

Final Project

Write a program based on Monte Carlo methods that simulates the transport of photons from a monoenergetic gamma point source inside a scintillation detector. The source is located in \mathbf{r}_s and photons with E_γ energy are released isotropically. The detector crystal is a solid NaI (Sodium Iodide) cylinder centred around the origin and parallel to the z-axis, characterised by its radius R , height h , and density ρ . The rest of the detector equipment such as the protective housing and photomultiplier tube (PMT), as well as the air between the source and the crystal is ignored, i.e.: the model geometry is virtually a NaI cylinder in vacuum. The interactions of the photons inside the crystal result in free electrons/positrons, that could escape the detector, resulting in some energy deposited by the photon "missing" from what is detected. Use the approximation that the charged particles path in the crystal is negligible, and consequently the annihilation of a positron following a pair production happens at the same location. The *resolution*/uncertainty of the whole detector system is modelled by applying a Gaussian noise with a variance described by the *full width at half maximum* (FWHM) to the final energy deposited by a particle.

The program has to satisfy the following requirements:

- The input arguments of the program are the \mathbf{r}_s 3D coordinates of the gamma source, E_γ source energy of the gamma photons, R , h , and ρ parameters of the NaI crystal, and FWHM full width at half maximum describing the detector resolution.
- The program has to account for the following photon-matter interactions: Compton-scattering, photoelectric absorption, and pair production. The energy dependent cross sections in a tabular form (at discrete energy values) are to be obtained from the XCOM database (<https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html>, details in the appendix), and for energies different from the discrete values the cross sections are to be determined by linear interpolation.
- The program has to produce a gamma spectrum from the deposited energies registered by the detector using 1024 energy channels that should contain most characteristics of a real spectrum (e.g.: photopeak, Compton edge, escape peak). The channels should be scaled so that the whole photo peak is visible (remember that a Gaussian noise is applied)
- Apart from producing a spectrum the program has to calculate the η_{tot} total and η_{int} intrinsic efficiency of the detector defined as

$$\eta_{tot} = \frac{E_{det}}{E_{tot}} \quad \text{and} \quad \eta_{int} = \frac{E_{det}}{E_{int}}$$

where E_{det} is the total energy deposited in the detector by the particles, E_{tot} is the total energy released from the source, and E_{int} is the total energy of particles that reached the detector.

Tasks

- (i) Record a gamma spectrum with the following input parameters:

Parameter	Unit	Spectrum "A"	Spectrum "B"
r_s	cm	(3; -3; 2)	(4; 4; 0)
E_γ	keV	661.7	1332.5
R	cm	2.5	3.0
h	cm	3.0	5.0
ρ	g/cm ³	3.67	3.67
FWHM	keV	6.0	8.0

And study the recorded spectra, especially the following aspects:

- Identify the characteristics of the spectra. Which processes are responsible for the different peaks?
 - Determine the location of the Compton edge, and compare the theoretical value to the result of the simulation
 - Consider the interval between the Compton edge and the photopeak. What process causes the counts in this energy range?
- (ii) Record 11 spectra using the input parameters for Spectrum "A" while the coordinate of the source is moved from point (1.0; 3.5; 2.0) to (-4.0; -1.5; 2.0) in uniform steps. Plot the efficiencies η_{tot} and η_{int} as a function of the position number and discuss the resulting dependency.
- (iii) Record 10 spectra using the input parameters for Spectrum "B" while the source energy is increased from 0.4 MeV to 4 MeV in equal steps. Plot the efficiencies η_{tot} and η_{int} as a function of the source energy and discuss the resulting dependency.

The program has to be accompanied by a documentation that briefly describes the structure of the program, the used algorithms and functions, along with the recorded spectra for the "A" and "B" cases, as well as the efficiency analyses, along with the required answers and discussions described above.

A. Photon Cross Sections from XCOM

Visit the <https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html> url, where you can download photon cross sections for different elements, compounds, or mixtures. For the project we need the cross sections for sodium iodide, which is a compound. After choosing compound, by clicking the "Submit Information" button on the lower left, you will be able to specify the compound by its formula, "NaI" for us, the energy range, from 0.001 MeV to 10 MeV for our purposes, and optionally can choose which cross sections to visualise (it is informative to choose all, but will not affect the data we need). Clicking "Submit Information" again you will see a plot of the chosen cross sections, followed by

a table of cross sections from which you can choose columns to download. We will need the cross sections for incoherent scattering (Compton scattering), photoelectric absorption, and pair production both in the nuclear and electron field (their sum will be the cross section for pair production for us), the energy column is always included. After clicking "Download data" you can either right click and use the "Save as" feature, or copy and paste the relevant part in a text file in order to save the data for use in your program. Screenshots of each step are shown in Figures 1 to 4.

Element/Compound/Mixture Selection

In this database, it is possible to obtain photon cross section data for a single element, compound, or mixture (a combination of elements and compounds). Please fill out the following information:

[Help](#)

Identify material by:

- Element
- Compound
- Mixture

Method of entering additional energies: (optional)

- Enter additional energies by hand
- Additional energies from file (*Note: Your browser must be file-upload compatible*)

Figure 1: XCOM select what kind of material you need

Fill out the form to select the data to be displayed:

[Help](#)

Formula for compound (e.g. H₂O for water):

Optional output title:

Graph options: <ul style="list-style-type: none"> <input checked="" type="checkbox"/> Total Attenuation with Coherent Scattering <input checked="" type="checkbox"/> Total Attenuation without Coherent Scattering <input checked="" type="checkbox"/> Coherent Scattering <input checked="" type="checkbox"/> Incoherent Scattering <input checked="" type="checkbox"/> Photoelectric Absorption <input checked="" type="checkbox"/> Pair Production in Nuclear Field <input type="checkbox"/> Pair Production in Electron Field <input type="checkbox"/> None 	Additional energies in MeV: (optional) (up to 100 allowed) <small>Note: Energies must be between 0.001 - 100000 MeV (1 keV - 100 GeV) (only 4 significant figures will be used). One energy per line. Blank lines will be ignored.</small> <input type="text"/> <input checked="" type="checkbox"/> Include the standard grid Energy Range: <input type="text"/> Minimum: 0.001 MeV <input type="text"/> Maximum: 10 MeV
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Return to [previous](#) document.

Figure 2: XCOM choosing energy ranges and material

To download data in spreadsheet (array) form, choose a delimiter and use the checkboxes in the table heading. After downloading, save the output by using your browser's **Save As** feature.

Delimiter:

- space
- | (vertical bar)
- tab
- newline

[Download data](#) [Reset](#)

Edge	(required) Photon Energy	Scattering		<input checked="" type="checkbox"/> Photoelectric Absorption	Pair Production		Total Attenuation	
		<input type="checkbox"/> Coherent	<input checked="" type="checkbox"/> Incoherent		<input checked="" type="checkbox"/> In Nuclear Field	<input checked="" type="checkbox"/> In Electron Field	<input type="checkbox"/> With Coherent Scattering	<input type="checkbox"/> Without Coherent Scattering
		MeV	cm ² /g		cm ² /g	cm ² /g	cm ² /g	cm ² /g
	1.000E-03	7.422E+00	5.916E-03	7.794E+03	0.000E+00	0.000E+00	7.801E+03	7.794E+03
	1.035E-03	7.394E+00	6.244E-03	7.245E+03	0.000E+00	0.000E+00	7.252E+03	7.245E+03
	1.072E-03	7.366E+00	6.586E-03	6.736E+03	0.000E+00	0.000E+00	6.744E+03	6.736E+03
53 M ₁	1.072E-03	7.366E+00	6.586E-03	7.021E+03	0.000E+00	0.000E+00	7.029E+03	7.021E+03
	1.072E-03	7.366E+00	6.586E-03	7.925E+03	0.000E+00	0.000E+00	7.932E+03	7.925E+03
	1.072E-03	7.366E+00	6.587E-03	7.021E+03	0.000E+00	0.000E+00	7.028E+03	7.021E+03
11 K	1.072E-03	7.366E+00	6.587E-03	7.924E+03	0.000E+00	0.000E+00	7.932E+03	7.924E+03
	1.500E-03	7.010E+00	1.065E-02	3.801E+03	0.000E+00	0.000E+00	3.808E+03	3.801E+03
	2.000E-03	6.555E+00	1.541E-02	1.917E+03	0.000E+00	0.000E+00	1.924E+03	1.917E+03
	3.000E-03	5.687E+00	2.459E-02	7.003E+02	0.000E+00	0.000E+00	7.060E+02	7.003E+02
	4.000E-03	4.947E+00	3.292E-02	3.351E+02	0.000E+00	0.000E+00	3.401E+02	3.352E+02
	4.557E-03	4.592E+00	3.712E-02	2.387E+02	0.000E+00	0.000E+00	2.433E+02	2.387E+02

Figure 3: XCOM cross section table

<head><title>NIST XCOM database</title><!-- Google Analytics 4 --><script async src="https://www.googletagmanager.com/gtag/js?id=G-95LN1VEEJ2"></script>					
<script>window.dataLayer = window.dataLayer []; function gtag(){dataLayer.push(arguments);} gtag('js', new Date()); gtag('config', 'G-95LN1VEEJ2');</script><!-- End of Google Analytics 4 --><SCRIPT async type="text/javascript" id="_fed_an_ua_tag" src="https://dap.digitalgov.gov/Universal-Federated-Analytics-Min.js?agency=DOC&subagency=NIST&pua=UA-37115410-4&t=false&exts=ppsx,pps,f90,sch,rtf,wrl,txz,m1v,xlsm,msi,xsd,f,tif,eps,mpg,xml,pl,xlt,c"></script></head>Photon Incoher. Photoel. Nuclear Electron					
Energy	Scatter.	Absorb.	Pr. Prd.	Pr. Prd.	
1.000E-03	5.916E-03	7.794E+03	0.000E+00	0.000E+00	
1.035E-03	6.244E-03	7.245E+03	0.000E+00	0.000E+00	
1.072E-03	6.586E-03	6.736E+03	0.000E+00	0.000E+00	
1.072E-03	6.586E-03	7.021E+03	0.000E+00	0.000E+00	
1.072E-03	6.586E-03	7.925E+03	0.000E+00	0.000E+00	
1.072E-03	6.587E-03	7.021E+03	0.000E+00	0.000E+00	
1.072E-03	6.587E-03	7.924E+03	0.000E+00	0.000E+00	
1.072E-03	6.587E-03	7.924E+03	0.000E+00	0.000E+00	
1.500E-03	1.065E-02	3.801E+03	0.000E+00	0.000E+00	
2.000E-03	1.541E-02	1.917E+03	0.000E+00	0.000E+00	
3.000E-03	2.459E-02	7.003E+02	0.000E+00	0.000E+00	
4.000E-03	3.292E-02	3.351E+02	0.000E+00	0.000E+00	
4.557E-03	3.712E-02	2.387E+02	0.000E+00	0.000E+00	
4.557E-03	3.712E-02	6.585E+02	0.000E+00	0.000E+00	
4.702E-03	3.816E-02	6.166E+02	0.000E+00	0.000E+00	
4.702E-03	3.822E-02	6.334E+02	0.000E+00	0.000E+00	

Figure 4: XCOM download data