

GEANT4 simulations on argon transparency to neutrons

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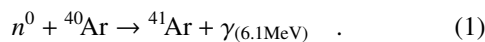
Abstract. As the largest neutrino experiment to date, the DUNE experiment will have record-sized detectors, of which some will be liquid argon time projection chambers (LArTPC). One of the candidate calibration methods for these detectors is the pulsed neutron source (PNS) calibration, which relies on an anti-resonance peak in the cross section of argon-40. The upcoming Argon Resonance Transport Interaction Experiment (ARTIE) seeks to confirm the existence of such anti-resonance peak and, thus, the feasibility of the PNS method. In this project, GEANT4 simulation results for the ARTIE experiment are presented. The results show the accurate reconstruction of the initial energy profile from the time signal, even with a 150 ns time smearing of the energy resolution. This reconstruction principle is the basis for ARTIE, thus indicating the upcoming experiment's robustness regarding its setup and methodology.

KEYWORDS: cross section, anti-resonance, scattering length

1 Introduction

One of the major oncoming physics experiment is the Deep Underground Neutrino Experiment (DUNE), the largest ever neutrino experiment. The proton accelerator at Fermilab will ensure a neutrino production, which will travel 1300 kilometres towards the Sanford Underground Research Facility (SURF). The experiment will have two main sets of detectors: near detectors (right after the neutrino production) and far detectors (underground at SURF). The latter will be a collection of record-sizes liquid argon time projection chambers (LArTPC).

Even though LArTPC technology is approaching maturity, the sheer size of the detector at DUNE means that there are several novel engineering problems involved in their development and operation. One of these issues is calibrating the detectors, for which a candidate method is the so-called pulsed neutron source (PNS) calibration. In such method, a source emits neutrons into the LArTPC, which, after being elastically scattered and losing its energy through Brownian motion, will be captured by the argon atoms through the following nuclear reaction:



The LArTPC itself then measures the emitted gammas, which allows for the determination and correction of the energy response across the volume.

To effectively calibrate the entire argon chamber through the PNS method, the neutrons need to be able to travel dozens of meters before being captured. Thus, the PNS calibration method relies on an extremely low value for argon's cross-section. As such, nuclear theory indicates that there is an anti-resonance peak in the cross-section for ${}^{40}\text{Ar}$ at 57 keV. However, the only experimental data available [2] focused on measuring resonance peaks and, thus, used less dense argon (in gaseous form) and had a precision of around 10^{-1} barns – far too high to record the anti-resonance phenomena (Fig. 1). As shown

in Tab. 1, estimating the anti-resonance peak of ${}^{40}\text{Ar}$ to be $\sigma = 10^{-3}$ barns yields a scattering length of 343 meters in pure ${}^{40}\text{Ar}$ and of 29 meters in natural argon [1].

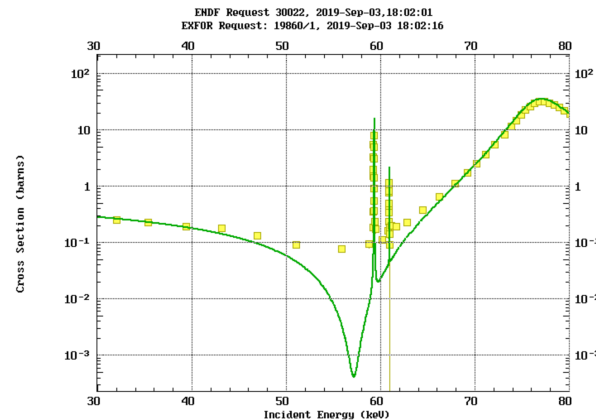


Figure 1. Total neutron cross-section data for ${}^{40}\text{Ar}$, including theoretical (green line) and experimental [2] (yellow markers).

The goal of the Argon Resonance Transport Interaction Experiment (ARTIE) at Los Alamos National Laboratory is exactly to confirm the existence of and characterize the anti-resonance peak at 57 keV and to determine natural argon's scattering length, thus confirming the feasibility of the PNS calibration method for DUNE's LArTPC far detectors. At the center of the setup is a 2-meter target filled with natural liquid argon – therefore much denser than in Winters's experiment [2] – surrounded by a vacuum jacket; kapton windows will be placed on each interface (Fig. 2). At 60 meters from the beam origin, there will be a neutron counter which records the time for each hit.

This project seeks to provide initial estimations for the ARTIE experiment and, by such, identify possible issues in its setup, data acquisition strategy, and reconstruction

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Isotope	Abundance (%)	σ at 57 keV (barns)	Contribution to σ (barns)	Scattering length (meters)
^{40}Ar	99.6035	1×10^{-3}	0.996×10^{-3}	343
^{38}Ar	0.0629	1.0	6.29×10^{-4}	542
^{36}Ar	0.3336	3.0	1.00×10^{-2}	34
Total			1.16×10^{-2}	29

Table 1. Argon isotopes and contributions to scattering length at 57 keV [1].

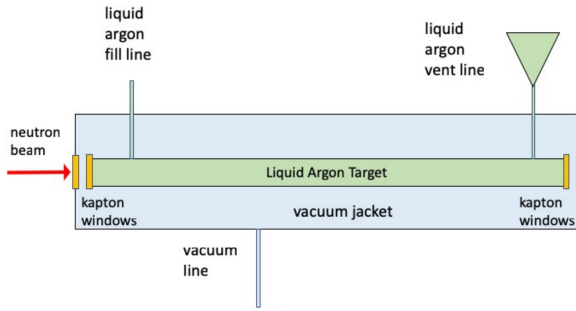


Figure 2. Illustration of ARTIE target setup [1].

methodology. All simulations were performed using a GEANT4-based program, developed in this project. GEANT4 is a detector-based simulation toolkit, especially focused on particle-matter interactions. This toolkit provides a C++ framework where the geometry, physics, and runtime behavior of particles and data can be customized.

2 Methods

As previously stated, this project's purpose was to predict ARTIE experimental results and identify possible issues with its setup. The GEANT4 simulations used the QGSP_BIC_HP¹ Reference Physics List, with subsequent analysis being done *a posteriori* on ROOT.

2.1 Geometry

The guiding point of the simulation's geometry was to include the main elements – gauged by their potential to affect the final result – of ARTIE's setup: the liquid argon target, six kapton windows, the surrounding air, and the aluminum envelopment structures (for the vacuum jacket and argon target).

The target dimensions followed ARTIE's proposal specifications [1], having 1.6 m in length and 25 mm in inner diameter. For the benchmark simulations, the target was vacuum. However, for the full simulations, the target was natural liquid argon, with its temperature and density defined as 87 K and 1.395 g/cm^3 , respectively.

The kapton windows were 4 mm-thick, following usual dimensions. The surrounding air amounted to a total of 2 m lengthwise, with equal parts before and after the target. The aluminum envelopes had a thickness of 4 mm.

¹Precompound *quark gluon string* model (QGSP), with GEANT4 Binary cascade (BIC) and high-precision neutron tracking (HP).

2.2 Sensitive Detectors

There were three sets of sensitive detectors (SD's) defined in the simulation: Counter, Target, and Windows. The Counter SD was positioned 30 m after the center of the argon target; since its purpose was to record arriving neutrons – and not their interaction with other particles – it was defined as 4 mm-thick vacuum. The two Target SD's consisted exclusively of the liquid argon part of the experimental target, divided in two SD's for easier profiling of the neutrons at the center of the target. The six kapton windows formed the remaining set of SD's, thus allowing for comprehensive profiling along the setup.

2.3 Beam configuration

The setup included a 5 mm-diameter neutron beam originating from 30 m before the center of target – i.e. 60 m away from the neutron counter. The beam emitted 10^7 neutrons per run, with their initial energy being linearly distributed on the 25 keV - 85 keV spectrum

2.4 Analysis method

Result analysis from the simulations focused on determining the accuracy to which the initial energy profile could be reconstructed from the time signal. A simple kinematics derivation from kinetic energy,

$$E_0 = \frac{1}{2}mv^2 \quad \text{and} \quad v = Lt^{-1} \quad ,$$

yields the framework for the energy-time relationship,

$$\hat{E}_0(t) = kt^{-2}, \quad k \equiv \frac{1}{2}mL^2 \quad . \quad (2)$$

Using benchmark simulations where the target's interior was vacuum, the time-energy data profile was fitted with a $f(x) = p_0x^{-2}$ function, where p_0 was the varying parameter. The resulting p_0 value was then compared to the theoretical value of $k = 1.8817 \times 10^{10} \text{ keV}\cdot\text{ns}^2$. Afterwards, the full simulation – with the target's interior as liquid argon – yielded the relevant time signal. In order to test for robustness, this time signal was contaminated with a 150 ns noise, following a uniform distribution in terms of E_0 . The modified time signal was then input into the reconstruction function $\hat{E}_0(t)$. A statistical comparison between the resulting \hat{E}_0 and the original E_0 profiles determined the accuracy of the reconstruction method.

3 Results

The main simulation results are hereto presented, focusing on five main topics: the evolution of the undisturbed beam's profile along the setup; neutron-capture reactions on the liquid argon target; the nature of neutrons that reach the counter; the initial energy and time-of-flight of these neutrons, including the correlation between these two variables; and time-energy reconstruction results.

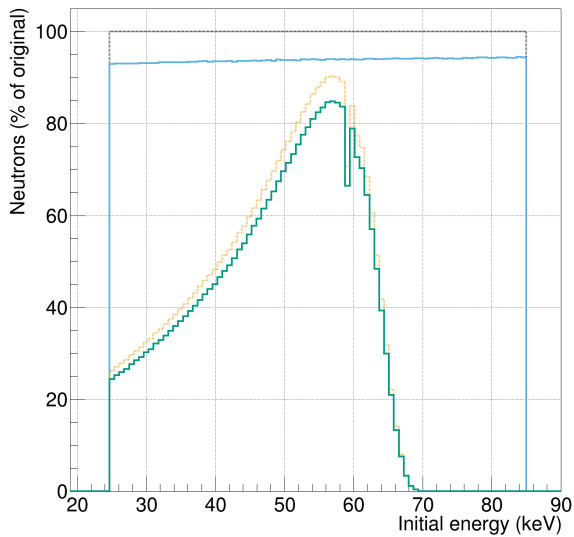


Figure 3. Initial energy of non-interacting neutrons at different locations: initial (*dashed black*), beginning of argon target (*solid blue*), end of argon target (*dashed orange*), and counter (*solid green*).

The nine SD's positioned along the setup allowed for a comprehensive profiling of the beam at different locations. Each component of the setup acts as a filter on the beam, rejecting – i.e. interacting with – neutrons of certain energies, while bypassing – i.e. not interacting with – neutrons of other energies. Fig. 3 highlights this effect by showing the initial energy profile of undisturbed neutrons (normalized in respect to the initial beam profile) at four important locations: first kapton window, entrance of liquid argon target, exit of liquid argon target, and neutron counter.

As mentioned in Sec. 1, neutron-capture reactions emit gamma particles, which may negatively affect experimental readings. Figs. 4 and 5 show, respectively, the position of these emissions and the initial energy of the captured neutrons. Out of the 10^7 original neutrons, a total of 1.4×10^4 underwent this reaction.

The main variables of interest for this project were the initial energy (E_0) of neutrons that reached the counter and their time-of-flight (T). Their correlation is shown as a profile – for full simulations (Fig. 6) – fitted with the $\hat{E}_0(t)$ estimator (Eq. 2). As shown, the fitted value $\hat{k} = 1.8799 \times 10^{10}$ is 0.1% off the theoretical value k . Fig. 7 shows the reconstructed energy profile (\hat{E}_0), with the original energy profile (E_0) in the background for visual com-

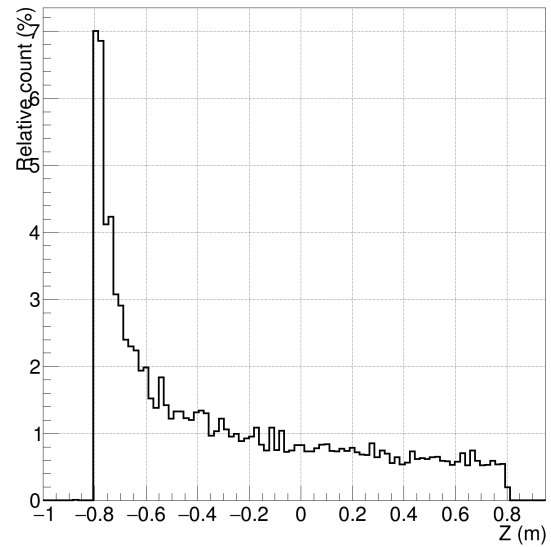


Figure 4. Position of gamma emissions inside target.

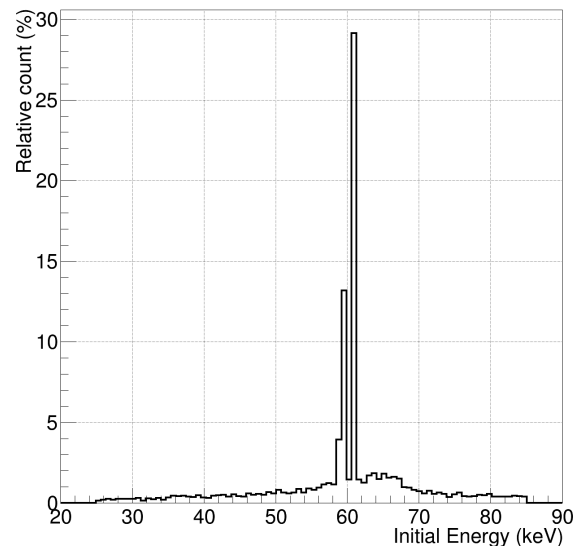


Figure 5. Initial energy of captured neutrons.

parison. Lastly, Fig. 8 plots the absolute and relative bias in performing this reconstruction.

4 Discussion

As the beam needed to travel through kapton and air, one of the main concerns before the simulations was the possibility of these materials significantly altering the energy profile of the beam through scattering mechanisms, thus introducing a bias in the beam's profile that could mask or disrupt the liquid argon's effects – which itself was the experiment's goal. The beam filtering effects from both kapton and air have almost no energy dependence and are relatively small ($\leq 5\%$).

The neutron-capture data relative to the liquid argon target (Figs. 4 and 5) show that the corresponding nuclear

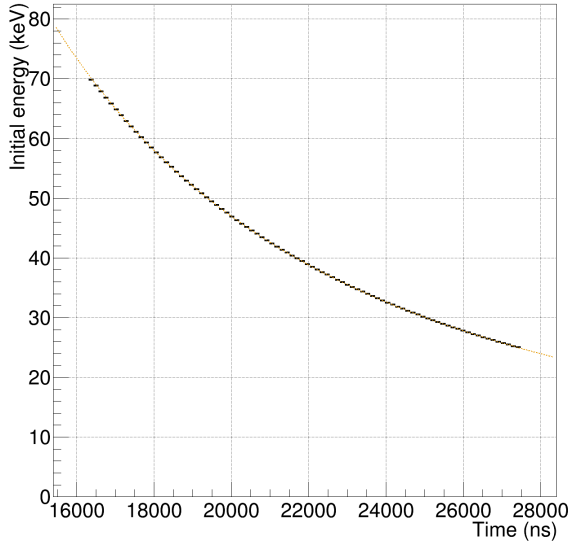


Figure 6. Time-energy profile of neutrons at counter, with fit $f(x) = \hat{k}x^{-2}$, $\hat{k} = 1.8799 \times 10^{10}$.

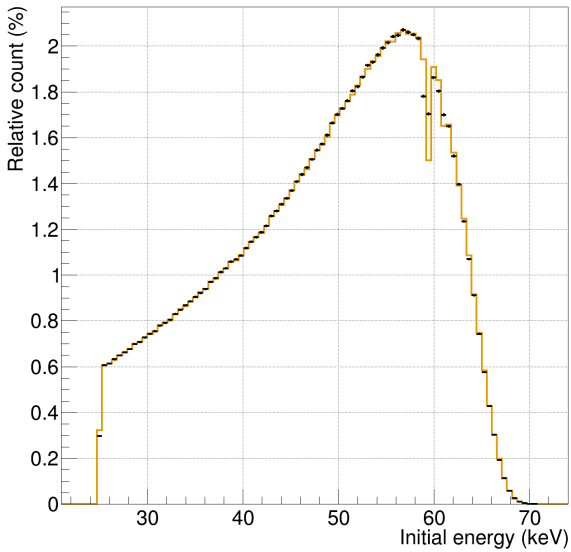
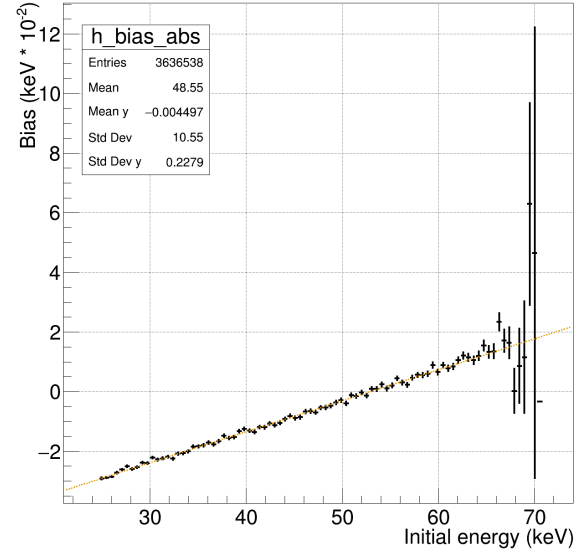


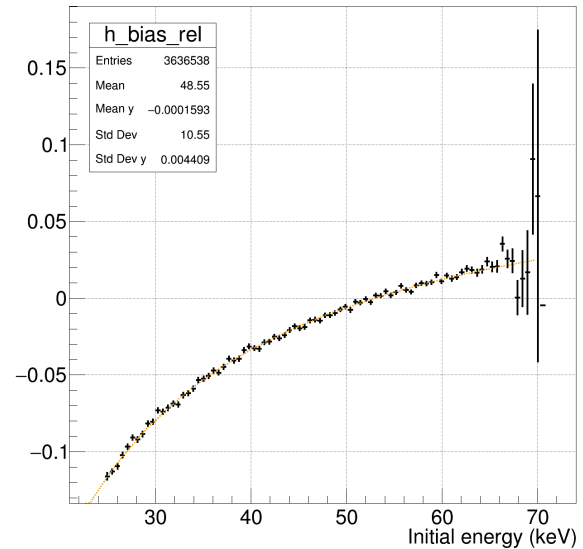
Figure 7. Reconstructed energy \hat{E}_0 (black markers) and initial energy E_0 (orange line) profiles.

reaction (Eq. 1) rarely happens, and when it does, it occurs at the beginning of the target, far from any sensitive equipment that could be disrupted by the resulting gamma rays. The two peaks in Fig. 5 show that most of these neutron-capture reactions result from neutrons with an initial energy of 59 keV and 61 keV, thus corresponding to the resonance peaks in the ^{40}Ar cross-section data (Fig. 1). These peaks in turn result in corresponding troughs in the E_0 profile after the beam passes through the argon target (Fig. 3).

An important goal of the experiment setup is to avoid the contamination of the counter data with neutrons that had previous interactions. A trivial analysis of the `fNhits` variable² and the radial position for counter hits indicated



(a) Fit: $f(x) = p_0 + p_1x$, $p_0 = -5.5005$, $p_1 = 1.0397 \times 10^{-1}$



(b) Fit: $f(x) = p_0x^{-1} + p_1$, $p_0 = -5.4994$, $p_1 = 1.0395 \times 10^{-1}$

Figure 8. Bias plots for \hat{E}_0 : (a) absolute, (b) relative.

that all hits were direct, which helps ensure a cleaner data set for the actual experiment.

As shown in Fig. 7, the reconstruction method manages to obtain values for \hat{E}_0 that closely reach the actual E_0 profile, having an average bias of -4.5×10^{-5} keV (1.6×10^{-4} %). Even though there is noticeable smearing of the 59 keV and 61 keV resonance peaks, both continue to be well identified. The absolute and relative bias plots shown in Fig.8 indicate that the lowest bias occurs for neutrons in the 50 keV -60 keV range, which ends up being a very positive result, since it coincides with the 57 keV region of interest.

²The `fNhits` variable records the numbers of interactions per run, i.e. of each neutron emitted and other subsequent particles created. For these simulations, full particle tracking (i.e. not only for creation events) was set up only for neutrons.

5 Conclusion

The main goal of this project was to obtain simulation estimations of the oncoming ARTIE experiment, thus identifying possible issues in the setup, data acquisition, or reconstruction method. As such, the simulations did not raise alarms in the aforementioned areas, but rather indicated their robustness. The initial energy profile was accurately reconstructed – even after introducing 150 ns noise in the time signal – clearly showing natural argon’s anti-resonance peak. Therefore, the authors are optimistic that ARTIE will experimentally confirm and measure this anti-resonance.

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