Neutron kinematics write-up

August 11, 2023

1 Motivation

The goal of the neutron kinematics study is to take an in-depth look at the muon-induced neutron behavior in and around the solid neutron moderator shield in the LEGEND-1000@LNGS baseline design. This is a late-stage exploratory study which is not looking to solve a specific problem or iterate on the current design parameters. Rather, it is aimed at identifying important information which might have been neglected or overlooked previously which could have a significant impact on our understanding of the implementation of the shield. If any other potential modifications are necessary or beneficial, they should be proposed as soon as possible, as the collaboration is narrowing in on a final design for the shield in preparation of the CDR.

2 Simulation setup

As of the time of writing, the simulation setup is fairly 'standard' for cosmogenic simulations for LEGEND-1000 within the collaboration. warwick-legend, or WLGD, is a simulation module written using Geant4 10.7. A branched repository of WLGD is maintained and developed by some members of the LEGEND simulations effort who are largely based out of Italy, hence the repository is known as 'ItalSim'. This study uses a modified version of the ItalSim repository, which collects additional neutron information which is not available in WLGD or the current commit of ItalSim.

As part of the 'standard' cosmogenics simulation, a LEGEND-1000 cryostat with a single, large copper reentrant tube is implemented. The neutron shield is a hollow cylinder with solid caps on the top and bottom, much in the shape of a closed tin can. This can has an inner diameter of 4 meters, an inner height of 2 meters, and a thickness of 10 cm. The selected shield material is pure PMMA, with no dopant or coatings added. The primary muons which are simulated for the generation of the muon-induced neutrons are sampled from a large collection of input muons generated by the MUSUN simulation software, based on experimental data which has been collected at LNGS regarding muon kinetic energies and angular distributions at laboratory depth. 10^7 muons were simulated, which required about 20 hours of processing time on the computing cluster utilized, and resulted in about 600 MB of data.

3 Data collection and analysis

Please refer to the glossary for some terms and references which are used in this paper which might not be intuitive or well-known outside of a small section of the L1000 collaboration.

This section is rather technical, and not important to the final results, but is written for documentation purposes and can be skipped.

As a reminder, in Geant4, the hierarchy of complexity is Run - Event - Track - Step. A run typically contains many events, an event is defined as the track of a 'primary particle' plus the track of all secondaries. Each particle has one track, which is typically comprised of several steps, which propagate the particle in the simulation world. If the particle is destroyed, absorbed, or exits the world, its track ends.

The current version of ItalSim uses the data collection and output methods implemented previously in WLGD. In this data collection scheme, a ROOT ntuple is created at the run-level. The ntuple is filled with data at the event level. Since one event can contain many tracks, data which is collected at the track-level has to be stored in a vector. Since one track can contain many steps, the only options for data collection at the step-level using this method are to store the data in a 2D vector, or to aggregate the step-level data into a single parameter, for example by summing all of the energy depositions, and then store them in the same fashion in which tracks are stored. Furthermore, vectors of strings are not available for this use until Geant4 version 11, and ItalSim uses Geant4 10.7. So, to summarize: the current ItalSim version collects information at the event-level, and so is mostly limited to track-level and event-level information, and cannot store strings. To circumvent this, a second ntuple was added. This ntuple uses no vectors, enabling the storage of strings, and also collects information directly at the step-level. By doing so, the data requires additional processing following simulation, but is more flexible.

To limit file size, step-level data was collected only for neutrons and only within the cryostat. The following parameters were collected: position (x,y,z), time, kinetic energy, step ID (unique for each step), track ID, process (i.e. the physical process in simulation which the particle is currently experiencing), and finally the names of the material and the simulation volume which the particle is currently propagating through. Any parameters which are not listed were not used for this study and are unavailable, but could be added at the cost of fractional increases in file size and processing times.

Previous recent studies have already focused on the production mechanisms and initial parameters for muon-induced neutrons, so those are not studied here. Rather, the main focus is on neutron behavior at the boundaries of and inside of the shield, with a secondary focus on neutron behavior within the liquid argon.

The inclusion of the 'process' and 'material' variables are essential to this data analysis. When a neutron in the simulation moves from one material to another, Geant4 is forced to end the current step as part of the propagation algorithm. This is known as a *boundary crossing*. Steps are typically ended by physical processes, such as the occurrence of a scattering event. Since the boundary crossing is unphysical, the process which is assigned to the step is "Transportation", an artificial process used in Geant4 for bookkeeping. By searching for boundary crossings, and using the current material and track ID of the neutron, it is always possible to identify a neutron entering or exiting the shield.

With the step-level information in hand, there are multiple avenues for processing and analyzing the data, which are somewhat abstract and are best explained with an example. It might be beneficial to plot the total energy loss of a neutron which has entered and then exited the shield. This could be accomplished simply by recording the neutron's energy when it enters the shield, and comparing this to the value when it exits the shield, using the boundary crossing method in the previous paragraph. However, some neutrons will be created inside of the shield, and some will be absorbed inside of the shield, and cannot be included in this analysis. The main work in this type of analysis is accounting for many less obvious cases such as these, and maintaining consistency when using multiple processing avenues to compile results.

4 Results

4.1 Neutron reflection and transmission

Some final terminology must be introduced in order for the kinematic study to be understood. As neutral particles, neutrons do not lose energy in matter continuously through electromagnetic processes. Because of this, they have a tendency to scatter dozens or even hundreds of times before finally being absorbed via neutron capture (Fig. 1). The multiple scatters may cause neutrons to change their direction dramatically, or even reverse direction.

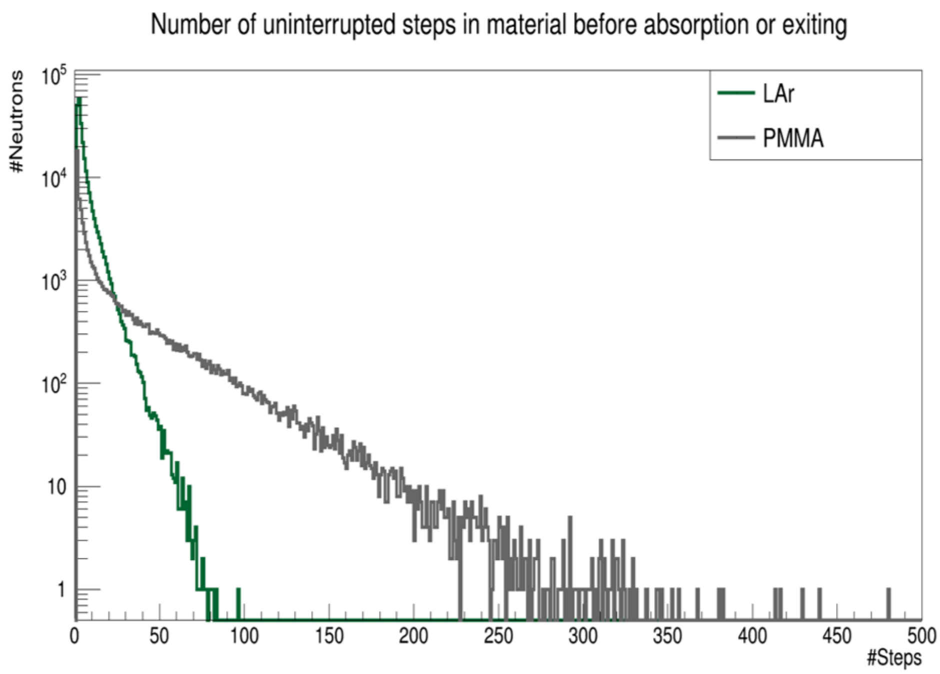

Figure 1: Number of uninterrupted steps neutrons experience in each material before absorption or exiting the material. A neutron may have more than one entry on the plot if it re-enters the materials multiple times.

So, a neutron which enters the shield may scatter multiple times, reverse direction, and exit the shield without traversing its entire length. This is visualized in Fig. 2. When this happens, the neutron is *reflected* - although this is not a precisely correct usage of the mechanics of reflection, the meaning can be understood well enough. If, instead, the neutron travels 'through' the shield, it is transmitted. Because of the scattering nature of neutrons, the same neutron can be reflected or transmitted multiple times. Fig. 3 plots the number of times each neutron experienced a shield boundary crossing, if one was experienced at all. The shield is a moderator, not an absorber, so the majority of neutrons will cross the boundary twice each time - once when entering, and once when exiting. Hence, odd-numbered total boundary crossings are less frequent. Future sections will rely heavily on the concepts of reflection and transmission to explore the neutron behavior. One note to be made for future significance - on average, neutrons are about four times more likely to reflect than to transmit, due to the short mean free path length in the moderator.

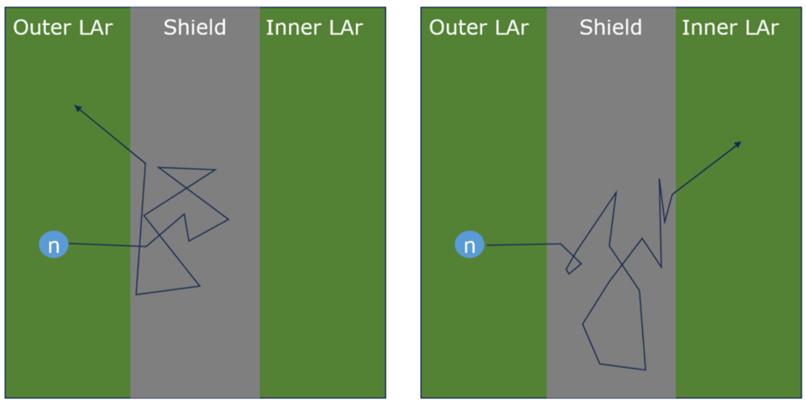

Figure 2: Illustrations of the concept of neutron reflection (left) and transmission (right).

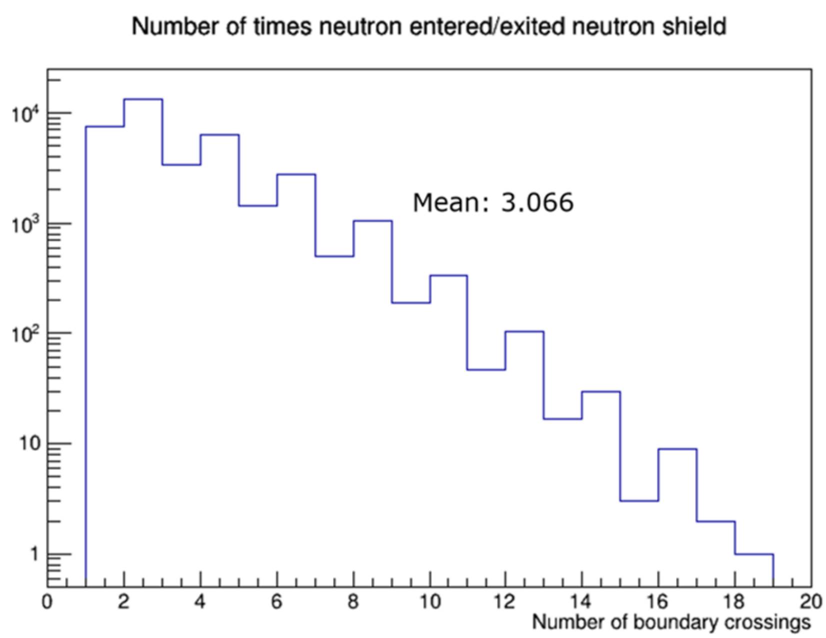

Figure 3: The number of times each neutron crossed the boundary between argon and PMMA, if it crossed at least once. The stepwise behavior is explained in text.

4.2 Scattering angles

The likelihood for a neutron to scatter depends on the nuclei available in the current material. Over 99% of liquid argon consists of the isotope ^{40}Ar. A PMMA monomer has a chemical formula of C5O2H8, so the available target nuclei are primarily ^{1}H, ^{12}C, and ^{16}O, with the largest secondary isotope being ^{18}O at about 2% natural abundance. Along with a relatively high scattering cross-section across a broad energy range, the nucleus of hydrogen is very close in mass to a neutron, which allows a greater maximum exchange of energy per scatter.

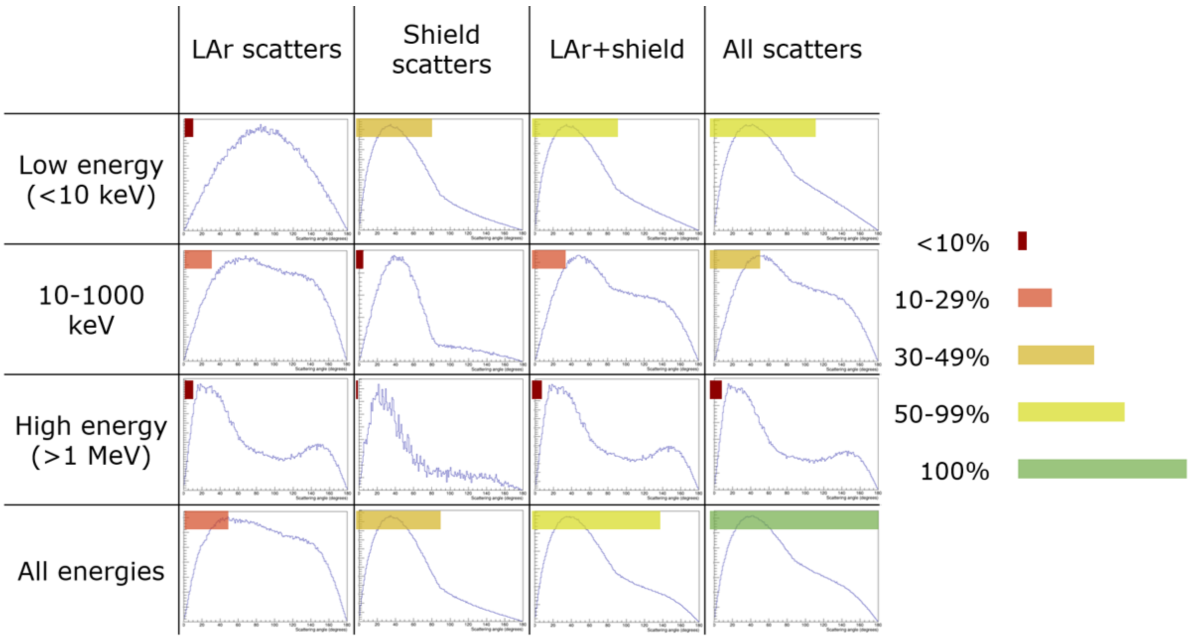

Figure 4: Plots for scattering angles in various materials and neutron energy ranges. Plots are from 0 to 180 degrees. The size of the colored bar represents its relative fraction of total scatters in the cryostat.

Fig. 4 summarizes the scattering angle distribution for neutrons in the liquid argon and in the shield, and the colored bars denote which fraction of all scatters each plot represents. A scattering angle of 0 represents nearly no deflection, and a scattering angle of 180 degrees represents total reversal of direction. Despite having a significantly smaller total volume than the LAr, almost half of scatters within the cryostat occur inside the shield. The mean scattering angle in the shield tends to be smaller than that of the liquid argon. This is again because of the similar masses - the hydrogen atom is forward-scattered along with the neutron, so to follow the principles of conservation of momentum, there is a maximum momentum transfer. In the case of the shield scatters, the tail at higher scattering angles is from scatters with the oxygen and carbon atoms, which can deflect the neutrons' momentum more strongly, but which have a lower cross-section. Statistics for scattering of higher energy neutrons are lower in the shield because neutrons tend to lose more energy per scatter, so high energy neutrons drop to a lower energy tier rather quickly. Finally, it should be noted that the top-left plot represents isotropic scattering. The reason the value seems to peak around 90 degrees is because the number of possible scattering directions is greatest at this value. To see the isotropic scattering more clearly would require a look at the post-scatter momentum of the neutrons.

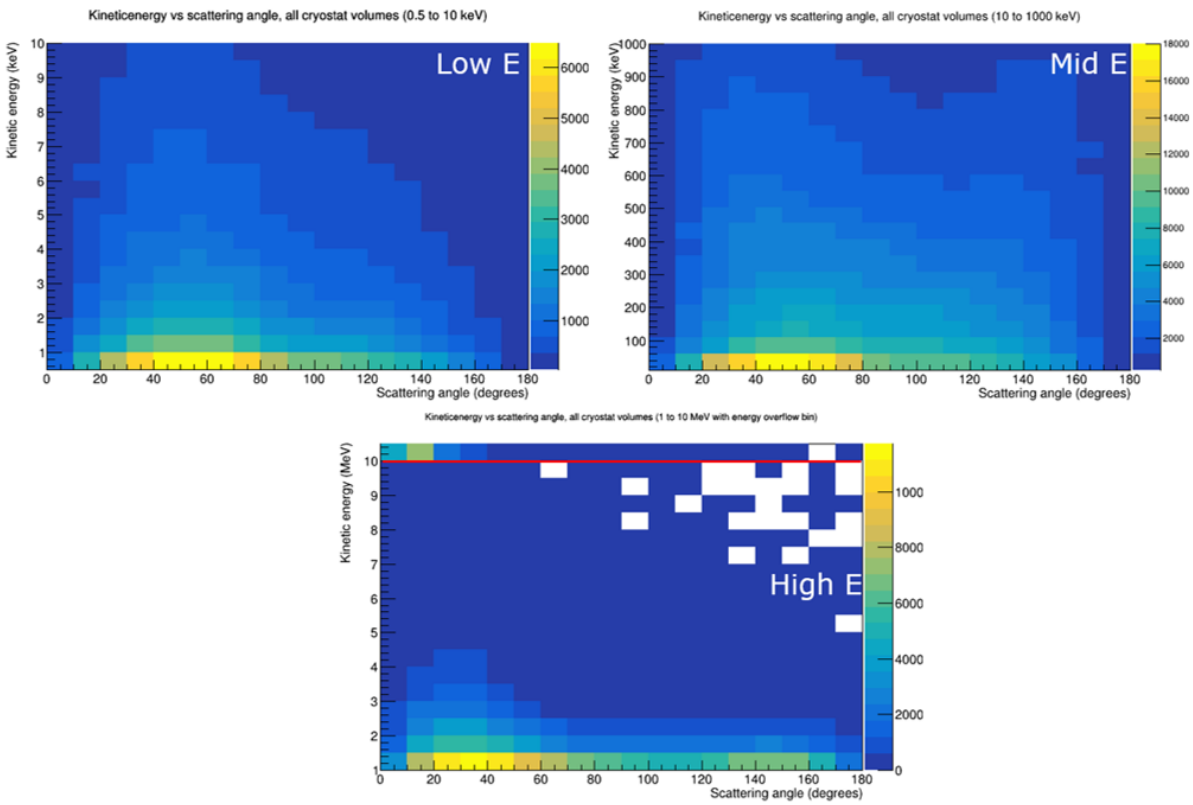

Figure 5: Scattering angle vs. kinetic energy (post-scatter) for neutrons up to 10 MeV. Neutrons above 10 MeV are included in the top row of the bottom plot as an overflow bin (above the red line).

The relationship between kinetic energy, energy transfer, and scattering angle is rather simple, but can be examined as well, in Figs. 5 and 6. The first is the post-scatter kinetic energy vs scattering angle distribution, and the second is the fraction of energy lost (or $\frac{\Delta E}{E}$) as a function of scattering angle in both materials. The first of these confirms the results of Fig. 4, and does not provide much more information, except for the overflow bin at the top of the third plot, which provides scattering angles for 10+ MeV neutrons which scatter elastically. These are predictably small, as the neutrons at these high energies are difficult to deflect elastically (inelastic scatters are not included). The second figure, however, shows a clear separation of the hydrogen, carbon, and oxygen scatters in the PMMA, as well as the mostly well-defined relationship between total energy loss and scattering angle. The 'fuzziness' of the values in the first plot must be due to the low kinetic energies of the incident neutrons in this region, but the precise cause of this is unclear.

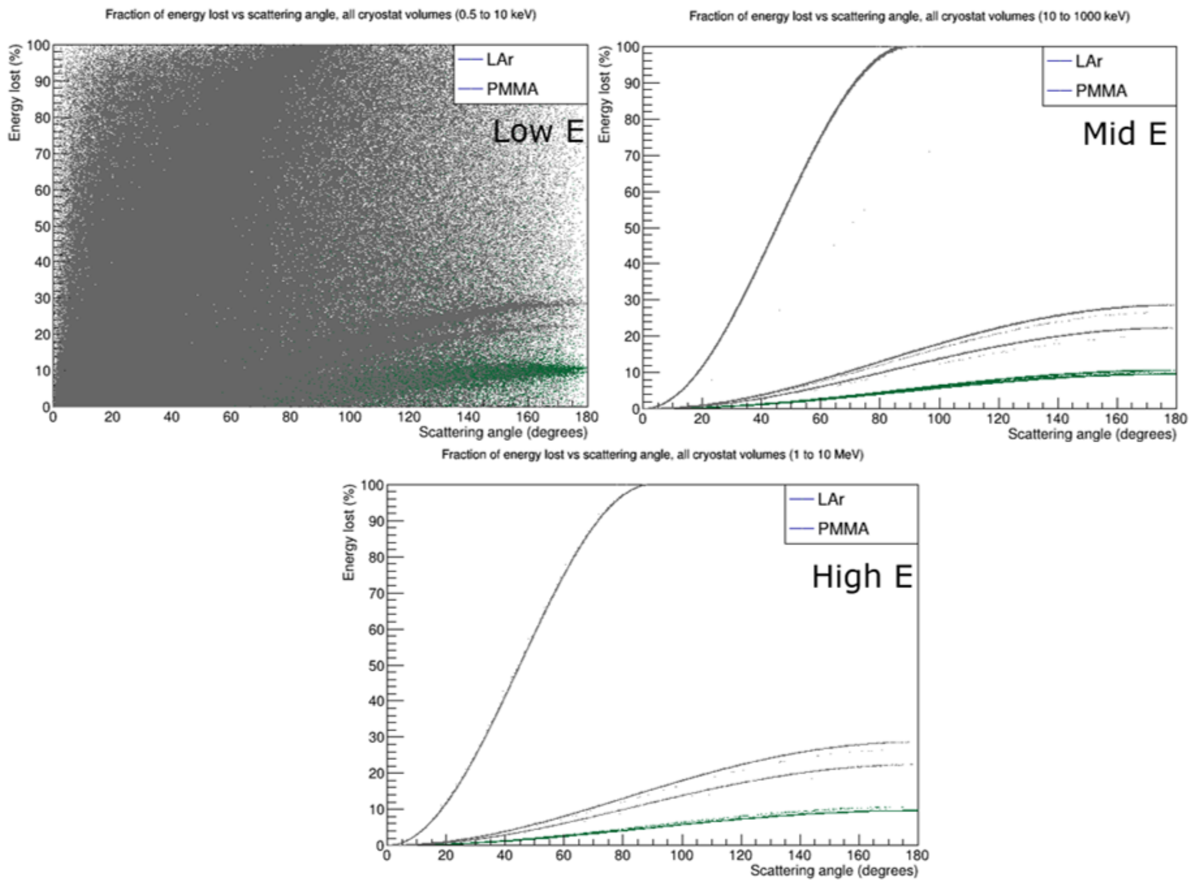

Figure 6: Fraction of energy lost as a function of scattering angle. The amount of energy loss for a given scattering angle is greatest for two equal mass particles (hydrogen), and decreases steadily from there to the heaviest participant (argon).

4.3 Neutron paths

Next, it can be instructive to study the paths of the neutrons - free path lengths (Fig. 7), total path lengths before absorption or exiting the cryostat (Fig. 8), and of course the distance which reflected neutrons penetrate into the shield (Fig. 9, transmitted neutrons are included for completeness, but these neutrons always make it through the full 100 mm thickness of the shield).

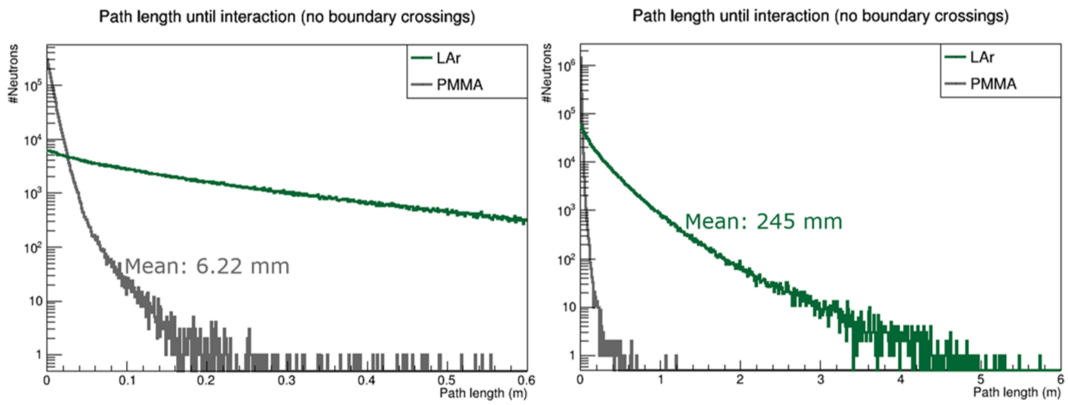

Figure 7: Path length between scatter events in each material. The mean free path is so different that it is difficult to visualize both curves on a single plot.

Of these, Fig. 7 provides the most clear information, especially regarding the mean free path of a muon-induced neutron in the PMMA shield. As expected, the free path follows an exponential distribution, due to the probabilistic nature of scattering. However, it is nonetheless important to not the very small value of the mean free path in the PMMA, as a result of the high scattering cross-section. It is possible for a neutron to travel more than 10 cm through the shield without interacting if it enters at certain positions and angles which result in propagating parallel to one of the walls of the shield, rather than towards the argon volume on the other side, although this is rare due to the specific requirements necessary.

Fig. 8 is related to both Fig. 1 and Fig. 7, with an essential distinction to be made. Fig. 1 represents the number of steps a neutron has in each material *uninterrupted*, i.e. without any boundary crossings. One neutron may have multiple entries in this plot. Some related distributions, such as the displacement from its creation point which a neutron may travel before capture, have been studied previously.

Fig. 9 confirms indirectly the important note made at the end of Sec. 4.1. Due to the nature of the random walk and the relatively short mean free path, neutrons are much more likely to reflect than to transmit through the shield. This is a double-edged sword - on the one hand, neutrons outside of the inner argon volume tend to stay outside, and away from the sensitive detectors. On the other hand, neutrons generated in the inner argon volume are more likely to reflect as well, and stay in the area where they threaten to capture on the germanium. This has a heavy impact on understanding the optimization of the shield dimensions.

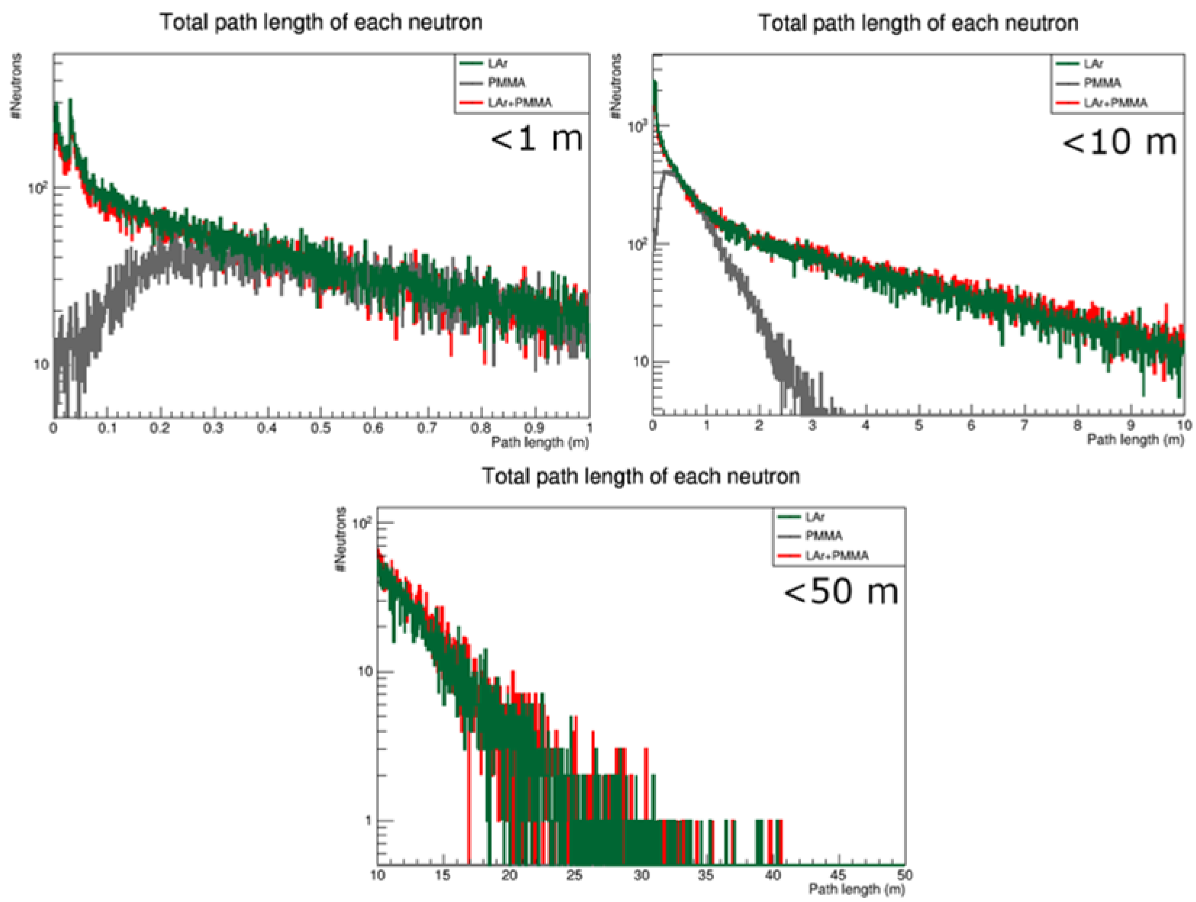

Figure 8: Total path lengths of neutrons within the cryostat. As with Fig. 7, it is difficult to visualize the two very different ranges one one plot without resorting to logarithmic scaling.

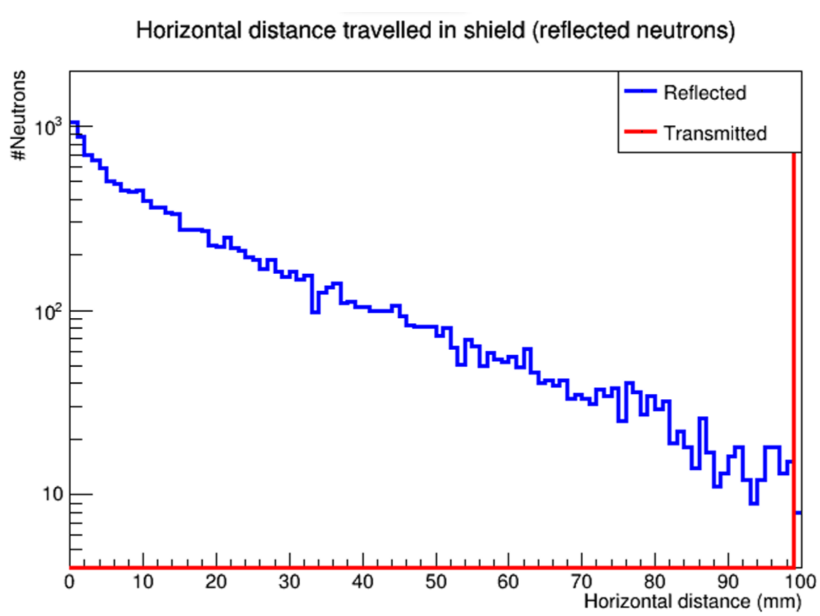

Figure 9: Maximum horizontal distance through the shield achieved by each neutron. A smaller subset was used, to discard less well-behaved events.

4.4 Energy loss

Finally, the energy loss of the neutrons in the cryostat will be examined. Here, some of the conclusions will be the most difficult to intuitively understand, so extra information will be provided as it is deemed necessary.

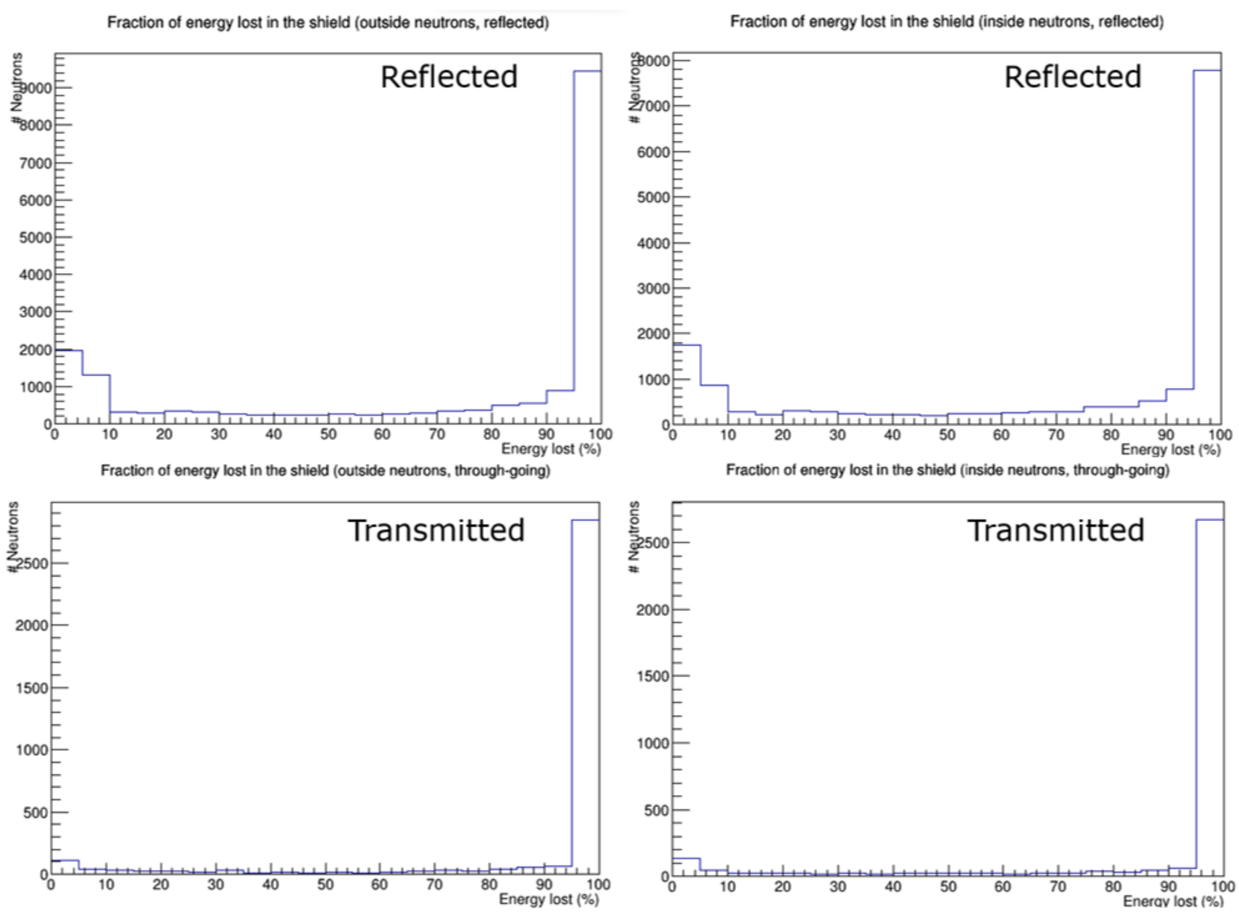

Figure 10: Fraction of total energy lost by each neutron which enters the shield.

The loss of energy by neutrons in the shield may be examined in a few different ways. Fig. 10 presents the fraction of energy lost by reflected and transmitted neutrons after traversing the shield. Again, neutrons which enter/exit the shield more than once will have more than one entry. An 'inside' neutron enters the shield from the inside wall; an 'outside' neutron enters the shield from the outside wall. As can be seen, transmitted (or through-going, in the plot) neutrons are moderated very effectively, although a very small fraction traverse the shield without losing very much energy, if any. It has been seen in Fig. 1 that reflected neutrons are highly likely to scatter only once or a few times prior to exiting. For this reason, it is understandable to have a population of neutrons which did not lose very much energy in the shield. However, even for this population, many neutrons lose most or all of their kinetic energy while in the shield. In both cases, the neutrons are still more likely to exit the shield than to be absorbed while in the shield.

At this point, it is necessary to include some context from plots presented by Michele

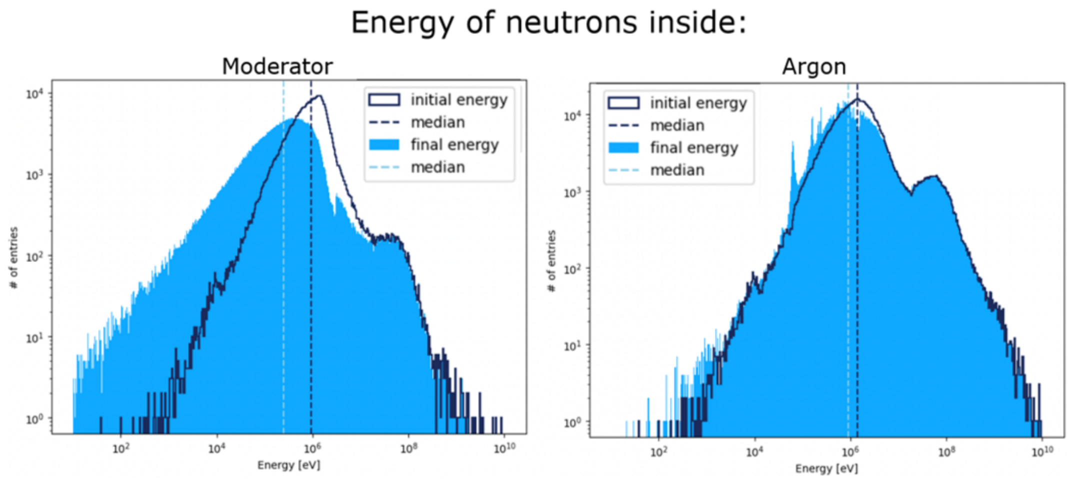

Figure 11: Neutron initial and final energies upon entering or exiting either volume of interest. Again, one neutron may have one, two, or more entries, depending on how many boundary crossings it experiences.

Morella from GSSI, who has been working on this effort in parallel via another branch of ItalSim. First, Fig. 11 plots the initial and final energies of neutrons while traversing either the argon or the moderator. The 'knee' which appears at high energies may be a result of competing processes of hadronic interactions for high-energy muons. Note the energy peaks and valleys in the final energy plots (blue). For the liquid argon, these correspond to neutron scattering resonances and antiresonances. A neutron which is propagating in the argon near a resonance energy is very likely to scatter again, so its final state upon exiting the argon is unlikely to be near a resonance energy. More importantly, the opposite is true for neutrons near antiresonance energies - the neutrons metaphorically fall into a 'well' where the argon is nearly transparent for them, and they can traverse great distances in the argon without interacting. Hence, it is very important to have a moderator material with a high scattering cross-section near the argon scattering antiresonances.

Next, Fig. 12 plots the *total* energy lost for neutrons while in each material, rather than the fraction of energy lost which was shown in Fig. 10. Here, there is a reversal from the previous paragraph - the energy loss curve is somewhat smooth in the argon, but there are noticeable peaks and valleys in the PMMA curve. Moreover, it is strange to observe these peaks when the neutrons may experience dozens of scatters within the shield, which should effectively smooth out any stochastic effects. This can be reconciled by once again considering the results in Fig. 10. A large majority of neutrons lose >95% of their total energy after traversing the shield. There are peaks and valleys in the final energy spectrum of neutrons exiting the liquid argon, in the previous paragraph. These neutrons which exit the argon are either entering the steel wall of the cryostat, or they are entering the shield. These neutrons enter the shield and lose >95% of their energy, creating the peaks and valleys observed in the most recent figures. If this seems confusing, consider that if Fig. 11 (right) was placed on top of Fig. 12 (left) with a matching x axis range, the peaks and valleys in each would match.

Another way to examine this is to plot the fraction of energy lost vs the initial kinetic

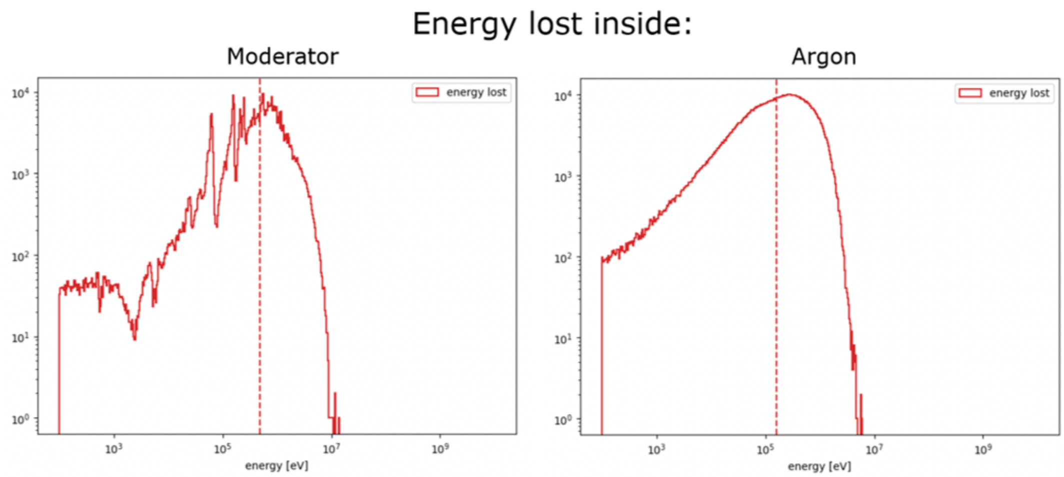

Figure 12: Absolute values of energy lost by each neutron as it traverses one of the relevant materials.

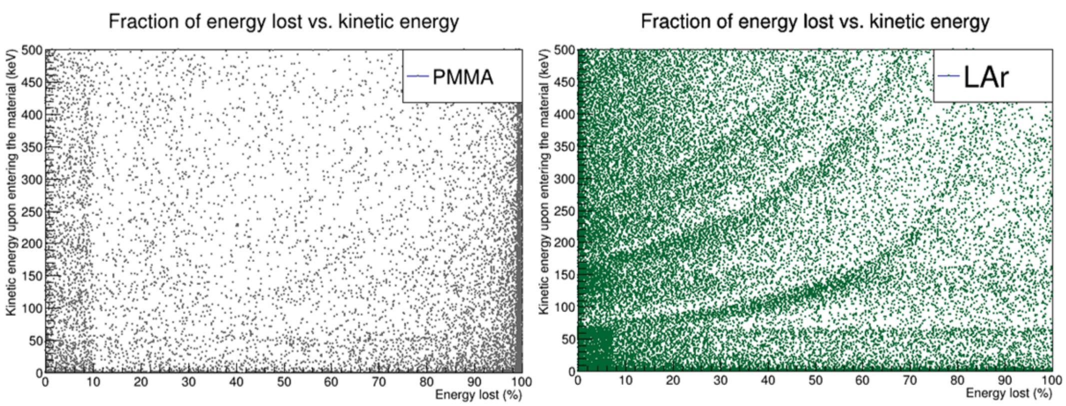

Figure 13: Neutron initial energy upon entering a material vs. the fraction of its total energy lost. The PMMA results confirm previous assumptions; the LAr results are discussed further elsewhere.

energy of the neutrons each time they enter one of the materials of interest, as in Fig. 13. The results for the PMMA are predictable: most neutrons lose almost all of their energy, while the remainder mostly lose only a small fraction, making this effectively a 2D projection of Fig. 10. However, there are visible features in the results for the argon. For visibility and completeness, this plot has been enlarged and included again in Fig. 14. However, this time a plot of the scattering cross-section on ^{40}Ar (from the Nuclear Energy Agency website) has been included along the side, and the energy ranges of the axes have been aligned. The magenta lines are at the center of the four strongest scattering antiresonances in the ENDF plot. The orange lines follow the trends for neutrons that fall into each scattering 'well'. For example, if a neutron with an initial energy of 115 keV (y axis) loses 50% of its energy (x axis), it will have an energy of 57.5 keV, and fall into the antiresonance centered at 57.1 keV. All of this is to say: the behavior of the neutrons around the scattering (anti)resonance energies plays a vital role in understanding the neutron propagation in the system, and the most direct effect this has is that the shield must have a high scattering cross section at all of the antiresonance energies.

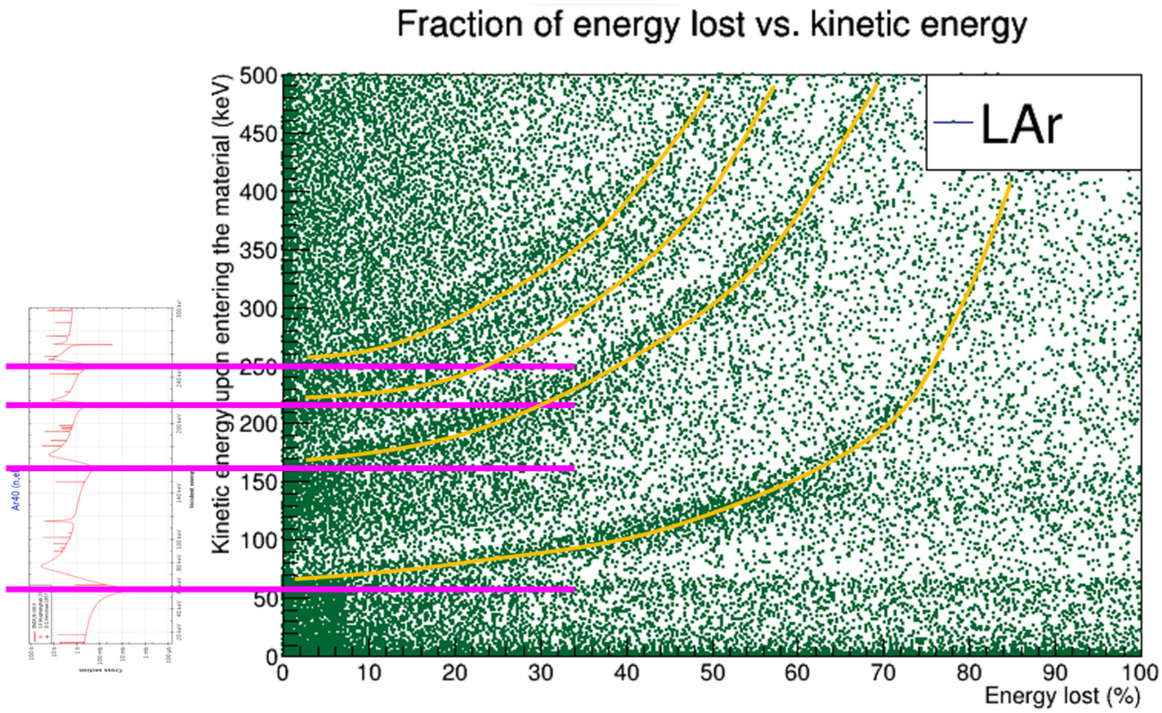

Figure 14: A larger version of Fig. 13 (right), emphasizing the relation between the antiresonance energies and the neutron final states upon exiting the argon.

A Glossary

Boundary crossing - In Geant4, when a particle moves from one material to another.
Cryostat - All LEGEND-1000 components which are inside of the outer water shield. This includes the double-walled steel cryostat, the copper reentrant tube, the ICPC germanium detector array, and the focal materials of this study, the liquid argon shielding and the PMMA moderator. Minor materials such as the fiber shroud and detector holders are not included.
Geant4 - A particle simulation framework based in C++ and maintained by SLAC, with ROOT integration. Link
Inside neutron - A neutron which originates, or enters the shield, from the inner liquid argon volume encapsulated by the shield.
ItalSim - See warwick-legend
MUSUN - MUon Simulations UNderground, a program designed to use the results of muon transport through rock/water to generate muons in or around underground laboratories taking into account their energy spectrum and angular distributions. Link
Outside neutron - A neutron which originates, or enters the shield, from the liquid argon volume outside of the shield.
Reflection - In this study, a neutron is reflected if it exits the shield from the same 'side' it entered. See Sec. 4.1 for more detail.
ROOT - A package written in C++ and maintained by CERN, useful for large-scale data collection and analysis. Link
Scattering (anti)resonance - A specific energy in a material in which neutrons are extremely likely (less likely) to scatter.
Shield - a.k.a. neutron shield, the solid plastic shield which is included in the LEGEND-1000@LNGS baseline design for the express purpose of moderating the muon-induced neutrons. The reasons for the dimensions and material choice of the shield have been extensively discussed in other LEGEND presentations.
Transmission - In this study, a neutron is transmitted if it travels fully through the shield. See Sec. 4.1 for more detail.
warwick-legend (WLGD) - A simulation module written in Geant4 10.7 which is used to simulate and analyze cosmogenic interactions for LEGEND. Github link A more recent repository has been developed and maintained by Moritz Neuberger on behalf of the Technical University of Munich group Github link And finally, the ItalSim version has been branched from the previous link Github link

B Unused plots

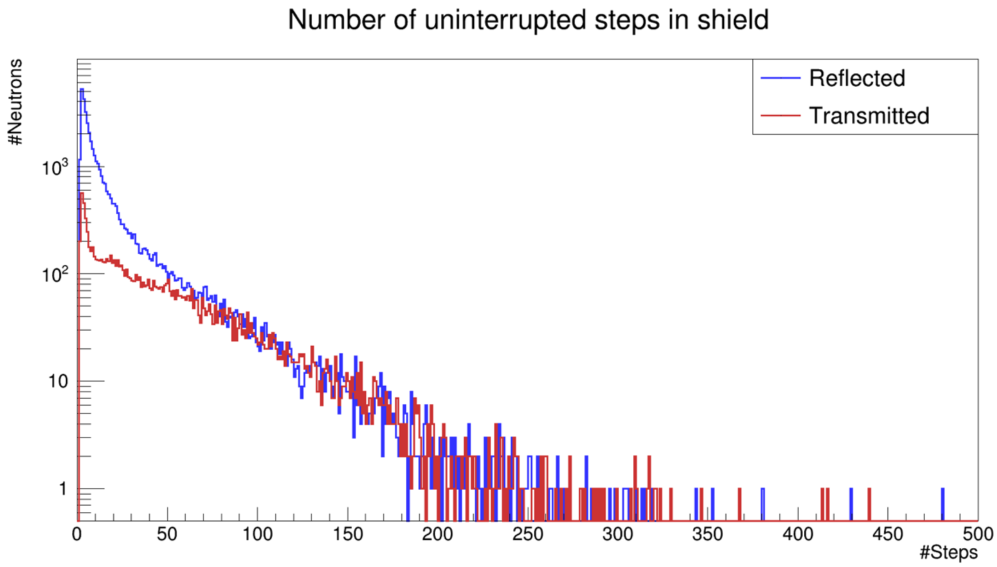

Figure 15: Similar to Fig. 1, except only for the shield, and the reflected/transmitted neutrons have been plotted separately.

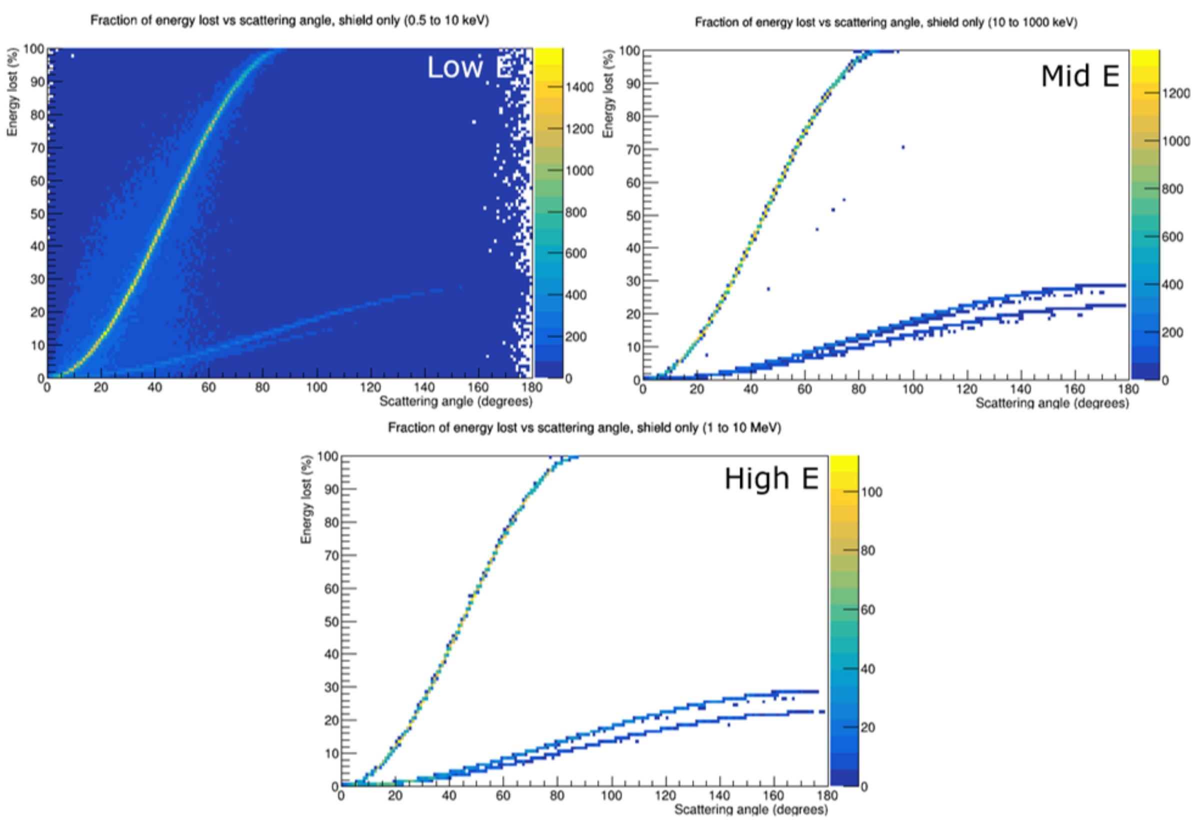

Figure 16: A "colz" version of Fig. 6, to check how many neutrons were actually creating all the fuzz in the first plot. Turns out they're quite a minority.

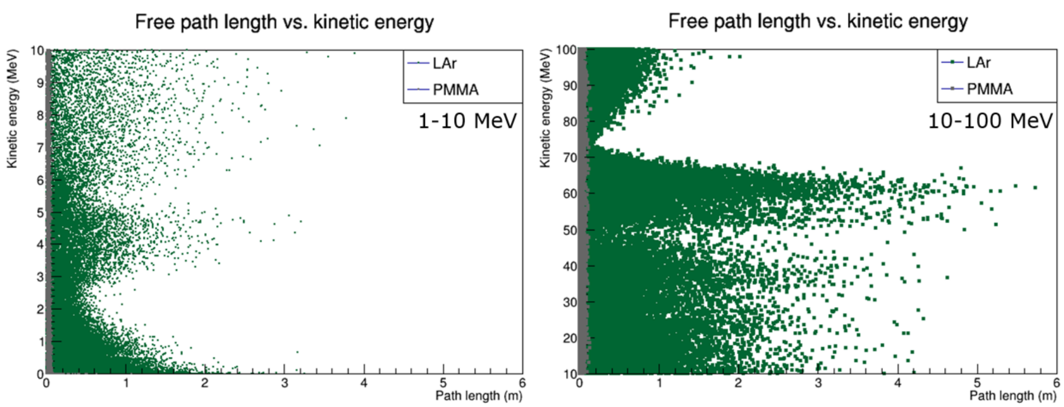

Figure 17: Path length between scatters vs. the neutron energy at the time of the scatter. I don't have much input for this one, and I especially don't want to get into a protracted discussion on the behavior of 10+ MeV neutrons in Geant4, so this plot is relegated to the appendices.