Developing Monte Carlo simulations of the GAINS spectrometer

University of Groningen

Gefré Wortelboer

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Abstract

The GAINS spectrometer at GELINA was built to measure cross sections of inelastic neutron reactions. The study of such reactions is of crucial importance to reactor simulations. The measurements are performed using prompt γ-rays: the γ radiation emitted by excited nuclei. In the present paper we use the Monte Carlo package Geant4 to develop simulations capable of reproducing the spectra measured by GAINS. Ultimately it should be able to model the decay of any element, given its decay scheme. In order to produce reliable spectra it is necessary to calibrate the photopeak efficiencies and energy resolution. In doing so, the measured spectrum of ^{152}Eu was used. After fitting several parameters, the agreement between the simulated and measured efficiencies was found to be good. The energy resolution was fitted using a simple polynomial, resulting in a reasonable fit for most detectors. Finally, the procedure of simulating nuclear decay is discussed and the spectrum of ^{152}Eu is used as a performance test. Several features of the measured spectra can be observed in the simulated spectra. This includes the positions of photopeaks as well as their relative intensities.

Contents

1 Introduction

The cross sections of inelastic neutron reactions (n, xn) are currently lacking in data [1]. The reason for this is mostly the small amount of neutron facilities and the difficulties of the measurement process. These difficulties include for instance poor detector efficiencies and the need to distinguish between different emission processes. Measurements of neutron cross sections are of importance to reactor core simulations. These simulations require an accuracy of less than 8%.

Several methods exist to investigate (n, xn) reactions. Direct detection involves studying the neutrons that emerge from (n, xn) reactions. This requires the ability to distinguish between different reaction channels. Neutron activation analysis studies the reaction products of neutron-induced radioactivity [2]. Consequently, this technique excludes long-lived isotopes or isotopes whose radioactive decay paths are poorly understood. The detectors situated at the GELINA Neutron time-of-flight facility use prompt γ-ray spectroscopy. In this technique the γ radiation emitted by excited nuclei is detected. However, this usually only gives a lower bound of the cross sections, since the ground state may be achieved if several neutrons are produced (and hence no γ is emitted) [1]. Despite this limitation, the results can still be used to validate theoretical models. To perform these prompt γ-ray measurements, the GELINA facility uses two HPGe arrays (GAINS and GRAPhEME). The GAINS spectrometer will be described in more detail in section 1.1.

The cross sections themselves are inferred from the measured number of counts in the detectors' spectra and the efficiencies of the detectors. It is therefore necessary to obtain these efficiencies as precisely as possible. In order to gain a better understanding of the effect that certain parameters and processes have on the data, we will make use of Monte Carlo simulations. Such simulations are especially useful for complicated detector setups and nuclear decays.

The main goal is to produce simulations capable of replicating the spectra obtained by the GAINS setup. The C++ library Geant4 will be used for these simulations (section 1.2). We start by calibrating the efficiency and energy resolution using the spectrum of ^{152}Eu (section 2). To properly reproduce the spectra it is necessary to take into account the nuclear structure of the elements involved. This is described in section 3.

1.1 The GAINS spectrometer

The GELINA (Geel Electron Linear Accelerator) neutron time of flight facility uses a neutron beam with energies up to 15 MeV [3]. To produce the neutrons, an accelerated electron beam is directed onto a target [4]. Neutrons emerge from this mainly through (γ, n) and (γ, f) reactions. The neutron flux is determined using a fission chamber placed inside the beam. The chamber is coated with ^{235}U deposits. If a neutron interacts with the ^{235}U sample, fission might take place. The fission products will have

enough energy to ionize the surrounding material, which produces a signal.

200 m away from the neutron source, a target containing the nucleus of interest is placed [1]. To investigate inelastic neutron reactions, GELINA uses the GAINS (Gamma Array for Inelastic Neutron Scattering) spectrometer. It consists of an array of 12 HPGe detectors (figure 1). They are placed at angles 125°, 110° and 150° with respect to the incoming neutrons. The spectrometer measures the γ-rays that are emitted through (n, xnγ) reactions. The intensity of the radiation can then be used to calculate cross sections.
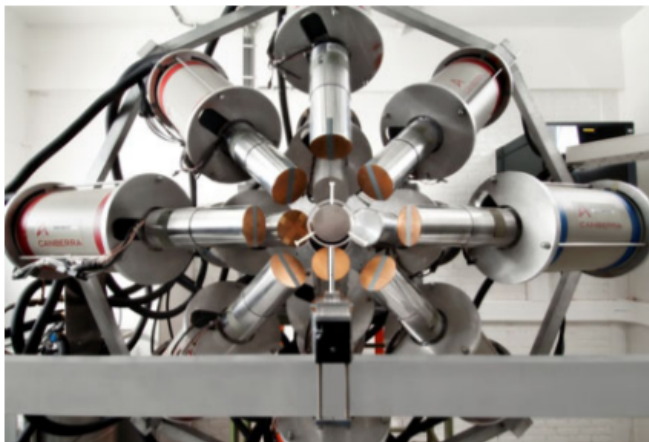

Figure 1: The GAINS spectrometer [1].

Each detector has the following components:

- A cylindrical HPGe crystal with a hole at its back. This comprises the sensitive volume of the detector.

- A circular window consisting of either carbon or aluminum. It serves as an absorber for low energy γ-rays.

- An aluminum cap.

The precise sizes, distances and materials vary for each detector and were obtained from the specifications provided by the facility. A schematic drawing of the listed components is shown in figure 2.

1.2   The Geant4 simulation package

Geant4 (GEometry ANd Tracking) is a C++ library that can be used to perform Monte Carlo simulations of a wide range of physical phenomena [5]. It uses existing (evaluated) databases to model the interactions. The transportation of particles is
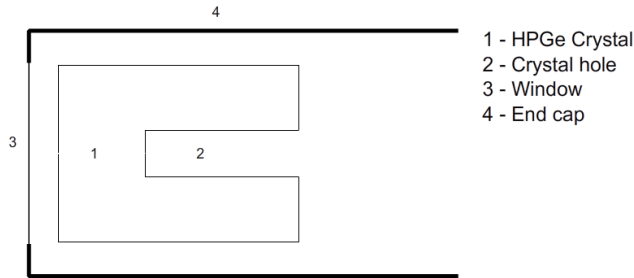
Figure 2: A schematic drawing of a detector.

divided into small steps. At each iteration the package uses the mean free paths of the surrounding materials to randomly sample a step length. After this step length interactions take place and energy is deposited[1]. Only the energy that is deposited in a detector's sensitive volume is recorded.

To simulate prompt γ-rays we require electromagnetic interactions down to low energies and detailed simulations of decay schemes. The most prevalent types of γ-ray interactions are the photoelectric effect, Compton scattering and pair production. Geant4's QBBC physics list will be used to model these interactions. It is most suitable for radiation experiments in the energy range below 1 GeV [6]. To be able to handle nuclear decay as well, Geant4's radioactivation package was used. This package is able to simulate nuclear decay according to a given decay scheme.

Geant4 allows the simulated geometry and materials to be specified very precisely. Based on the components listed in section 1.1, a virtual detector was built for each of the 12 detectors in order to mimic the geometry of the GAINS spectrometer. A drawing of a simulated event is shown in figure 3.

2 Calibration

The detector efficiencies and energy resolutions must be carefully calibrated. The former is especially important for the determination of cross sections. In this paper we will however only be interested in photopeak efficiencies. To determine the efficiencies necessary for the calculation of cross sections, a more sophisticated treatment than the one presented here will be required. For the calibration the spectrum of ^{152}Eu was used. ^{152}Eu was chosen due to the high number of the transitions and the wide range they cover, increasing the reliability of the calibration. The measured γ spectrum of ^{152}Eu is shown in figure 4.

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[1]Interactions can also take place continously throughout a step (e.g. interactions with electric fields). Here we will however mostly be concerned with discrete processes that occur at the end of a step.
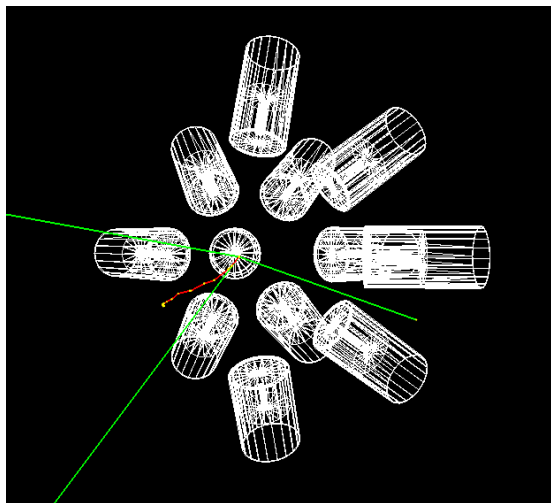
Figure 3: A drawing of a simulated event. In this example both γ-rays (green) and electrons (red) were emitted. Yellow dots signify that an interaction took place at that position.
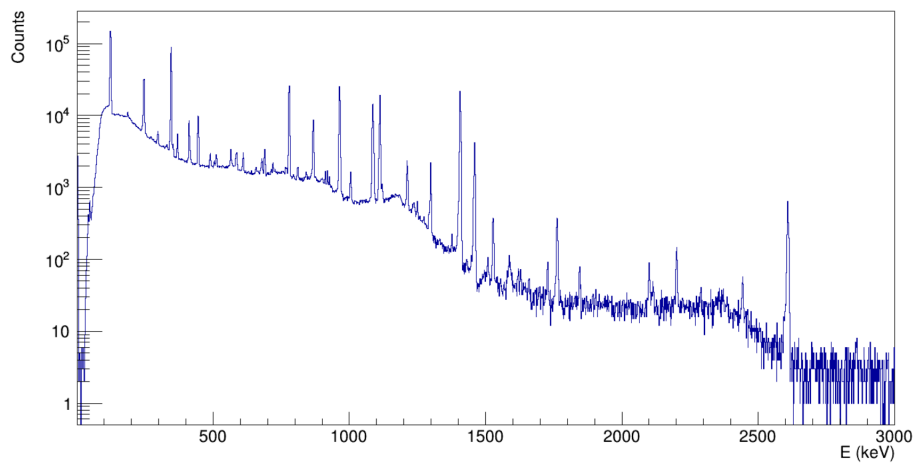

Figure 4: The measured γ spectrum of ^{152}Eu.

2.1 Efficiency calibration

The calibration of the efficiency was based on the eight most intense photopeaks of ^{152}Eu. The efficiencies of these peaks were measured by the facility. In this context the efficiency of a photopeak corresponds to the fraction of photons with the energy of that photopeak, that are fully absorbed. In order to determine the simulation's efficiencies the setup shown in section 1.2 was used. A point-like source that emitted mono-energetic gamma-rays isotropically was placed at the center. For each photopeak energy 10^7 events were simulated. The 1408 keV spectrum is shown in figure 5.
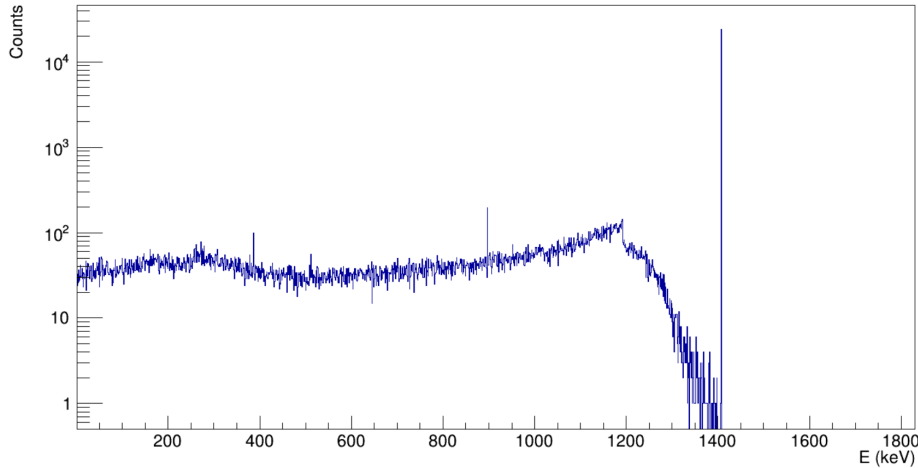

Figure 5: The simulated 1408 keV γ spectrum of detector 1. Note that the finite resolution of the detector is not included in this spectrum.

In addition to the photopeak, two other peaks can be observed, separated by 511 keV and 1022 keV from the photopeak. These occur whenever at least one photon produced by e^+e^- annihilation escapes the detector. The remaining continuous part of the spectrum can be attributed to Compton scattering. The maximum in front of the photopeak is the Compton edge. It's energy is the maximum energy that a photon can transfer to an electron through Compton scattering and is given by

$$E_{\text{Compton}} = E_\gamma \left(1 - \frac{1}{1 + \frac{2E_\gamma}{m_e c^2}} \right). \tag{1}$$

For $E_\gamma = 1408$ keV this evaluates to 1192 keV. Although it is possible, with a rather small probability, to deposit more energy through multiple scattering.

Initially when setting up the geometry of the simulation, the specifications were closely followed. Whenever discrepancies between the simulated and measured efficiencies were observed, several parameters were tweaked. These included the window thickness and

the distance of the detectors. As the window acts as an absorber for low energy photons, it has a significant influence on the shape of the graph. Moreover, most of the windows consisted of carbon epoxy fibers, whose exact composition is unknown to us. The material of the simulated windows was set to pure carbon, making it unsurprising that the window thickness needed to be fitted.

Finally, if the simulated and experimental graphs differed only by a multiplicative factor, the distance was fitted. To obtain a reasonably good fit, the surface of the detector was approximated to lie across a sphere with a radius equal to the distance. In that case, the efficiency will be inversely proportional to the square of the distance. The average of the simulated efficiency divided by the measured efficiency was calculated and the distance was multiplied by the square root of that value.

The parameters that were adjusted are displayed in table 1. Graphs comparing the simulated and measured photopeak efficiencies are shown in figure 6. We estimate the statistical error in the simulated efficiency by assuming that the number of counts in the photopeak follows a binomial distribution. The standard deviation, for low efficiencies, is $\sqrt{N}$, with N the number of counts in the photopeak. The simulated number of counts was at least 10^4, giving an error of less than 1%.

Detector number	Distance (cm)	Window thickness (mm)
1	18.76 $\longrightarrow$ 17.97	0.5 $\longrightarrow$ 1
2	18.11 $\longrightarrow$ 18.35	0.5 $\longrightarrow$ 0.5
3	18.22 $\longrightarrow$ 19.75	0.5 $\longrightarrow$ 0.05
4	17.51 $\longrightarrow$ 18.09	0.5 $\longrightarrow$ 0.5
5	18.43 $\longrightarrow$ 19.13	0.5 $\longrightarrow$ 0.5
6	18.40 $\longrightarrow$ 18.63	0.5 $\longrightarrow$ 0.5
7	17.65 $\longrightarrow$ 18.00	0.5 $\longrightarrow$ 0.5
8	18.18 $\longrightarrow$ 18.51	0.5 $\longrightarrow$ 0.5
9	18.03 $\longrightarrow$ 19.95	0.5 $\longrightarrow$ 0.5
10	18.56 $\longrightarrow$ 18.81	0.5 $\longrightarrow$ 0.5
11	18.19 $\longrightarrow$ 18.97	0.5 $\longrightarrow$ 0.05
12	17.35 $\longrightarrow$ 17.65	0.5 $\longrightarrow$ 0.5

Table 1: The parameters that were tweaked. Both the values from the specifications (before arrow) and the fitted values (after arrow) are shown.

The overall agreement between the simulated and experimental graphs is good. Despite adjusting the window thickness, small discrepancies can be seen at lower energies for detectors 1, 2, 3 and 11. As mentioned before, the source used in the simulations was point-like. It would however be more realistic to take into account the finite size of the ^{152}Eu sample and use an extended source (see for instance [7]).
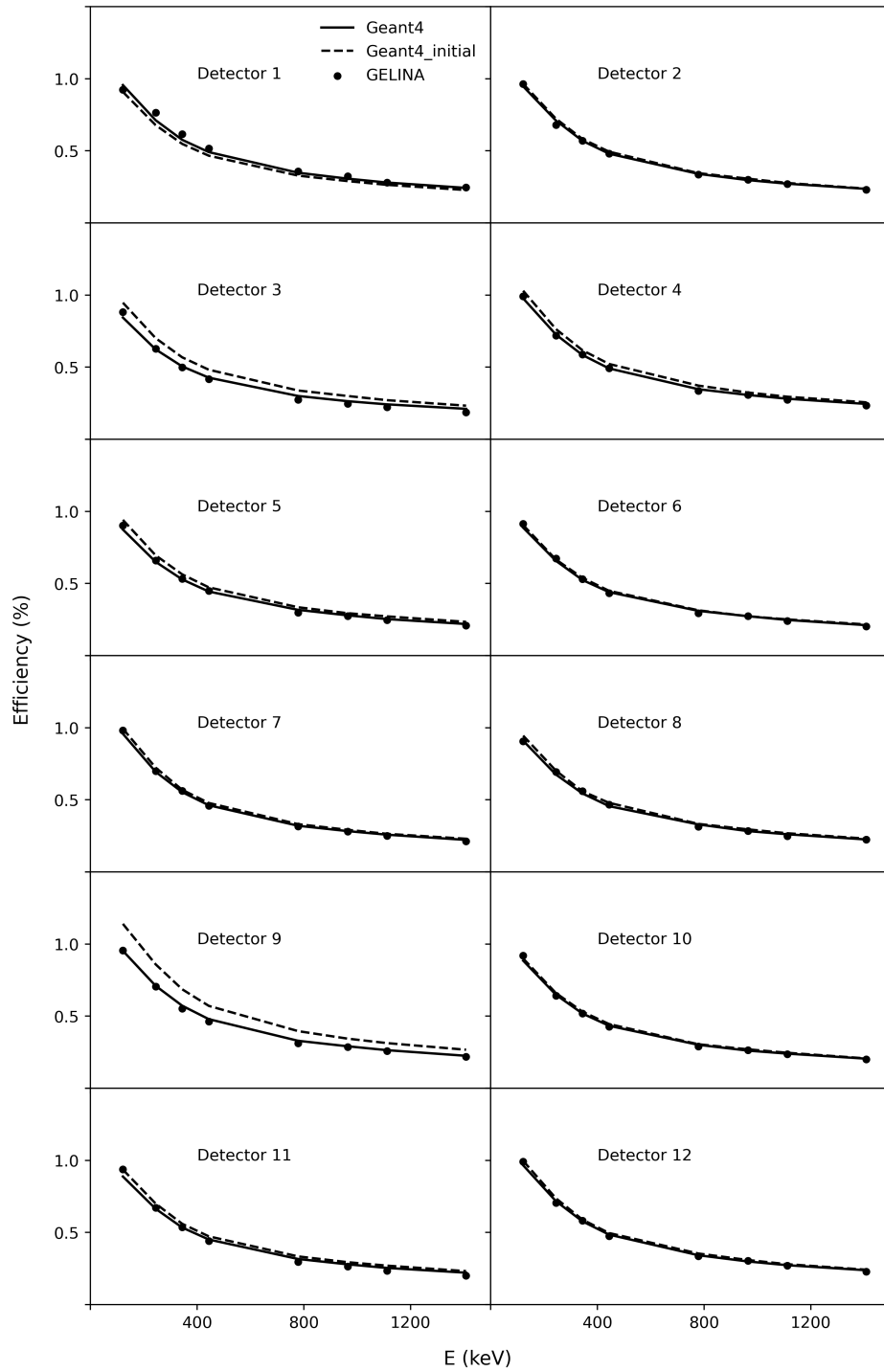
Figure 6: The photopeak efficiencies of each detector. The graphs show the simulated efficiencies, the measured efficiencies and the efficiencies before fitting the parameters.

2.2 Energy resolution calibration

By default Geant4 does not model the energy resolution of the detectors. A spread in the energy spectrum was included manually after the simulation had been run. This spread in energy arises due to the statistical nature of the creation of electron-hole pairs in semiconductors [8]. The uncertainty can be estimated by taking the rms deviation $\sqrt{N}$, where N is the number of electron-hole pairs. Generally the uncertainty is reduced because of energy conservation. This is characterized by the Fano factor F, giving an uncertainty of

$$\sigma = \sqrt{NF} \tag{2}$$

In practise however, a worse resolution is usually obtained due to uncertainties in the collection of charges.

In order to obtain the energy dependence of the resolution, the spectrum of ^{152}Eu was used once again. The shape of the photopeaks can be approximated well by a Gaussian distribution. Its standard deviation was interpreted as the resolution at the energy of the peak. The remainder of the spectrum was fitted using a third degree polynomial. The complete fitting procedure is shown in figure 7.
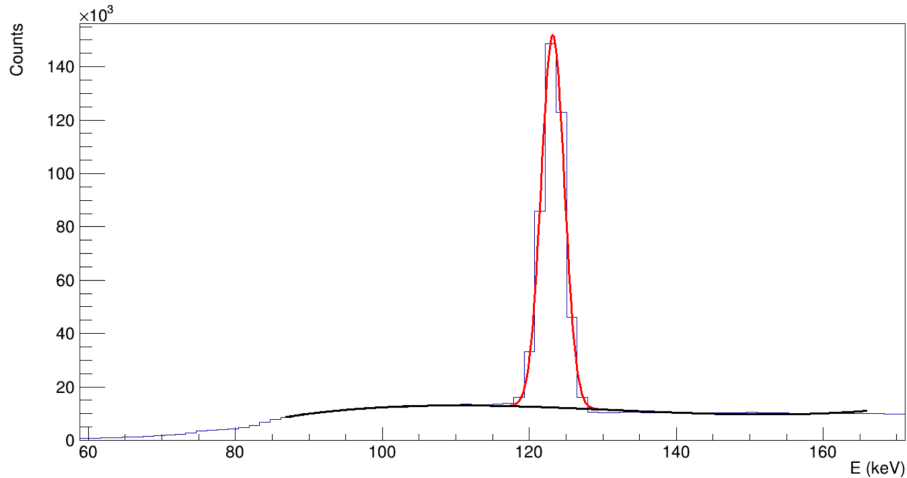

Figure 7: The photopeak fitting procedure. The fit (shown in red) consists of the sum of a third degree polynomial (black) and a Gaussian.

In cases where two peaks overlap, the previously mentioned model (convolution of a polynomial and a Gaussian) will not give accurate results. This may be the case if a photopeak's position coincides with that of a Compton edge. More complicated models would have to applied to get a good fit. With the current model, the resolutions of such peaks will considerably deviate from the general trend for each detector. To keep the complexity of the models low, these have been left out. The results are shown in

9

figure 8.

In order to fit the data points, a second degree polynomial seemed suitable. However, as the detector crystals consisted of identical material, the shape of the fit was kept the same for each detector. The fit functions only differed from each other by a constant term:

$$\sigma_i(E) = aE^2 + bE + c_i, \tag{3}$$

where i denotes the detector number and a, b, c_i are fit parameters. This resulted in a reasonable fit for most detectors. The fit was particularly bad for detector 8. For this detector the width of the peaks appears to fluctuate significantly more than the other detectors, making it impractical to remove outliers.

3   Nuclear decay simulations

The previous sections have been dedicated to calibrating the simulation in order to produce reliable spectra. In this section this will be combined with simulations of nuclear decay. Ultimately the application should be able to simulate the decay of any element, given its decay scheme. Currently these decay schemes are provided through regular text files. As a performance test the decay of ^{152}Eu will be simulated. In its ground state, ^{152}Eu decays radioactively through β-decay and electron capture into either ^{152}Gd or ^{152}Sm respectively. Both these processes may leave the daughter nucleus in an excited state, causing the nucleus to relax to its ground state through gamma decays. Once the ground state has been reached, further decay is possible. Although most features of ^{152}Eu's spectrum are a result of the decays into ^{152}Gd or ^{152}Sm. Their decay schemes are shown in figures 9 and 10.

The information necessary to properly simulate these decays includes the lifetime and excitation energy of each possible level and the types and intensities of each transition. The datasets provided by Geant4 retrieve this information from ENSDF files [10]. Since ^{152}Eu can decay through electron capture, information about the binding energies of the shell electrons is needed as well. This data is derived from Livermore data libraries [11].

The simulation is carried out by placing a point-like ^{152}Eu's source at the center of the setup. Based on the provided datasets, a decay channel is picked with a probability proportional to its intensity. The program then determines which daughter particles need to be created and calculates their kinetic energies. A crucial issue arises due to the fact that the source is point-like. To speed up the simulation, the setup is embedded in vacuum instead of air. However, as the lifetime of ^{152}Eu is very long, even the smallest amount of energy will be enough to launch the source out of the volume, cutting the simulation short. To circumvent this, one could use a more realistic source where the sample is surrounded by a plastic shield. The ^{152}Eu sample will then be confined to this
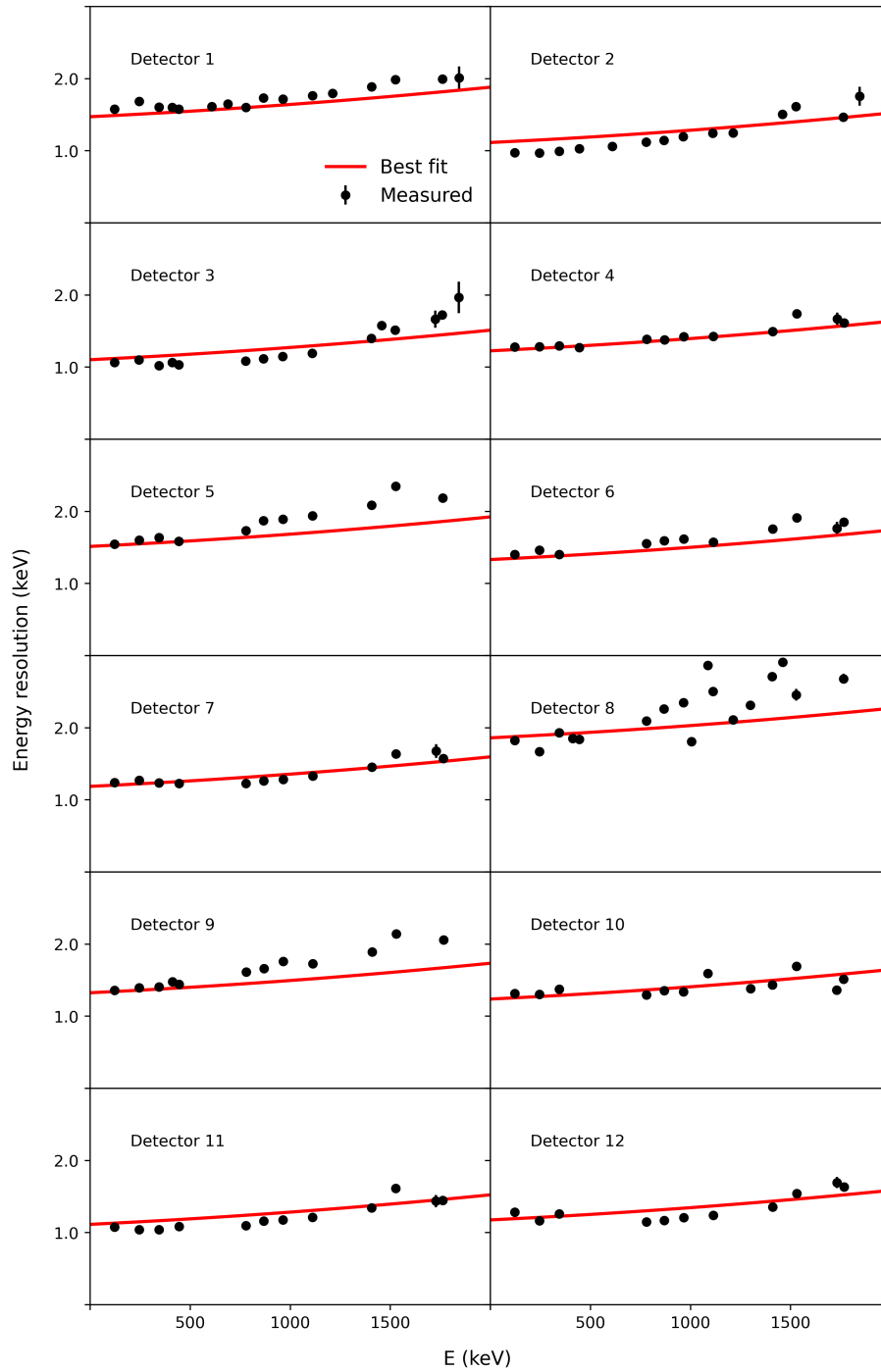
Figure 8: The energy dependence of each detector's resolution. For the fit (obtained by minimising the χ^2-value) of the data, a second degree polynomial was used where only the constant term varied per detector.
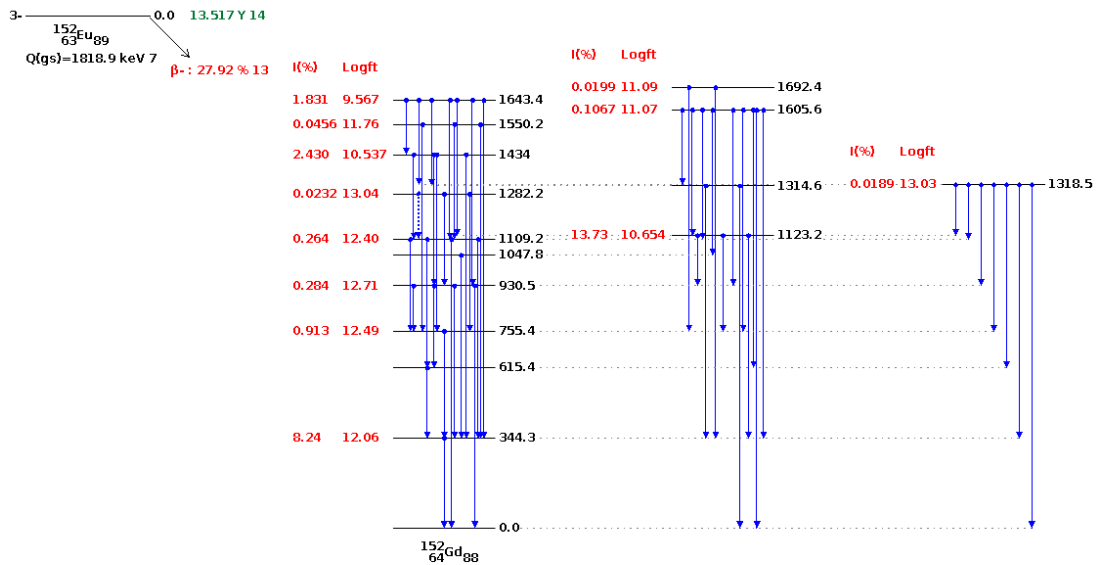
Figure 9: The decay scheme of ^{152}Eu's β^--decay channel [9]. For each level the figure shows the intensities (red), excitation energy in keV (black) and the possible transitions (blue arrows).
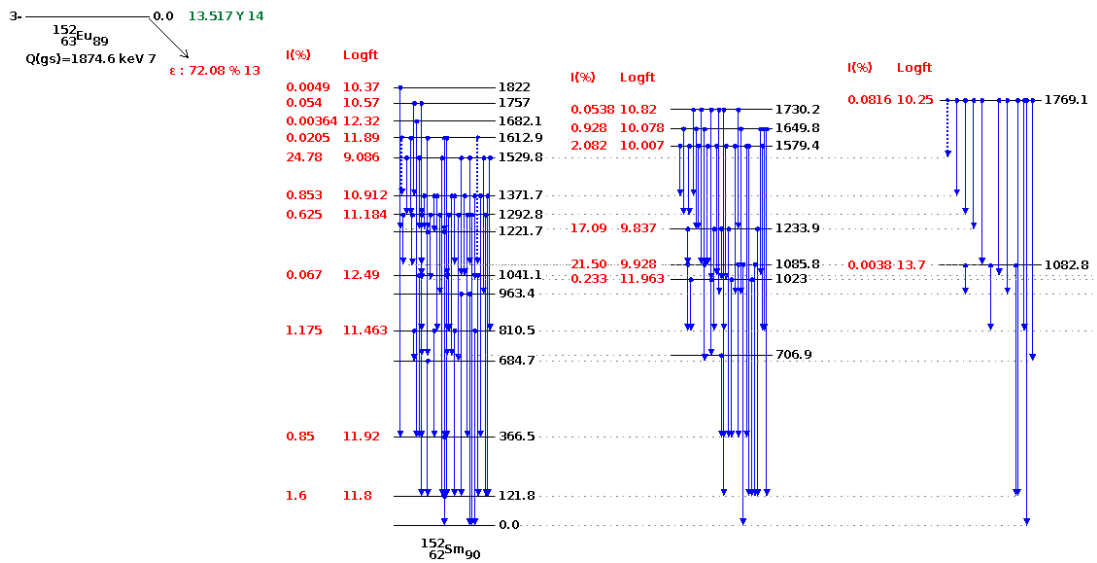

Figure 10: Part of the decay scheme of ^{152}Eu's electron capture channel [9]. For each level the figure shows the intensities (red), excitation energy in keV (black) and the possible transitions (blue arrows).

region. Another option is to keep air as the surrounding material, making it nearly impossible for the sample to move around much. Currently this latter option is being used.

The simulated spectrum of ^{152}Eu is shown in figure 11. It exhibits several features that the measured spectrum has. This includes the positions of the photopeaks as well as their relative intensities. Beyond roughly 1500 keV on the other hand, various photopeaks can be observed in the measured spectrum that are missing in the simulated spectrum. Some of these (e.g. the 2600 keV peak) can be attributed to background radiation, as their energies do not appear in the spectrum of ^{152}Eu. The simulation only models the gamma-rays originating from the ^{152}Eu sample, neglecting any other sources of radiation. The remaining missing photopeaks peaks are generally not a direct result of the decay of ^{152}Eu. The 2121 keV peak for instance arises due to internal conversion of ^{152}Sm [10]. To obtain such photopeaks, the simulation would have to be run for a much longer time.
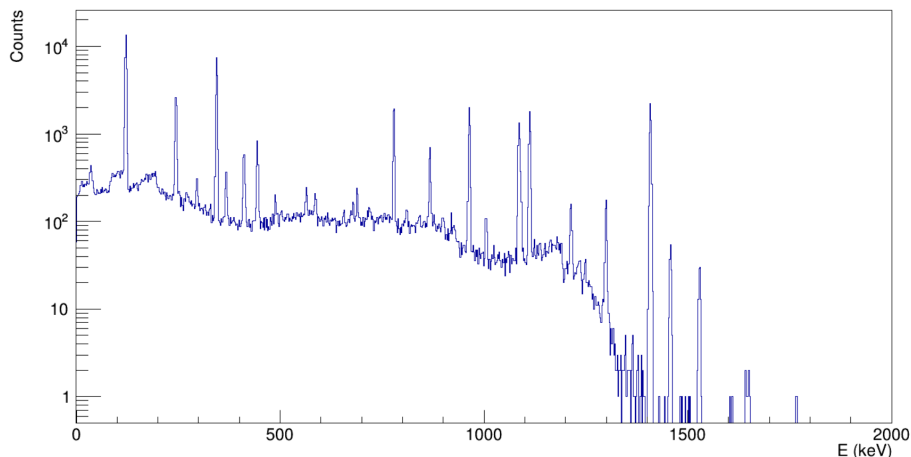

Figure 11: The simulated spectrum of ^{152}Eu

4 Conclusions

The study of inelastic neutron reactions is of utmost importance to reactor studies. To this end, the GAINS spectrometer at GELINA was built to measure cross sections of (n, xn) reactions. These cross sections are determined using prompt γ-ray spectroscopy. To better understand how certain parameters influence the measurements, simulations have been built. The Monte Carlo package Geant4 was used to develop these simulations. The efficiencies of each detector must be known very precisely, as the calculation of the cross sections depends on the their values. In the present paper however, we

have only shown the process of determining photopeak efficiencies. In a future project, more detailed procedures can be implemented to obtain the detector efficiencies. Small discrepancies could still be observed between the simulated and measured photopeak efficiencies at low energies. An extended source, as opposed to a point source, could possibly improve the agreement as it takes into account the geometry of the sample.

By default Geant4 does not model the energy resolution of the HPGe detectors. A spread in the deposited energy was included manually based on the spectrum of ^{152}Eu. The width of photopeaks present in the measured spectra was taken as a measure of the energy resolution. A second degree polynomial seemed to produce a reasonable fit of the data. The resolution of the eight detector on the other hand, yielded a particularly bad fit. Future efforts could be dedicated to investigating the cause of this.

Simulations of nuclear decay were subsequently implemented. As a performance test, ^{152}Eu's spectrum was used once again. The spectra produced by the simulation exhibited many of the features that the measured spectra have. The photopeak positions and their relative intensities for instance, showed good agreement. For higher energies, discrepancies can be found. The reasons are that the background radiation currently is not included and that the simulation would have to be run for a much longer time.

In conclusion, the package that has been developed is capable of simulating detailed nuclear decay schemes as well as the energy resolution and photopeak efficiencies of each detector. It should be emphasized that only one particular Monte Carlo package has been used. As a consistency check, the same simulations could be carried out with frameworks other than Geant4.

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