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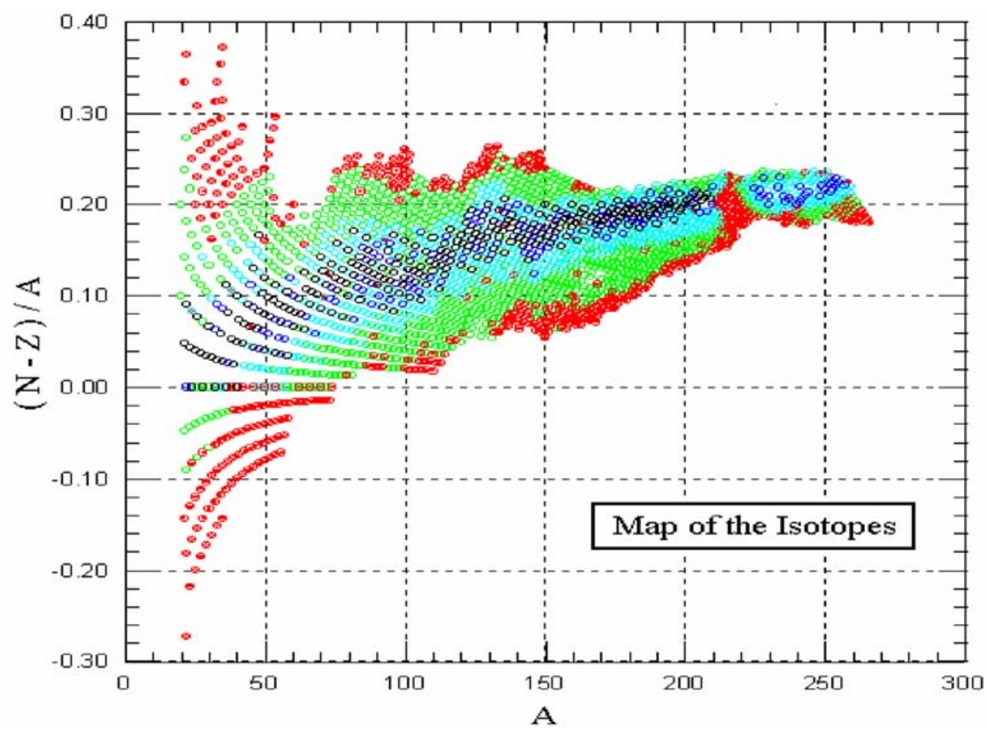

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by
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Total Absorption Gamma-ray Spectrometer (TAGS) Simulations with GEANT4

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Abstract

This project aims to study the structure of neutron-rich fission products of importance to Advanced Fuel Cycle applications. The measurement of β-decay feeding intensities is made possible through the use of the Total Absorption Gamma-ray Spectrometer (TAGS) method, utilising a large NaI scintillator detector. The method relies heavily on the modelling of the detector response using a Monte Carlo model. This report looks at the progress of developing such a model (using Geant4) and the other considerations required to implement the TAGS method.

I. INTRODUCTION

The TAGS method is used to measure the β-decay branching ratios of neutron-rich fission fragments and is largely dependent upon Monte-Carlo simulations for the interpretation of experimental data.

This document outlines the development of a Monte-Carlo (MC) model to simulate the response of a Total Absorption Gamma-ray Spectrometer (TAGS) using Geant4. In this project, fission fragments will be supplied by the CAlifornium Rare Isotope Breeder Upgrade (CARIBU), currently being developed at the Argonne Tandem Linac Accelerator System (ATLAS) [Car]. The measurement of the neutron-rich fission products will provide data for decay heat calculations used in the Advanced Fuel Cycle (AFC) project, information on nuclei approaching the r-process for the astrophysics community and new nuclear structure information for the basic nuclear physics community.

A. The Total Absorption Gamma Spectroscopy (TAGS) Method

Far from stability, where the Q value for β-decay is large, the daughter nuclei which follow β-decay can be populated in regions of high level density and at high excitation energy. This leads to a fragmented decay, with many weak β-decay branches and multiple gamma-ray decay pathways from each of the high-lying daughter levels to the daughter ground state. The identification of these many branches is almost impossible with conventional γ-spectroscopy, as demonstrated by Hardy [Har77].

During the 1990s, a research group at the Idaho National Engineering Laboratory (INEL) developed a Total Absorption Gamma-ray Spectrometer (TAGS) (FIG 1) and applied it to the measurement of 45 fission products [Gre92a, Gre92b, Gre95, Gre97]. Their method involved a large well-type sodium iodide (NaI(Tl)) detector that measured simultaneously all of the γ-ray decays emitted into the detector-volume following a β-decay. This was made possible by placing the source at the bottom of the well in the detector, so as to give close to 4π angular coverage. In this scenario it doesn't matter how fragmented the decay pathway might be, summing all the γ-rays gives you the same signal independent of the different paths that are followed in the decay to the ground state. This provides a gamma signature of the β-feeding to each level, enabling identification of the beta decay branching ratios.

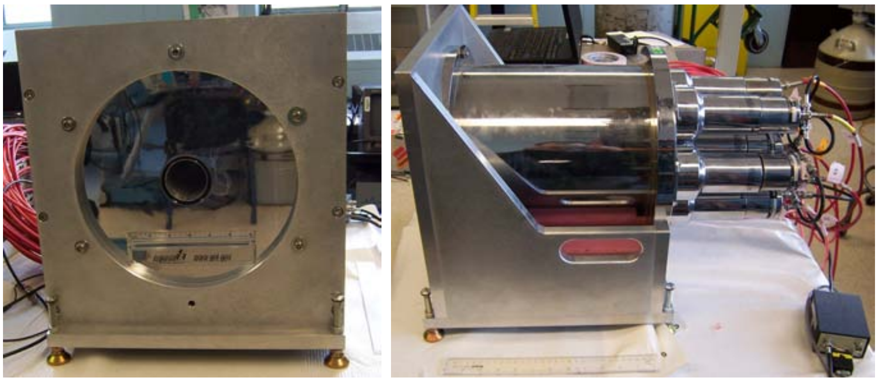


FIG. 1: Front and side views of the Total Absorption Gamma-ray Spectrometer (TAGS) detector, a large well-type NaI(Tl) crystal

NaI(Tl) has a high efficiency and fast detector response, but suffers from a poor energy resolution. These intrinsic detector properties, combined with the large number of β-feeding levels, produces a complex detector response. As such, the TAGS method relies heavily on Monte-Carlo simulation for the unfolding of the individual β-feeding level signatures from the observed spectrum.

More recent work employing the TAGS method was done by the Instituto de Fisca Corpuscular, CSIC-university, Valencia [Can99a, Rub07].

B. CAlifornium Rare Isotope Breeder Upgrade (CARIBU)

A major focus of the international nuclear physics community over the last decade has been the development of radioactive beam capabilities for the study of neutron-rich nuclei. While very large scale (billion dollar) facilities such as FRIB in the USA [FRww] and FAIR in Europe [Fww] are in the advanced planning stages, smaller scale facilities are either in production or being built. The CAlifornium Rare Isotope Breeder Upgrade (CARIBU) at ATLAS at ANL is a unique example that is currently in the implementation and testing phase. The fission fragments from a 1 Ci spontaneous fission source of ^{252}Cf will be mass separated so as to provide almost isotopically pure radioactive ion beams. These can be post accelerated to use for the initiation of secondary reactions, or the radioactive products can be studied directly.

C. Decay Heat

The decay heat produced in nuclear fuel is due to the radioactive decay of products resulting from fission. The time behaviour of this quantity is critical to the design and operation of nuclear reactors and affects fuel removal and reloading processes, safety after accidents (such as a loss of coolant incident), as well as the storage, transport and reprocessing requirements for spent fuel.

Calculation of the time evolution of the decay heat requires knowledge of the fission yields, beta-decay lifetimes, as well as the beta and gamma-ray decay schemes for all of the fission products and their subsequent daughter decays back to the line of stability. The difficulty in getting access to many of these neutron-rich fission fragments, together with the complications of measurement with conventional γ-spectroscopy methods, has hindered experimental measurements. As a result, much of the information currently used to determine the decay heat comes from theory and this has been shown to be inaccurate. The result is less efficient designs to compensate for the large uncertainties in this information.

The International Atomic Energy Agency has noted that there are a number of nuclei for which a lack of experimental information on the β-decay branching ratios has important implications for the design of Gen IV reactors [Dwww] and has requested that priority be given to studies of these nuclei.

D. Nuclear structure and r-process

The astrophysical r-process is a rapid sequence of successive neutron captures, interspersed by beta-decays, that occurs in explosive stellar events such as supernovae, and is responsible for the formation of many heavy nuclei above iron. The path of the r-process lies through neutron-rich nuclei that are not very well studied and CARIBU promises to be a unique source for a range of nuclei that will not be available elsewhere. While measurements of masses and lifetimes are critical for our general understanding of the r-process, the measurements of beta-decay branching ratios and well-understood level schemes, for which TAGS will play an essential role, will be very important for making detailed predictions of the r-process.

II. INTRODUCTION TO GEANT4

Monte-Carlo (MC) simulations are commonly used in many areas of physics research. Developed around 1930, they were first used to model the transport of nuclear particles and radiation through matter [Met49]. A MC model is essentially a random number generator providing bounded variable inputs to a physics based model. For example, modelling the path of a γ-ray in a detector would use a random number as input to the calculation of the mean free path in the first step. Individually, these steps do not provide much information nor does the single whole scattering path, but looking at the statistical distribution of many paths can provide a good basis for comparison with experiment.

GEometry ANd Tracking 4 (GEANT4) is a MC transportation code that was developed in the late 1990's as a CERN collaboration [Agn03]. Based on object oriented C++, GEANT4 is a re-write of the fortran based GEANT3 and was developed initially by the high energy physics community. GEANT4 allows for a generic framework within which a number of models covering a range of energies, can be applied to many areas including high energy and medical physics.

GEANT4 was chosen for the modelling of the TAGS detector due to the flexibility of the code and the suitability of the physics classes that it employs [Gww]. Many other projects involving the modelling of γ-ray intensities in detectors have used Geant including AGATA [Aww], GRETA [GRww] and other TAGS type detectors [Can99a].

III. PHYSICS ASPECTS

A. Scintillator non-proportionality

Scintillator non-proportionality is the name associated with a non-linear energy response typical of scintillators. This non-proportionality is best observed with measurements of nuclides that include a number of gamma transitions in a cascade, creating a sum peak. The gamma transitions in such a decay generally have a half life of the order of pico-seconds (or less) and as such are detected simultaneously relative to a typical detector's response time. One might first expect to have a pulse height equal to the sum of the component single pulse heights. If an energy calibration were performed, based on the centroid positions of single gamma peaks only, the summation peak is often found at a centroid position higher than expected. The shift in position of the sum peak to higher energy is attributed to the non-proportionality of the scintillator.

The first observation of a non-linear response in NaI(Tl) detectors can be traced back to the 1950s [Pri50]. In 1956, Engelikemeir investigated a number of different NaI(Tl) detectors of various geometries produced by the same manufacturer [Eng56]. Deviations of up to 20% from linearity were found for the low energy regions. The non-observation of this effect prior to this time, was attributed to insufficient sensitivity.

Observation of the non-proportionality was made more apparent by a method introduced by Peelle et al in 1960 [Pee60]. The method observed the shift in position of the sum peaks produced by sources decaying via cascading gamma transitions. Using a 3" x 3" NaI(Tl) detector, deviations of 27 keV (^{88}Y sum peak from 898 keV and 1836 keV transitions) and 44 keV (^{207}Bi sum peak from 569.6 keV and 1063.7 keV transitions) were observed from the expected sum peak positions, relative to a calibration of energy using only single-gamma energy peaks.

The method of measuring the shifts in sum gamma transitions was extended upon by Kantele [Kan61]. A 4π geometry was created by placing two 3" x 3" NaI(Tl) detectors together, face to face and passively adding the output into a single acquisition system. The larger solid angle increased the probability of detecting a sum event and thereby increased the statistics of non-proportionality measurements. A consistent non-proportionality deviation was observed when one of the detectors was removed, suggesting that non-proportionality is geometry independent.

In 1961, Zerby et al created a Monte Carlo model of a 2.5" x 2" NaI(Tl) scintillator by looking at the specific interaction processes in the crystal and not simply the energy deposition [Zer61]. They modelled the non-proportionality in the gamma response $L(E_\gamma)/E_\gamma$, where $L(E_\gamma)$ is the light response from the scintillator due to a gamma event of energy E_γ. They concluded that the non-proportionality effects are not exclusive of the gamma processes but are also caused by electron processes. Using this model and a measured gamma response, they deduced the non-proportional response for different energy electrons.

A direct measurement of the electron response is difficult due to the attenuation of beta particles by the glass envelope encasing the hygroscopic NaI(Tl) as well as the light-tight aluminium can. An indirect method is made possible by use of the Compton Coincidence Technique (CCT).

The CCT method uses a collimated beam of mono-energetic gammas that illuminate the scintillator. Mono-energetic gamma-rays can undergo Compton scattering in the scintillator, producing a Compton electron and a scattered gamma-ray. In the event that the scattered gamma-ray exits the scintillator without any further interactions, the Compton scattered electron is the only event that deposits energy in the scintillator. By use of an external collimated detector, (usually HPGe), the scattered gamma-ray can be detected and used as a trigger for the Compton electron event in the scintillator.

Although there has been much research into this phenomenon [Mos08], the origins of non-proportionality are still largely unknown. There has been a renewed interest into the cause of non-proportionality in recent years, with the prospect of improving the overall energy resolution of scintillator detectors.

B. Pile-up

Pile-up effects are an inherit problem of the finite processing times of electronic acquisition systems and ultimately, the rate of the events in a detector [Ten84]. To retrieve information from the collected charge, preamplifiers integrate this charge, then are reset (more commonly by means of resistive feedback). The result is a sharp rising function followed by a long tail, known as a tail pulse. Amplifiers then integrate and differentiate this signal to produce a Gaussian like function whose pulse height is proportional to the collected charge of the tail pulse.

If events are occurring at great frequency in the detector, there is an increased probability of another pulse arriving whilst the first event is being processed. If the event arrival is close enough in time, the peaks will ride on top of each other. This is seen by the acquisition system as one pulse that has an amplitude that is the sum of the two individual pulse component heights. If the two events occur such that the second event arrives on the tail of the first (before this can be fully reset), then the result is a slightly reduced or increased second pulse.

The motivation for understanding and accounting for the effects introduced by pile-up, is to accurately model all aspects of the detector in order to understand the complex number of processes and interactions that will be measured by TAGS. Pile-up effects are a significant component of the detector response, producing tails on peaks or shifting peak positions in the spectrum. This is particularly important when dealing with large count rate, as will be the case with the large volume, high-efficiency TAGS. Monte Carlo simulations typically work on an event by event basis, and produce only discrete data for each separate event. In the present case, G4 does not directly model pile-up so that the effects must be taken into account outside of G4.

IV. EXPERIMENTAL ASPECTS

The main detector that we are concerned with in this project is the Total Absorption Gamma-ray Spectrometer (TAGS) detector (FIG 1). This is a 20 cm (diameter) by 20 cm (length) well-type thallium doped NaI detector, that covers approximately 99% of 4π solid angle for a source located in the bottom of the well [Gre92a].

The TAGS detector was acquired from INEL in 2007, after the retirement of key personnel. The past performance of the detector can be seen from publications of the former owners [Gre92a]. However, since receiving the detector, it has not operated in a predictable fashion and seems to have a degraded energy resolution compared to these earlier published results.

A. Count Rate and Non-proportionality

The high solid angle coverage required for the TAGS method can be a disadvantage since even a weak source can result in a large detector count rate causing pile-up effects. The contribution of background is also significant, with many cosmic pulses saturating the preamplifier. Shielding the detector is important when the detector is placed at an experimental station for use.

The effect of count rate on the TAGS detector can be seen by measuring the central PMT response to a ^{60}Co source as a function of source position along the central axis (FIG 2). The 1173 keV and 1332 keV lines form a single un-resolved peak. For the higher count rates, there is a notable broadening and shift of the first peak position. The response of the central tube is believed to resemble a ^{60}Co spectrum with poor resolution due to incomplete light collection. The peak located at channel 300 is the summing peak, this is identified by its decrease in magnitude as the source is removed from the well.

In addition to measurements undertaken with TAGS, several other NaI(Tl) detectors were used to measure properties of basic crystals before moving to the more complex TAGS geometry. These detectors included a 3" x 3" cylindrical detector located at Argonne (ANL3x3), a 5" x 5" cylindrical detector from the Australian National University (ANU5x5) and a 6" x 5" well type cylindrical detector from the Australian Nuclear Science and Technology Organisation (ANSTOwell).

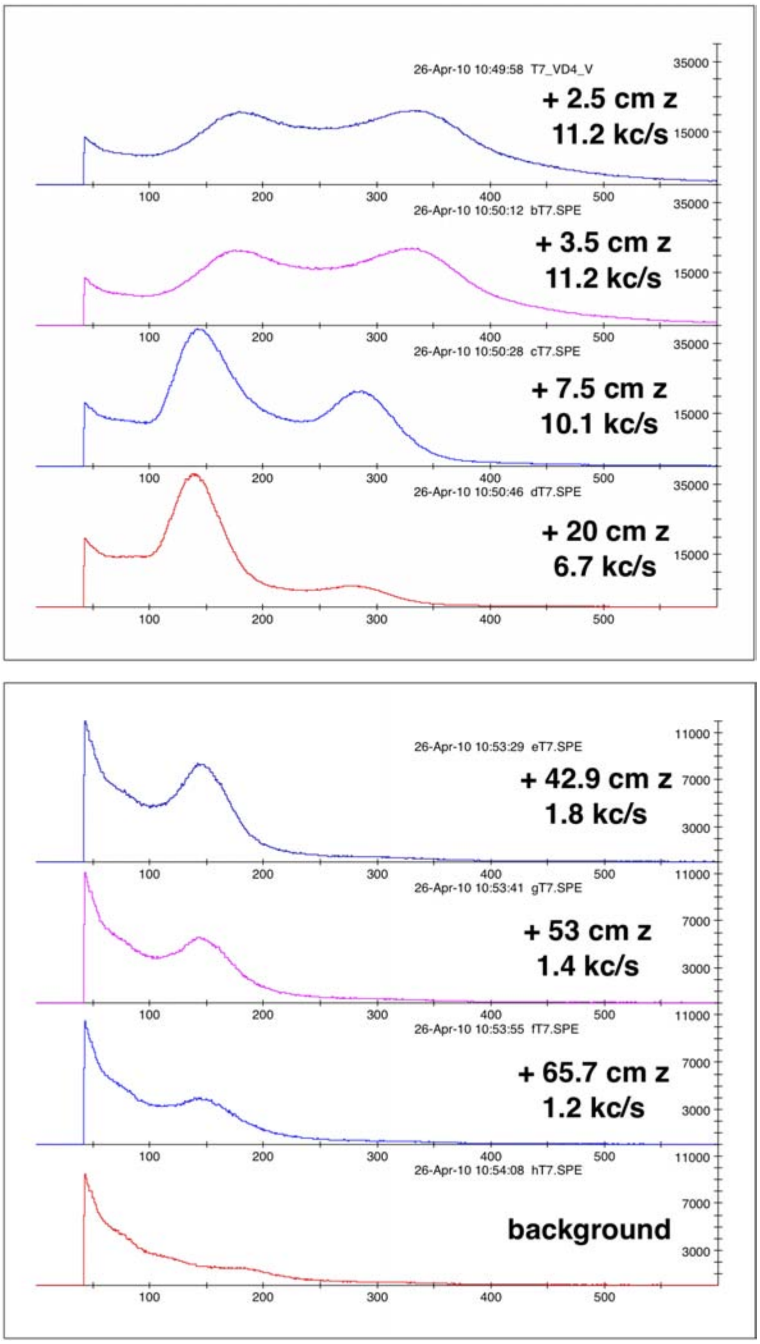


FIG. 2: Count rate effects observed in the TAGS central PMT in response to a ^{60}Co source placed at various points along the detector axis, background spectrum shown at bottom

Using the ANL3x3 detector, three ^{60}Co sources of decreasing activities were measured with the source placed against the detector face (FIG 3). There is a significant shift in the peak positions with a change in count rate, the background spectrum is shown at the

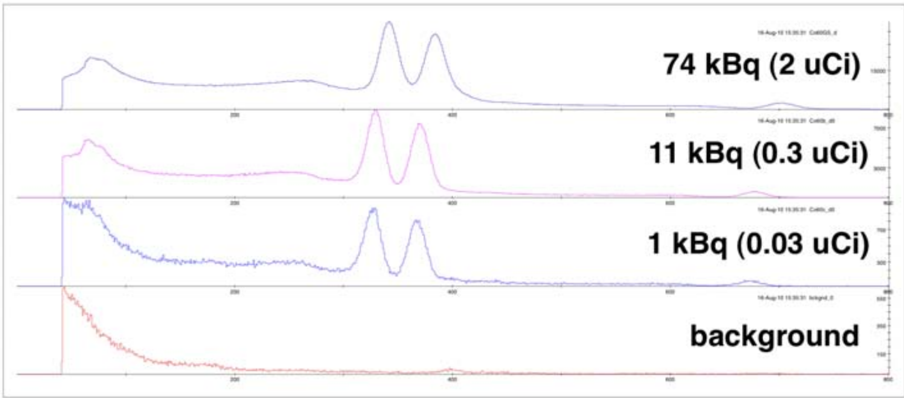


FIG. 3: ANL3x3 measurement of three ^{60}Co sources with different activities, placed against the detector face

bottom for comparison.

The sum peak is also visible in each case. As mentioned previously, one method employed to measure the non-proportional response of scintillators is to calibrate the spectrum to the singles peaks alone, then measure the displacement of the sum peak position from the expected value. Using this method, very little non-proportional effects are seen for this detector.

A count rate dependent shift is seen for the ANU5x5 detector, this time from the same ^{60}Co source at varying distances from the detector (FIG 4). In the case of this detector, calibration using the singles peaks gives a non-proportional deviation of up to 45 keV for the sum peak.

A similar energy shift with count rate is seen for two different activity ^{137}Cs sources at a distance of 10 cm from the detector (FIG 5).

Moving to the slightly larger ANSTOwell detector, measurements were made with a different set of sources placed at the bottom of the well and at the top of the well for ^{60}Co (FIG 6) and ^{137}Cs (FIG 7). These spectra show the expected increase in intensity in the 2505 keV sum peak with the increase in detection geometry resulting from the source lying in the well. The non-proportional shifts here are around 10 keV.

What is interesting is the shape change in all of the peaks with different count rates. It is not clear what causes this shape and position shifting of the measured spectra with count rate, however the effect is significant. It is present in the individual PMT response (FIG 2)

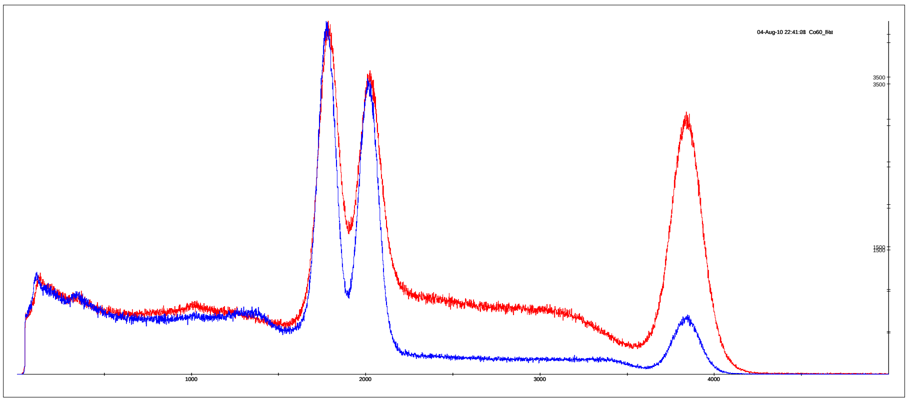


FIG. 6: ANSTOwell detector with ^{60}Co source placed at the top of the well (blue) and at the bottom of the well (red)

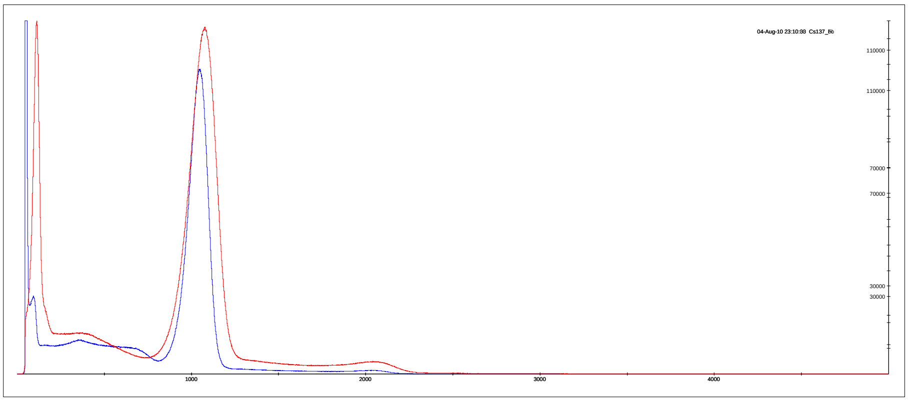


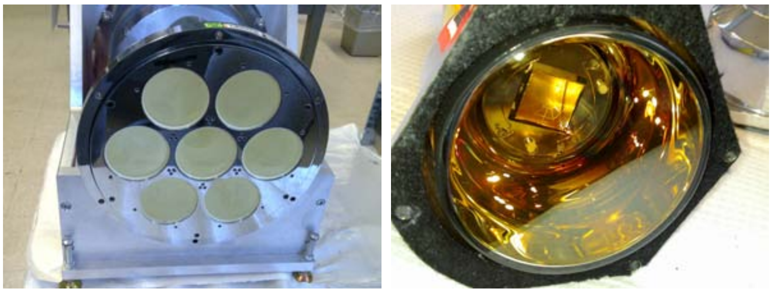
FIG. 7: ANSTOwell detector with ^{137}Cs source placed at top of the well (blue) and at the bottom of the well (red)

B. General check of TAGS performance

The measurements of single and double line γ-sources using TAGS, indicated a poor energy resolution.

The PMTs of TAGS were removed to visually inspect both the scintillator and tubes. The scintillator was found to be transparent and showed no fractures or dislocations from its glass envelope (FIG 8 (a)). The PMT photocathodes are clearly intact and show no signs of stripping or damage (FIG 8 (b)).

The optical coupling had dried up, requiring application of optical grease to all of the



(a) (b)

FIG. 8: TAGS with PMTs removed showing (a) no major problems visually with the crystal and (b) the photocathode coating of one of the removed tubes

tubes. However, there was no significant improvement in the resolution of TAGS after the optical coupling was replaced and the detector re-assembled.

C. PMT gain matching

An added complication with large scintillator crystals is the large light collection area required. Increasing the size of a PMT is an option, however the response properties of a large single tube can be degraded and the tube itself would be fragile. As a result, multiple smaller PMTs are required to cover the window and maximise the collection of light. Figure 9 is a picture of the TAGS tubes and the adopted name for each tube position. To get a uniform response across the scintillator window, ideally, tubes that are manufactured in the same batch are employed.

The response of a PMT is strongly dependent on the applied bias. For a detector employing a single PMT, this is less of an issue. However, for large detectors comprising of multiple PMTs, the final signal is the summed response of the individual tubes. Therefore, if one tube has a higher gain than the rest, the measured total response will result in a poor resolution or, in the extreme case, an unrecognisable spectrum. As such, an important issue with the operation of these detectors is the gain matching of the PMTs. The voltage dividers provided for this application have an additional bias adjustment potentiometer to offset the main bias for this purpose.

Using a mono-energetic γ-ray source such as ^{137}Cs, a method to gain match the tubes would be to align the single peak positions for a fixed bias. This assumes that the response is

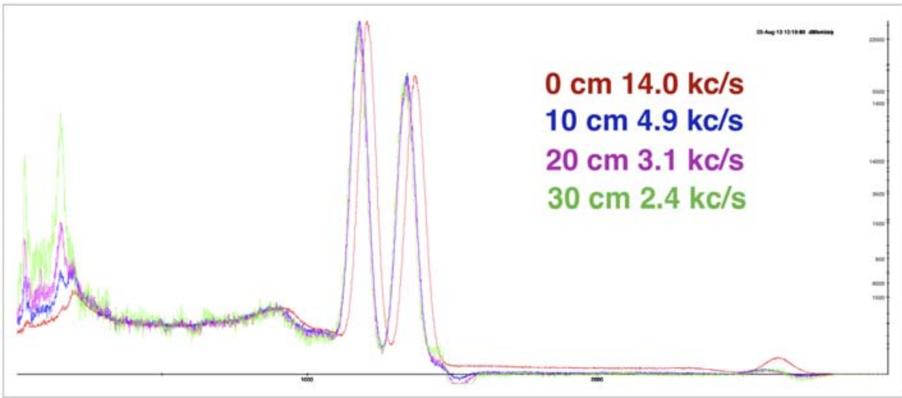


FIG. 4: Shift of peak position with count rate - ANU5x5 detector with ^{60}Co source at different distances from detector, background subtracted spectra

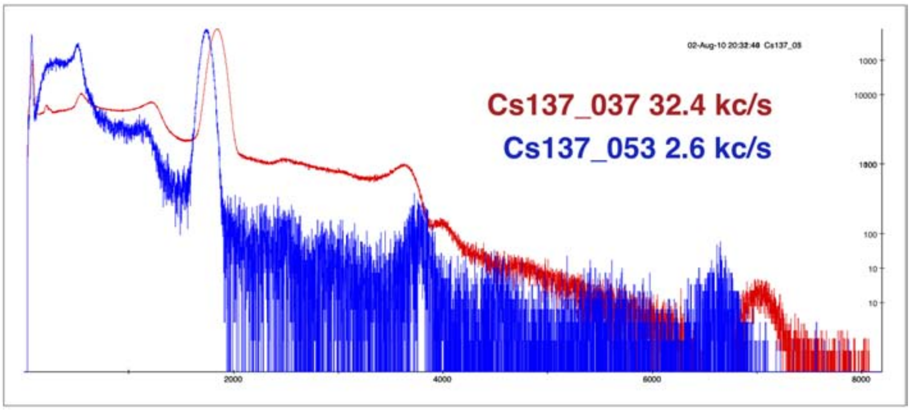


FIG. 5: Shift of peak position with count rate - ANU5x5 detector with two different ^{137}Cs sources at 10 cm distance from detector, background subtracted spectra

and will most likely be present in the total TAGS detector response.

To mitigate these effects, measurements will have to be undertaken within a strict count rate window within which these effects are well known and can be accounted for. Greenwood et al used 4000 counts per second as an upper limit for experiments measuring the β-feeding intensities [Gre92a].

To allow for flexibility of the experiment, several such count rate regions should be measured and characterised, up to the limit where pile-up effects become significant. The above measurements highlight the importance of maintaining a low, constant count rate during a measurement.

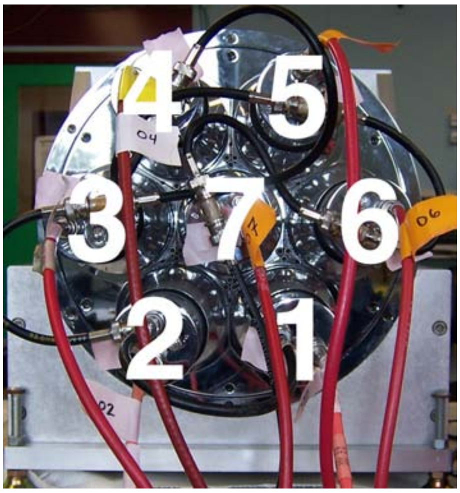


FIG. 9: Adopted positions of the TAGS PMTs

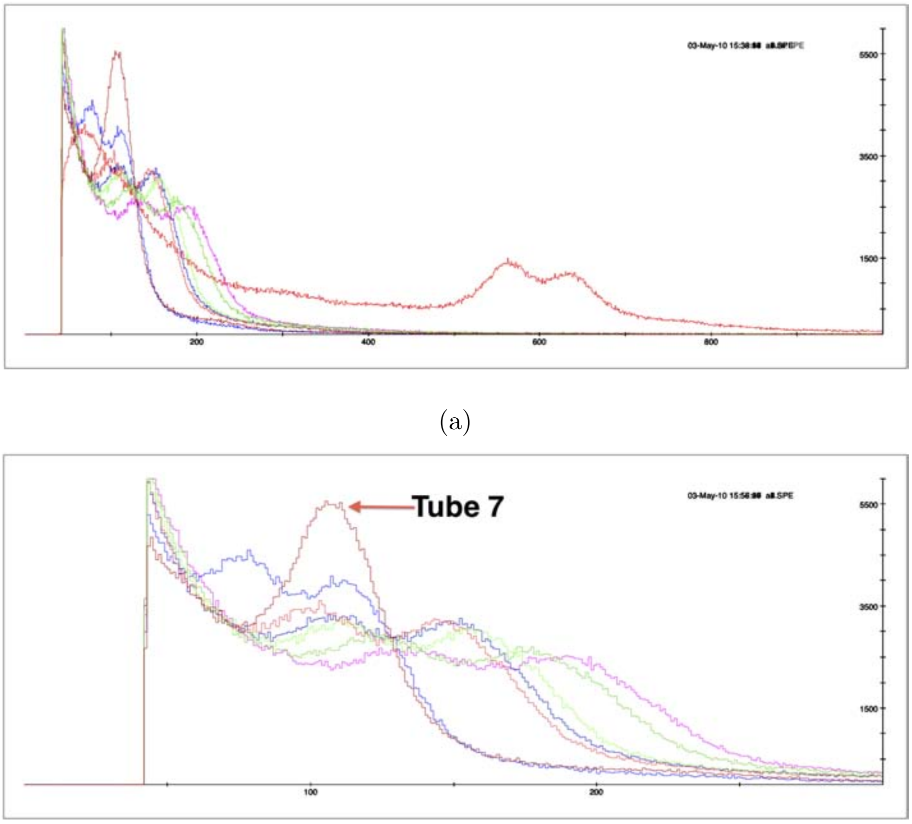
the same for each PMT, which would be the case for a symmetric scintillator. The question becomes, how does one best gain match for a scintillator that is not expected to produce a symmetric response for each PMT?

To demonstrate this point, a ^{60}Co source was placed 22.9 cm from the front face of TAGS positioned on the central axis. The response from each tube was measured and the final response produced by passively summing each individual tube (red curve in fig 10).

A consistent response was found for the peripheral tubes, giving a double peak feature that resembles a ^{60}Co spectrum with very poor resolution. The central tube response shows a single peak (brown in fig 10). The peripheral tubes share the same geometry when the source is placed on the axis, as in this case. A similar shaped double-peaked response for the central tube is achieved by moving the source position off axis.

The method used to gain match the PMTs in this case, consisted of using a ^{60}Co source positioned off axis (above the detector), to produce a consistent individual tube response from the tube furthest from the source. This response was very similar to the features shown by the central tube with the source placed in the well. By moving the source systematically, the same individual tube feature can be matched in position for all of the peripheral tubes. Figure 11 shows the result of the attempt at matching with the source positioned 22.9 cm above the detector. This does not produce a consistent summed response. In fact, the summed response varies with source position (figure 12).

A second method involved matching the individual tube count rates, (using a count-rate



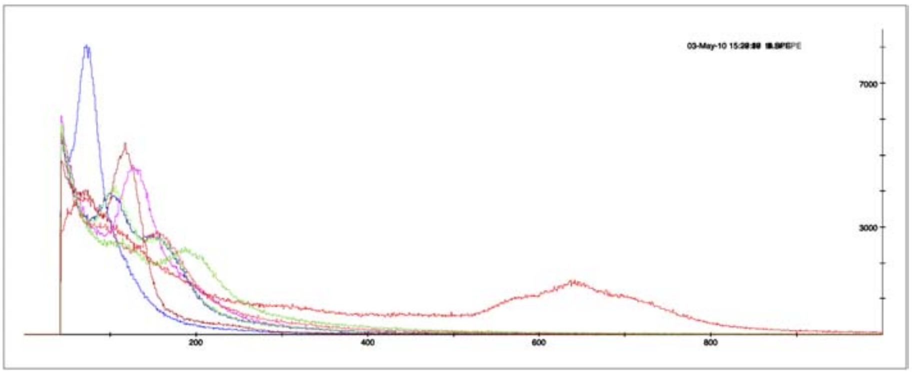
(a)

(b)

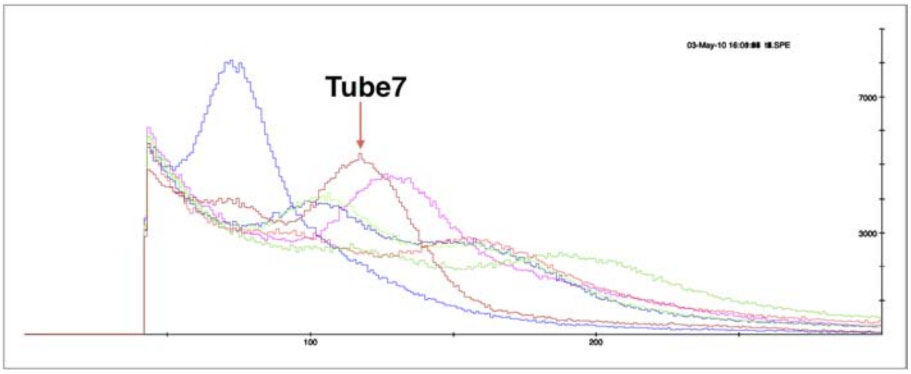
FIG. 10: Measurement of ^{60}Co at 22.9 cm distance from the front face of TAGS (a) individual tubes shown with the passively summed result in red (b) expanded view of PMT components; 1-blue, 2- pink, 3- dark blue, 4- orange, 5- dark green, 6- light green, 7- brown

meter), for a source placed in a fixed axial position. The central tube was then adjusted to minimise the summed-response resolution. The final technique used in the attempt to improve the gain matching, consisted of using a common voltage divider and systematically matching the main peak feature positions for the peripheral tubes. The best resolution achieved using any of these techniques was 15 - 20 % for the 1173 keV ^{60}Co γ-ray. The detectors response in 1992 [Gre92a] was reported to be 5.95 %, and measured from figure 3 of this reference to be 8 %.

Similar attempts at gain matching were made with a lower activity source, but no improvements in the resolution resulted. From this information and other measurements, it is believed that the currently used PMTs are damaged and will be replaced by modern equivalent tubes manufactured by Hamamatsu.



(a)



(b)

FIG. 11: Measurement of ^{60}Co at 22.9 cm distance above long axis in the centre of the detector (a) individual tubes shown with the passively summed result in red (b) expanded view of PMT components; 1-blue, 2- pink, 3- dark blue, 4- orange, 5- dark green, 6- light green, 7- brown

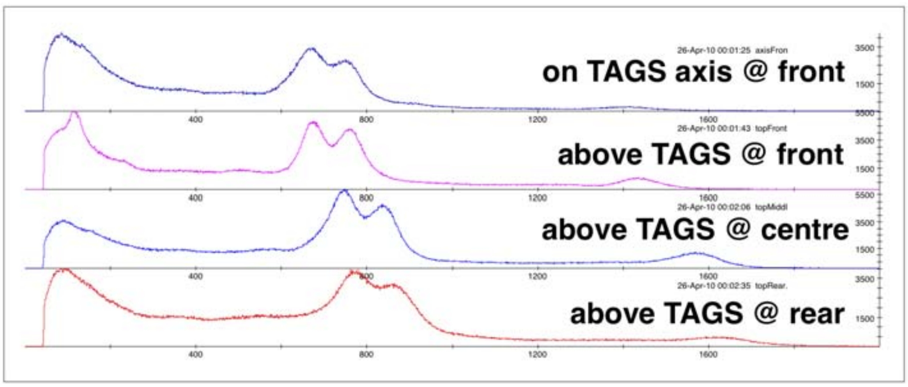


FIG. 12: Passively summed response of TAGS to a ^{60}Co source as a function of source position

A more consistent method of gain matching that has been used elsewhere, involves the use of a single reference light pulsar, at a frequency suitable for the photocathode, carried to each of a detector's PMTs by means of fibre optic cables. The single peak produced is used for gain matching and this can often be done automatically by computer controlled adjustment of each tube bias [Kar97].

V. GEANT4 MODEL OF ARGONNE TAGS DETECTOR

The main purpose of this project is to model the response of the TAGS detector using GEANT4. This model will be used to interpret the experimental data, so that it needs to be accurate and reproduce as many features as possible. Many versions of the TAGS simulation have been developed over the course of this project with increasing complexity as more physical properties are included. The development of the model is anticipated to continue beyond the work described in this report.

This section is intended as a brief overview of the most recent model features. Further general information about GEANT4 can be found in reference [Gww]. The simulation code is written in C++ and the components described below are generally C++ classes.

A. DetectorConstruction

DetectorConstruction is the class where the elements and materials used in the simulation are described and are built. Starting from elements such as Na and I, the materials or compounds in the detector are described (NaI). The materials are then assigned to make up the logical volumes of objects that are constructed using various built-in shapes. These objects are then placed in the "World" volume. In this way, complex geometries and materials can be produced from basic shapes and elements.

A common problem with building models of detectors is the inability to measure internal dimensions of components, particularly when there is no documentation. In the case of TAGS, all of the dimensions have been taken from reference [Gre92a].

The NaI material in the present model makes up the bulk of the detector volume. A future improvement would be the addition of the thallium doping. The NaI is enclosed in an aluminium can on three sides and a glass SiO_2 window on the rear of the detector. A silicon detector is placed in the well while a section of aluminium plate placed adjacent to the SiO_2 window acts as a simulated photocathode. The DetectorConstruction is also the place where the active detector volumes (SensitiveDetectors) are defined, (see section D below). The OpenGL rendering of this constructed detector is shown in figure 13.

The most recent model includes the possibility to directly simulate the optical photons from scintillation light. To accommodate this, additional properties such as the refractive

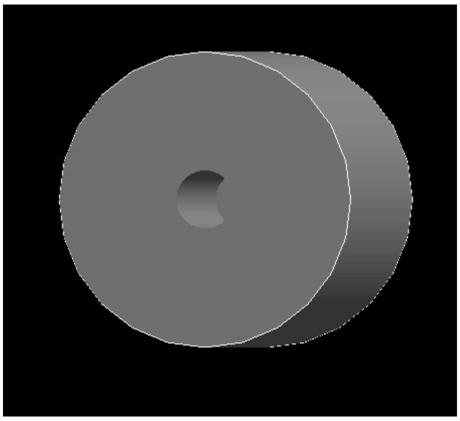


FIG. 13: OpenGL rendering of the TAGS geometry showing the outer aluminium casing

index as a function of the photon energy are manually defined for each material and boundary interface.

B. PhysicsList and PrimaryGeneratorAction

The PrimaryGeneratorAction is a mandatory class defining the method by which particles are generated. The base class is a gun that fires mono-energetic particles in a defined direction. The current model utilises the General Particle Source (GPS) class that allows the user to fully define the energy and direction of the emitted particles.

The PhysicsList class allows the user to define the properties and behaviour of the particles or photons that will be used in the simulation. For example, an electron is first defined using either the provided particle details or a modified version, then the physical behaviour of this particle is associated to physics modules, for example multiple scattering.

There are a wide variety of physics modules available, usually written by groups that focus on a particular energy range. For the current model, the low energy Penelope physics module is employed. Also implemented in the PhysicsList is the Radioactive Decay Module (RDM). This is a module that allows the creation of a radioactive ion as the source of particles, it uses input files to define the decay paths and intensities and an additional file to handle the subsequent transition(s). The data contained in the RDM input files are sourced from the Brookhaven National Laboratories' Evaluated Nuclear Structure Data Format (ENSDF) database. The advantage of using the RDM, is that the total response to a decay is treated in a single "event" (see EventAction and SteppingAction for the description of a "event"), with all of the particles emitted in the decay (γ's, β's, IC e^-'s etc) handled without the need for them to be defined explicitly.

C. SensitiveDetector

A SensitiveDetector is a specified material or volume in the geometry that is of particular interest. For example, the NaI volume would be defined as a SensitiveDetector allowing information on the interactions and processes occurring in that volume to be extracted. It is first defined in the DetectorConstruction and usually follows a particular logical volume, such as the silicon detector. When a particle or photon interacts with this volume, the associated SensitiveDetector class will be called. In this class, information about the interaction or hit (for example, energy deposition) can be accumulated.

The TAGS model contains sensitive volumes for the NaI, the silicon detector and the aluminium plate that acts as a simulated PMT. The NaI SensitiveDetector uses an energy deposited method from the step class (see below) to determine the detector response to a particle interacting within it.

D. EventAction and SteppingAction

A"step" in the simulation is a single transport of a particle or photon followed by an interaction. An event consists of the variable number of steps that result from the initial particles or photons. For example, if we take the case of a γ-ray of initial energy E_0, then the first step may involve Compton scattering and the production of a Compton electron together with the scattered γ-ray. The following step could consist of another Compton scatter or a photoelectric absorption and so on until there are no more interactions. The simulation will then back track and pick up the first Compton electron and systematically follow this through all of its steps. The resultant total steps from the initial and secondary particles are defined as an event.

The EventAction and SteppingAction classes are user classes that are called after each event and step respectively. They allow for the addition or extraction of information at these levels. In the case of the TAGS model, information that is produced by the RDM is

[Decay Index] *(0-Other, 1-β-, 2-β+, 3- e^--capture, 4-α, 9- Error)*
[Feeding Energy from RDM]
[γ1 from RDM]
[γ2 from RDM]
[γ3 from RDM]
[TAGS energy deposited]
[Si detector energy deposited]
[spare data field]
[PMT1 light counted] *double*
[PMT2 light counted] *double*
[PMT3 light counted] *double*
[PMT4 light counted] *double*
[PMT5 light counted] *double*
[PMT6 light counted] *double*
[PMT7 light counted] *double*

FIG. 14: Event Data structure, all values are unsigned short except the PMT values

extracted at the step level and passed to the EventAction. The EventAction accumulates all of the relevant information from the SensitiveDetector classes and the SteppingAction, and passes this bundle to the RunAction where it can be written to file.

E. RunAction and Output

RunAction is the final user action class called in this model. Its main purpose is to collate the data and write the results to an output file. Information is written in binary format to minimise the size of the output file.

The output consists of a header for the file, this names the data and gives the number of events that were simulated. The rest of the information is given on an event by event basis like experimentally obtained data. The structure of the data is shown in figure 14.

The RDM does not have direct access to the events that it is producing. Some extra code has been put in place to draw out this information. The first field in the data structure is a decay index, indicating the type of decay that the RDM has selected from the decay input file. Next is the energy of the emitted decay. The following three fields give the individual γ-transitions that have been emitted by the RDM.

The TAGS and Silicon detector energy deposited fields are the accumulated energy deposited in the respective sensitive detectors (in units of keV). The PMT light counted fields give the number of photons that hit the individual pseudo photocathodes. These fields are used for the light activated version of the simulation.

VI. TAGS SIMULATIONS

A. Detector Efficiency

Using an earlier version of the TAGS simulation, the total and Full Energy Peak (FEP) efficiencies were determined by simulation. This was undertaken as a test of the basic functioning of the model and to establish the best source position (in terms of efficiency), along the axis from the bottom of the well. The total (a) and FEP (b) efficiencies are shown in figure 15. The results confirm that the optimum position for a source is 2.5 cm from the bottom of the well and that a maximum total efficiency of 99% for an energy of 200 keV can be achieved, in agreement with reference [Gre92a].

B. Resolution

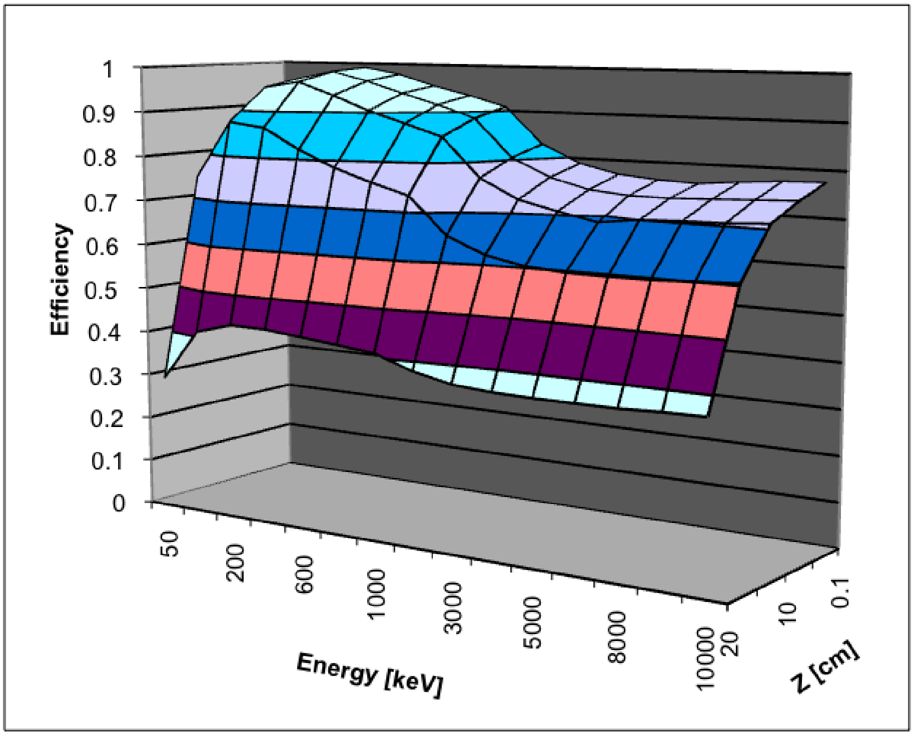
The resolution of a detector is composed of contributions from many physical factors, for example noise in the analogue electronics. Many of these physical processes are not modelled in the simulation, the most significant of these is from the data acquisition system. The G4 simulation produces discrete data that models only the most significant physical properties of a detector. In place of modelling all processes and extending simulation run times, some of the more dominant properties can be added post-simulation.

One such property is the detector resolution. A gaussian broadening is applied to the simulation results, where the properties of the broadening can be determined from experiment.

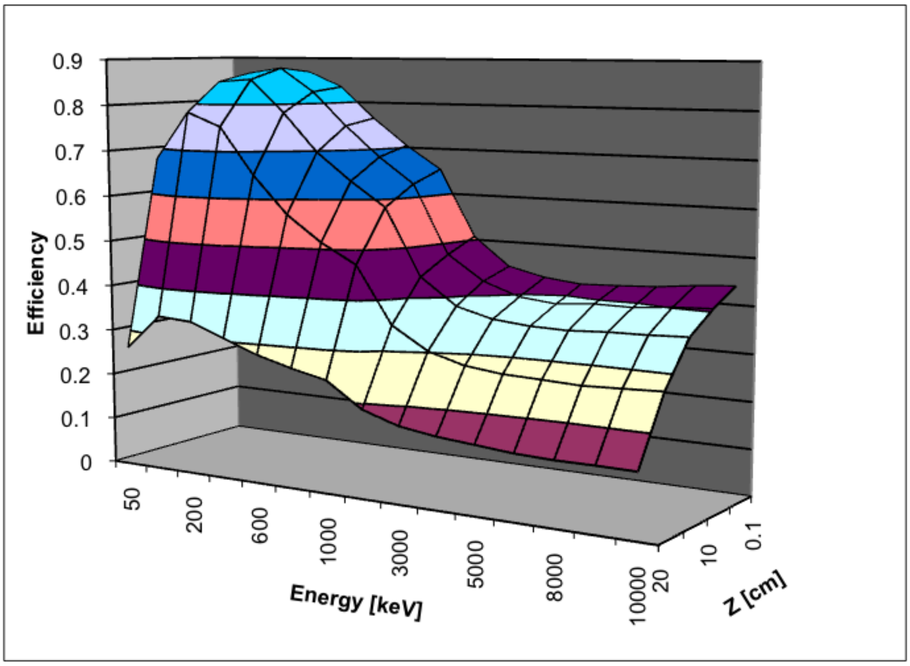
C. Non-proportionality of light

The problem of non-proportionality is treated in recent TAGS work undertaken by the Valencia group [Can99a]. They use a collection of NaI(Tl) data from various references, under the assumption that the data is applicable, and use this to derive an expression for the detector response to electrons. This expression is then utilised in the simulation to determine the overall non-proportional shift from an interaction in the detector.

A method of dealing with and modelling the non-proportional response has not been implemented in the model. This is being investigated and is the subject of future work.

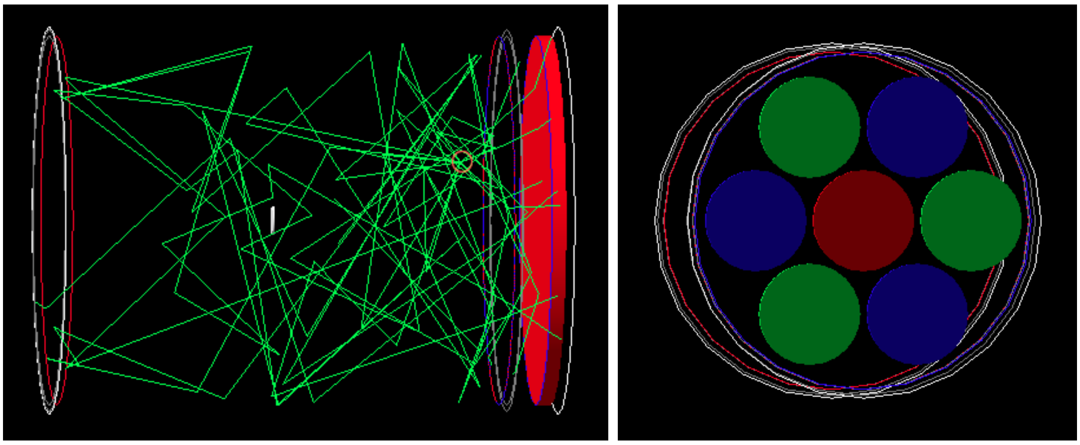


(a)



(b)

FIG. 15: Simulation of (a) the TAGS total efficiency and (b) the TAGS Full Energy Peak efficiency as a function of source position from the bottom of the well, z



(a) (b)

FIG. 16: OpenGL rendering of TAGS geometry showing (a) a 250 eV electron deposited in the sensitive detector (indicated by the red circle) and the resulting optical photons hitting a single large pseudo PMT (b) update of model to include individual PMT sensitive detectors

D. Simulation of Light

To investigate the fundamental reason for non-proportionality, some different approaches were used with varying complexity in the level of modelling. The first approach taken was the energy deposited method, that records the interactions of electrons for the TAGS sensitive detector.

An alternative method employs the scintillation module in G4. The model follows the light produced in the scintillator crystal and tracks the photons until they hit the aluminium PMT pseudo-cathode. Figure 16 (a) shows an OpenGL rendering of light produced from a 250 eV electron deposited in the TAGS volume. The pseudo PMT is simply used as a sensitive region to count the amount of light (number of photons) that reach the material, so there is no reflection at that boundary. Figure 17 shows a comparison of simulated data with and without simulation of the optical photons.

An update to the model was the separation of the single pseudo PMT into seven PMTs positioned in the same arrangement as the TAGS PMTs. This separation can be seen in figure 16 (b). What is of interest is the individual tube response to light, as measured in the section "PMT gain matching". The simulated individual tube response to a ^{60}Co source (fig 18) gives the same general trends as the measured individual responses, though with very

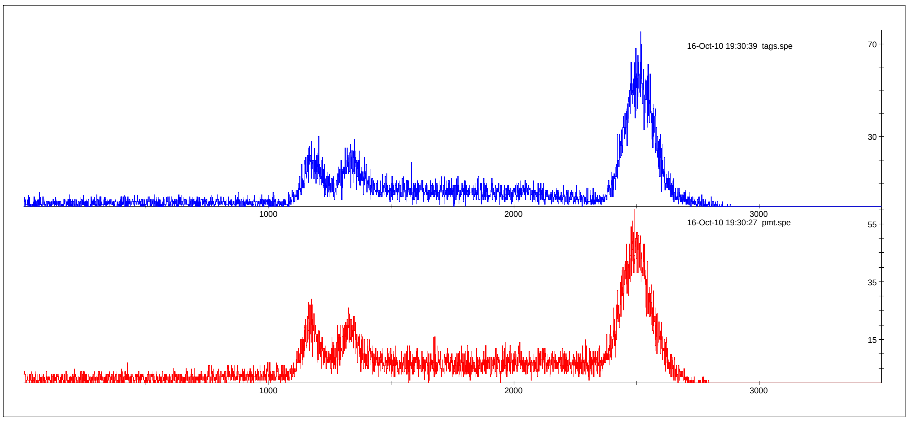
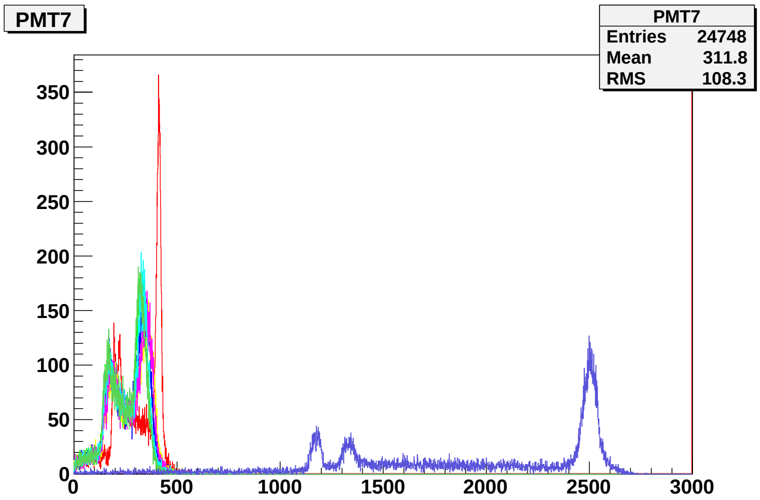


FIG. 17: Simulation of TAGS detector with a ^{60}Co source, comparison of results using the energy deposited method (blue) and tracking of scintillator photons (red)

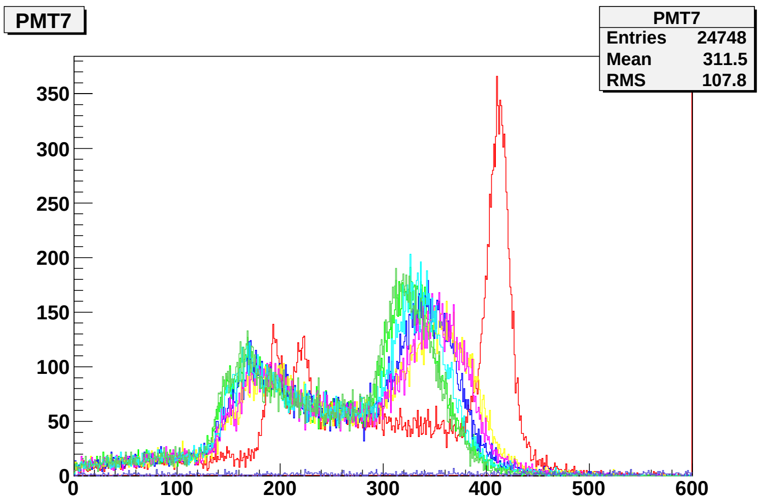
poor resolution (fig 10). This information can be used to better understand how to obtain gain matching of the tubes. What is interesting from the simulation, is the resemblance of the central tube response to the the total response observed. It would be expected that the central tube position, being the most symmetric, would have a response most similar to the expected total response, only with insufficient light collection. This was further evidence to suggest that the existing PMT's were not functioning properly.

The other noteworthy comment here is that the individual tube responses are clumped in the low energy region where detector noise typically occurs. These components add event-by-event to produce a total response that occurs at a much higher energy, away from this low-energy noise region. The implications are that the total response is only obtained by summing of all of the tube components at the time of measurement. Post measurement of the individual tube events would require time stamping of the information. Time stamping would be an advantage in the case of a gain drift of an individual tube as adjustments could be made post-collection, where as in the instantaneous method, resolution may be compromised and data would be lost.

In the model, the extra information available with the simulation of light, comes at the cost of greatly increased simulation time. For every step where energy is deposited, many optical photons are generated, which are then tracked until they are either absorbed and killed or they leave the volume of interest. As a rough indicator, simulations can take 100-1000 times longer to complete compared to the non-light simulations. Due to this fact



(a) components



(b) zoom on components

FIG. 18: TAGS simulation of ^{60}Co showing (a) the individual PMT components with the summed result (b) zoom in on individual components

alone, the selection of this option for simulations is not a favourable one for general purposes although it holds promise for a more fundamental understanding of how the TAGS detector works.

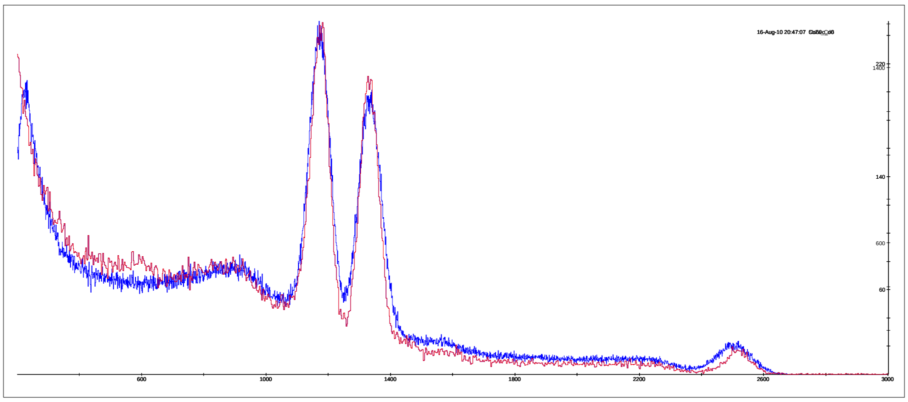


FIG. 19: ANL3x3 detector with ^{60}Co source placed against face of detector. Simulation (blue) Experiment (red)

E. Basic simulation comparisons

The basic energy summing model was tested against three NaI(Tl) detectors, a 3” x 3” cylindrical detector (ANL3x3), a 5” x 5” cylindrical detector (ANU5x5) and a 6” x 5” well type detector (ANSTOwell). The dimensions of the simulation were altered from the basic model in order to verify the functioning of the model components. In increasing the size and complexity of the detectors being modelled, the progress of the model at handling the properties found in a large well type TAGS detector can be evaluated.

A ^{60}Co source was placed against the face of the ANL3x3 detector and measured, the setup was then simulated. Figure 19 shows a comparison of the experimental results (red) to the simulation result (blue). Good agreement is found with the main spectral features with the exception of the ^{60}Co sum-peak positions. The slight differences here are due to light non-proportionality not being implemented in the basic simulation model.

A similar comparison was undertaken using ^{88}Y (fig 20), with a source detector distance of 15 mm. The experimental result (red), is compared to the basic simulation (blue) and also a version of the simulation incorporating background materials in order to reproduce the backscatter feature (green). Once again the overall trend is modelled well. The largest discrepancy is the backscatter peak. Improvement is likely to be possible by more accurately modelling the materials surrounding the detector in the experiment.

Figure 21 shows the measurement of a ^{60}Co source placed against the face of the ANU5x5

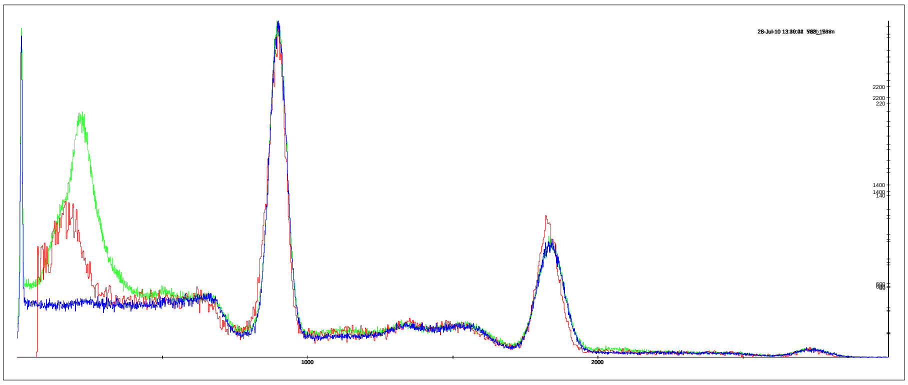


FIG. 20: ANL3x3 detector with ^{88}Y source placed 15 mm from face of detector. Experiment (red), Simulation (blue), Simulation with backscatter materials added (green)

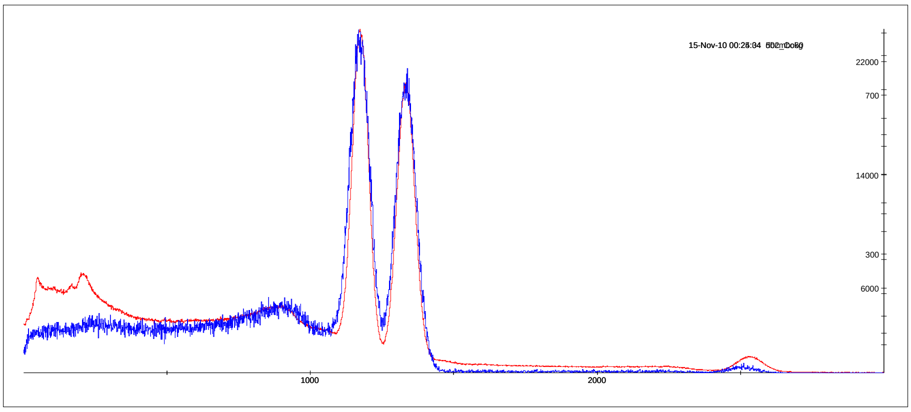


FIG. 21: ANU5x5 detector with ^{60}Co source placed against face of detector. Experiment (red), Simulation (blue)

detector (red) compared to the simulations (blue). The notable difference in this comparison is due to back-scattering, which is not modelled here. There is also a larger non-proportionality shift in the ^{60}Co sum-peak, which can also be attributed to the larger detector crystal. The dimensions used for the simulation and the source detector distance were estimated, giving poor agreement on the magnitude of the sum-peak.

Figure 22 shows the measurement of ^{60}Co using the ANSTOwell detector with the source at the bottom of the well (red). The main features of the simulation (blue), agree with experiment, in particular the increased magnitude of the ^{60}Co sum-peak. The shift of the the sum-peak position is similar to the non-proportional shift of the ANU5x5 detector, which

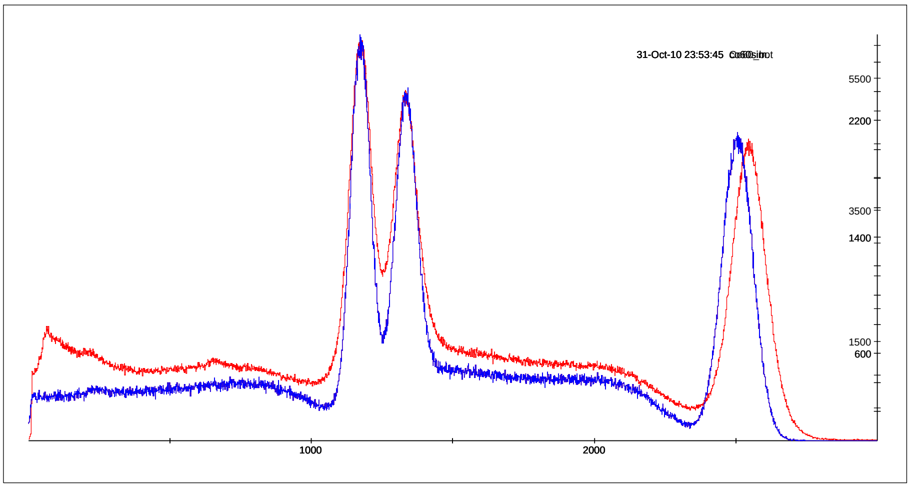


FIG. 22: ANSTOwell detector with ^{60}Co source placed against face of detector. Experiment (red), Simulation (blue).

is of comparable size.

F. Pileup Generator Script

Pile-up can cause effects such as tailing and summation which are not simulated in G4. These effects will need to be accounted for in order to accurately model the detector response, particularly when measurements are made under high count-rate conditions. There are two general approaches to dealing with pile-up. The first approach involves removing the effects from the experimental data, based on a statistical approach [Wie76, Ten84].

A second approach is to produce pileup in the simulation data. The generation of pile-up to this discrete data is achieved through a pileup generator script written in C++. The script randomly selects events in the given file and creates new "piled up" data based on an experimental count rate. This concept has been tested and is currently under development. This approach allows for greater separation of the individual processes involved in creating an accurate detector response and is the preferred direction at present.

G. TAGS response generation: RDM vs GPS vs Mixing script

To unfold TAGS experimental data requires a simulated detector response using the proposed decay scheme as input. If the measurement and simulation agree, then it is possible that the decay scheme proposed is the correct one. If they do not agree, then the decay scheme is changed by adjusting existing β-decay feeding intensities or through the addition of new β-levels. A simulation response based on the new decay scheme would then need to be generated and the process repeated until agreement is found.

The most efficient process for achieving agreement has not been finalised. Several alternative methods are being considered, involving (i) the use of the Radioactive Decay Module (RDM), (ii) the General Particle Source (GPS), or (iii) a mixing script.

1. Radioactive Decay Module (RDM)

As previously mentioned (PhysicsList and PrimaryGeneratorAction), the RDM is treated as an ion that undergoes radioactive decay determined by input from two text files. The first text file contains the decay information for the specified species, the second file contains information about the transitions that result and is used as input by a photon-evaporation module. The standard input files come as a package with GEANT4 and are sourced originally from ENSDF data.

The control of the RDM is via command line at the user interface or macro file for batch mode. The advantage of using the RDM, is that all of the response for a particular β-feeding level is given in a single event, which takes care of summing of γ-transitions in cascade. Furthermore, these files can be modified to suit any changes required and could possibly be done using a conversion script to pull information from a more standard format such as an ENSDF file.

Some disadvantages are the requirement of a specific file name for the input files, (eg z27.a60 for ^{60}Co), resulting in the constant writing over of the one file which could lead to mistakes. The RDM creates a single response for a complete decay to the ground state, separation of the components for analysis is not a straight-forward task. Iteration of the level scheme, eg adding a β-level, may require the time consuming re-running of the simulation.

2. General Particle source (GPS)

A similar approach is possible through the use of the GPS module. In this case, the total response can be produced by means of a multiple vertex option that allows several mono-energetic particles or photons to be defined and emitted in a single event. The advantage is the flexibility of being able to get a single total response for the defined β-feeding branch including cascade summing effects, while retaining the ability to simply separate the components for analysis.

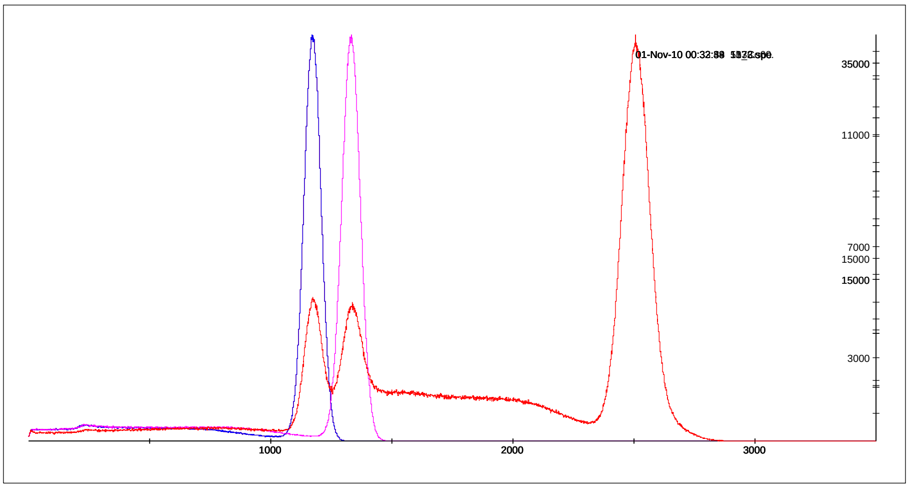
This approach has the requirement to define all of the transitions in macro input-files which could be tedious, but has the advantage of being more flexible than the RDM. The value of this method is currently being investigated.

3. Folding script

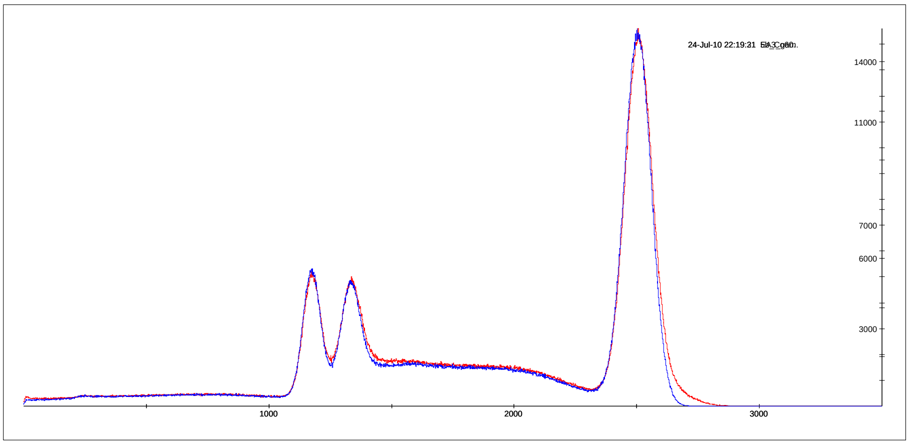
In the approach reported by the Valencia group [Can99a], all mono-energetic γ-transitions for the decay scheme are modelled individually. The detector response to a β-feeding level is determined by folding these individual γ-transitions.

A stand-alone script has been written in C++ to fold γ-responses by randomly selecting components from two individual γ-response input files. This is done in a way so as to maintain the geometry properties (detection efficiency) of the detector responses. Figure 23 (a) shows an example of a ^{60}Co source simulated using the RDM (main β-branch), compared to the mono-energetically produced components. These components are folded using the script and compared to the RDM produced result in figure 23 (b). The slight discrepancy is due to not including the bremsstrahlung or direct observation of β.

The advantage of this method, is the one time use of the simulation code to produce all of the required β and γ transitions. If a β-level is added, only this added level is required to be simulated. Any gain of time in not re-doing simulations may be taken up with the time to run the mixing code for each convolution, although this is quicker.



(a)



(b)

FIG. 23: Folding script used to fold individually simulated responses. (a) ^{60}Co main β-branch simulated using RDM (red) compared to the individual components (b) individual components folded (blue)

VII. CONCLUSION

This work has resulted in a basic working model of the TAGS detector at Argonne, written using Geant4. Future work will be to model and better understand the detectors' non-proportional response to light, test and benchmark the pile-up generator script against a working TAGS detector, and to fine tune to accommodate the analysis method for TAGS data.

Step-by-step instructions on how to operate the current version of the model are given in an appendix that is separate to this report.

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[FRww] FRIB - Facility for Rare Isotope Beam (US facility, see http://www.frib.msu.edu)

[Gww] GEANT4 webpage (http://geant4.cern.ch/)

[GRww] Gamma-Ray Energy Tracking Array (GRETA) (see http://grfs1.lbl.gov)

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