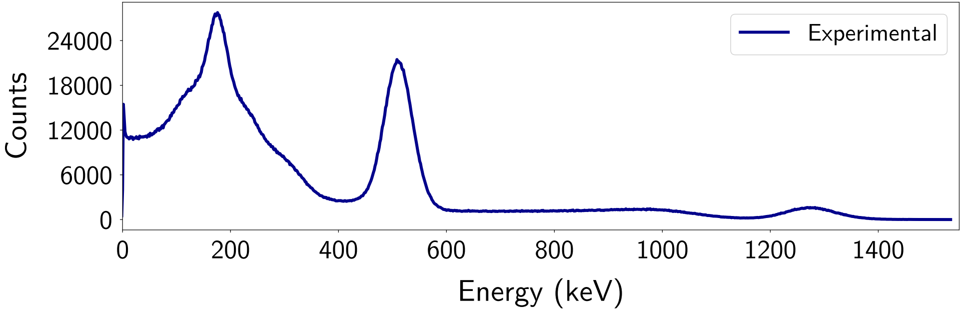
A significant (and complex) contribution to the gamma spectrum is the backscatter peak, which can only be properly understood by reconstructing the physical environment surrounding the experiment.

Mandatory decisions

To fulfill our main objective, we need to redefine the scope of our work. Therefore, we decided to exclude the following:

^{22}Na Source

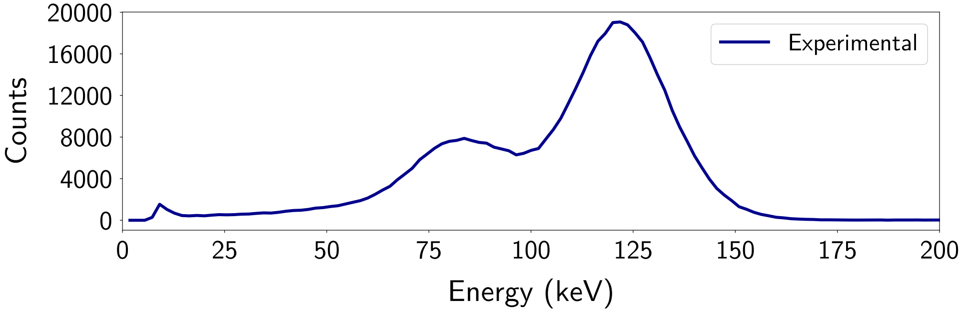
Although this source presents a well-known 511 keV photopeak, it originates from positron annihilation (pair production), a mechanism outside standard gamma interactions.



Mandatory decisions

^{57}Co Source

Photon interactions in the scintillator can emit a fluorescence photon, producing an escape peak. However, this peak is not part of the true gamma spectrum, as it results from a residual detector interaction.



Mandatory decisions

Outdoor experimental arrangement

To properly understand backscattering, it must be studied under immutable experimental conditions.

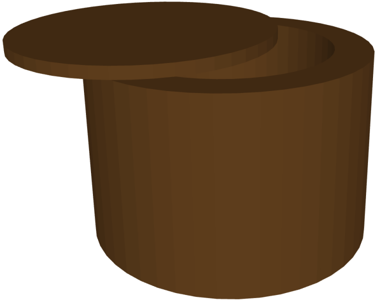


Figure: Lead barrel containing the detector and the radioactive source

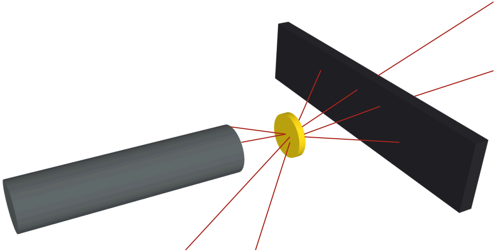


Figure: Outdoor arrangement involving the detector, the radioactive source and external objects

Code Architecture

Modules / Layer	Language	Main Responsibility
Physics and Geometry Engine (`PhysicsEngine`, `KleinNishina`, `VectorRotator`, `GeometryNavigator`)	C++	High-performance core: NIST attenuation coefficients, Compton scattering sampling, vector rotations, and full navigation through Pb/CsI geometry.
Photon Transport Orchestrators (`SinglePhotonTransporter`, `MultiPhotonTransporter`)	Python + C++	Controls the complete photon loop: step-by-step propagation, boundary checks, interaction sampling, and accumulation of deposited energy.
Source and Spectrum Builders (`SourceSampler`, `Spectrum`, `EnergyResolution`)	Python	Samples initial energies, constructs the raw spectrum, and applies the detector's instrumental resolution (FWHM model).

Conditions for photon propagation

We now have build all the essential components required for the simulation to begin:

1. Initial photon energy:
$$E = E_0$$
2. Initial photon direction (unit vector):
$$\hat{u} = (u,\ v,\ w)$$
3. Position of the radioactive source:
$$(x, y, z) = (0,\ 0,\ 9.45)$$
4. Spatial region through which the photon will propagate

Elements of the experimental setup

1. Radioactive source
2. Lead shielding (Model 747)
3. Miniaturized CsI scintillation detector (1×5)

Geometry visualization

Let's take a look from different perspectives

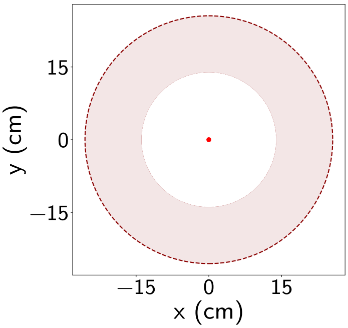


Figure: Top view

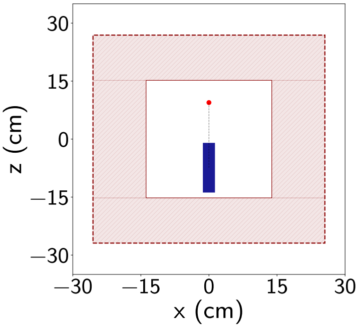


Figure: Side view

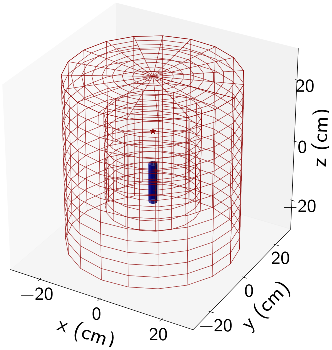


Figure: 3D view

Deepening into photon movement

Once the initial photon parameters have been defined, we must address two key questions:

In which material is the photon located?
At what distance is the next geometric boundary?

Determining the current material

To determine whether the photon is in vacuum, inside the detector or within the barrel, we perform a series of geometric checks.

The photon is inside the detector if

$$x^2 + y^2 \leq R_{\mathrm{det}}^2, \qquad z_{\mathrm{min}}^{\mathrm{det}} \leq z \leq z_{\mathrm{max}}^{\mathrm{det}}.$$

The photon is inside the barrel if

$$r = \sqrt{x^2 + y^2} \leq R_{\mathrm{out}}, \qquad |z| \leq \frac{H_{\mathrm{tot}}}{2}, \qquad \text{and not} \qquad r < R_{\mathrm{in}}, \quad |z| < \frac{H_{\mathrm{in}}}{2}.$$

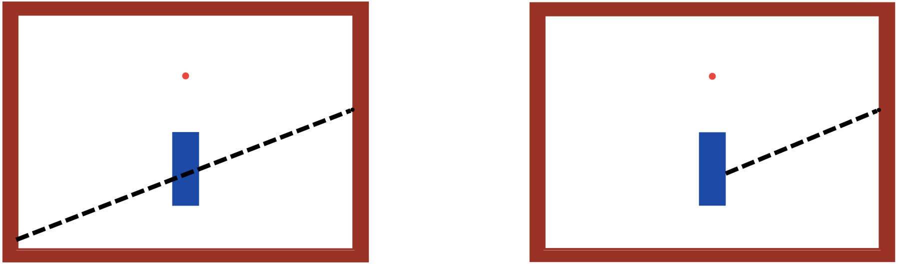
Deepening into photon movement

Determining the next geometric boundary

At each step, the photon has a well-defined position and direction. Together, these specify a parametric trajectory,

$$\vec{r}(t) = \vec{r}_0 + t\,\hat{\Omega}, \qquad t \geq 0,$$

which allows us to determine where the photon **intends** to go next.



Probability of interaction

When the photon reaches a surface (either the barrel or the detector) the first step is to determine whether it interacts or not. This decision is governed by the statistics of a homogeneous Poisson process.

Probability of an interaction in a differential segment ds

$$P(\text{interaction in } [s, s + ds]) = \mu_{\text{tot}}(E)\, ds,$$

where $\mu_{\text{tot}}(E)$ is the linear attenuation coefficient, interpolated from NIST data.

The probability that the photon has *not* interacted after traveling a distance s is then given by

$$P(\text{survive up to } s) = \exp[-\mu_{\text{tot}}(E)\, s],$$

which corresponds to the standard survival function of a homogeneous Poisson process.

How is the final decision made?

Let $\xi \sim U(0,1)$ be a uniform random variable. We want to sample an interaction distance s_{int} whose survival function is

$$P(s_{\text{int}} > s) = \exp[-\mu_{\text{tot}}\, s].$$

Sampling rule

We set the survival function equal to a uniform variable:

$$\xi = \exp[-\mu_{\text{tot}}\, s_{\text{int}}].$$

Taking logarithms:

$$-\ln \xi = \mu_{\text{tot}}\, s_{\text{int}},$$

which directly gives

$$s_{\text{int}} = \frac{-\ln \xi}{\mu_{\text{tot}}}.$$

What happens if the photon interacts?

Only two possible interaction types

1. Photoelectric effect
2. Compton scattering

How is the interaction type selected?

If the distance to the next boundary satisfies $s = s_{\text{int}}$, a physical interaction occurs. Its type is chosen according to the probabilities

$$P_{\text{photo}} = \frac{\mu_{\text{photo}}}{\mu_{\text{tot}}}, \qquad P_{\text{Compton}} = \frac{\mu_{\text{Compton}}}{\mu_{\text{tot}}}.$$

Using a new random number $r \sim U(0,1)$, we select:

$$\text{photoelectric if } r < P_{\text{photo}}, \qquad \text{Compton otherwise.}$$

Compton scattering: what must be sampled?

Once the interaction type has been selected as **Compton**, the photon does not disappear. Instead, it changes:

1. its **direction** (scattering angle θ),
2. its **energy** (from E to E').

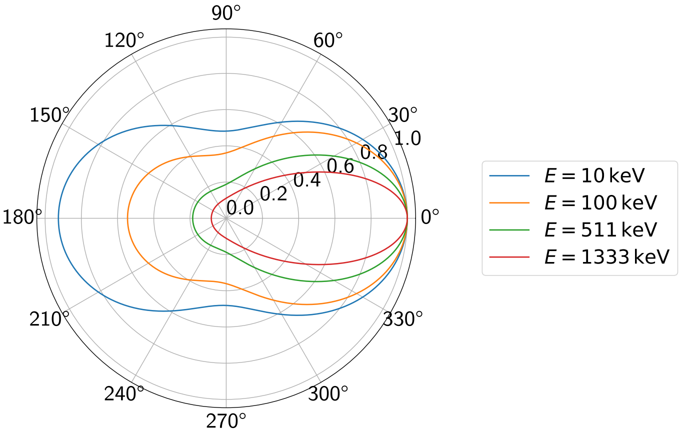
Key question

Given a photon of energy E, what is the probability of scattering at angle θ?

This angular probability is not uniform. It is dictated by the **Klein–Nishina differential cross section**, which follows from relativistic quantum electrodynamics.

Klein–Nishina differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2}\left(\frac{E'}{E}\right)^2\left[\frac{E'}{E} + \frac{E}{E'} - \sin^2\theta\right], \qquad E' = \frac{E}{1 + \frac{E}{m_e c^2}(1-\cos\theta)}$$



Why acceptance–rejection?

Once a photon has undergone a Compton interaction, the next step is to sample the scattering angle θ. The probability of scattering into a direction is governed by the Klein–Nishina differential cross section, which defines a **non-trivial** probability density:

$$f(\cos\theta) \propto \left(\frac{E'}{E}\right)^2 \left[\frac{E'}{E} + \frac{E}{E'} - \sin^2\theta\right].$$

This PDF:

- is strongly asymmetric,
- depends on the incoming energy,
- cannot be inverted analytically.

Therefore, an **acceptance–rejection algorithm** is required.

Acceptance–Rejection Algorithm

We aim to sample a variable x (here $x = \cos\theta$) from a target PDF $f(x)$ for which the CDF cannot be analytically inverted.

Basic idea

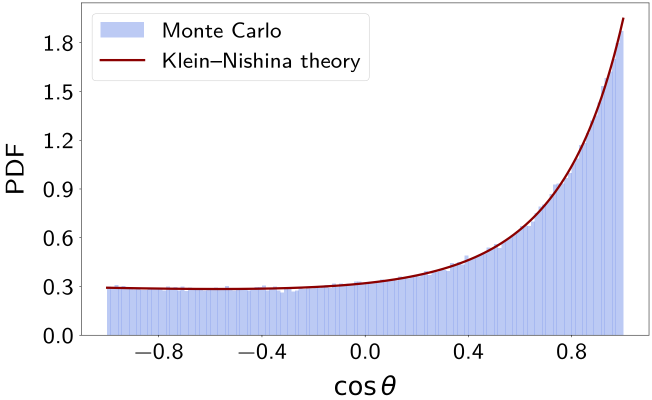
Select an easy-to-sample proposal distribution $g(x)$ and accept or reject candidate values according to the ratio $f(x)/g(x)$.

1. Choose a proposal PDF $g(x)$ and a constant M such that
$$f(x) \le M\, g(x) \qquad \forall\, x.$$
2. Sample a candidate value x^* from $g(x)$.
3. Draw a uniform random number $u \sim U(0,1)$.
4. Accept x^* if
$$u \le \frac{f(x^*)}{M\, g(x^*)};$$
otherwise reject it and return to step 2.

Validation of Klein–Nishina Sampling

To verify that the Monte Carlo sampling of Compton angles is correct, we compare:

1. The **Monte Carlo histogram** of $\cos\theta$ obtained from $N = 2 \times 10^5$ sampled events
2. The **normalized Klein–Nishina theoretical PDF**.



Why do we need a `VectorRotator`?

When a photon undergoes a Compton interaction, Klein–Nishina only gives the **polar angle** θ between the initial and final directions.
However, a full 3D direction requires two angles:

$$(\theta,\, \phi).$$

Key facts

- θ comes from Klein–Nishina.
- ϕ is always **uniform in** $[0, 2\pi)$ due to azimuthal symmetry.
- We must rotate the incoming direction $\hat{\Omega}$ into a new direction $\hat{\Omega}'$ separated by angle θ.

The module `VectorRotator` performs exactly this 3D rotation in a numerically stable way.

Rotation formula used in `VectorRotator`

Given a unit incoming direction $\hat{\Omega}$, we build two orthonormal vectors $\hat{u}$ and $\hat{v}$ perpendicular to it. Then the scattered direction is:

$$\boxed{\hat{\Omega}' = \cos\theta\,\hat{\Omega} + \sin\theta\,\big(\cos\phi\,\hat{u} + \sin\phi\,\hat{v}\big)}$$

- The term $\cos\theta\,\hat{\Omega}$ fixes the projection required by physics.
- The term $\sin\theta(\cos\phi\hat{u} + \sin\phi\hat{v})$ sweeps the circle of radius $\sin\theta$ around $\hat{\Omega}$.
- ϕ ensures uniform sampling around the axis.

This is the same rotation scheme used in PENELOPE and Geant4.

`PhysicsEngine` Interpolation

The attenuation coefficients $\mu(E)$ do not vary linearly with energy. From a physical standpoint, both the photoelectric effect and Compton scattering exhibit approximate power-law behaviors:

$$\mu_{\text{photo}}(E) \propto Z^n \, E^{-3}, \qquad \mu_{\text{Compton}}(E) \propto \frac{Z}{E}.$$

For this reason, the coefficients are evaluated using logarithmic interpolation:

$$\log \mu(E) \approx \log \mu(E_i) + \frac{\log E - \log E_i}{\log E_{i+1} - \log E_i} \left[\log \mu(E_{i+1}) - \log \mu(E_i)\right].$$

Quick note

The NIST database does not specify the functional form of the interpolation nor does it state that it should be logarithmic. This choice was made after observing that the values exhibit a logarithmic trend.

`SinglePhotonTransporter`: photon loop

After updating $(E', \hat{\Omega}')$, the photon re-enters the transport loop:

1. **Material check**: vacuum / Pb / CsI.
2. **Update attenuation** via `PhysicsEngine`:

$$\mu_{\text{photo}},\ \mu_{\text{Compton}},\ \mu_{\text{tot}}.$$

3. **Two distances**:

$$t_{\mathrm{int}} = -\ln\xi/\mu_{\mathrm{tot}}, \qquad t_{\mathrm{bnd}} = \text{next boundary}.$$

4. **Decision**:

$$t_{\mathrm{int}} < t_{\mathrm{bnd}} \Rightarrow \text{interaction}, \qquad t_{\mathrm{bnd}} < t_{\mathrm{int}} \Rightarrow \text{cross region}.$$

5. **If interaction in CsI**:
   - Photoelectric $\rightarrow$ full deposit $\rightarrow$ stop.
   - Compton $\rightarrow$ partial deposit, update $(E, \hat{\Omega})$ $\rightarrow$ continue.
6. **If in Pb or air**: update position/direction $\rightarrow$ continue loop.

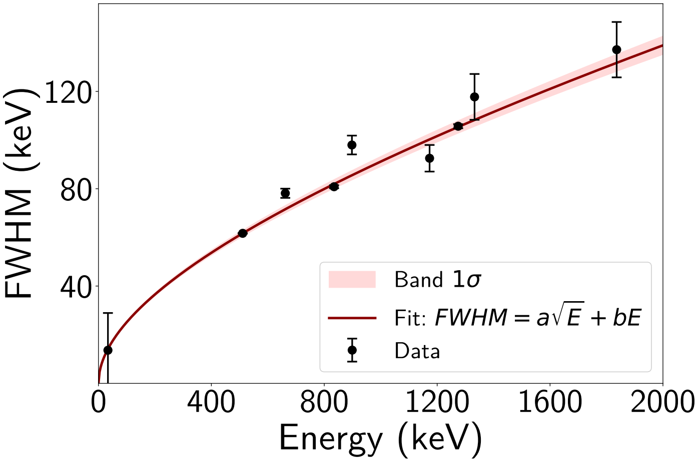
`MultiPhotonTransporter`: core idea

The `MultiPhotonTransporter` simply repeats the full single–photon transport loop millions of times and builds the final energy spectrum.

- Samples an initial energy from the radioactive source.
- Calls the `SinglePhotonTransporter` to obtain the deposited energy.
- Fills the spectrum histogram.
- Tracks statistics: photoelectric, Compton, backscatter, efficiency.
- Applies the detector energy–resolution model at the end.

This produces the simulated spectrum to be later compared with experiment through the FWHM curve.

Energy Resolution Curve (FWHM)

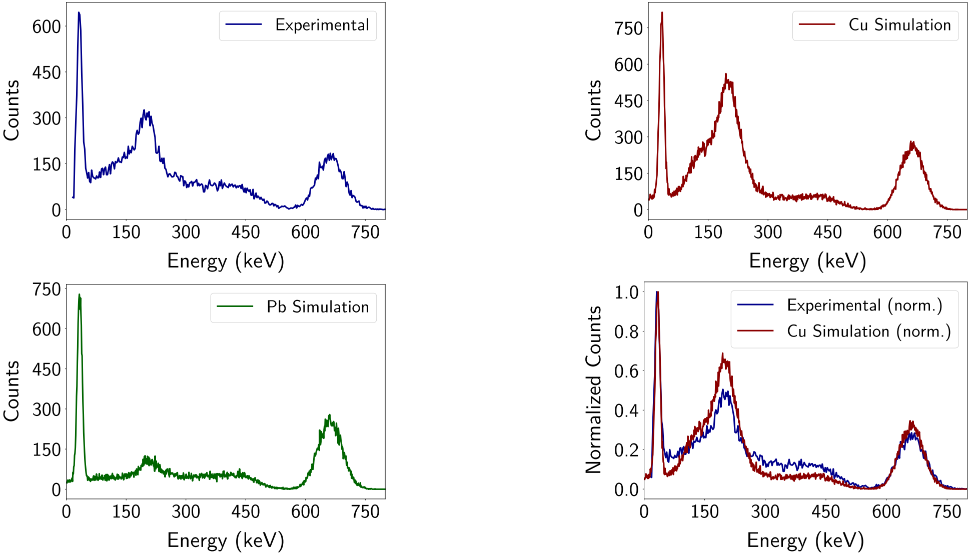


How the points were obtained

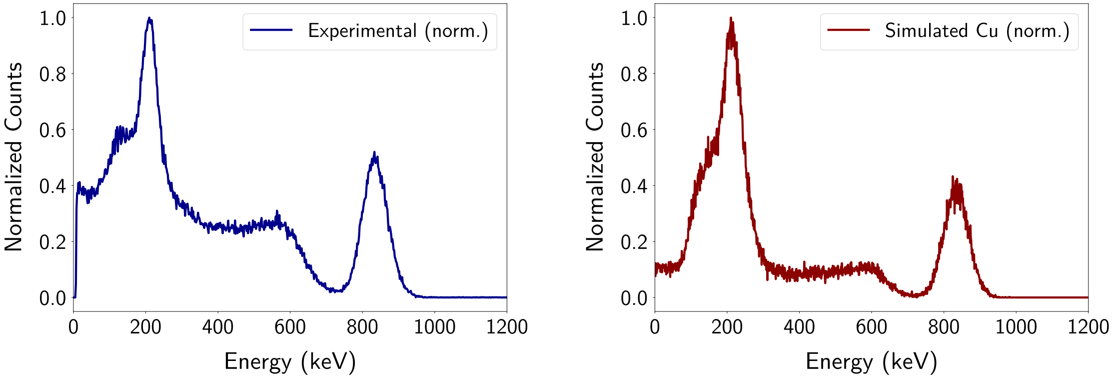
FWHM values were extracted from Gaussian fits to the photopeaks of:

- Cs-137
- Na-22
- Y-88
- Co-60
- Mn-54

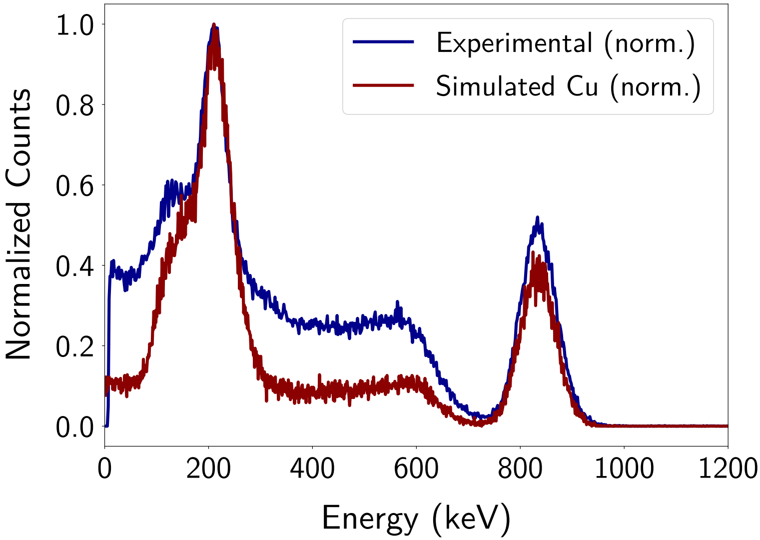
137Cs spectrum



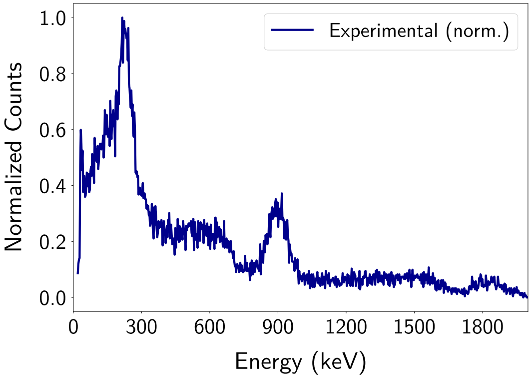
Mn54 spectrum

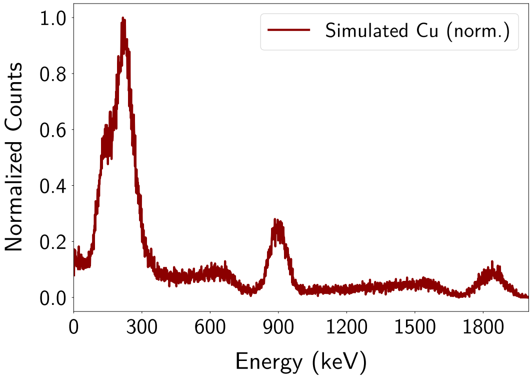


Mn54 spectrum

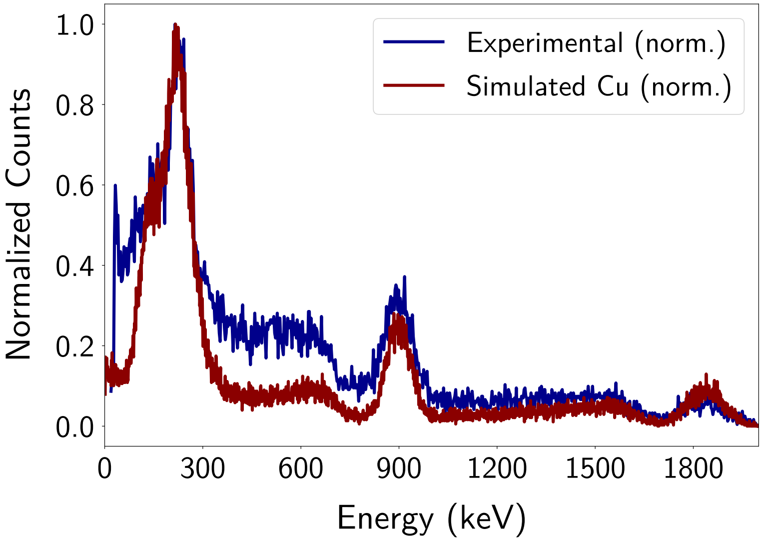


88Y spectrum

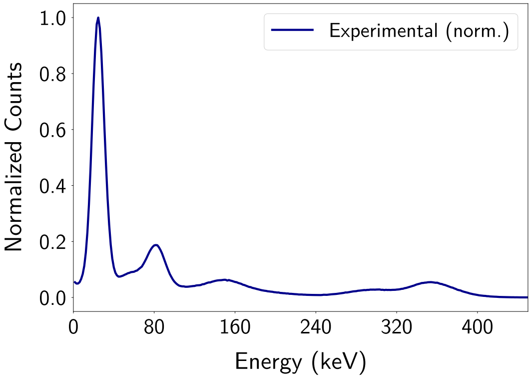


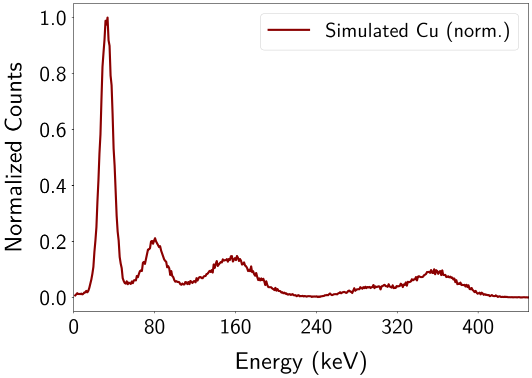


88Y spectrum

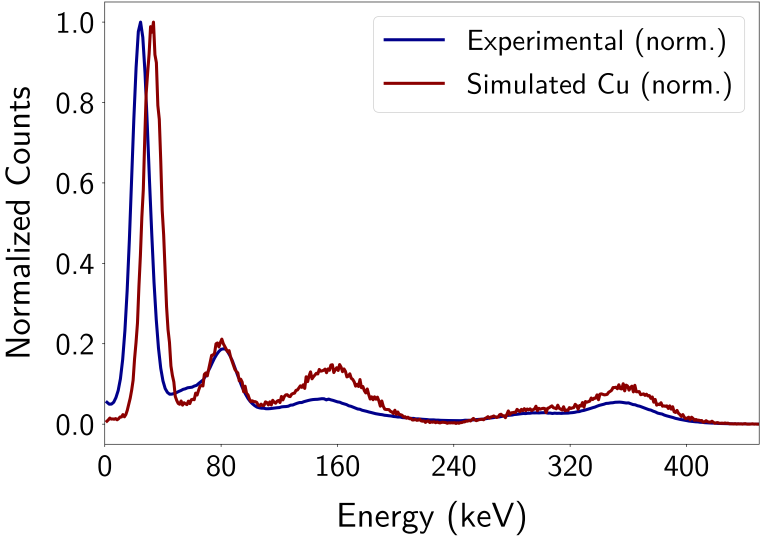


133Ba spectrum





Ba133 spectrum



Conclusions

At the end of the project, the following conclusions were reached:

1. A solid understanding of the physics behind all regions of a typical gamma spectrum was achieved.

2. Regarding the backscatter peak, it was found that it strongly depends on the attenuation coefficients of the materials involved, on the geometry surrounding the source, and on the initial activity of the source.

3. The difficulties that arose during the progress presentation were successfully resolved.

Project potential

Of course, this work has been done before, gamma spectroscopy has been used for more than a century. Therefore, an additional challenge for us was to identify what aspects of our approach were truly novel, and we would like to briefly highlight those contributions.

Detection system geometry

CsI Scintillation Detector

The detector is a cylindrical crystal defined by:

1. Diameter: 2.54 cm,
2. Length: 12.7 cm,
3. Center position: $z = -7.40$ cm,

Lead Shield

The lead cylinder has:

1. Inner radius: $R_{\text{in}} = 13.85$ cm,
2. Thickness: 11.7 cm,
3. Outer radius: $R_{\text{out}} = 25.55$ cm,
4. Inner cavity height: $H_{\text{in}} = 30.4$ cm,

Initial energy sampler `SourceSampler`

Since radioactive sources are not monoenergetic, each emits photons at discrete energies E_i with relative probabilities P_i. A source with n gamma lines is therefore described by

$$\{(E_1, P_1), (E_2, P_2), \dots, (E_n, P_n)\}.$$

Normalizing these probabilities,

$$p_i = \frac{P_i}{\sum_{j=1}^{n} P_j},$$

one obtains a cumulative distribution function (CDF):

$$\mathrm{CDF}(k) = \sum_{i=1}^{k} p_i.$$

This CDF allows mapping a uniform random number $u \in [0, 1]$ to an energy index through

$$\mathrm{CDF}(k-1) < u \leq \mathrm{CDF}(k).$$

A more realistic model

A proper selection of the initial emission direction is essential for accurately reproducing the spectra. In this new 3D model, the source is assumed to be point-like and uncollimated, so the radiation is treated as an isotropic field over 4π steradians.

What does an isotropic field mean?

A real isotropic field, in this context, implies that every area element on the surface of a sphere receives the same probability. This corresponds to a uniform distribution over the solid angle,

$$dP = \frac{1}{4\pi}\, d\Omega.$$

Two properties of this distribution

The polar angle θ cannot be sampled uniformly, whereas the azimuthal angle ϕ can:

$$\cos\theta \sim U(-1,\, 1), \qquad \phi \sim U(0,\, 2\pi).$$