Simulating Gamma Scintillator Detectors
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1   Introduction

The TRINAT group is working on a time-reversal experiment that attempts to measure the time-reversal symmetry violation by observing the products of a beta decay. The products observed are the nuclear recoil, the emitted beta and the gamma rays. The gamma rays are counted in two scintillating crystals as seen in Figure 1. If the counts in the scintillating crystals are not equal, this would be an indication of time-reversal symmetry breaking.
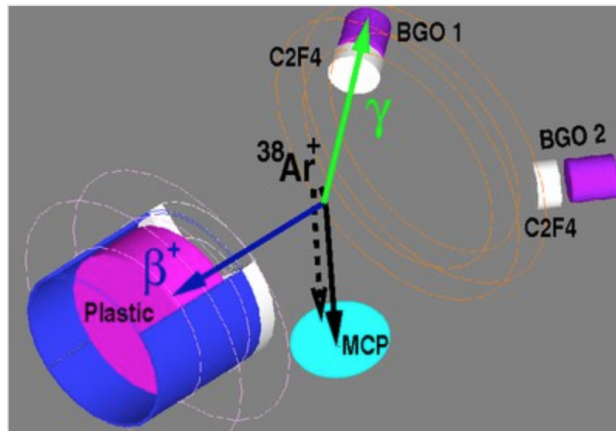

Figure 1: Drawing of experimental setup for time-reversal experiment. The gamma scintillator detectors are labeled as BGO1 and BGO2. [1]

My focus for this term was simulating scintillation crystals that can be used for the gamma detectors. Specifically, I looked at BGO and GAGG crystals to see how well they would work as detectors. The report will cover the simulations I used and the results from the simulations. It will compare the simulations to sample data that was taken of an existing crystal. It will also explore a method of creating a scintillator detector out of a combination of two crystals. This would allow for gamma detection at lower energies in the presence of the largest expected background.

Contents

2 EGSnrc

2.1 Getting Started

EGSnrc is a tool for simulating "electron gamma showers". I used this to simulate a monoenergetic point source of gamma rays incident on a few different scintillating crystals. I was then able to measure the energy deposited in the crystals to predict the scintillator's ability to detect gamma rays.

The instructions to download and install EGSnrc can be found here: https://github.com/nrc-cnrc/EGSnrc/wiki/Installation-overview. The instructions are very straightforward and easy to follow.

On the HPElite laptop I was using, EGSnrc was installed in /home/trinat/EGSnrc. Within /EGSnrc, there are two folders: /egs_home and /HEN_HOUSE. /egs_home contains most of the code that is manipulated by the user. /HEN_HOUSE contains most of the physics information such as data on some existing materials. When adding custom materials for detectors it might be required to add a density correction file to /HEN_HOUSE/pegs4/density_corrections, information on how to do this can be found here: https://github.com/nrc-cnrc/EGSnrc/wiki/Generating-density-correction-files.

There are a few manuals containing documentation for EGSnrc every manual can be found here: https://nrc-cnrc.github.io/EGSnrc/. The Getting Started Manual is great for learning how to use EGSnrc. Section 4 of this manual walks you through running a program and changing a few parameters. It primarily uses tutor codes which are useful for getting started, but I was not able to adapt the tutor codes for my purposes so I used a different method explained in the next section.

The PIRS701 manual is the core manual and contains information on the physics and technical specifications of EGSnrc as well as some guidance on writing input files. The PIRS702 manual goes into more detail on the DOSRZnrc routines which allow for making a custom material that is cylindrical. I had PIRS701 and PIRS702 open at the same time whenever I was using EGSnrc because they have everything needed to help with writing the input files that I was using. The next section covers what part of EGSnrc I was using and how to manipulate the input files to get the desired information.

2.2 DOSRZnrc

Within /EGSnrc/egs_home there is a folder /dosrznrc in which I did my programming. There are many files in this folder and the extension of the file indicates it's purpose. Input files end in .egsinp, this is where modifications need to be made. The file called depth_dose_example.egsinp, is an example file that can be modified to suit the needs of the simulation. The file is heavily annotated and every section of the code is clearly described in the PIRS 701 and 702 manuals. Wherever clairification on any part of the code is needed, one can search the two manuals and an indepth explanantion will be found.

In order to run the dosrznrc executable once the input file has been written one must simply

type: "dosrznrc -i myfile.egsinp". One of the input files I wrote was GAGG25rz.egsinp, this has a GAGG crystal of radius 2.5cm and length 5cm and the source is a point source of monoenergetic gammas 24cm away from the crystal.

In order to check the geometry of your detector you can type "previewRZ myfile.egsinp" and the output will look like Figure 2, allowing you to ensure that the geometry is correctly input. In the example case GAGG25rz is a simple geometry so the image is not very interesting but this feature becomes useful when making more complicated geometries.
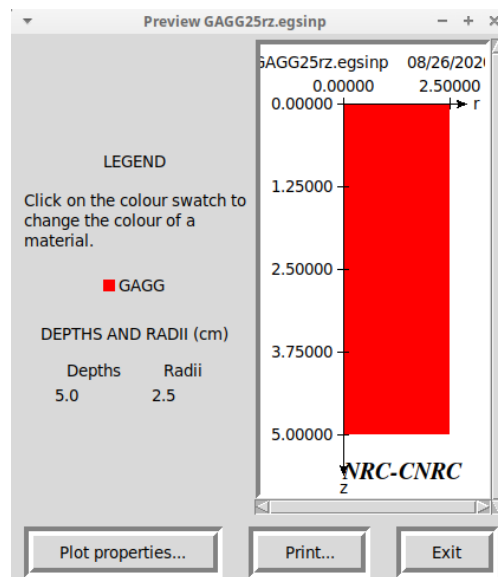

Figure 2: PreviewRZ output showing the detector geometry from EGSnrc. The x-axis shows the radius of the detector while the y-axis shows the length.

2.3 Reading Outputs

Once dosrznrc is run with this input file, a few files will be made all called GAGG25rz with various extentions. The file of interest is GAGG25rz.plotphd, this contains the information for a pulse height distribution. The data in plotphd is a comma separated file that can be read by a plotting program such as python. The results in this file are normalized to make a histogram with a total area equal to 1. The bin size can be adjusted in the .egsinp file. An example of the pulse height distribution results from this input file can be seen in Figure 3.

This method of finding the energy deposited in the crystal worked well when I had only one material, however once I introduced a second material this method did not work. I was only able to make a pulse height distribution for one material at a time. So I could have run the code twice and modified it to check the GAGG crystal in one case and the BGO crystal in the other case, but this did not allow me to follow each event and the relationship between each gamma's route through GAGG and then BGO.

In order to achieve the results in Figures 14 and 15 I used a less practical method that achieved

my goal. In the file 4mmGBGOwview.egsinp, I have a geometry with 4mm of GAGG followed by 5cm of BGO and there is a 3.5cm viewport. In the I/O control portion of the input file, I set IWATCH = deposited and OUTPUT OPTIONS = dose summary. This printed every small deposition of energy to the terminal as the simulation was running. This greatly increased the computation time as expected. I was able to print the terminal output to a file and then use a python script to read the important information from the output. The python code to do this can be found in /aafanassieva-jupyter/Spring2020/EGSnrc/Energy in BGO and GAGG and the file is called Energy in BGO and GAGG. The python code takes 5-10 minutes to run because the output files from EGSnrc in this setup are very large. There is likely a more efficient way of achieving the same results but this would involve hacking the source code which was more risky than creatively reading the output in python.
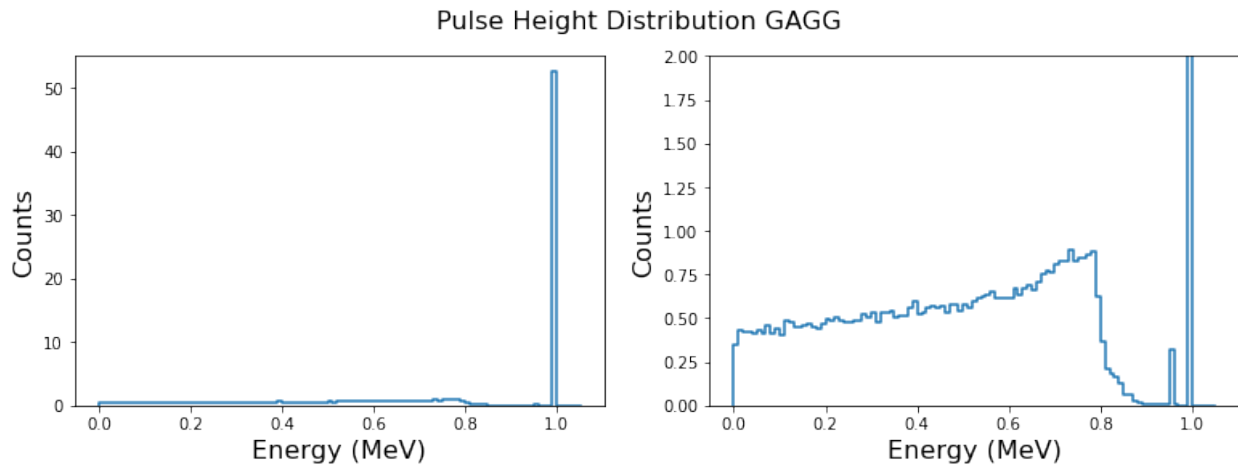

Figure 3: Pulse height distribution from EGSnrc for a cylinder of GAGG with a 2.5cm radius and a 5cm height. The source is a point source of 1MeV photons.

3   GEANT4

3.1   Quick Overview

To access GEANT4, I went to the folder /home/trinat/geant4 and I created a folder B3myscint (a duplicate of GEANT4's example B3). Within B3myscint there are three folders. The /src folder contains many .cc files. For every .cc file in /src there is a corresponding .hh file in /include. /B3_build is where the code is run and compiled.

The code in GEANT4 code is very well organised so that each component of the simulation is kept in a different file. For example: the geometery of the detector is contained in B3DetectorConstruction.cc and the particle source is contained in B3PrimaryGeneratorAction.cc. When manipulating the simulation to do what I needed I sometimes found that it was difficult to find information on the internet pertaining to my specific needs. While there is documentation for GEANT4, it is sometimes cumbersome and there are so many people using the simulation package that there is too much information and it is hard to narrow it down to what I was actually looking for. I found that looking at the examples given in GEANT4 was the best method of learning what to add to my simulation.

In order to compile the code, go to file /geant4/B3myscint/B3_build/. In this folder there is a file called READMECOMPILE that explains how to compile the code. There are a few steps that are written out and once they are followed, type make B3example to make the executable. If there are any errors that the compiler finds it will display them at this stage and indicate which .cc or .hh file needs to be fixed. To run the executable with a gui type: ./exampleB3. To run the executable with a macro without any visualization type: ./exampleB3 testrun.mac . My macro testrun.mac contains a few simple lines that tell the code how many events to simulate. When initially testing the simulation it helps to use the gui to visualize what is happening. To run the beam in the gui type /run/beamOn 100 in the command line of the gui to run 100 events. An example of what the visualization will look like is shown in Figure 4. To run a larger number of events it is necessary to use the macro, otherwise the visualisation will crash or never finishing running.
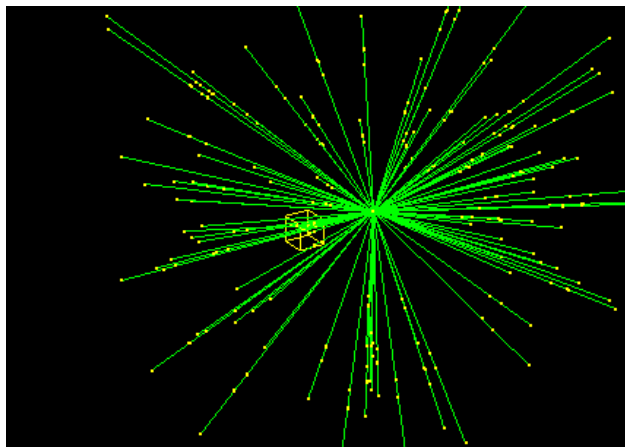

Figure 4: Example of GEANT4 run with a 5x5x5cm GAGG cube 10cm away from a point source of gammas.

3.2 My Modifications

I based my simulation on example B3 given in GEANT4 because I thought it most closely resembled the simulation I needed to look at. Whenever I made any changes I looked at other GEANT4 examples. For example, when I wanted to measure the energy deposited in the crystal, I took the scoring components of example B1 and adapted them to my simulation.

The biggest changes I made were to the source and the detector geometry. Example B3 has an array of rectangular crystals arranged to make a cylinder as a PET scanner. I changed these crystals to vacuum since I did not need them in my simulation but deleting them entirely gave me many errors. I changed the geometry of the "patient" in example B3 to be a scintillator of GAGG or BGO depending on which crystal I was testing. I also changed the source from a fluorine decay to a point source of gamma rays.

Another big change that I had to do was writing the energy deposited in the crystal for every event. This was difficult to do since I could not find an example given by GEANT4 that did this. I did find a power point that went through the steps required to output the desired results to a csv and linked it here. [3] This process required me to make an additional .cc file called B3SteppingAction.cc as well as a corresponding header file. This created a routine which wrote to a file every time an event was recorded in the simulation. In RunAction.cc I also needed to write code to create, open and close the csv file to which information would be written. I was then able to use this file to plot the resulting pulse height distributions that I was interested in. I was not, however, able to make this work for two crystals, so the results for two crystal simulations in this report are all from EGSnrc.

4 Python and Jupyter Notebooks

All of my data processing was done in Jupter Notebooks over the course of the term. To access the Jupyter Notebooks, go to jupyter.triumf.ca and sign in with the trinat trcomp account. Then go to /aafanassieva-jupyter/ and all my files are there. To open a notebook or file simply click on the name. To run a notebook you can click "Run" near the top of the page and this will run every cell in order, from the top of the page to the bottom. Alternatively, you can run individual cells by selecting the cell and pressing "Shift+Enter". Note that when running cell by cell, the cells preceding the selected cell will not be run automatically. If a variable in one cell depends on something that was written in a previous cell, all the cells should be run in order.

There is an introductory python course that can be found on trcomp, in /group/scicompy/Lecture Notes. There, you will find pdf worksheets as well as powerpoints and extremely detailed python notebooks. This folder is useful for getting started learning python.

5 Simulation Comparisons to Data

5.1 Cs 137

To test the accuracy of the simulations, we made comparisons to test data that was made with a 1x1x1cm GAGG a few years ago. The first source I compared the simulated results to was ^{137}Cs because the decay is simply monoenergetic 662keV gammas. In the simulations that were compared to real data, I placed the particle source 10cm away from the crystal. The pulse height distributions from EGSnrc and GEANT4 are shown in Figure 5. Both plots show the same results except that on the right, the plot is magnified to highlight the lower energy results.

A key difference between the GEANT4 and EGSnrc data is the peak at 0.6MeV is much bigger in EGSnrc than in GEANT4. The reason is likely that the EGSnrc code is treating the escaping k-shell x-rays differently than GEANT4. The k-shell x-ray in Gd (the heaviest component of GAGG) is 50.2 keV. This agrees with the plot, as there is a small peak at 0.61 MeV, 0.05 keV below the photo-peak at 0.662MeV. When the photo-peak fraction (the ratio between the photo-peak and the total interactions), that of EGSnrc was lower than that of GEANT4.
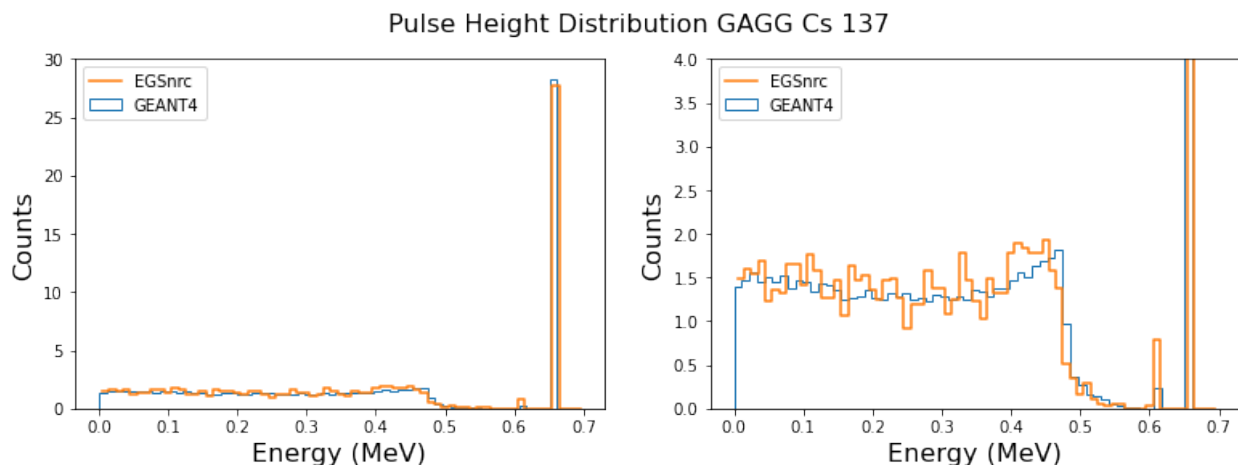

Figure 5: Pulse height distributions for a 1x1x1 cm cube of GAGG from GEANT4 and EGSnrc. Source is a Cs 137 point source emitting 662keV gamma rays.

To compare to the data I needed to add a Gaussian convolution to the data. This can be seen in Figure 6. The cutoff point for the data was at 0.2MeV which explains why the data goes to 0 there where the simulations did not. It is also important to note that the data has some noise at lower energies which could account for the rise in counts around 0.3MeV. It looks like the EGSnrc simulation more closely follows the data than GEANT4. Both simulations have a very similar shape although the Compton edge in EGSnrc has more counts than in GEANT4. This can be attributed to the fact that EGSnrc has a lower photo-peak fraction than does GEANT4.
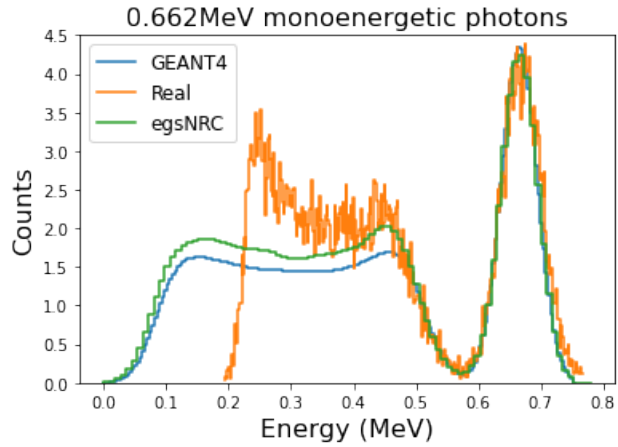
Figure 6: The same pulse height distributions from Figure 5 but with a single width Gaussian convolution. This is being compared to data taken of a 1x1x1 cube of GAGG shown in the orange line.

5.2 Ba 133

Another source I tried to compare the simulations to was Ba^{133}. This proved to be difficult to fit well because there are multiple decays and photo-peaks in the spectrum. Figure 7 shows the results given by GEANT4 for a Ba^{133} decay convoluted with a single width Gaussian. There should be multiple widths in this convolution and I was not able to make this work in my python code. In EGSnrc it was not trivial to make a radioactive source so I did not run EGSnrc for a Barium source.
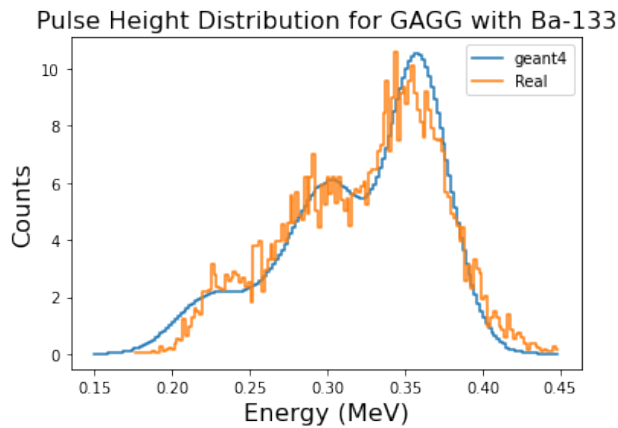

Figure 7: Pulse height distribution for a 1x1x1 cm crystal of GAGG with results taken from GEANT4 convoluted with a single-width Gaussian. Ba 133 source 10cm from the crystal.

5.3 Na 22

The ^{22}Na decay is shown in Figure 8. The EGSnrc results look very different from the GEANT4 and real data because I was unable to make a radioactive source in EGSnrc. Instead, I put monoenergetic 1274 keV gamma rays from a point source. I tried to convolute the GEANT4 data with two Gaussian functions of two different widths. The flat blue line around 1.1 MeV is where the two Gaussians overlap. To make a quantitative comparison between the data and the simulations, I made a calculation of the ratio between the compton edge and the photo peak. To do this, I summed the counts between 1.1 and 1.4 MeV in all three cases, and divided this sum by the sum of counts between 0.6 and 1.1MeV. The results of this calculation are shown in the Table 1 below.

Table 1: Photopeak/ Compton Edge Ratio in ^{22}Na

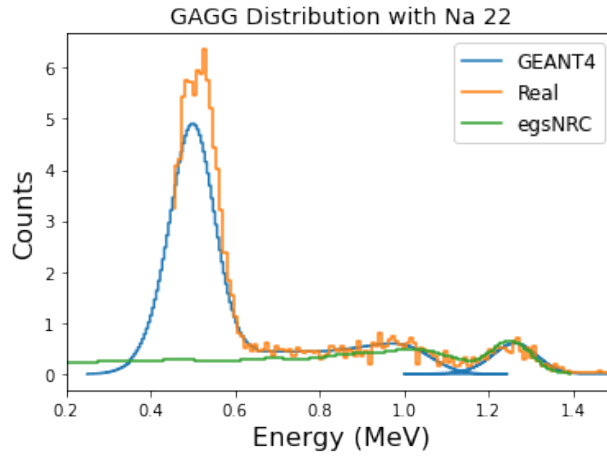| Results	Photopeak/Compton Ratio
Real Data	$0.315 \pm .050$
GEANT4	0.298
EGSnrc	0.293

Figure 8: Pulse height distribution for a 1x1x1cm cube of GAGG with a Na 22 source 10cm from the crystal.

5.4 Physics Lists in GEANT4

A parameter that I tried adjusting in GEANT4 was the physics lists. The physics lists are what determine the way that the physics interactions occur in the simulations. In Ben Fenker's thesis he states that he used the physics packages: emstandard_opt3, em_livermore and em_penelope for his simulations. To see how these packages would affect the simulation I ran them separately and the results can be seen in Figure 9. In this simulation I ran a GAGG crystal with a radius of 2.5cm and a length of 5cm with a 1MeV point source of gammas. As can be seen in the figure, there are statistical fluctuations in the data but the resulting photo-peak fractions are similar. The photo-peak fractions for the different physics lists are shown in Table 2.

In an attempt to see if EGSnrc's lower photo-peak fraction could be accounted for by the larger peak at 0.995 MeV due to kshell x-ray escapes, I added the smaller peak to the photo-peak and divided it by the total number of interactions. This did not increase the photo-peak fraction significantly, when I added this smaller peak to the calculation, the photo-peak fraction was equal to .529 .
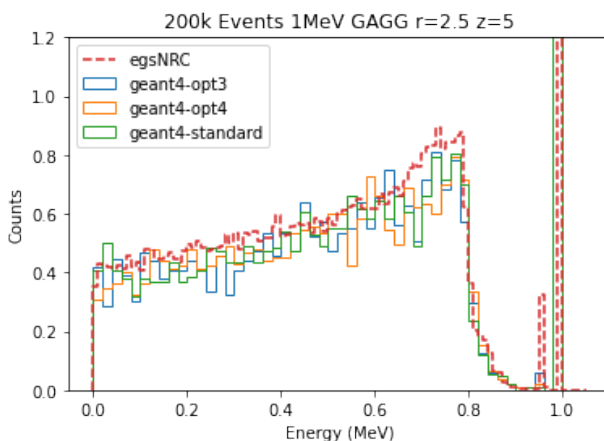

Figure 9: Plot comparing a few physics lists in GEANT4 using a crystal of GAGG with radius 2.5cm and length 5cm, 25cm away from a 1MeV point source.

Table 2: Photo-peak fractions calculated from results in Figure 9

	Photo-peak Fraction
standard	$0.576 \pm 1\%$
opt3	$0.579 \pm 1\%$
opt4	$0.579 \pm 1\%$
EGSnrc	0.527

6 BGO and GAGG Comparisons

The two crystals I simulated were BGO and GAGG. The geometry of the simulation consisted of a crystal that had a radius of 2.5 cm and a length of 5cm located 25cm away from a point source of monoenergetic gamma rays. The reason for this distance is because it is the distance away from the radioactive source in the experiment.

The pulse height distributions for BGO and GAGG with 1MeV gammas can be seen in Figures 10 and 11. The photo-peak fraction for BGO at 1MeV is 0.72 and for GAGG it is 0.53. The photo-peak fraction was calculated by dividing the counts in the peak (in this case at 1MeV) by the total interactions in the crystal.
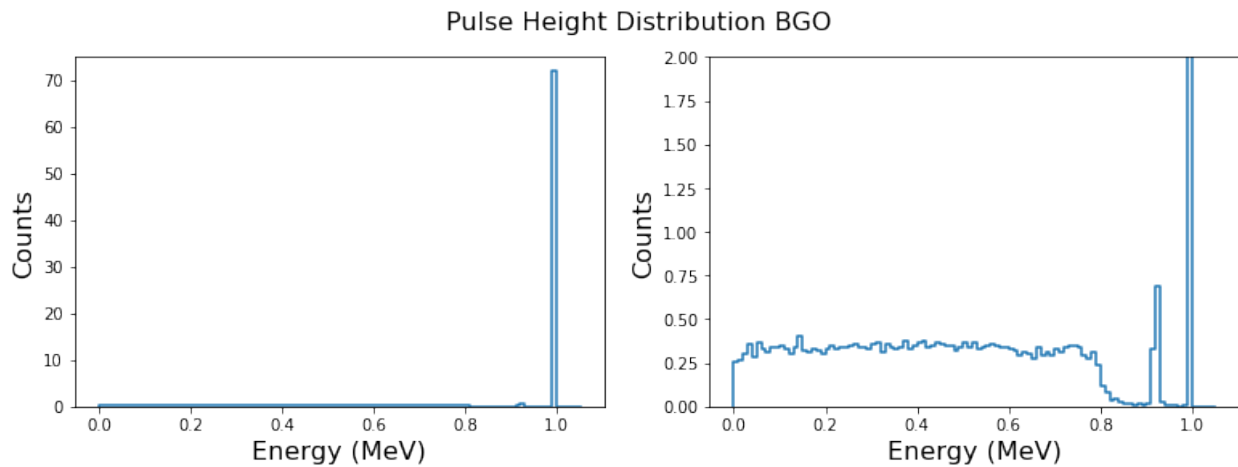

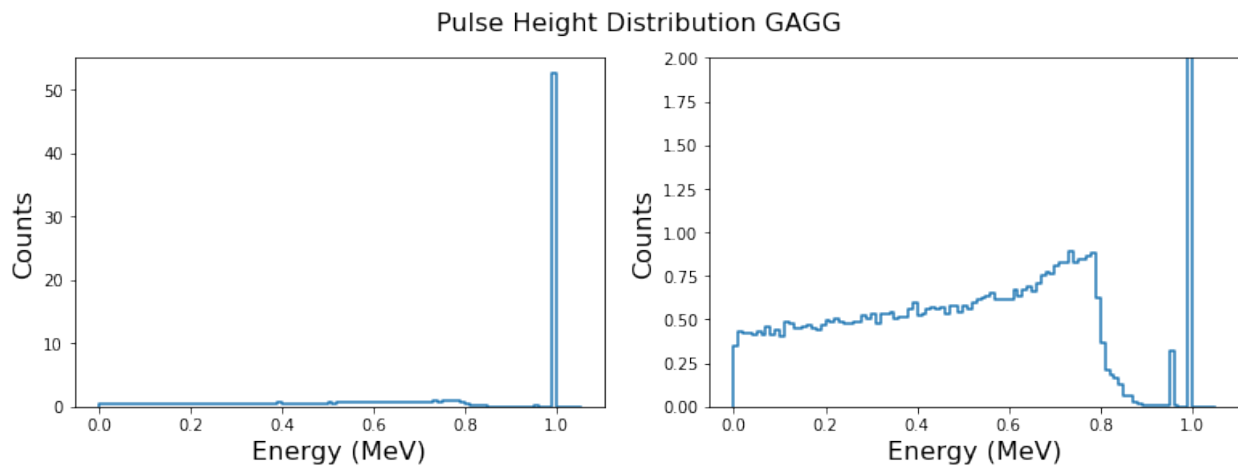Figure 10: Pulse height distribution for a BGO crystal with r=2.5cm and z=5cm. A point source of 1MeV gamma rays. Results from EGSnrc.

Figure 11: Pulse height distribution for a GAGG crystal with r=2.5cm and z=5cm. A point source of 1MeV gamma rays. Results from EGSnrc.

Figure 12 shows the photo-peak fraction at multiple energies for GAGG and BGO with both crystals having the same geometry.
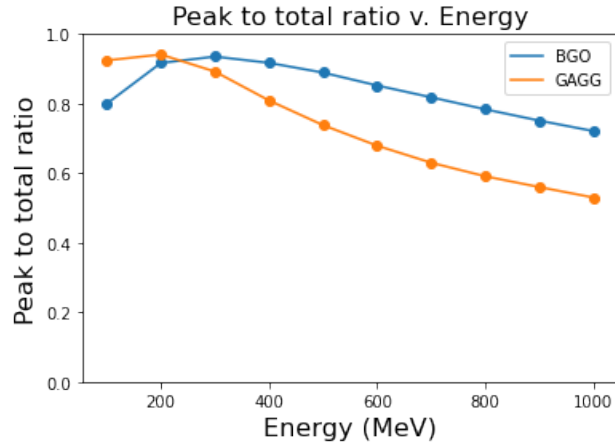

Figure 12: Photo-peak fraction with respect to energy for GAGG and BGO crystals both with radius 2.5cm and length 5cm. The source is monoenergetic point gamma source 25cm away from the crystal.

7 BGO and GAGG Sandwich

7.1 Motivation

The decays the experiment will be measuring will have an abundance of positrons. This means that there will be a significant amount of annihilations resulting in 511keV gamma rays. This means that with a single crystal, it will be difficult to distinguish any gamma rays below 511 keV since there will be such a high number of counts attributed to the annihilation gammas. To try to account for this, we want to place a thin layer of GAGG in front of a larger BGO crystal. The GAGG will ideally detect most of the lower energy photons while the BGO will collect any higher energy photons.

Figure 13 shows the photo-peak fractions at multiple energies for a 4mm thick GAGG crystal compared to a 5cm thick BGO crystal, both with a radius equal to 2.5cm . In this geometery, when the photo-peak of the BGO is measured, there is a 4mm GAGG crystal directly in front of it. The photo-peak fraction in GAGG notably declines from 100keV to 1MeV where the curve begins to flatten. We can take advantage of the high photo-peak fraction at low energies.
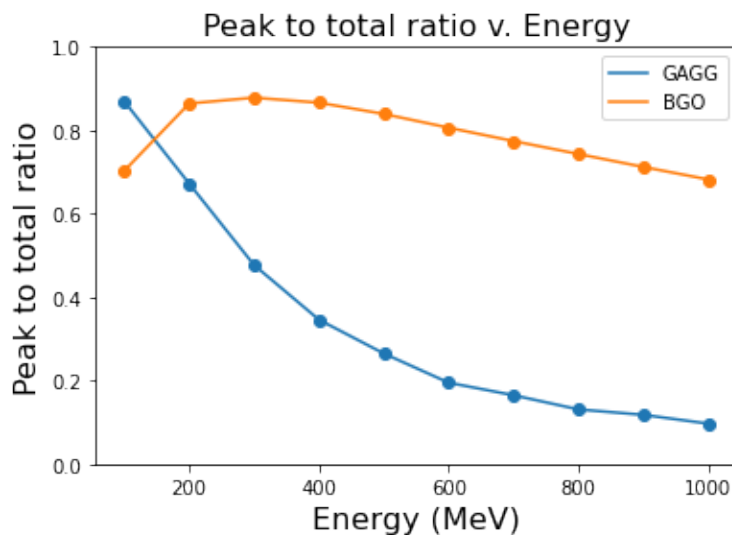

Figure 13: Peak to total ratios at multiple energies for 4mm GAGG and 5cm BGO. There is no fit function the points are connected by a line to be seen more easily.

7.2 Results at Multiple Energies

Figures 14 and 15 show the energy deposited in GAGG and BGO at 100keV and 500keV respectively. In the scatter plot, each point represents one event, and its position on the plot shows how much energy was deposited in the GAGG and in the BGO crystals. The points are transparent so that the more points there are on a spot the darker it becomes. At 100keV we can see that almost all of the gamma rays fully interact in the thin GAGG crystal. In the 500keV crystal the opposite

is true. This achieves our goal of detecting low energy gamma rays in the GAGG without being overwhelmed by the abundant 511keV gamma rays.
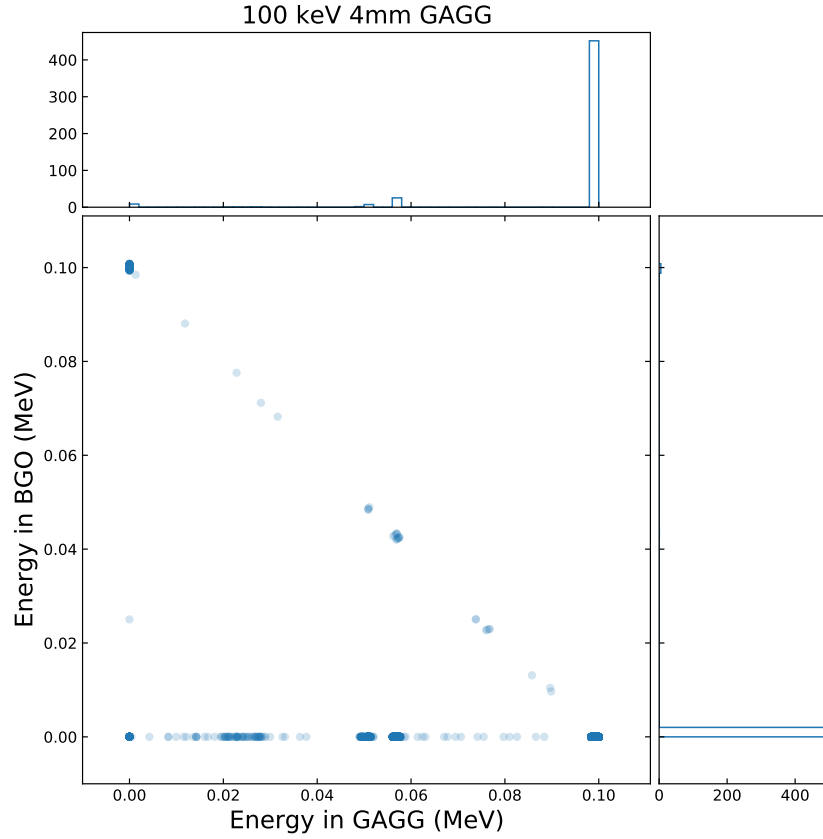

Figure 14: Scatter plot showing the energy deposited in GAGG (x-axis) and BGO (y-axis) from a point source of 100 keV monoenergetic gamma rays. Each point represents one particle and the histogram projections have been normalized to have a total area of 1.
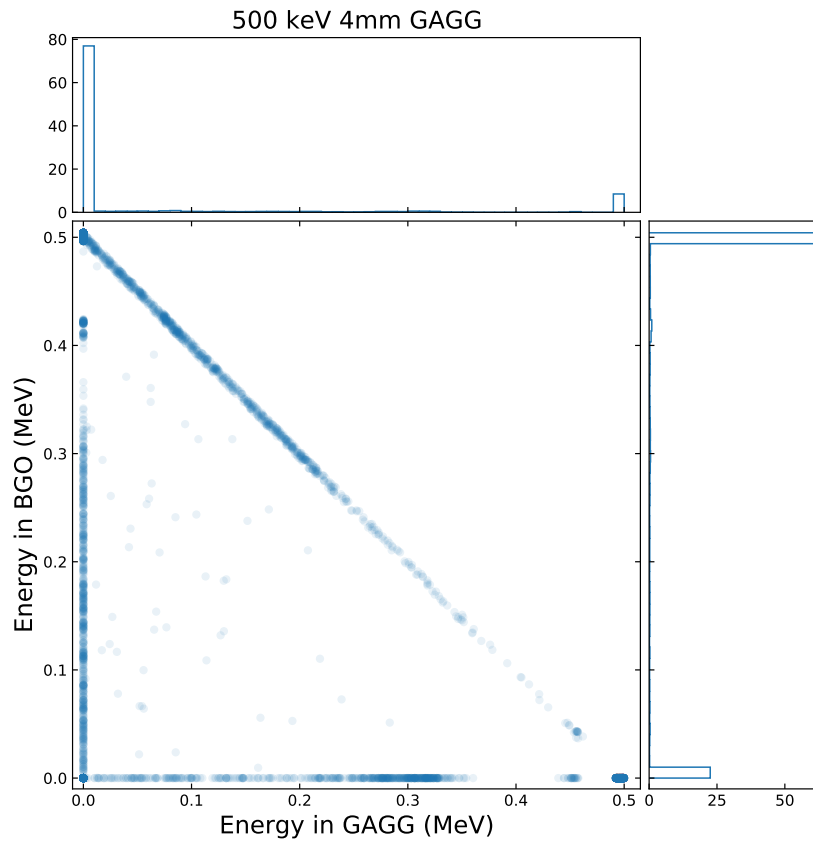
Figure 15: Scatter plot showing the energy deposited in GAGG (x-axis) and BGO (y-axis) from a point source of 500 keV monoenergetic gamma rays. Each point represents one particle and the histogram projections have been normalized to have a total area of 1.

8 Semrock Filters

In order to distinguish between the scintillation of GAGG and that of BGO, we explored the idea of using filters that would separate the GAGG scintillation light from the BGO. Semrock has a wide range of filters that can select which wavelengths to transmit while the rest are reflected. One of the difficulties with these filters is that they have a large angle dependence. As can be seen in Figure 16, changing the angle of incidence changes the wavelengths transmitted by the filter. The geometry of our system will result in photons being incident on the Silicon PM at all angles not just 45 degrees. This would not be a problem if the scintillation spectra of GAGG and BGO were significantly separated. As can be seen in Figures 17 and 18, the scintillation spectra overlap enough that even a perfect filter at 500nm would not be able to distinguish between both crystals. A configuration that could work would be Cerium Bromide and GAGG but Cerium Bromide is hygroscopic and would not be compatible in our system. Instead of using filters, the difference in the decay time of the two scintillations can be used to distinguish between both crystals.
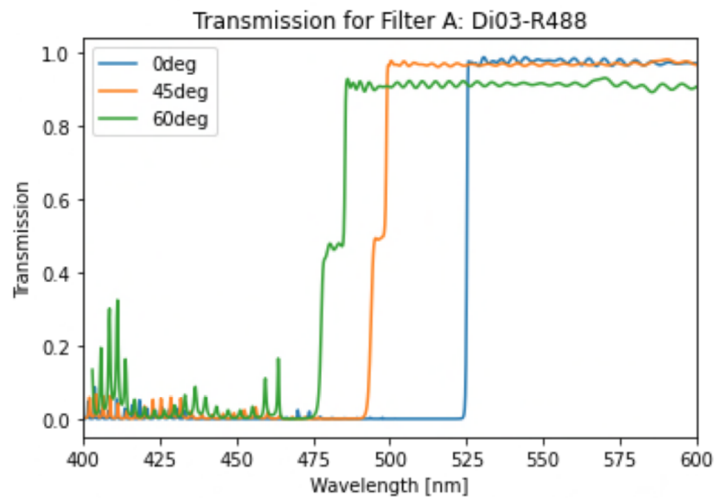

Figure 16: Filter Di03-R488 from Semrock Inc designed for transmitting wavelengths above 488nm with an angle of incidence of 45.
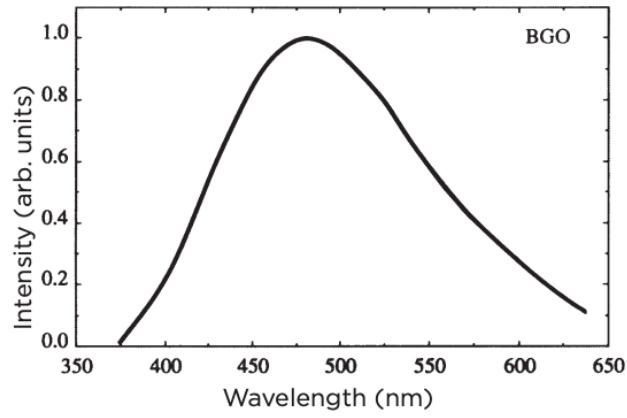
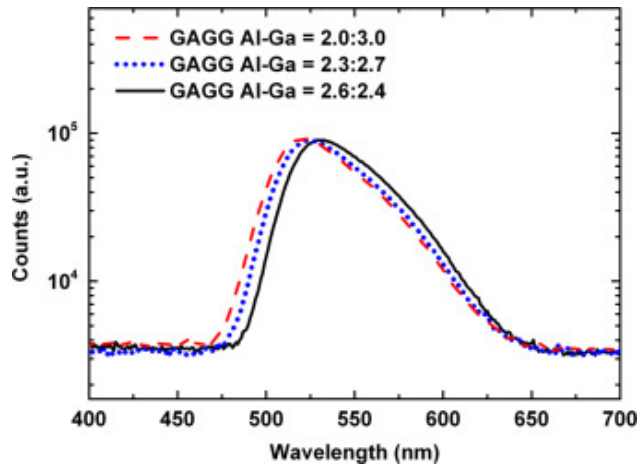Figure 17: BGO Scintillation spectrum taken from Saint-Gobain Crystals [2]

Figure 18: GAGG Scintillation spectrum[4]

9 Conclusions and Next Steps

Based on the comparisons of the simulations to the data, the simulations are a close approximation to what should be expected from a real experiment using the chosen scintillating crystals. On a larger GAGG crystal (r=2.5cm and z=5cm) with 1MeV gammas, there is a disagreement in the photo-peak to Compton ratio between GEANT4 and EGSnrc of roughly 10% with EGSnrc being a closer approximation to the data. This disagreement is not seen in the smaller GAGG crystal when looking at the sodium peak to Compton ratio. The different GEANT4 physics lists packages give results for pulse height distributions that agree within their uncertainty.

The method of using a thin layer of GAGG in front of a thicker BGO crystal is worth testing in the lab. Using wavelength filters to distinguish between GAGG and BGO scintillation is not a reliable method because of the overlapping scintillation spectra and the large angle dependance of the Semrock filters. More work would need to be done in order to determine how to differentiate between the scintillation in GAGG and in BGO.

References

[1] Time-reversal test in radiative beta: progress. *APS Bulletin Abstract E01.00158 DAMOP 2020*. J.A. Behr, A. Gorelov, J. McNeil, D. Melconian, M. Anholm, G. Gwinner, T. Valencic, A. Afanassieva.

[2] Saint-Gobain Crystals. BGO bismuth germanate material data sheet, Aug 2016. `https://www.crystals.saint-gobain.com/sites/imdf.crystals.com/files/documents/bgo-material-data-sheet.pdf`.

[3] Mihaly Novak. *GEANT4 Analysis*, 2019. `https://indico.cern.ch/event/776050/contributions/3241822/attachments/1789267/2921102/Analysis-v3.pdf`.

[4] Pawel Sibczynski, Joanna Iwanowska-Hanke, Marek Moszyński, Lukasz Swiderski, Marek Szawłowski, Martyna Grodzicka, Tomasz Szcześniak, Kei Kamada, and Akira Yoshikawa. Characterization of GAGG: Ce scintillators with various al-to-ga ratio. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 772:112–117, 2015.