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Investigating the Simulation of Inelastic Neutron Scatters in the LUX-ZEPLIN Dark Matter Experiment

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1 Introduction

1.1 Dark Matter

Dark matter is one of the biggest remaining mysteries in modern physics. Despite conclusive evidence that dark matter exists we still don't know what it is despite decades of theories and experiments.

As early as the 1930s, J. H. Oort observed that stars in the Milky Way were moving faster then possible given the amount of visible mass [1] and F. Zwicky observed that galaxies in the Coma Cluster were moving in such a way that their mass must be much greater than their visible mass [2]. In the 1970s, V. Rubin and collaborators conducted an extensive survey of galaxies. Stars in these galaxies were observed to move at at a constant speed as distance from the galactic centre increased and as visible matter decreased [3]. This contradicts the decrease in velocity expected if only visible matter existed and lead to the conclusion that there must be invisible matter or 'dark matter' contributing to the gravitational pull.

Further evidence comes from the Cosmic Microwave Background (CMB). Although it is a highly uniform temperature at 2.73K the CMB contains fundamental temperature fluctuations. These fluctuations contribute to structure formation in the universe however, given the small size of CMB fluctuations the current structure of the universe wouldn't have had time to form based solely on these. This leads to the conclusion that an electrically-neutral form of matter i.e. dark matter must have been present in the early universe to kick-start structure formation [4]. The total and baryonic matter densities can be calculated from the CMB fluctuations, showing that the majority of the matter in the universe is actually dark matter at around 85% [4]. The effects of dark matter can also be seen in gravitational lensing and galaxy clusters, in other words there is no lack of evidence for dark matter. All that remains is to detect and identify it which is the aim of experiments such as LUX-ZEPLIN (LZ).

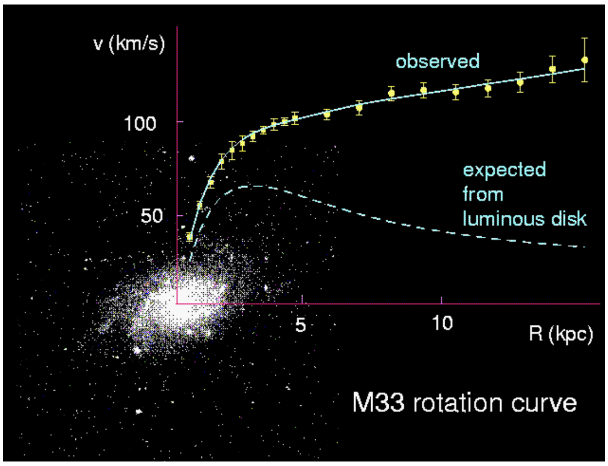

Figure 1: Image of M33 galaxy overlaid with graph of the observed rotational velocity against distance from galactic centre and the theoretical prediction calculated using only visible matter. The discrepancy between observation and theory indicates the existence of dark matter. Figure from [5].

1.2 WIMP Model

Weakly interacting massive particles (WIMPs) are a class of dark matter candidates. WIMPs have masses in the range roughly 1 GeV − 1 TeV, are electrically-neutral and only interact with matter via the weak force. They are non-baryonic (not made of quarks) and are produced thermally in the early universe. Although no WIMPs exist in the Standard Model there are several potential candidates in extensions to the Standard Model such as the neutralino in the supersymmetric extension. Statistical thermodynamic models allow the abundances of WIMPs to be predicted which have been found to be consistent with cosmological dark matter measurements, strengthening the position of WIMPs as the most prominent dark matter candidate [4]. Many experiments are attempting to find WIMPs through direct and indirect detection and through particle colliders. Direct detection experiments, such as LZ, aim to detect WIMPs from our own galactic dark matter halo as they pass through the Earth and interact with matter. WIMPs should undergo detectable nuclear recoils however, these would deposit such a low energy (1-100keV) that extremely sensitive detectors are needed to detect them. The nature of WIMPs also means these interactions would be very rare, meaning detectors need long exposure times to see any events.

1.3 LUX-ZEPLIN Experiment

The LUX-ZEPLIN (LZ) experiment is located 4850ft underground at the Sanford Underground Research Facility in South Dakota, USA. Its main aim is to directly detect WIMPs using a low background, multiple-detector set-up centered around a dual-phase time projection chamber (TPC) filled with 10 tonnes of liquid xenon (LXe) [6]. A dual phase TPC is shown in figure 2, when particles pass through the 7 tonne active region of the LZ TPC they interact with the LXe to produce scintillation photons and ionisation electrons. The scintillation photons are detected by photomultiplier tubes (PMTs) surrounding the TPC producing what is known as the S1 signal. An electric field causes the electrons to drift upwards where they produce a second scintillation on the xenon gas known as the S2 signal. Using the S1 and S2 signals a lot of information about the interaction can be determined such as the location within the TPC, if it is a nuclear or electron recoil and if it is a single or multiple scatter. The TPC is located deep underground to shield from cosmogenic radiation and submersed in a water tank for further shielding. It is surrounded by inner and outer detectors to produce veto signals for external and internal backgrounds which come from intrinsic radioactivity in the detector components, impurities in the LXe and environmental and cosmogenic radiation.

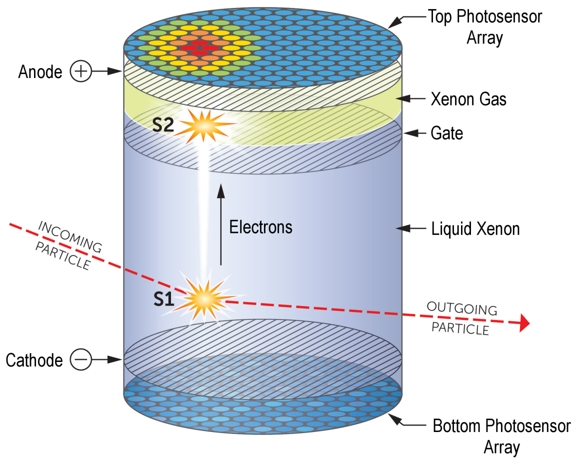

Figure 2: Diagram of a dual phase time projection chamber (TPC) showing the S1 and S2 signals produced by a particle interacting in the liquid xenon volume.

To achieve the sensitivity needed to detect WIMP signals, backgrounds must be completely accounted for. Calibration is performed to measure the detector responses to different background sources and inform a background model. Neutrons are a particularly dangerous background because low energy elastic neutron scatters can look identical to a WIMP signal. Neutron calibration is performed using a deuterium-deuterium (DD) generator, 2.45MeV mono-energetic neutrons are produced and sent down a conduit into the TPC as shown in figure 3. This allows the detector response to nuclear recoils to be calibrated which is where the WIMP signal will be found.

1.4 Project Aim

In previous research it has been found that there are 10 times as many single inelastic neutron scatters in data compared to simulation [8]. This suggests that there is an issue in the simulation of neutron scattering in the TPC which could have an impact on the neutron background predictions. A potential consequence of the modelling issue could be that a WIMP signal is mistaken for a neutron signal or vice versa. The aim of this project is to investigate the simulation of neutron inelastic scatters to try to determine and fix this issue.

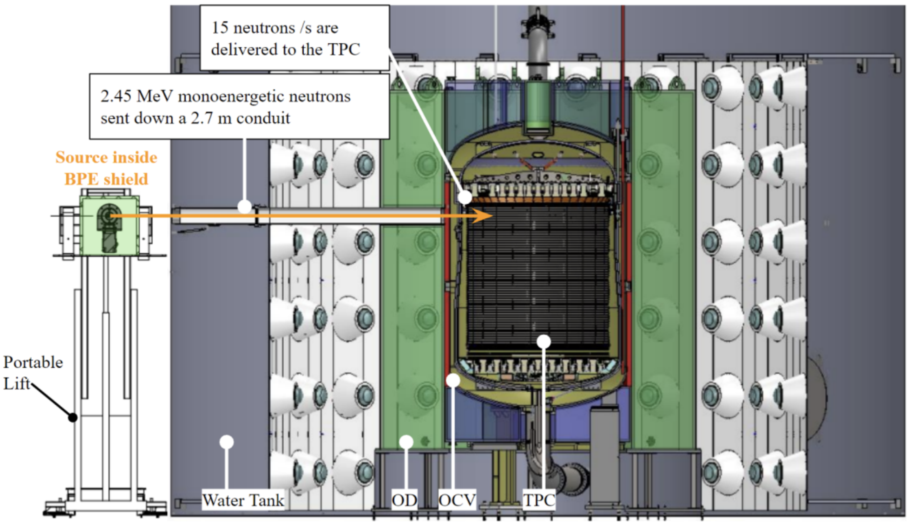

Figure 3: Diagram of LZ experiment showing neutron calibration set-up using DD generator. Figure from [7].

2 Methods

2.1 Simulation

BACCARAT (Basically, A Component-Centric Analog Response to AnyThing) is the LZ software for simulating particles and their interactions in the experiment. BACCARAT is based on Geant4 which is a set computation libraries for the Monte Carlo simulation of particle physics interactions. BACCARAT adds various packages to improve and tailor the simulation for LZ such as adding an improved xenon response [9]. Simulation allows the prediction and estimation of backgrounds which is extremely important in the detection of dark matter as discussed in the introduction. This project is interested specifically in the simulation of inelastic neutron scatters within the LXe TPC which will impact any neutron background model.

2.1.1 Installation and running

LZ uses the Perlmutter supercomputer at NERSC (National Energy Research Scientific Computing Centre) which is accessed remotely using a Secure Shell protocol (ssh). LZ uses GitLab to store all their software and BACCARAT can be cloned from the LZ repository to your user directory using `git clone git@gitlab.com:luxzeplin/sim/baccarat.git`. Once cloned and navigated to the baccarat directory, a specific environment must be used to run BACCARAT which is setup using shifter (`shifterLZ`) and `source setup.sh`. Finally it must be compiled using `make`. BACCARAT only needs to be compiled once unless the code is updated.

To run a simulation a macro is used and the command `BACCARATExecutable </path/to/macro.mac>`. The macro specifies many different simulation parameters. This project was interested in inelastic neutron scatters within the LXe TPC, therefore the macro was set to only record information in this volume using the line `/Bacc/io/setVolumeToRecord LiquidXenonTarget record=deposits,volumes, tracks`. The DD calibration neutron source was set as the generator of neutrons using the command `/Bacc/source/set DD 1.5 kBq`, the activity of 1.5kBq is irrelevant and has no effect. Additional commands for the DD source specify the experimental setup `/LZ/StraightNeutronTubeEmpty true` sets the straight conduit to be empty of water and `/LZ/UseNeutronTubeSmallBranch true` sets the small branch conduit to be used for Direct mode which is 2.45MeV neutrons [7]. Finally, the command `/Bacc/beamOn 500000` sets the number of events to 500000. Simulations were run for varying numbers of events but to get good statistics a large number like 500000 had to used since only around 2% of those neutrons actually reach the LXe TPC without interacting i.e. with 2.45MeV energy.

2.2 Data Analysis

BACCARAT outputs a ROOT file with the simulation data, JupyterLab was then used to analyse the simulation data. Firstly the LZ kernel was set up so all the packages needed were installed and the correct versions. The ROOT file was read in using the uproot library. The file contains 2 'trees' Run-Header, which stores the run-level information, and Events, which stores all the information specific to each event. Each event is uniquely labelled by an event id. For energy-only simulations, i.e. photon tracking off, Events stores header, primaries, tracks, deposits and volumes information. Initial processing was carried out on the data to find the events in which the neutron arrived at the LXe volume without losing energy, i.e. no interactions outside the volume, and underwent at least one inelastic scatter inside the volume. The BACCARAT output quantities that were used for this analysis are listed in appendix A.

To check the accuracy of the simulation, the energies of gammas released in inelastic scatters, the emission times of the gammas, the energy conservation of inelastic scatters, the total reaction cross sections and the number of scatters per event were investigated.

2.2.1 Gamma Energies

The gammas created from the de-excitation of xenon nuclei in inelastic neutron scatters are tagged as having a 'neutronInelastic' particle creator process in the simulation data so can be identified and traced back to the xenon isotope they were emitted from. The gamma energies should correspond to allowed nuclear transitions for the given isotope. Therefore the comparison of the gamma energies produced by the simulation with known values from nuclear databases such as NuDat3 allows the simulation to be checked. The maximum possible gamma energy is 2.45MeV since this is the initial neutron energy, this value is theoretically possible but highly unlikely since it represents the total transfer of energy from incoming neutron to xenon nuclear excitation and then to gamma ray.

2.2.2 Gamma Emission Times

The time between when the xenon nucleus is excited and the gamma ray(s) emitted can also be compared to known values. Certain states have a known half-life which allows the potential gamma emission times to be modelled and compared to the simulation data. For example, the most abundant isotope Xe129 has a first excited state of 39.6keV which decays to the ground state releasing a 39.6keV gamma, this has a known half-life of 0.97ns. By selecting the emission times of 39.6keV gammas and comparing the distribution to that found by using the exponential decay law and the half-life it can be checked whether the simulation is modelling emission times correctly. Some isotopes have long-lived states which are also known as meta-stable states. These states can have very long life-times such as Xe129m and Xe131m which have half-lives of 8.88 and 11.9 days respectively.

2.2.3 Energy Conservation

Another important thing to check was if energy was conserved in inelastic scatters. The incoming neutron energy should be equal to the sum of the outgoing neutron energy, the xenon recoil energy and the energy of any gammas emitted from xenon. The incoming energy is found by looking at the kinetic energy of the final step of the neutron, this is because when the neutron undergoes an inelastic scatter its tracking ends in the simulation data and becomes a 'new' neutrons i.e. it starts a new track with a new trackID. The outgoing energy is then found by summing the kinetic energies of the initial step of the product particles, these can be found as they will have a particle creator process 'neutronInelastic' and their parentID will match the trackID of the incoming neutron.

2.2.4 Reaction Cross Sections

Simulation reaction rates were compared to cross-section data from the ENDF/B-VIII.0 database by calculating weighted cross sections for elastic scatter, inelastic scatter and neutron capture reactions which take into account the abundance of each xenon isotope in the LXe volume. These abundances are given in table 4. For each isotope the cross section in barns for 2.45MeV neutrons for each reaction was taken from the database and then each multiplied by the abundance, then the weighted cross sections for each reaction added together to get 3 values which were then normalised. This can then be compared to simulation data by looking at the first step of each event and counting if one of the 3 reactions occurs, the numbers of each reaction are then normalised to compare to the weighted cross sections.

2.2.5 Single and Multiple Scatters

LZLAMA stands for LZ Light Analysis Montecarlo Application and it is software which is used to simulate the detector response given the volume energy deposits for example from the BACCARAT output. It can take the BACCARAT output and produce the S1 and S2 observables furthermore, it can classify each event as single scatter (SS) or multiple scatter (MS). If something isn't being simulated correctly, this could have a knock on effect in the LZLAMA output. To check if LZLAMA was classifying events correctly, an alternative method of classifying events as SS or MS was used. A clustering algorithm was implemented to group together energy deposits for each event. If the energy deposits are close enough together in time and space then they are classified as coming from the same scatter, if the total energy of the cluster is above a certain energy it is a detectable scatter. The parameters for this are given by the detector resolutions given in table 1. The specifics of the clustering algorithm used in this project closely followed that developed by P. Antonopoulos [10]. Once the energy deposits for each event are clustered, then each event can be classifies as SS or MS depending on the number of clusters it has and the results compared to LZLAMA.

z resolution	10mm
energy threshold	5keV
timescale	7μs

Table 1: Parameters for clustering algorithm.

3 Results and Discussion

The values of gamma energies produced by each isotope were found not to always match database values. Particularly in the case of Xe129 and Xe131, a lot of gamma energies that don't correspond to allowed nuclear transitions, i.e. 'fake' gammas, were produced by the simulation which are shown in figures 4. The results for other isotopes are shown in figure 8. The significance of Xe129 and Xe131 gamma energies being simulated incorrectly may be due to the fact that they have meta-stable states.

Analysis of gamma emission times shows that these meta-states aren't simulated correctly, in fact gamma emission times aren't simulated correctly in general. There are no gamma emission times longer than around 70ns as shown in figure 5 where we would expect some of a few seconds and even hours and days when taking into account the meta-stable states. Specifically looking at the meta-stable state of Xe131 which decays to the ground state with a single 163.9keV gamma, the emission times of this gammas are of the order of a few tens of picoseconds instead of days as expected (see figure 6). In general, the most common occurrence is the almost immediate emission time of a gamma ray and otherwise the emission times are generally very short. For example, the most common gamma ray in the simulation data is 39.6keV from the transition in Xe129. Figure 7 shows the gamma emission times from the simulation data next to a theoretical sample of gamma emission times demonstrating that the simulated emission times are all much too short.

When checking energy conservation in inelastic scatters, it was found that in 70.2% of inelastic scatters energy was conserved exactly and in 98.9% of inelastic scatters energy was conserved within $\pm$1keV. In the few cases where energy wasn't conserved within $\pm$1keV, the energy almost doubled which was caused by the total energy of the gammas being too large. These cases always occurred for inelastic scatters off Xe131 which produced almost all fake gamma energies. In most inelastic scatters even if fake gamma energies were produced, these added up to conserve energy but in these few cases they didn't.

The reaction cross sections showed good agreement with the ENDF data, the results can be seen in table 2.

The results of the single scatter (SS) and multiple scatter (MS) analysis are shown in table 3. The LZLAMA results showed that the majority of events were classified as MS. Although more MS events are expected given the interaction length of the neutron and the size of the LXe TPC, LZLAMA classifies almost all as MS which isn't accurate. This can be attributed to the gamma emission timing being incorrect, prompt emission of gamma rays causes LZLAMA to classify events incorrectly. Comparing to

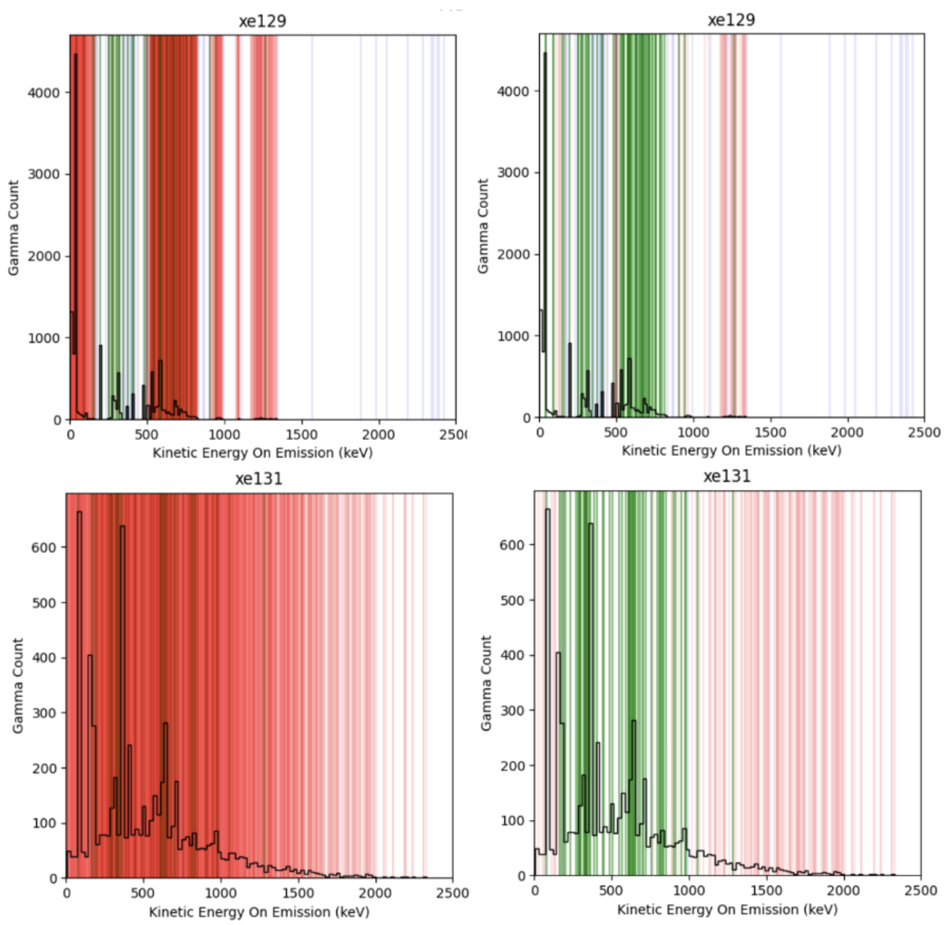

Figure 4: Histograms showing the distribution of energies of gamma rays emitted in the de-excitation of xenon isotopes Xe129 and Xe131 from the simulation of neutron inelastic scatters in the LXe TPC. The overplotted vertical lines classify the gama energies. Green shows gamma energies which correspond to allowed transitions from nuclear databases, red shows 'fake' energies and blue shows allowed energies which don't appear in the simulation data. The plots on the left define fake lines as those which don't match exactly a known energy and the plots on the right as those which are outside ±1keV of a known energy where the energies are rounded to integers. As the prevalence of red shows, the simulation is incorrectly modelling the gamma energies.

Reaction	ENDF	Simulation
Elastic Scatter	0.677	0.677
Inelastic Scatter	0.320	0.319
Neutron Capture	0.00264	0.00248

Table 2: Isotope weighted xenon cross section ratio comparison.

the results from clustering, there is a 9% more SS events from clustering confirming that LZLAMA isn't classifying the events correctly for this simulation.

Method	Single Scatters	Multiple Scatters
LZLAMA	1	99
Clustering	10	90

Table 3: Percentages of single scatter and multiple scatter events using 2 methods of classification LZLAMA and clustering.

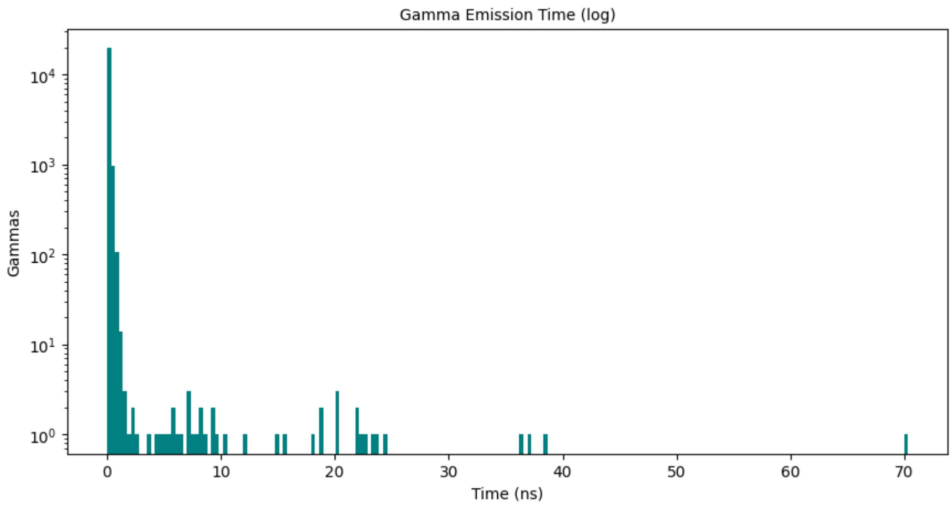

Figure 5: Histogram showing the distribution of gamma emission times for the first inelastic neutron scatter in each event. The emission times are all very low, with the majority of gammas emitted immediately after the inelastic scatter.

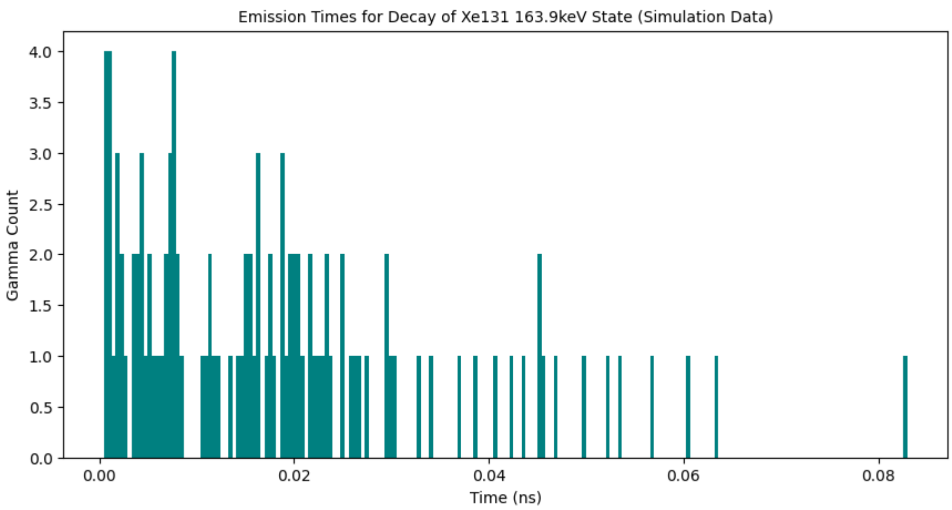

Figure 6: Histogram showing the distribution of emission times for 163.9keV gammas (decay of Xe131m). This transition has a half-life of 11.9 days which is not being simulated correctly as shown by the low emission times.

3.1 Updating Geant4

Further research shows that meta-stable states not being simulated properly in neutron inelastic scatters is a known problem. BACCARAT currently uses Geant4 v10.3. This issue is supposed to be fixed beyond Geant4 v10.4 however, after running another simulation using Geant4 v11.0 it was discovered that the meta-stable states are still not simulated correctly. The problem is that this isn't fixed if using the NeutronHP package which is what LZ uses in BACCARAT for a precise treatment of low energy (0-20MeV) neutrons. In order for the meta-stable states to be created and decayed correctly with appropriate decay times the RadioactiveDecay package must be used. Updating Geant4 did improve the simulation results in other ways; the energy conservation issue was fixed so that energy is always conserved over inelastic scatters and the overall number of fake gamma energies produced by the simulation was reduced, particularly in the low energy range. Plots for of the gamma energies using updated Geant4 are shown in figure 9.

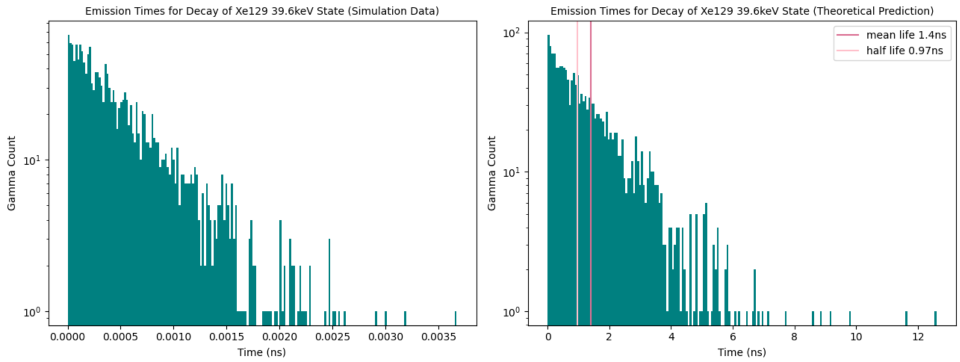

Figure 7: The histogram on the left shows the distribution of emission times for 39.6keV gammas (first excited state of Xe129) and the histogram on the right shows what this plot should look like based on the known half-life of the state 0.97ns. The simulated emission times are much lower than what they should be.

4 Conclusion

The cause of the discrepancy between data and simulation in the number of single inelastic neutron scatters was found. BACCARAT isn't simulating inelastic neutron scatters correctly, there are incorrect gamma energies, too short decay times and energy isn't always conserved. The meta-stable states of Xe129 and Xe131 aren't simulated properly, producing many incorrect gamma energies for these isotopes and prompt decay times which cause LZLAMA to wrongly classify events as multiple scatter. This issue isn't automatically fixed by updating Geant4, although this does improve some aspects of the simulation such as energy conservation. To simulate meta-stable states correctly, the RadioactiveDecay package must be used. Further work could look at testing this package and incorporating it into BACCARAT to improve simulation of neutron inelastic scatters and check its effect on neutron background predictions.

5 Acknowledgements

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A BACCARAT Output Quantities Used in Analysis

RunHeader Tree

- runHeader.processNames - Vector containing the processes name.
- runHeader.processIndexes - Vector containing the processes index to reconstruct the process name.

Event Tree

- header.eventId - ID of the event.
- track.particleNames - Particle name of the current track.
- track.particleIDs - PID of the current track for type of particle.
- track.particleTrackIDs - ID of the current track (i.e. index).
- track.particleParentIDs - Parent track ID of the current track.
- track.particleCreatorProcess - Creator process of the current track.
- track.step.processesID - Index of the Geant4 process name called at the end of the step, given by runHeader.processIndexes.
- track.step.kinEnergies_keV - Particle kinetic energy at the beginning of the step in keV.
- track.step.times_ns - Global Geant4 time of the step in ns.
- track.step.positions_x_mm - x position in mm.
- track.step.positions_y_mm - y position in mm.
- track.step.positions_z_mm - z position in mm.

B Liquid Xenon Composition

Xenon Isotope (Mass Number)	Abundance (%)
124	0.09
126	0.09
128	1.92
129	26.44
130	4.08
131	21.18
132	26.89
134	10.44
136	8.87

Table 4: Abundances of each xenon isotope within the liquid xenon taken from BACCARAT documentation.

C Gamma Energies For All Isotopes

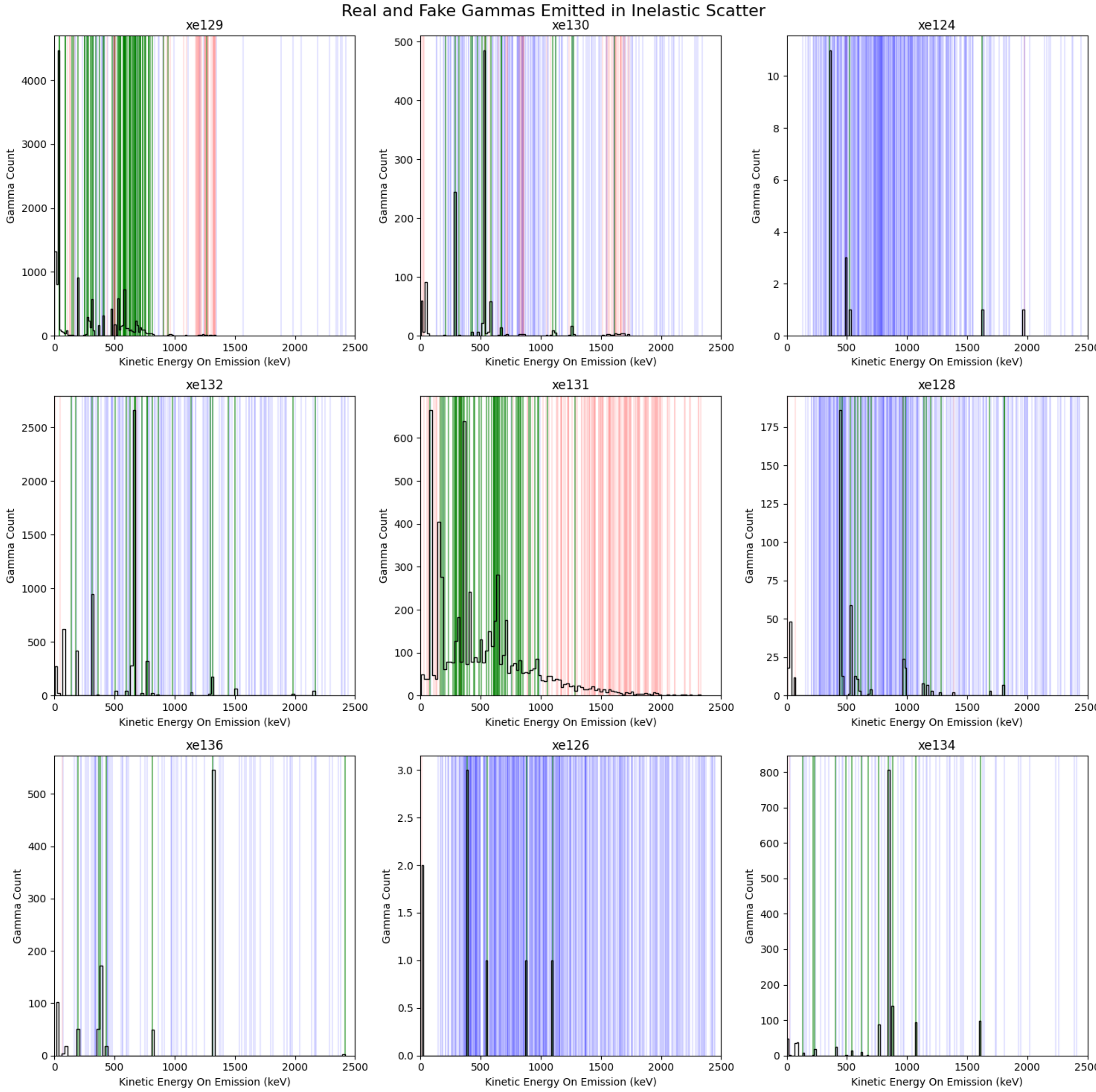

Figure 8: Histograms showing the distribution of energies of gamma rays emitted in the de-excitation of xenon isotopes from the simulation of neutron inelastic scatters in the LXe TPC. The overplotted vertical lines classify the gamma energies. Green shows gamma energies which correspond to allowed transitions from nuclear databases, red shows 'fake' energies and blue shows allowed energies which don't appear in the simulation data. In these plots the fake lines as those which are outside ± 1keV of a known energy where the energies are rounded to integers. Xe130 has a few fake gamma rays throughout and the other isotopes have fake gammas concentrated on low energies.

D Gamma Energies For All Isotopes with update to Geant4 v11.0

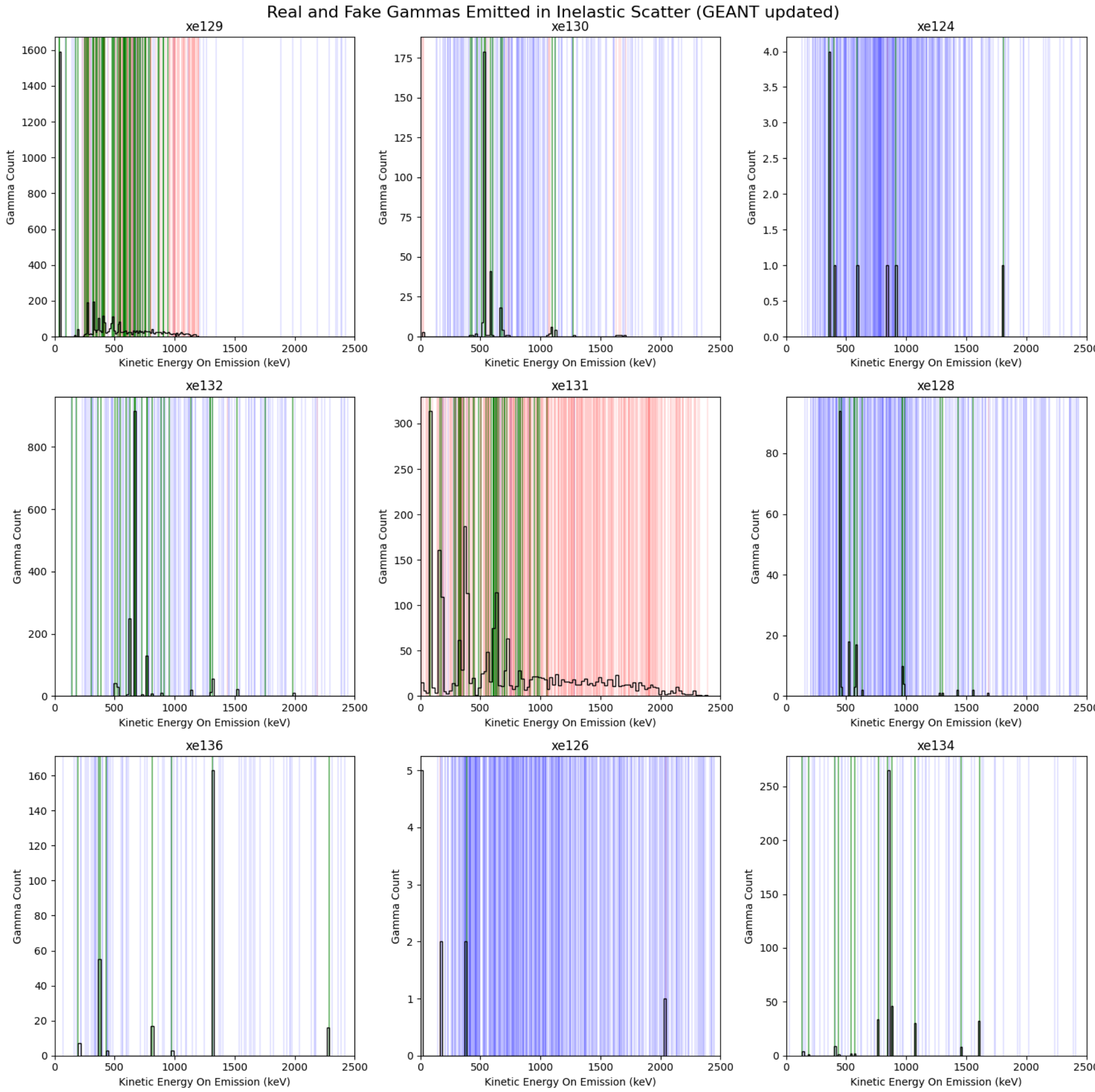

Figure 9: Same plots as figure 8 but using BACCARAT updated to Geant4 v11.0. Xe129 and Xe131 still have many fake gamma energies but the quantity of low energy fake gammas for other isotopes has decreased.

Personal Statement
This project helped me to develop several useful technical, as well as general, skills and experience. Technical skills such as using Linux terminal, using remote computers and Python programming were developed and improved. I gained experience with simulation, particularly in the context of particle physics experiments the important role Monte Carlo simulations play. I also learnt about being involved in large collaborations such as LZ, how they function and how to work as a team with people all over the world. I had to use my timetabling skills to complete the project on time and do my tasks. Problem solving was also developed, trying to fix issues without help and then working through issues with my supervisor and others and identifying paths forward. Finally, I gained further experience writing my report on how to write academically and succinctly and had my first experience making an academic poster.

Lay Summary
The LUZ-ZEPLIN (LZ) experiment aims to directly detect dark matter. Dark matter is an unknown substance that makes up around 85% of our universe but interacts so weakly that it's very difficult to detect and as of yet hasn't been detected. Since dark matter interacts so weakly experiments need to be extremely sensitive to detect these interactions. Background radiation passes through the LZ detector which can cover up the dark matter signal. Simulations are used to model these backgrounds. Neutrons can look like exactly like a dark matter signal making them an important background to quantify. This project investigated an issue with the LZ simulation of inelastic neutron scatters which could influence the background predictions. Simulations were performed and analysed, and it was found that the simulation was producing erroneous gamma ray energies and releasing them at incorrect times. A potential fix was identified in the computation packages.