Search for Higgs Portal Scalars and Heavy Neutral Leptons Decaying in the MicroBooNE Detector

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Abstract

This thesis presents a search for Higgs Portal Scalars (HPS) and Heavy Neutral Leptons (HNL) decaying in the MicroBooNE liquid argon time projection chamber (LArTPC). The measurement was performed using data collected in-time with the Neutrino at the Main Injector (NuMI) beam with a total exposure corresponding to $7.01 \times 10^{20}$ protons on target. Mono-energetic HPS and HNL would be produced from kaons decaying at rest in the NuMI hadron absorber, before travelling $\sim 100$ m to the MicroBooNE detector where they decay. A single selection and search strategy is used to target decays of HPS to $\mu\mu$ pairs and HNL to $\mu\pi$ pairs. The results are expressed as limits, at the 90% confidence level, on the mixing angles that control the rates of production and decay for each new particle. For the HNL model, upper limits are set on the mixing parameter $|U_{\mu 4}|^2$ in the range $[12.9 \times 10^{-8}, 0.54 \times 10^{-8}]$ for HNL with masses in the region 246–385 MeV. For the HPS model, limits on the scalar-Higgs mixing angle $\theta^2$ are set, excluding a region with a lower boundary between $[31.3 \times 10^{-9}, 1.09 \times 10^{-9}]$ and an upper boundary between $[2.50 \times 10^{-5}, 5.05 \times 10^{-9}]$ for scalars with a mass of 212–275 MeV. These results set the first constraints in this region of parameter space from a dedicated experimental search for HPS.
Declaration

I declare that no portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.
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I am especially grateful to Davide Porzio, who passed away last year. The work performed in this thesis would not have been possible without his ingenuity and determination in pioneering MicroBooNE’s first HNL search. His passion and patience made him as good a mentor in the first years of my PhD as anyone could have hoped for. More importantly, I am grateful to him for his kindness, his generosity, for making sure I (and everyone else) were always included in the social life of the department, and for the many interesting conversations we shared.

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1 Introduction

The existence of dark matter, neutrino mass and the matter-antimatter asymmetry of the universe are not explained by the Standard Model (SM) of particle physics. An extension to the SM is therefore required. Two minimal extensions to the SM are considered in this thesis, Heavy Neutral Leptons (HNL) and Higgs Portal Scalars (HPS). Each of the corresponding models introduces a hidden-sector—new particles with highly-suppressed interactions with the SM—which account for the unexplained phenomena while maintaining consistency with the extensive experimental tests of the SM.

The two models considered are theoretically distinct, but produce similar phenomenology at the MeV to GeV energy scale that is relevant for neutrino experiments. In both cases, new unstable particles are produced in meson decay. These particles have lifetimes long enough to travel $10^2$-$10^3$ m from their production point before they decay to SM particles. These new particles are collectively referred to as Long-Lived Particles (LLPs). This work is a search, using the MicroBooNE detector, for a shared detector signature which is produced both by HNL decaying to muon-pion ($\mu^\pm \pi^\mp$) pairs and HPS decaying to muon-muon ($\mu^+ \mu^-$) pairs.

The MicroBooNE detector, located at Fermilab, is a liquid argon time projection chamber (LArTPC) which collected accelerator neutrino beam data between 2015 and 2020. The detector received an on-axis neutrino flux from the “Booster Neutrino Beam” (BNB) and a highly off-axis flux from the “Neutrinos at the Main Injector” (NuMI) beam. HPS and HNL could be produced alongside neutrinos in both beams.

This thesis focuses on potential LLP production in the NuMI hadron absorber via kaons decaying at rest. The hadron absorber is located downstream of MicroBooNE at the end of the NuMI decay pipe. LLPs in the absorber would approach the detector in almost the opposite direction to the vast majority of neutrinos, which come from the beam target. Since the LLPs are produced by two-body decays of kaons at-
SECTION 1. INTRODUCTION

rest, they will be mono-energetic. These two features are used to discriminate the
potential LLP decays from the large neutrino background and increase MicroBooNE’s
sensitivity to the models.

Section 2 describes the theoretical motivation and phenomenology of the two
models in more detail. The detection principles, design and operation of LArTPCs, as
well as a description of the MicroBooNE detector, are outlined in section 3. Section
4 describes the NuMI neutrino beam, including the simulation of the neutrino flux
that MicroBooNE receives and the modeling of the kaon decays in the absorber.
The methods and software used for simulating and reconstruction of MicroBooNE
data are described in section 5. The section also covers the tools specific to LLP
generation and the data samples produced and used for this analysis. Section 6
describes the techniques used to identify LLP decays and the first stages of the
selection of LLPs from the neutrino and cosmic-ray background. Boosted Decision
Trees (BDTs), described in Section 7, are used to further distinguish signal from
background and construct the final variables on which a search is performed for
an excess of data over background prediction. In section 8, the methods used to
estimate the various systematic uncertainties which impact the results of the analysis
are discussed. Section 9 presents the final results and exclusion region contours for
both models.

In addition to the LLP search which makes up the main body of this thesis, a
selection and analysis of ProtoDUNE-SP test beam data was also conducted. The
analysis, which is described in section 3.4, was published in the first data results
paper from the DUNE collaboration [1]. Although not included in this thesis, the
author produced the HNL flux simulation and associated uncertainty estimates for
the previous MicroBooNE HNL search, developed primarily by Davide Porzio. The
results of the search were published in a paper in Physical Review D [2].
2 Hidden Sector Searches

This section details the theoretical background of the two LLP models considered in this thesis, with a focus on the phenomenology relevant to developing a search strategy. The experimental methods which have been used to probe these models and pre-existing constraints on the parameter space are discussed.

2.1 Higgs Portal Scalars

The majority ($\approx 84\%$) of the matter in our universe is not accounted for in the SM [3]. A large number of astrophysical and cosmological observations suggest the existence of large amounts of non-baryonic matter which appears to only interact gravitationally. This matter is referred to as dark matter. Observations require the dark matter to be stable and non-relativistic and therefore there is no particle candidate in the current SM. Many particle-based dark matter models require a depletion mechanism of dark matter in the early universe to account for the current relic abundance. This mechanism motivates the search for small but appreciable non-gravitational interactions between dark and visible matter [4].

One possible source of interactions between the SM and dark matter particles is via a new electrically-neutral real singlet scalar boson ($S$) that interacts through the Higgs portal [5]. The extended Lagrangian of the model can be expressed as

$$
\mathcal{L} = \mathcal{L}_{SM} + \mathcal{L}_{DS} - (AS + \lambda S^2) H^\dagger H,
$$

(2.1)

where $\mathcal{L}_{SM}$ is the SM Lagrangian and $\mathcal{L}_{DS}$ is the Lagrangian of any new dark sector containing one or more new dark matter particles ($\chi$). The Lagrangian $\mathcal{L}_{DS}$ can then include interaction terms between dark matter and the Higgs Portal Scalar (HPS). Here, $A$ and $\lambda$ are two renormalisable portal couplings between the scalars and the SM Higgs field doublet ($H$) [6].
The new scalar particle acquires small couplings to Standard Model particles via mass mixing with the Higgs boson. After electro-weak symmetry breaking and diagonalisation, the Lagrangian of the scalar interactions appears as

\[
\mathcal{L} \supset -\frac{1}{2}m_S^2 S^2 + \sin(\theta) S \left( \frac{2m_W^2}{v} W^\mu W^\mu + \frac{m_Z^2}{v} Z^\mu Z^\mu - \sum_f \frac{m_f}{v} \bar{f} f \right),
\]

where the two relevant parameters, \( m_S \), the mass of the scalar and \( \theta \), the coupling constant which governs the magnitude of the scalar-Higgs mixing, are introduced.

For scalar masses \( m_S \geq 2m_\chi \), nearly all viable dark matter scenarios have been ruled out by existing experimental constraints on invisible scalar production [4]. We therefore assume that there are no additional particles with mass less than \( m_S/2 \), and any decays of the HPS must be to SM particles via the Higgs mixing. Existing experimental constraints on this scenario restrict the available parameter space to values of \( \theta \ll 1 \), i.e. the scalar is long-lived. The phenomenology of the HPS at the energy scales relevant to neutrino experiments is described in Ref. [7].

### 2.1.1 Production

At MicroBooNE the dominant production channel will be through the decay of kaons to pions, \( K \rightarrow \pi S \). The decay proceeds via the penguin diagram shown in fig. 2.1, where, due to the mass dependence in the S coupling, the dominant contribution comes from the loop including the top quark. The scalar is emitted by a virtual quark in the quark-W-boson loop. The partial width for this decay is given by

![Figure 2.1: A kaon decaying to a pion and Higgs portal scalar via a penguin process. The scalar later decays into pairs of SM particles.](image-url)
SECTION 2. HIDDEN SECTOR SEARCHES

\[ \Gamma (K^\pm \to \pi^\pm S) \simeq \frac{\theta^2}{16\pi m_K} \left| \frac{3V_{td}^* V_{ts} m_t^2 m_K^2}{32\pi^2 v^3} \right|^2 \lambda^{1/2} \left( 1, \frac{m_S^2}{m_K^2}, \frac{m_S^2}{m_K^2} \right), \]  

where \( m_K, m_\pi, m_t \) are the masses of the kaon, pion and top quark, respectively, \( V_{td} \) and \( V_{ts} \) are the relevant CKM matrix elements and \( v \) is the vacuum expectation value of the Higgs field. Finally, \( \lambda \) is the Källén function,

\[ \lambda(x, y, z) \equiv x^2 + y^2 + z^2 - 2xy - 2yz - 2zx. \]  

2.1.2 Decay

Since the HPS interacts with the SM in the same fashion as the Higgs boson, except with an additional \( \theta \) suppression, its decay properties are the same as that of a light Higgs boson. For HPS produced via kaon decay, the maximum allowed mass is \( m_k - m_\pi \simeq 354 \text{ MeV} \). For masses below this value, the allowed decays are \( S \to e^+e^-, \mu^+\mu^-, \pi^0\pi^0, \pi^+\pi^- \), where each decay channel becomes accessible in turn for increasing \( m_S \). The partial decay widths can be computed from eq. (2.2). The width for the decay to charged leptons is given by

\[ \Gamma (S \to \ell^+\ell^-) = \theta^2 \frac{m_t^2 m_S}{8\pi v^2} \left( 1 - \frac{4m_\ell^2}{m_S^2} \right)^{3/2}, \]  

and to pions by

\[ \Gamma (S \to \pi^0\pi^0) = \frac{1}{2} \Gamma (S \to \pi^+\pi^-) = \theta^2 \frac{|G_\pi^* (m_S^2)|^2}{32\pi^2 v^2 m_S^2} \left( 1 - \frac{4m_\pi^2}{m_S^2} \right)^{1/2}, \]  

where \( G_\pi(x) = \frac{2}{\pi}x + \frac{11}{9}m_\pi^2 \) describes the form factor at tree level \( [8] \). A derivation of a more complete hadronic form factor can be found in Ref. \( [9] \). Any differences from the tree level approximation are negligible in the mass range close to the pion threshold which is considered here. The total branching width to \( S \to \pi^+\pi^- \) is twice that of \( S \to \pi^0\pi^0 \) due to the two possible charge conjugations.

Figure 2.2 shows how the branching ratios to the various decay modes change as a function of HPS mass. As this analysis is a search for two tracks, we are interested in \( m_S > 211.3 \text{ MeV} \), where the decay to a muon-antimuon pair becomes accessible.
Figure 2.2: The branching ratio of the various decay modes of the HPS as a function of its mass.

MicroBooNE has already published a search for HPS decaying to $e^+e^-$ pairs [10], setting limits for HPS masses below 210 MeV. For an HPS with mass $2m_\mu < m_S < 2m_{\pi^0}$, the branching ratio $BR(S \rightarrow \mu^+\mu^-) \simeq 1$. For $m_S > 269.0$ MeV, the decay $S \rightarrow \pi^0\pi^0$ becomes accessible and the charged pion decays at $m_S > 279.1$ MeV. We do not consider decays to neutral pion pairs as part of our signal since the detector signature differs significantly. While the $S \rightarrow \pi^+\pi^-$ decay signatures appear very similar to the $S \rightarrow \mu^+\mu^-$ decays, the lifetime of the HPS becomes too short for this analysis to be sensitive to decays above the $\pi^+\pi^-$ threshold.

### 2.2 Heavy Neutral Leptons

The existence of three flavour neutrino oscillation is well established. The oscillation directly implies the existence of small but non-zero mass for at least two of the neutrino states. There is no mechanism for neutrino mass generation in the SM. The absence of a right-handed chiral partner to the left-handed neutrino means it is not possible to construct a Dirac mass term as for the charged fermions.

This motivates the introduction of additional right-handed singlet fields which would not interact via the weak force. These new particles allow for the generation of neutrino masses via either Dirac or Majorana mass terms [11]. Furthermore, right-handed neutrinos with large mass provide a natural explanation for the extreme
lightness of the active neutrinos, via “See-saw” mechanisms \([12]\).

By construction, all the SM charges of the new states are zero. They therefore will not interact directly via the strong, electromagnetic, or weak forces. The only possible interactions with SM particles occur via mass mixing with the SM neutrinos. These weaker-than-weak interactions often lead the new right-handed states to be referred to as \textit{sterile neutrinos}. The term \textit{Heavy Neutral Leptons} (HNLs), named for their significantly greater masses than active neutrinos, is also common in the literature, and will be used in this thesis.

One particular model is the \textit{Neutrino Minimal Extension of the SM} \((\nu\text{MSM})\) \([13]\), which introduces three HNLs. The lightest of these, with a mass the order of KeV, is a viable dark matter candidate. The other two are predicted to have masses \(\mathcal{O}(100 \text{ MeV})\) to \(\mathcal{O}(10 \text{ GeV})\). The new HNLs can simultaneously account for the neutrino masses and the matter-antimatter asymmetry observed today through participation in leptogenesis in the early universe \([14]\).

We follow a generic phenomenological approach. The addition of HNLs to the SM is modelled via an extension of the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix with a single additional heavy mass eigenstate, which mixes very weakly with the active neutrino states. Then the three flavour eigenstates of the left-handed neutrinos \(\nu_\alpha\) exist as a linear combination of the SM neutrino mass eigenstates \(\nu_i\) \((i = 1, 2, 3)\) and the new heavy neutral lepton state, \(N\), in the form

\[
\nu_\alpha = \sum_i U_{\alpha i} \nu_i + U_{\alpha 4} N, \tag{2.7}
\]

where \(U_{\alpha i}\) \((i = 1, 2, 3, 4\) and \(\alpha = e, \mu, \tau\) are elements of the extended PMNS matrix. Four new parameters are introduced: the HNL mass \((m_N)\) and the elements of the extended PMNS matrix \(U_{\alpha 4}\) \((\alpha = e, \mu, \tau)\).

The possible range of HNL mass spans many orders of magnitude. In this thesis, we will explore the existence of HNLs in the mass range that can be produced and directly detected by the MicroBooNE experiment \((m_N = \mathcal{O}(100 \text{ MeV}))\). In this mass range the HNLs lose coherence with active neutrinos and thus produce no
new oscillatory effects [15]. The HNLs instead propagate for long distances before decaying to SM particles through mass mixing.

2.2.1 Production

HNLs can be produced through mixing-mediated interactions with SM gauge bosons. Phenomenologically this means that HNLs can be produced in place of a neutrino in any neutrino-producing process, with a rate suppressed by the mixing angle $|U_{\alpha 4}|^2$, provided the final state is kinematically allowed. Figure 2.3(b) shows an example of such a substitution.

Figure 2.3: Diagrams showing a positively charged kaon decaying to an anti-muon and (a) a muon neutrino or (b) a heavy neutral lepton via mixing.

HNLs with $m_N < 494$ MeV could be produced via kaon and pion decay in the BNB and NuMI beams (see section 4), before travelling to the MicroBooNE detector and decaying into SM particles. The dominant production channels in the BNB and NuMI beams are

$$\pi^\pm \rightarrow N\ell^\pm \quad \text{and} \quad K^\pm \rightarrow N\ell^\pm,$$

(2.8)

where $\ell$ is an electron or a muon. Decays of neutral kaons also contribute a small portion of the HNL flux, but their contribution from the NuMI absorber is negligible.

Meson Decay Rates

The HNL mass modifies the meson’s rate of decay, relative to that of the decay to a SM neutrino. Firstly, there is an alteration to the phase space of the meson’s decay due to the differing masses of a HNL and an active neutrino. In addition, an adjustment must be made since the helicity suppression which occurs in meson decays to the light active neutrinos has minimal effect in decays to HNLs due to the larger HNL mass. This leads to significant enhancement of certain channels, in particular
Figure 2.4: The kinematic enhancement of meson decay rates to HNLs as a function of the HNL mass.

The rate of $\pi^+ \to e^+ N$ is increased by a factor of up to $10^5$. For two-body meson decays, this modification can be described by a kinematic factor dependent on the mass of the parent meson and its two daughter particles, the HNL and accompanying lepton. This kinematic factor $K^M_{a4}$ [16, 17] is given by

$$K^M_{a4} = \frac{F_M(\delta^N_M, \delta^N_M)}{\delta^2_M(1 - \delta^2_M)} \lambda^2 \left(1, \delta^N_M, \delta^N_M\right),$$

(2.9)

where $F_M(a, b) = a + b - (a - b)^2$, and $\delta^N_M = m^2_N/m^2_M$ and $\delta^a_M = m^2_{\ell a}/m^2_M$ are the squared ratios of the daughter masses to the parent meson mass. Figure 2.4 shows this factor as a function of $m_N$ for each of the two-body production decays. For the decay $K^\pm \to N\mu^\pm$, the source of HNLs we are interested in, the kinematic factor varies between 1.5 and 4. The final branching width of two-body kaon decays to HNLs can therefore be expressed as a modification of the equivalent SM decay to neutrinos,

$$\Gamma \left( K^+ \to N\ell^+ \right) = |U_{a4}|^2 K^M_{a4} \Gamma \left( K^+ \to \nu_\alpha \ell^+ \right).$$

(2.10)

2.2.2 Decay

The HNLs are unstable and therefore decay in flight with a lifetime dependent again on the mixing parameters $|U_{a4}|^2$ where $\alpha = e, \mu, \tau$. The existing limits on this mixing [18] imply that an HNL with a coupling not already excluded would
be long-lived enough to travel to MicroBooNE and potentially decay there. The possible decays for a HNL with mass $\mathcal{O}(100 \text{ MeV})$ are \[15\]

\[
\begin{align*}
N \to e^− \pi^+, \quad N \to μ^− \pi^+, \quad N \to νπ^0, \quad N \to νγ, \\
N \to e^- e^+ ν, \quad N \to μ^- μ^+ ν, \quad N \to μ^- e^+ ν, \quad N \to 3 ν.
\end{align*}
\] (2.11)

If the HNL is taken to be a Majorana particle, the charge conjugates of these decays are also possible.

![Figure 2.5: The branching ratios of the various decay modes of the HNL as a function of its mass. The ratios shown are for a Majorana HNL and are taken from Ref. \[19\]. Solid lines show the entirely muon-like coupling case ([$U_{e4} : U_{μ4} : U_{τ4}$] = [0 : 1 : 0]) and dashed lines the entirely electron-like coupling case ([$U_{e4} : U_{μ4} : U_{τ4}$] = [1 : 0 : 0]).](image)

The branching ratios to the various modes are shown in fig. \[2.5\] For $m_N < m_π$, the dominant decay mode is to three neutrinos. This channel is experimentally unobservable, and the decay to $N \to e^- e^+ ν$ is the best prospect for observing HNLs in this mass range. For higher $m_N$, decays to $N \to e^- π^+$ and $N \to μ^- π^+$ dominate \[20\]. These decay channels are particularly promising for a search using a LArTPC with a clear experimental signature of a charged pion track and either a muon track or electron shower originating from the same vertex. Charged-current neutrino interactions can replicate the same final-state particles and are therefore a
background. However, the differing kinematics, detailed in section 6.1, between a HNL decay and neutrino interaction should allow for good separation.

This search focuses on the two-track signature $N \rightarrow \mu^\pm \pi^\mp$, shown in fig. 2.6 — a decay which requires non-zero $|U_{\mu 4}|$. Assuming $|U_{e 4}| = |U_{\tau 4}| = 0$, the HNL production rates and the $\mu \pi$ decay width are both proportional to $|U_{\mu 4}|^2$ only. The decay width can be expressed as [19]:

$$
\Gamma(N \rightarrow \mu \pi) = |U_{\mu 4}|^2 \frac{2f_\pi^2|V_{ud}|^2m_N^3}{32\pi v^4} I\left(\frac{m_\mu^2}{m_N^2}, \frac{m_\pi^2}{m_N^2}\right),
$$

(2.12)

with

$$
I(y, z) = [(1+y+z)(1+y) - 4y] \lambda^2(1, y, z),
$$

(2.13)

where $f_\pi$ is the pion decay constant, $V_{ud}$ is the relevant CKM matrix element and $\lambda(x, y, z)$ is the same two-body phase space factor encountered in eq. (2.3). The quantity $v$ is the Higgs vacuum expectation value and is often expressed in terms of the Fermi coupling constant as $v = \left(\sqrt{2}G_F\right)^{-1/2}$. The factor of two arises from the sum over the two charge conjugate decay channels.

The available HNL mass ($m_N$) values are limited by the kinematic restriction of decay and production, that is, $m_K - m_\mu > m_N > m_\mu + m_\pi$. The selection could also be sensitive to the three-body decay, $N \rightarrow \mu^- \mu^+ \nu$ but the kinematics differ significantly, and this decay is therefore not considered here.

### 2.2.3 Dirac or Majorana Nature and Polarisation Effects

The HNL states can be either Dirac and Majorana in nature. Majorana HNLs would decay in equal numbers into $\mu^+ \pi^-$ and $\mu^- \pi^+$ final states, whereas Dirac HNLs would only decay through the process that preserves lepton number. Therefore the expected event rate for Majorana HNLs is double the rate of Dirac HNLs. The absorber flux
considered here comes predominately from positively charged kaons. Therefore the HNLs are “neutrino-like” and the Dirac decay is \( N \rightarrow \mu^+\pi^- \). The assumption in this thesis is that HNLs are Majorana particles. The limits in the Dirac case will also be derived.

Unlike for HPS decays, the products of the \( N \rightarrow \mu\pi \) decay are not isotropic in the HNL rest frame due to polarisation effects. Instead, the angular distribution of the decay products for each charge conjugation (\( \mu^\mp\pi^\pm \)) are described by a function of the form \( A \pm hB\cos\theta \) \cite{21, 22}. The angle \( \theta \) is between the polarization vector of the HNL and the momentum of the charged muon in the HNL rest frame. The HNL helicity \( h \) can take values of either \( +1 \) or \( -1 \). The fraction of HNL in each helicity state (\( F^+ \) and \( F^- \)) is determined by the HNL production decay (\( K^+ \rightarrow N\mu^+ \)) dynamics and is dependent on \( m_N \). In the limit \( m_N \rightarrow 0 \) the fractions are \( F_+ \rightarrow 0 \) and \( F_- \rightarrow 1 \), i.e. like SM neutrinos, all the HNLs are produced with a negative helicity. For the \( m_N \) considered here \( 0.6 < F^+ < 0.775 \).

The angular distributions for the two charge conjugations (\( \mu^+\pi^- \) and \( \mu^-\pi^+ \)) add up to an isotropic distribution. As the MicroBooNE detector is largely insensitive to the charge of muons and pions, it does not discriminate between the two channels and would observe the combined isotropic distribution. If the HNL is Dirac, it decays via \( N \rightarrow \mu^-\pi^+ \) and the decays that produce forward-going muons will be enhanced due to polarisation effects. The maximum amount by which the rest frame angular distributions differ from the isotropic distribution is \( \approx 30\% \).

### 2.3 Previous Experimental Searches

No direct experimental evidence has been observed for either of the models considered. The anomalies involving excesses of electron-neutrino like events observed in both LSND \cite{23} and MiniBooNE \cite{24} have been interpreted as being caused by HNL but the minimal model and final states considered here produce events inconsistent with the kinematics of the excess \cite{25}.

HPS decaying into \( e^+e^- \) were proposed as an explanation for the observation of four events by the kaon decay experiment KOTO, reported in the channel "\( K^0_L \rightarrow \)"
\( \pi^0 + Invisible^\prime \), with a rate two orders of magnitude above the SM prediction of \( K^0 \rightarrow \pi^0 \nu \bar{\nu} \) decays \cite{26}. A more recent publication (Ref. \cite{27}) rejected one of the data candidates as being caused by an upstream background decay. The background prediction was also revised upwards to 1.22 \( \pm \) 0.26 giving an excess of 1.78 counts. The previous MicroBooNE search for HPS \cite{10} excluded the range of values in the HPS parameter space which could have been responsible for causing such an excess.

In the absence of evidence for their existence, experiments set limits on the upper rate of production and decay of the LLPs. Both the production rate and the decay rate of the LLPs scale with the square of the relevant mixing parameter (\( \theta^2 \) or \( |U_{\mu 4}|^2 \)). The limits are expressed in the corresponding parameter space.

Here, the existing experimental limits on the relevant mixing parameters for the two models will be discussed. Only searches for LLP with masses in the MeV scale are considered. Searches for both particles have been performed across much larger mass ranges, with experimental signatures varying greatly with mass. In particular, both oscillation experiments and end point measurements of \( \beta \) decays can probe eV to KeV scale HNLs \cite{18}, while collider experiments have set limits for mass ranges on the order of GeV and above for both HNL and HPS searches \cite{28}.

### 2.3.1 Experimental Methods

In the MeV mass scale, there are two types of LLP search technique available, peak searches which probe only the LLP production rate, and decay signature searches which probe both the LLP production and decay rates. The experimental methods employed are largely the same for HPS and HNL signatures.

**Peak Searches**

In a peak search experiment, the possible existence of an LLP is inferred by measuring the decays that would produce it, \( P \rightarrow d + Invisible \). Here \( P \) is the parent meson (a pion or kaon) and \( d \) is the daughter particle (a pion or lepton). Any LLPs produced would exit the detector without decaying and so are labeled Invisible. Neutrinos, or pairs of neutrinos, produced in the SM decays of \( P \) would also exit the detector.
without interacting, so represent backgrounds to the search. If the momentum values of $P$ and $d$ are measured, the missing invariant mass can be calculated as $m_{\text{mis}}^2 = (P_P - P_d)^2$, where $P_P$ and $P_d$ are the parent and daughter 4-momenta. If LLPs, with mass $m_{\text{LLP}}$, are present in the decay, an excess over the background prediction will be observed at $m_{\text{mis}} = m_{\text{LLP}}$.

For example, the NA62 collaboration \cite{29} measures the process with a parent kaon and daughter muon, $K^+ \rightarrow \mu^+ + \text{Invisible}$. An HNL search is performed by searching for an excess over the “background” SM process $K^+ \rightarrow \mu^+ \nu_\mu$. The NA62 experiment measures the momentum of kaons before they decay in flight. Peak searches are also carried out where the LLP parent is slowed to rest, and therefore its momentum is known to be zero. One such experiment is the E949 experiment \cite{30} which analysed stopped kaons decay to both $K^+ \rightarrow \pi^+ + \text{Invisible}$ and $K^+ \rightarrow \mu^+ + \text{Invisible}$ which are sensitive to HPS and HNL respectively.

**Decay Signature Searches**

Decay signature searches look for the decay products of the LLPs. The LLPs are typically produced outside the detector before propagating to the detector, where they may decay to visible SM particles. The expected event rate depends on the mixing angle at both production and decay. Decay searches often occur in beam-dump experiments, which are explicitly designed for rare decay searches. They therefore employ methods to reduce the background from SM neutrinos produced alongside the LLPs. For example the PS191 \cite{31} and CHARM \cite{32} experiments utilise low-density decay chambers to minimise the rate of neutrino interaction. Recently, the improved resolution of modern neutrino experiments allows them to function as competitive beam-dump experiments alongside their neutrino physics programme goals, with no or minimal modifications.
2.3.2 Existing Limits

Heavy Neutral Leptons

Existing experimental limits on the relevant HNL mixing parameter ($|U_{\mu 4}|^2$) in the mass range surrounding our region of interest are given below. The excluded regions are shown in fig. 2.7. All limits are given at the 90% confidence level (CL).

- The MicroBooNE collaboration has published an analysis searching for the same decay channel as this work ($K^\pm \rightarrow N\mu^\pm$ and $N \rightarrow \mu^\pm\pi^\mp$) [2]. The analysis was performed on data collected from $2 \times 10^{20}$ protons on target (POT) from the on-axis BNB beam. A specialised trigger window was used to capture HNL events that arrived at the detector after the SM neutrino background. The data in this trigger window was used to produce limits on $|U_{\mu 4}|^2$ in the range $(4.7 - 0.7) \times 10^{-7}$ for masses in the range 260 to 385 MeV. The results set the first limits on HNLs using a LArTPC.

- The neutrino experiment T2K set limits in this same channel ($K^\pm \rightarrow N\mu^\pm$ and $N \rightarrow \mu^\pm\pi^\mp$) alongside other channels [33]. The analysis uses data collected using the off-axis near detector ND280, with an exposure of $\approx 2 \times 10^{21}$ POT.
The ND280 detector is located 280 m from the beam target at an angle of 2.04°. The search is restricted to events occurring in three argon gas TPC volumes. Due to the low density of the gas, the search has minimal neutrino background. After a kinematic selection for events consistent with HNL decay, no signal candidates were observed. The limit shown in fig. 2.7 is the single-channel limit that is directly comparable to this search. The limit constrains $|U_{\mu 4}|^2$ at the level $10^{-8} - 10^{-9}$ in the HNL mass range 250 – 380 MeV. The T2K collaboration has also presented more stringent limits on $|U_{\mu 4}|$ in the case that $|U_{e 4}|$ and $|U_{\tau 4}|$ are not assumed to be zero and are instead marginalized using the results from other channels.

- **PS191**, an experiment at CERN, was specifically designed to search for massive decaying neutrinos [31]. Data was taken in 1984 with an exposure of $\approx 10^{19}$ POT where 19.2 GeV protons were directed at a beryllium target. The detector was located 128 m from the target and 2.3° off-axis. It comprised a detector volume (12 m long, with a cross-sectional area of 18 m²) sparsely instrumented with scintillator planes and filled with helium. The large volume provides high potential HNL rates, while the low density prevents a large background from SM neutrino interactions. Events were triggered by deposits consistent with two particles crossing the hodoscope at the rear of the detector simultaneously. The $\sim120,000$ triggered events were checked for compatibility with an HNL decay signature by first filtering with a microprocessor and then visual inspection of the remaining events. No candidates consistent with signal were observed and limits were produced on $|U_{\mu 4}|^2$ in the range $10^{-5} - 10^{-9}$ for the mass range 120 to 350 MeV [34].

- The **NuTeV** collaboration performed a search using the high energy neutrino beam produced by protons accelerated in the Tevatron ring at Fermilab. NuTeV received $3 \times 10^{18}$ POT with an energy of 800 GeV while the detector was configured for a HNL search. The high energy protons produce significant numbers of charmed mesons in collisions with the target, allowing the production of higher mass HNLs than the other beam-dump style experiments described here. Limits on $|U_{\mu 4}|^2$ in the range $10^{-6} - 10^{-7}$ were placed in the mass range
225 to 2000 MeV [35].

- **NA62**, a kaon decay experiment at the CERN super proton synchrotron (SPS), performed a peak search for $K^+ \rightarrow \mu^+ N$. The initial result [36] used data collected in 2015 to set limits on $|U_{\mu4}|^2$ at the level $10^{-7}$ to $10^{-6}$ for masses in the range 250 to 373 MeV. Updated results using the larger 2016-2018 dataset have since been published. They improve the sensitivity by an order of magnitude to $10^{-8} - 10^{-7}$ and extend the mass range to 250 to 384 MeV [37].

- The **E949** experiment, a kaon decay experiment which ran at Brookhaven National Lab in 2002, analysed the decays of $2 \times 10^{12}$ stopped kaons produced from 21.5 GeV protons. Using the peak search method, limits on $|U_{\mu4}|^2$ were set in the mass range 175 to 300 MeV at the level of $10^{-7} - 10^{-9}$ [38].

- In 1982, an experiment located at **KEK** analysed the decays of stopped kaons produced using a 0.5 GeV proton beam. The momentum spectrum of $3 \times 10^6$ produced muons was used to set limits on $|U_{\mu4}|^2$ in the mass range 70 to 300 MeV at the level of $10^{-4} - 10^{-6}$ [39, 40].

- The Swiss Institute for Nuclear Research (**SIN**) performed a peak search using stopped pions decaying via $\pi^+ \rightarrow \mu^+ + \text{Invisible}$. The experiment was performed using a scintillator detector in 1981 [41], and then a germanium detector in 1987 [42, 43]. Upper limits were set on $|U_{\mu4}|^2$ in the mass range 1 to 30 MeV at the level $\approx 2 \times 10^{-5}$.

- The **PIENU** collaboration also performed an HNL peak production search using stopped pions. The experiment was performed in the TRIUMF M13 beamline and used plastic scintillator to stop the pions and measure the muon kinematics. The most recent and stringent limits were published in 2019 [44] and set limits on $|U_{\mu4}|^2 \approx 3 \times 10^{-6}$ for 15 to 30 MeV and $\approx 10^{-5}$ for 30 to 34 MeV, extending the mass range beyond that of SIN.
Higgs Portal Scalars

The existing experimental limits on the HPS mixing parameter $\theta$ in the mass range surrounding our region of interest are listed below. The excluded regions are shown in fig. 2.8. The HPS limits are at the 90% CL unless otherwise stated.

Figure 2.8: The existing experimental limits on the HPS parameter space. Dedicated searches are indicated with solid lines. Reinterpretations of historical data are shown with dashed lines.

- The MicroBooNE collaboration has published a search for HPS decaying to $e^+e^-$ pairs \cite{10}. The analysis focuses on scalars from kaons decaying at rest after being produced at the NuMI absorber, and uses data corresponding to $1.93 \times 10^{20}$ POT. This produces limits on $\theta^2$ in the range $10^{-6} - 10^{-7}$ at the 95% CL for the mass range directly below our considered range ($0 < m_S < 211$ MeV).

- The E949 collaboration produced limits on the branching fraction of the decay $K^+ \rightarrow \pi^+ X$, where $X$ is a massive particle that exits the detector \cite{15}. This limit can be translated into a limit on the mixing parameter $\theta$ using the width of the kaon decay to HPS (eq. (2.3)). For masses up to 250 MeV, $\theta^2$ is constrained at the level $5 \times 10^{-8} - 10^{-6}$. The gap in the sensitivity surrounding
$m_{\pi_0} = 139.6$ MeV is due to the background from $K^+ \rightarrow \pi^+\pi^0$.

- The **NA62** collaboration used data collected in 2016-2018 to study $K^+ \rightarrow \pi^+\nu\bar{\nu}$ decays to produce limits on the branching fraction of the decay $K^+ \rightarrow \pi^+X$, where $X$ is a massive particle that exits the detector [46, 47]. As in the E949 analysis, the limit on the branching fraction is translated into a limit on the mixing parameter $\theta$. The limit is in the range $10^{-8} - 10^{-7}$ for masses up to 250 MeV. The gap in the sensitivity near the neutral pion mass is due to the $K^+ \rightarrow \pi^+\pi^0$ background.

- The **LHCb** collaboration set limits by looking for B mesons decaying to kaons and an accompanying HPS. For the HPS lifetimes considered ($0.1 < \tau(S) < 1000$ ps), the HPS quickly decays into a $\mu^+\mu^-$ pair inside the detector. Searches have been carried out for both $B^+ \rightarrow K^+S(\mu^+\mu^-)$ [48] and $B^0 \rightarrow K^{*0}S(\mu^+\mu^-)$ [49] giving limits on $\theta^2$ of order $\approx 10^{-6}$ over the mass range 250 to 4700 MeV. Figure 2.8 shows the joint coverage of the two limits at the 95% CL.

The following limits are reinterpretations of experimental results carried out by those outside the respective collaboration without access to the raw experimental data. Reinterpretations therefore depend on external beamline, flux and detector simulations. In cases where the topology differs from the original selection criteria, they also depend on estimated detection efficiencies. In the case of the CHARM experiment, different sensitivity estimates have been produced with near order-of-magnitude disagreements. For the PS191 and LSND experiments, only one such reinterpretation exists for each. The reinterpretations shown exclude regions which have meaningful upper limits as well as lower limits. This is due to the short decay lengths of the HPS for $m_S > 2m_\mu$, and will be discussed in section 2.4.

- The **CHARM** collaboration operated a beam-dump experiment at the CERN SPS with a 400 GeV proton beam impinged on a thick copper target. They performed a search for decays to $e^+e^-$ and $\mu^+\mu^-$ pairs of axion-like particles [32]. The axion-like particles are produced directly in the proton collisions with the
target. This is in contrast with the HPS studied here, which are produced in the decay of secondary mesons. Thus reinterpreting the result to apply a limit on $\theta^2$ relies on an estimation of the number of kaons which are produced in the proton-target collision and subsequently decay to HPS. In fig. 2.8 we use the recent result [50] which accounts for the significant kaon re-absorption in the thick target, weakening the limit with respect to previous analyses, for example Ref. [51]. The limit shown in fig. 2.8 is at 95% CL.

- The LSND experiment was a liquid scintillator detector located at the Los Alamos Neutrino Scattering Centre in the 1990s. In the early years of the experiment, 800 MeV protons were impinged on a water target and later a heavy metal target. A total of over $10^{23}$ POT were collected. Ref. [52] estimates the rate of potential HPS production at LSND, with the dominant channel being the proton bremsstrahlung process $p + p \rightarrow S + X$ where $X$ represents a hadronic final state. The authors then reinterpret LSND results with final state electrons and muons to produce limits on HPS in the mass regions below 211 MeV and 211 to 350 MeV respectively.

  The $e^+e^-$ limit uses the results of the electron neutrino appearance studies [53, 23]. The boosted $e^+e^-$ pair produced from HPS decays is deemed to be indistinguishable from single electron showers produced by electron neutrino interactions. They are reconstructed with the same efficiency of $\approx 0.1$.

  The $\mu^+\mu^-$ limit uses a search for excess muon neutrino interaction events produced by $\pi^0 \rightarrow \nu_\mu \bar{\nu}_\mu$ [54]. The authors assume that the $\mu^+\mu^-$ pair will be reconstructed as a single-muon event with an efficiency of $\approx 0.1$. They acknowledge the difficulty in estimating the true efficiency, due to the fact that the muons will be produced with less momentum and will therefore be more separated than the equivalent energy electron-like decay. An excess of data over prediction was in fact observed in the relevant energy range for both channels by LSND. The authors of the reinterpretation choose to place their limit at the values of $(m_S, \theta^2)$ which give 20 detected HPS decays in each channel. This is the limit shown in fig. 2.8.

- The HNL search results by PS191 have been recently reinterpreted in terms
of HPS decays \[ 55 \]. The HNL search channels \( N \rightarrow \nu e^+e^- \) and \( N \rightarrow \mu \pi \) are reinterpreted in terms of HPS decays \( S \rightarrow e^+e^- \) and \( S \rightarrow \mu^+\mu^- \), respectively. The authors assume the same triggering and detection efficiency conditions as the original HNL search, i.e., all HPS decays in which both daughters cross the hodoscope at the end of the decay volume are detectable. PS191 observed no events consistent with signal decays in either channel. The reinterpretation authors therefore produce limits that exclude values of \( \theta^2 \) that produce > 2.3 signal events (90% CL). The re-simulation of the beamline does not include the effects of the focusing horn on the kaons, which would increase the fraction of HPS reaching the decay volume. Hence, the limit is expected to be conservative. The authors provide limits on HPS in the mass region between 30 MeV and 310 MeV.

### 2.4 LLP Decay Lengths

There are some key phenomenological differences between the HPS and HNL models in terms of production and decay rates, which affect the relationship between mixing angle and final event rate in the detector. Discounting the additional suppression of \( \theta \) and \( |U_{\alpha 4}|^2 \), the decay length of HPS is much shorter than the decay length of HNL. This can be seen by comparing the respective coefficients of the decay width in eqs. (2.5) and (2.6) for HPS and eq. (2.12) for HNL. The additional factor \( f_\pi^2/v^2 \approx 2 \times 10^{-7} \), present in the HNL decay width but not the HPS decay width, drives this difference in magnitude.

Figure 2.9 shows decay length contours in the plane of \( m_{\text{LLP}} \) versus the mixing parameter for the two models. The HNL lifetime is calculated under the assumption it is a Majorana particle. For Dirac HNL the lifetime would be increased by a factor of two. The decay lengths are calculated accounting for the Lorentz dilation due to the lab frame LLP energy \( E_{\text{LLP}} \). For a LLP of mass \( m_{\text{LLP}} \) produced from kaon decay-at-rest (KDAR), \( E_{\text{LLP}} \) is determined by the two-body decay kinematics,

\[
E_{\text{LLP}} = \frac{m_K^2 + m_{\text{LLP}}^2 - m_\alpha^2}{2m_K},
\]  

(2.14)
Figure 2.9: Decay length contours as displayed as a function of the LLP mass and model mixing parameter for the HPS (left) and HNL (right) models.

where $m_K$ is the parent kaon mass and $m_d$ is the mass of the accompanying daughter particle ($\mu$ or $\pi$).

For HPS with $m_a > 2m_\mu$, the values of $\theta^2 (\approx 10^{-7}$ to $10^{-9})$ we are interested in produce decay lengths similar to the distance from the absorber to MicroBooNE (100 m). Therefore some HPS will decay before reaching the detector and the resulting reduction in the flux in MicroBooNE must be considered. For large values of $\theta^2$, only a small fraction of the produced HPS live long enough to reach the detector so the decay-signature search exclusion contours have an upper reach as well as a lower reach on the allowed values of $\theta^2$. This effect gives rise to the shape of the exclusion contours for the reinterpretations of PS191, LSND and CHARM data.

For HNL, in the range we are sensitive to, ($|U_{\mu d}|^2 \approx 10^{-7}$ to $10^{-9}$), the decay length is at least three orders of magnitude larger than the distance to the detector (100 m). The number of HNL decaying before reaching the detector is therefore negligible.

For the same mixing parameter values, HNL are produced much more copiously than HPS. This is because the HNL production channel ($K^\pm \rightarrow N\mu^\pm$) is a naturally large SM process suppressed by only the HNL mixing angle, whereas the HPS production involves a highly suppressed penguin process. This higher rate of HNL
production acts to offset the effect of the decay length difference on the event rate. Thus the ranges of mixing angles that we are sensitive to for the HNL and HPS models are similar.
3 Liquid-argon Time Projection Chamber

The liquid-argon time projection chamber (LArTPC) has become established as a technology for a range of modern accelerator neutrino experiments due to its excellent calorimetric reconstruction and spatial resolution. The current and near-future Fermilab neutrino programme utilises LArTPCs for neutrino oscillation measurements at both short and long neutrino baselines. Increasingly, the capabilities of the detectors have seen them deployed in exotic signatures searches allowing investigation of previously unexplored parameter space for scenarios that go beyond the Standard Model.

The MicroBooNE detector, operating since 2015, is part of the Short Baseline Neutrino Program (SBN) [56], along with the SBND and ICARUS detectors. The programme will perform an investigation into short baseline neutrino oscillations, an extensive programme of neutrino cross sections measurements, and R&D into the detector technology. The upcoming DUNE experiment [57] will construct several large (17 kt) LArTPC modules as its far detectors. They will be used to perform neutrino oscillation measurements over a long baseline. In particular, the neutrino mass ordering will be determined and a sensitivity to charge parity violation in the neutrino sector will be achieved for 75% of the possible values of the CP-violating phase $\delta_{CP}$. The experiment will also carry out an extensive range of beyond standard model probes including LLP searches using its near detectors [58].

This section will focus on two LArTPC detectors; MicroBooNE, the first large-scale LArTPC to take data at Fermilab, located in the BNB (on-axis) and NuMI (off-axis) neutrino beams, and the Phase I ProtoDUNE-SP detector which collected data from a charged particle test beam at CERN in 2018 to 2019. These detectors are both single-phase, horizontal drift LArTPCs and thus share many similarities in
Figure 3.1: Diagram showing the basic principle of charge readout in a LArTPC (from [59]). Charged particles produce ionisation electrons which are drifted by an electric field through wire panes at the anode. The wires on each plane have different orientations so each produce a different projection of the event.

3.1 LArTPCs overview

LArTPCs are large volumes filled with liquid argon. A homogeneous electric field is created across the volume between a cathode held at extremely high voltage ($\sim 100$ kV) and an anode. When a charged particle traverses the detector, it ionises the argon atoms. This produces a trail of ionisation electrons and positive ions in the particle’s path. The electric field causes the ionisation electrons to drift towards the anode where wire planes are located. The drifted electrons generate a current on the wires either by induction or collection as illustrated in fig. 3.1. The charge design and operation. Sections 3.1 to 3.3 will first illustrate the working principles of LArTPCs, and section 3.4 will demonstrate some of these principles with an analysis the author performed using test beam data in ProtoDUNE-SP to assess the prototype’s performance. Section 3.5 will lay out the particular specifications and operation of the MicroBooNE LArTPC, the detector which collected the data used in the main analysis of this work.
Figure 3.2: A pair of diagrams showing the signal created by ionisation electrons in a TPC (Adapted from Ref. [60]). The left plot shows the electric field lines through a small $x - y$ slice of the TPC. They show the paths ionisation electrons would follow (from top to bottom) across the TPC then around the negatively biased induction wires before finally being collected on the collection plane wires. The anode plane wires are shown in purple and dissect the page. The right-hand diagram shows example waveforms created on each wire plane.

Profiles on each wire can then be used to reconstruct the trajectories and energy deposition of the particles travelling through the liquid argon.

Scintillation light is also produced from the excitation and ionisation of the argon. This light is collected by a photon-detection system located behind the anode. The collected light can be used to ascertain prompt information about the timing of the interaction as well as provide additional information about the location and topology of an interaction. The collection of both charge and scintillation light requires high purity argon, and the argon is actively filtered by a system to remove electro-negative impurities such as oxygen and water, which would otherwise capture the drifting electrons.

### 3.1.1 Time Projection Chamber

The TPC consists of a field cage, cathode plane, and an anode plane assembly (APA) that define a cuboid volume inside a larger cryostat. A single APA comprises multiple planes of evenly spaced readout wires, with a typical spacing of 3-5 mm defining
the spatial resolution in the direction perpendicular to electron drift. The planes themselves are spaced at around 5 mm, and a voltage bias is applied to each of the planes so that electrons drift past the two induction planes (order -100 V and 0 V) before being collected on the positively biased final plane (order +100 V). An uninstrumented first grid layer is also sometimes used to shield the first induction layer from distant charge as it approaches.

The cathode is located at the opposite side of the TPC and is made up of one or more cathode planes held at a very large negative voltage (∼100 kV) to create the electric drift field inside the TPC. A field cage encloses the volume between the cathode plane(s) and the anode wire planes to create a region with a uniform electric field. The field cage is made up of series of loops each electrically connected to its neighbours via a resistor divider chain which in turn causes a series of voltage steps across the TPC maintaining a uniform electric field between the cathode and anode.

The signal induced on the induction planes as electrons approach is bipolar in shape. An example can be seen in fig. 3.2. A negative current is created as the electrons approach the wire before it becomes positive after the electrons pass. If no uninstrumented shielding plane is used, the negative peak on the first induction plane is shallow and broad as the charge induces a current at a large distance before reaching the plane. The second induction plane is shielded by the first plane to create a more symmetrical signal. The final plane is positively biased and collects the electrons producing peaked unipolar waveforms. The waveforms on each wire in a plane can be combined to produce a 2D projection of the particle interaction in the TPC.

The spatial location in the drift direction is determined by converting the electron drift time to distance using the $t_0$ of the interaction time. This $t_0$ can be inferred either from the associated light signal collected or an external triggering system, for example the beam delivery signal. The wires on each plane are orientated at different angles from vertical so that each 2D projection is different and 3D coordinates can be calculated.
3.1.2 Cryogenics and Argon Purity

Argon is a gas at room temperature. A cryostat surrounds the TPC and is kept at a temperature of 87 K to keep the argon in a liquid state. The temperature is maintained by continuously cooling and recirculating boiled off argon with a cryogenic system. Incorporated into this system is a number of filters to remove contaminants from the argon and maintain high purity. The impact of contaminants, such as water, oxygen, and nitrogen on the performance of the detector is discussed in sections 3.3.4 and 3.3.5.

3.1.3 Wire Readout and Signal Processing

The readout wires are connected to signal processing electronics located inside the cryostat, referred to as “cold electronics”. The analogue wire signals are first passed through front end Application Specific Integrated Circuits (ASICs) which pre-amplify and shape the signal. These ASICs have configurable gain and shaping time settings and are connected to cold motherboards which issue configuration commands and transfer the ASIC output. The signals are then passed to readout modules, where they are digitised and processed. A common final sampling frequency in the digitisation process is 2 MHz, defining a time “tick” as 0.5 µs. In MicroBooNE this digitisation happens outside the cryostat in the “warm”, in newer detectors such as ProtoDUNE-SP they are combined with the ASICs and placed inside the cryostat on front-end motherboards (FEMBs) to lower the noise level. The TPC information is then transferred to the data-acquisition (DAQ) system where it is saved and combined with the data from the other detector sub-systems.

The waveforms are processed off-line to make them suitable for high-level reconstruction. This involves noise filtering and accounting for the effect the detector has had on the waveforms. The signal processing attempts to recover the true ionisation electron signal which has become convolved with the field and electronics response. Fourier transforms are used to perform deconvolution and extract the signal waveform as a function of time. Section 5.4.2 details the noise filtering and deconvolution process used by MicroBooNE.
3.1.4 High-level Reconstruction

There are several possible tool kits used for performing “high-level reconstruction” for LArTPCs, i.e., the process of creating particle-like reconstructed objects from the processed waveforms. Both analyses in this thesis use versions of the Pandora pattern recognition framework \[61\]. The waveforms are scanned for peaks and then fitted with one or more Gaussian functions to form “hits”. Each hit has an associated time equal to the mean of the Gaussian and charge equal to the integral of the Gaussian which is proportional to the number of recorded electrons. Pandora uses a suite of algorithms to combine these hits, first clustered independently on each plane and then combined across planes to build 3-D reconstructed objects. Section 5.4 will describe the Pandora reconstruction algorithms in more detail.

Alternative frameworks include Wire-Cell 3D imaging \[62\], which uses the processed waveforms to directly reconstruct 3D images using tomographic techniques prior to any pattern recognition stage and a deep learning based approach \[63\] that makes pixel-level predictions of the nature of objects in 2D images using convolutional neural networks. Both frameworks are being applied in recent and current MicroBooNE analyses.

3.2 Particle Detection with LArTPCs

The lack of a magnetic field in LArTPCs mean particles travel in straight lines until they are captured or decay. For particles that lose energy primarily through ionisation, such as muons, charged pions, and protons, straight trails of ionisation electrons are collected by the detector. We refer to these as tracks or track-like objects. At the energies produced by neutrino beams (\(\sim\) GeV) the dominant energy loss of electrons and photons in LAr is through radiative processes. Unlike for ionisation losses, which appear continuous on the millimetre scale, radiative processes are stochastic and initiate electromagnetic (EM) cascades in the detector. We refer to these signatures as showers or shower-like objects.
SECTION 3. LIQUID-ARGON TIME PROJECTION CHAMBER

3.2.1 Track-like Signatures

As a charged particle traverses through liquid argon, small amounts of its energy are deposited along its trajectory in the form of ionisation electrons produced by Coulomb scattering with atomic electrons. The mean energy deposited per unit length for heavy charged particles in liquid argon can be described using the Bethe-Bloch equation [3],

\[
\left\langle -\frac{dE}{dx} \right\rangle = K z^2 Z A \beta^2 \left[ \frac{1}{2} \ln \left( \frac{2m_e^2c^2\beta^2\gamma^2 W_{\text{max}}}{I^2} \right) - \beta^2 - \frac{\delta(\beta\gamma)}{2} \right],
\]

where \( z \) is the charge of the travelling particle, \( Z \) and \( A \) are the atomic number and atomic mass of the medium and \( I \) is the mean excitation energy. Here \( \beta = v/c \) and \( \gamma = (1 - \beta^2)^{-\frac{1}{2}} \), where \( v \) is the speed of the particle. The constant \( K = 4\pi N_A r_e^2 m_e c^2 \), where \( N_A \) is Avogadro’s number, \( r_e \) is the classical electron radius and \( m_e c^2 \) is the electron rest mass energy. The variable \( W_{\text{max}} \) refers to the maximum possible energy transfer in a single collision which, in the low energy approximation relevant here, equals \( W_{\text{max}} = 2m_e c^2 \beta^2 \gamma^2 \). Finally, \( \delta(\beta\gamma)/2 \) is a correction factor to the energy loss related to the density of the medium [3].

Figure 3.4 illustrates two key features of particle energy loss which are important

Figure 3.3: Event display showing an example of a track-like topology; stopping proton candidate, with an initial momentum of 1 GeV, recorded by ProtoDUNE (from Ref. [1]).
to the physics capabilities of a LArTPC. Firstly, for all particles the energy loss rises rapidly at low momentum. As a particle slows its energy loss rises steeply until it comes to a stop. Secondly, there is a minimum in the energy loss for all particles located in the range of $\beta\gamma \approx 2 - 4$. Particles in this range are referred to as Minimum Ionising Particles (MIPs). The momentum a particle requires to be in this range depends on its mass. Equation (3.1) describes the mean energy loss, the process is stochastic, and the energy loss is described by a highly-skewed Landau or Landau-Vavilov distribution with rare large energy loss events driving the mean higher than the most probable value (MPV). It is the MPV rather than the mean which is most commonly measured in LArTPCs.

In LArTPCs, muons and charged pions are often produced within or close to the range of momentum (0.1 GeV - 1 GeV) corresponding to a MIP with a mean energy loss of $\approx 2.2$ MeV/cm. As a result, they travel large distances before losing energy increasingly rapidly at the end of their path and coming to an abrupt stop. This rapid energy loss at the end of a track is referred to as a Bragg peak. Because of the
Figure 3.5: Calibrated $dE/dx$ of a sample of test beam stopping protons with an initial momentum of 1 GeV (upper band) and stopping cosmic-ray muons (lower band) recorded with the ProtoDUNE-SP detector (from Ref. [1]). The residual range is a measure of the distance from the endpoint of the reconstructed track. The expected most probable values for both muons (blue) and protons (red) are shown as solid lines.

A proton's larger mass means they stop through ionisation energy loss more rapidly than the MIP-like pions and muons. The Bragg peak is visible in the final part of the proton track shown in fig. 3.3. The difference in the Bragg peak between protons and muons and pions allows them to be distinguished using calorimetric particle identification techniques. The difference in the Bragg peaks is illustrated in fig. 3.5, which shows the measured $dE/dx$ deposits of test beam protons and cosmic-ray muons in the final part of the track recorded by the ProtoDUNE-SP detector. Muons and pions are too close in mass to be reliably differentiated using this technique.

### 3.2.2 Shower-like Signatures

While both analyses discussed in this thesis focus on the track-like signatures of muons and pions, LArTPCs have excellent capabilities to reconstruct electrons and photons
– particles that are key to both the MicroBooNE and DUNE physics programmes. Backgrounds including photons and electrons from neutrino interactions must be rejected in the selection of LLPs.

High energy ($\gtrsim 100$ MeV) photons and electrons both initiate electromagnetic showers in LAr. Photons at this energy predominately lose energy via production of electron-positron ($e^+e^-$) pairs. The dominant energy loss of electrons is via radiation of photons. These processes combine to create a cascade with an increasing number of particles each with less energy as the shower progresses until a critical energy $E_c$ is reached. The energy $E_c$ is the point where radiation losses no longer dominate over collision-related losses. Figure 3.6 shows an example event display of an electromagnetic shower created by an electron with a momentum of 0.5 GeV in the ProtoDUNE-SP detector. This momentum is in the typical range of the electron-neutrino initiated electron showers observed in the MicroBooNE detector. The MIP-like stem of the shower is visible on the left of the display, before the radiation of a photon and its subsequent pair production create the shower of EM particles on the right.

The LArTPC technology allows discrimination of EM showers initiated by photons and electrons by considering the early stages of the shower development. For photons, the first step in showering is conversion into an electron-positron pair. Therefore
the earliest part of the visible shower will have an energy deposition matching two overlaid MIPs. Electron-initiated showers will start with a single MIP-like particle. Additionally, photons will travel some distance from their production point before converting to an $e^+e^-$ pair. If it is possible to determine the photon production point, using another particle produced by the same interaction, this gap is indicative of a photon-initiated shower.

### 3.2.3 Scintillation Light

Charged particles traversing LAr produce large amounts of scintillation light due to the ionisation and excitation of the argon atoms. This light is emitted isotropically by the radiative decay of excited argon dimers which are formed by one of two mechanisms: the recombination of an ionisation electron with an argon ion or self-trapped exciton luminescence where an excited argon atom combines with a ground state argon atom. The rates of both processes, and therefore the scintillation light yield, depend on the E-field strength. At a drift field of 500 V/cm, 24,000 photons are produced per MeV of energy deposited \[64\].

The two processes produce singlet and triplet excited states with distinct lifetimes before decaying to the ground state and releasing a photon. The singlet state has a very short mean lifetime of $\sim 6$ ns and produces what is called the fast component of scintillation light. The triplet state has a significantly longer lifetime of $\sim 1.6 \mu s$ and produces the slow component. The scintillation photons of both components are produced at the same wavelength of 128 nm, in the vacuum ultraviolet range (VUV). 128 nm wavelength photons cannot excite ground state argon. Hence liquid argon is transparent to its own scintillation light, allowing the light to travel large distances and be detected with reasonably high efficiencies. Both components are prompt in comparison to the millisecond level drift time of the electrons. This allows photon detection to be used to trigger on activity inside the detector and determine the time it took place at. Depending on the design of the photo-detection system the scintillation light can also be used to determine information about the location, energy and species of a particle.
3.3 Detector Effects

LArTPCs exhibit a number of effects that modify the recorded signal (ionisation electrons and scintillation photons) with respect to the signal produced. One MeV of deposited energy leads to $\approx 10^5$ ionisation electrons. These clouds of electrons drift through the electro-negative argon to the anode. A series of processes, including diffusion, electric field distortions and capture by either $\text{Ar}^+$ ions or impurities distort these drifting clouds before they arrive at the anode. In addition, scintillation photons undergo Rayleigh scattering and experience attenuation as a result of both quenching and absorption affecting the amount of light collected by the photon detection system. Understanding these effects is key to being able to calibrate the detector to provide an accurate energy, position, and time of detected particles, as well as providing the ability to model the systematic uncertainties on an analysis caused by these effects.
3.3.1 Space Charge Effect

$\text{Ar}^+$ ions are produced alongside the ionisation electrons. These heavy positively charged ions drift slowly towards the cathode. Surface detectors such as MicroBooNE and ProtoDUNE-SP experience very high rates of crossing cosmic rays ($\sim 5$ Hz). This creates large numbers of $\text{Ar}^+$ ions. Because of their slow drift (a few millimetres per second [1]), ions accumulate and distort the electric field across the detector creating non-uniformity. This is known as the Space Charge Effect (SCE). These electric field distortions affect the path of drifting electrons, which causes the charge to be reconstructed at a different position from where it was produced. The impact of the SCE on the reconstructed position of cosmic rays is shown in fig. 3.7. The distortions are greater near the cathode where the ions are collected. SCE-driven distortions in the electric field strength also affect the amount of recombination occurring across the detector and therefore affects the amount of measured charge.

3.3.2 Recombination

Ionisation electrons can be thermalised by the surrounding medium and recombine with nearby $\text{Ar}^+$ ions rather than completing their drift to the anode. The rate of recombination is dependent on the number of ions being created. This introduces a non-linear relationship between the amount of charge per cm which is measured at the anode ($dQ/dx$) and the true amount of deposited charge ($dE/dx$). A popular model used to describe recombination is the “Modified Box Model” developed by the ArgoNeuT collaboration [66]. It is used by both the MicroBooNE and ProtoDUNE-SP in the calibration of their detector. Within the model the relationship between ($dE/dx$) and ($dQ/dx$) is

$$\frac{dE}{dx} = \frac{\rho E}{\beta'} \left( \exp \left( \beta' W_{\text{ion}} (dQ/dx)/(\rho \mathcal{E}) \right) - \alpha \right), \quad (3.2)$$

where $\mathcal{E}$ is the electric field strength, $\rho$ the argon density and $W_{\text{ion}} = 23.6$ eV the energy required to ionise argon [67]. The model parameters $\alpha$ and $\beta'$ must be tuned to experimental data. ArgoNeuT extracted values of $\alpha = 0.93$ and $\beta' = 0.212$. These values are used as the nominal values for MicroBooNE and ProtoDUNE-SP [66].
3.3.3 Diffusion

Diffusion causes the clouds of electrons travelling towards the anode to spread out. The drift electric field causes anisotropic spreading, so diffusion is considered as two separate components, longitudinal diffusion in the drift direction, and transverse diffusion perpendicular to the drift direction. Longitudinal diffusion has the effect of widening the pulse measured on the wire, with clouds which have travelled furthest through the detector experiencing the greatest widening. The pulse width (in time) is given by

$$\sigma^2(t) \approx \sigma^2(0) + \left( \frac{2DL}{v_d^2} \right) t,$$

where $v_d$ is the drift velocity and $D_L$ is the constant which characterises the diffusion and can be determined by experiment. Transverse diffusion can cause charge to be detected on multiple neighbouring wires, creating smearing and reducing the position resolution. The transverse diffusion constant is given by $D_T = \frac{\mu \epsilon L}{e}$, where $\mu$ is the electron mobility, $e$ is the electron charge and $\epsilon L$ is the electron energy.

3.3.4 Argon Purity

Electro-negative contaminants in the argon such as water and oxygen capture a fraction of the drifting electrons, therefore reducing the measured $dQ/dx$ at the anode. The mean free electron lifetime is inversely proportional to the quantity of impurities present in the liquid argon at a given time. The total captured fraction of electrons is proportional to the drift time, and therefore inversely proportional to the electric field strength.

The electron-lifetime and therefore the purity of the argon can be monitored in a number of ways. One method is to use location and time-tagged cosmic-ray muon (MIPs) tracks to measure the ratio of measured charge from depositions that occur near the anode ($Q_A$) and the cathode ($Q_C$). The electron lifetime $\tau_e$ can then be extracted from

$$\frac{Q_A}{Q_C} = \exp \left( -\frac{t}{\tau_e} \right),$$

where $t$ is the drift time of charge from the cathode to the anode. Very small amounts of contaminants can have a significant impact on the electron lifetime. For
a drift distance of 2.56 m at an electric field of 0.273 kV/cm, an O\textsubscript{2} contamination as low as 60 parts per trillion can result in a 36\% signal loss \cite{69}. For this reason the lifetime and the performance of the liquid-argon filtration system are monitored continuously during data taking.

### 3.3.5 Rayleigh Scattering and Light Attenuation

While pure argon is transparent to the VUV scintillation produced, the photons have a high probability of Rayleigh Scattering. Each scattering changes the direction of the photons and therefore causes photons to travel a non-direct path to the light detection system, leading to a smearing of the time resolution of the photon detection \cite{70}. The value of the Rayleigh scattering length of $\lambda = 128$ nm photons in liquid argon remains under study with values in the literature ranging from 50 to 110 cm. A recent measurement of the scattering length performed with a dedicated experimental setup at CERN determined a value of $(99.1 \pm 2.3)$ cm \cite{71}. This differs from the calculated value of $(55 \pm 5)$ cm \cite{72} which was used to inform the default value in the light simulation of many LArTPC experiments.

Impurities in the liquid argon can create attenuation of the scintillation light through either quenching or absorption. Quenching occurs when excited dimers lose their energy via collisions with contaminants such as nitrogen or oxygen rather than de-exciting and releasing a photon. The slow component of the light is particularly affected by quenching. Scintillation photons can also be absorbed when nitrogen or other elements are present which have a higher cross-section for the VUV wavelength. Absorption results in an exponential decay of the number of photons as a function of distance travelled whereas quenching causes an overall decrease with no distance dependence.

### 3.4 ProtoDUNE

The ProtoDUNE-SP detector is a single-phase prototype of the DUNE Far Detector. It was operated at the CERN Neutrino Platform in 2018 and 2019, and serves as an important test-bed for full-scale components of the first far detector module to be constructed \cite{1}. The detector was exposed to a charged particle test beam
in September and October of 2018. The beam delivered momentum and species-tagged positively charged particles, predominantly charged pions, kaons, muons, and positrons. The proportion of each particle species depended on the target momentum setting of the beam which ranged from 0.3 GeV to 7 GeV.

The data set collected allows important tests of the reconstruction, calibration and analysis of particles as they would appear when produced in a neutrino interaction in the final DUNE modules. Furthermore, a program of hadron-argon cross-section measurements is currently being performed which will play an important role in understanding propagation of these particles through argon.

This section describes an analysis performed to select and perform calorimetric energy reconstruction of both 1 GeV pions and muons produced in the test beam. It was published as part of the first results paper from the ProtoDUNE-SP experiment [1]. The selection is important in assessing and validating the performance of the ProtoDUNE-SP detector and the full reconstruction, calibration and analysis chain which can be used to inform design and analysis choices for the future DUNE experiment. In addition, it serves as a platform for the charged pion cross-section measurements that are underway. The measurements, when completed, will provide a more precise understanding of neutrino interactions with argon that produce final-state pions, a key study channel of the DUNE experiment. The analysis, performed within the context of this thesis, illustrates many of the principles of particle detection in a LArTPC discussed in this section and so is included here.

3.4.1 ProtoDUNE-SP Detector

The ProtoDUNE-SP TPC is installed inside a membrane cryostat measuring 8.5 m in width and length and with a height of 7.9 m. The TPC is suspended inside the cryostat by a network of steel beams and is itself made up of two drift volumes sharing a central cathode. There are two anode planes on either side of the detector. Each anode plane is made up of three identical APAs sitting adjacent to one another as shown in figs. 3.8(a) and 3.8(b). Each APA is read out independently. A summary of the design and key nominal parameters of the TPC can be found in tab. 3.1.
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Figure 3.8: [a] A diagram showing the ProtoDUNE-SP TPC with the major components labelled. The coordinate system is labeled in the bottom right of the image (from Ref. [57]). [b] A photo taken inside one of the drift volumes before being filled with argon. The cathode can be seen on the right-hand side and the three neighbouring APAs on the left.

<table>
<thead>
<tr>
<th>TPC configuration</th>
<th>Anode-Cathode-Anode (2 separate volumes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TPC dimensions (one volume)</td>
<td>6.086 (h) × 3.597 (w) × 7.045 (l) m³</td>
</tr>
<tr>
<td>Active volume</td>
<td>2 ×154 m³</td>
</tr>
<tr>
<td>Instrumented LAr mass (87.65 K)</td>
<td>419 t</td>
</tr>
<tr>
<td>Number of TPC wire planes</td>
<td>4 (G, U, V, X)</td>
</tr>
<tr>
<td>Number of wires (total)</td>
<td>15360 (instrumented)</td>
</tr>
<tr>
<td>G: Grid plane</td>
<td>2 × 2880 (non-instrumented)</td>
</tr>
<tr>
<td>U: 1st induction plane</td>
<td>2 × 2400 (instrumented, wrapped)</td>
</tr>
<tr>
<td>V: 2nd induction plane</td>
<td>2 × 2400 (instrumented, wrapped)</td>
</tr>
<tr>
<td>Z: TPC-side collection plane</td>
<td>2 × 1440 (instrumented)</td>
</tr>
<tr>
<td>C: Cryostat-side collection plane</td>
<td>2 × 1440 (instrumented)</td>
</tr>
<tr>
<td>Wire orientation (w.r.t. vertical)</td>
<td>G: 0°, U: +35.7°, V: −35.7°, X: 0°</td>
</tr>
<tr>
<td>Wire spacing</td>
<td>4.79 mm (G, X); 4.67 mm (U, V)</td>
</tr>
<tr>
<td>Gap distance between planes</td>
<td>4.75 mm</td>
</tr>
<tr>
<td>Wire type</td>
<td>Cu-Be Alloy #25, diam. 150 µm</td>
</tr>
<tr>
<td>E-Field (nominal) in drift volume</td>
<td>500 V/cm</td>
</tr>
<tr>
<td>Cathode plane voltage</td>
<td>−180 kV</td>
</tr>
<tr>
<td>Anode plane bias voltages</td>
<td>G: −665 V, U: −370 V, V: 0 V, X: +820 V</td>
</tr>
<tr>
<td>Ground mesh</td>
<td>0 V</td>
</tr>
<tr>
<td>Max. drift length</td>
<td>3572 mm</td>
</tr>
<tr>
<td>(Cathode-to-G-plane distance at 87.65 K)</td>
<td></td>
</tr>
<tr>
<td>Drift velocity (nominal field, 87.65 K)</td>
<td>1.59 mm/µs</td>
</tr>
<tr>
<td>Max. drift time (nominal field, 87.65 K)</td>
<td>2.25 ms</td>
</tr>
</tbody>
</table>

Table 3.1: ProtoDUNE-SP TPC design and nominal parameters. Here, X refers to all collection planes, and Z and C refer to the collection planes on the sides of the TPC and cryostat, respectively. Adapted from Ref. [1].
The ProtoDUNE coordinate system as shown in fig. 3.8(a) is defined to be right-handed where the $y$ axis is vertical, increasing with height and the $z$ axis is horizontal and points approximately in the beam direction. The $x$ axis is also horizontal and is parallel to the electron drift with $x = 0$ taken to be the cathode in the centre of the detector.

In the current design of the first full-scale DUNE far detector module, the APAs are designed to be double sided. They are sandwiched between two separate drift volumes and read out charge from both sides. This is not the case for ProtoDUNE-SP where the APAs are positioned against the edge of the cryostat. Nevertheless, the same APA design is used in its role as a prototype. The centre of each APA contains two separate collection planes (each opaque to charge) separated by a mesh layer. The U and V induction planes use the same wires on both sides of the APA to minimise readout channels; they are wrapped around the APA. Finally, the outer layer is an uninstrumented grid plane, in place for pulse shaping purposes as described in section 3.1.

Electron diverters, designed with the motivation of mitigating the loss of charge in the vertical gaps between the APAs, were installed between the APAs on the negative-$x$ side of the TPC. These electron diverters are made up of two electrode strips mounted on an insulating board. When operating as designed, a voltage is applied to the electrodes to modify the electric field in the gaps such that electrons drift away from the gaps between APAs and into the active area. However during commissioning the electron diverters were seen to be drawing high currents due to one or more shorts in the cold volume. They were left unpowered and as a result of a resistive path to ground had a voltage close to zero. These grounded diverters collect charge produced near the gap and severely distort the drift paths of tracks passing the gaps. Electron diverters are not included in the design for the full-scale DUNE far detector modules.

The ProtoDUNE-SP photon detection system comprises 60 optical modules mounted within the APA frames. The modules are a mixture of three different photon collection systems proposed for DUNE. Each technology converts the incident LAr scintillation photons to a longer visible light wavelength using compounds referred
to as wavelength shifters, before trapping and directing some fraction of the light onto arrays of silicon photomultiplier photo-sensors (SiPMs) \(^73\). Of the 60 modules, 29 are double-shift light guides \(^74\), 29 are dip-coated light-guides \(^75\) \(^76\) and the final two are modules based on the ARAPUCA photon detector technology \(^77\). The photon detection system is not used in this analysis.

![Figure 3.9: A diagram showing the design of the ProtoDUNE-SP beamplug. The key components are labeled. Figure from Ref. \[1\].](image)

A “beam plug” is installed at the entry point of the test beam which extends from outside the cryostat through to \(\sim 5\) cm within the field cage boundary. The beam plug minimises energy loss of beam particles prior to reaching the active volume by providing a low density passage through the cryostat wall and the approximately 40 cm of argon between the cryostat wall and the TPC. The “beam plug”, shown in fig. 3.9, is constructed of alternating fibreglass and steel rings to form a cylinder. A series of resistors are connected to the steel rings to regulate the voltage from the field cage to the grounded cryostat membrane. The ends of the cylinder are capped with thin fibreglass plates. The cylinder extends from outside the cryostat to \(\approx 5\) cm within the field cage boundary and is filled with nitrogen at a nominal pressure of 1.3 bar.
3.4.2 Beam Line

The test beam ProtoDUNE-SP receives is delivered by an extension branch of the H4 beam line. Protons accelerated to 400 GeV by the CERN Super Proton Synchrotron (SPS) are extracted and directed onto a beryllium target, producing a beam consisting of a mixture of hadrons at 80 GeV. This beam of hadrons impinges on a second target of either copper or tungsten, to produce a very low energy (VLE) tertiary beam in the 0.3 to 7 GeV momentum range. Finally, the H4-VLE beam line momentum selects the particles and transports them to the ProtoDUNE-SP detector. For the 1 GeV momentum setting used in this analysis, the tungsten target was used to increase the hadron content of the beam. A full description of the beam line design can be found in Ref. [78]. The beamline enters in the right-hand side TPC volume (w.r.t beam direction) at around $x = -30$ cm and in the upper half of the TPC at approximation $y = 420$ cm (see fig. 3.8(a)). The beam points downwards (11° below horizontal) and towards the APAs on the negative x side (10° right from z-axis).

A series of detectors are located along the beam line which can be combined to give both a trigger for the TPC readout and particle identification for each event. There are eight scintillating fibre detectors that function as profile monitors (“XBPF”). Each measures the position of an intersecting particle in one dimension. Pairs of devices rotated at 90° from each other are used to monitor the beam position as it approaches the detector. The last two sets of XBPFs are used to measure a particle’s location and direction which are extrapolated to calculate the position and angle of entry to the detector. The momentum of the particles is calculated using the three XBPFs which surround the middle bending magnet as shown in fig. 3.10.
measured position of the particle at each monitor is combined with the knowledge of the magnetic field and distance between the monitors to calculate a particle’s momentum from the bending angle \[79\].

![Figure 3.11](image.png)

Figure 3.11: The 2D distribution of beamline particles’ Time of Flight and Momentum as measured by the beamline instrumentation. The red curves show the predictions for the various labeled particles.

Three trigger counters (“XBTF”) are used to determine the time of flight (TOF) of the particle. They are of a similar design to the XBPFs but all the fibres are readout together and therefore offer no position information. The upstream and downstream XBTFs are separated by 28.575 m and together give a timing resolution on the TOF of 900 ps \[79\]. Figure 3.11 shows the measured TOF of beamline particles as function of their measured momentum. Coincident signals between the middle and final XBTF are also used to trigger on beam particles when required.

Finally there are two threshold Cherenkov counters (“XCET”), one “low” and one “high” pressure. Cherenkov threshold counters detect the light produced if a particle is travelling at a velocity \((\beta)\) above the medium’s threshold velocity \(\beta_t = 1/n\) where \(n\) is the medium’s refractive index. The pressures of the two Cherenkov counters are tuned to produce threshold velocities so that when combined with the TOF
measurement they offer particle identification across the whole momentum spectrum.

3.4.3 Analysis Data and MC Samples

This analysis uses data corresponding to approximately 12 hours of exposure to a 1 GeV/c beam taken as part of a single run. The electron drift lifetime was approximately 14 ms as measured by the purity monitor throughout the run, which is significantly higher than required by the design specification. Data quality is assessed on an event by event basis with criteria for removing events in short periods of unstable drift voltage or where one or more of the TPC readout boards were inactive.

Monte Carlo (MC) simulations are produced in order to validate and understand the performance of the detector in the data results. A replica 1 GeV/c test beam sample is generated using the g4Beamline \[80\] and CORSIKA \[81\] packages to generate the beam particles and cosmic rays respectively. In this generation of the MC, the beam line instrumentation readout is not used in the simulation. Instead, a requirement is placed on beam MC that the true simulated beam particle is either a pion or muon.

3.4.4 Selection of Events With Reconstructed Beam Pions

The first step of selection involves using the beamline instrumentation to separate pion and muon events from the other species. For the 1 GeV beam energy run considered here, the beam line PID conditions stipulate that the recorded TOF is between 0 and 110 ns and there is no signal in the low-pressure Cherenkov detector. The time of flight criteria removes protons. At 1 GeV, the electrons are travelling fast enough to trigger the low-pressure Cherenkov detector. This leaves a pure sample of pion and muon interactions which are indistinguishable from each other at a beam momentum of 1 GeV with the beamline information.

The Pandora pattern recognition framework \[61\] is used to reconstruct the particle trajectories in the TPC. The framework then selects a single reconstructed particle as a likely candidate for the beam line track using a Boosted Decision Tree to
assess if a reconstructed topology is consistent with being of test beam origin. More information on the ProtoDUNE-SP specific adaptations to Pandora and its role in the reconstruction can be found in section 4.5 of Ref. [1]. The next stage of selection combines beam line and TPC information to remove events where a track has been incorrectly identified as the primary beam particle.

Figure 3.12: A series of data histograms of the beamline-TPC position differences at the start of the TPC track. The quantities are described in tab. 3.2. The offsets from zero are predominately due to the SCE. The greyed out areas indicate the events which are removed.

Figure 3.12 shows the distance and angle between the end of the beam line particle’s reconstructed trajectory and the start of the assigned reconstructed TPC beam particle track. The distance distributions are not centred around zero due to large distortions from SCE shifting the start points of the reconstructed TPC tracks. Events that fall in the shaded regions are removed, as they are not aligned with the measured beam line track. Hence they are likely to be either cosmic rays or secondary particles produced by the beam particle interacting upstream of the TPC.

For MC, the truth information of the beam particle is used in place of the beam line information. Figure 3.13 shows the equivalent distribution in MC. A log scale is used to show the different contributing components more clearly. The selection criteria for both Data and MC can be seen in tab. 3.2. The legend categorises the components based on the underlying truth information. The category an event falls into is determined according to the true particle that contributed most hits.
Figure 3.13: A series of MC histograms of the beamline-TPC position differences at the start of the TPC track. The quantities are described in tab. 3.2. The offsets from zero are predominately due to the SCE. The greyed out areas indicate the events which are removed.

<table>
<thead>
<tr>
<th>Beam Quality Criteria</th>
<th>Data</th>
<th>Monte Carlo</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cosine angle</td>
<td>&gt;0.93</td>
<td>&gt; 0.93</td>
</tr>
<tr>
<td>((X_{\text{Start}} - X_{\text{End}})) TPC</td>
<td>(0,10) cm</td>
<td>(-3,7) cm</td>
</tr>
<tr>
<td>((Y_{\text{Start}} - Y_{\text{End}})) TPC</td>
<td>(-5,10) cm</td>
<td>(-8,7) cm</td>
</tr>
<tr>
<td>((Z_{\text{Start}} - Z_{\text{End}})) TPC</td>
<td>(30,35) cm</td>
<td>(27.5,32.5) cm</td>
</tr>
</tbody>
</table>

Table 3.2: The criteria placed to select a purer sample of beam particles in both Data and MC. The Cosine angle is the angle between the direction of the TPC track and the direction of the true beam particle (MC) or beamline track (data). \(X_{\text{Start}}\) TPC is the start position in X of the reconstructed candidate beam track in the TPC before SCE corrections for both MC and data. For data, \(X_{\text{End}}\) Beam is the projected X location of the intersection of the track from the beam line instrumentation with the TPC. For MC, \(X_{\text{End}}\) Beam is the projected X location on the TPC of the true beam beam particle’s intersection with the TPC.
Table 3.3: A description of each of the categories based on the underlying truth information for the selected beam particles. The number of events falling into each of these categories is shown both at the reconstruction stage and after then beamline matching selection.

The MC distributions in fig. 3.13 illustrate the success of the beamline-TPC selection. The true beam particles are highly peaked in the selected region, whereas the long tails caused by cosmic rays and secondary particles not aligned with the beamline track are removed. The criteria used for the MC sample are listed in tab. 3.2. They are slightly offset from the data sample due to small differences in the SCE simulation from data.

Track length distribution after selection: Figure 3.14 shows the length of the reconstructed tracks which pass the selection above. The data spike at 230 cm is caused by tracks being incorrectly reconstructed as ending at the gap between the first and second APAs. As mentioned in section 3.4.1, the electron diverter in the gap
was grounded and this causes the tracks that cross the APA boundaries to become spatially distorted as well as a distortion of collected charge in that region. Both these effects can lead the Pandora reconstruction to split tracks at the APA boundary. In order to recover some of these events, a track stitching algorithm combines tracks that end at the APA boundary with tracks that start just after it within 10cm in the X and Y direction.

The pion track length distribution is roughly exponentially decaying driven by the pion cross-section. As 1 GeV pions have an expected interaction length in argon of ~1 m, the majority of pions will interact before coming to a stop via ionization energy loss. Conversely 1 GeV muons will stop predominantly via ionization energy losses (as described in section 3.2.1) with an expected path length of ~4 m, where the peak can be seen in both MC and data. The data and MC distributions are shown overlaid for illustration purposes only. They are not expected to agree well. For agreement the MC would need to be tuned to parameters that are unknown and must be determined from data in the first place.

The fractional muon component of the test beam is expected to be underestimated
in MC. The separation in length between pions and the peaked muon distribution means the muon fraction can be estimated from a distribution like fig. 3.14. Additionally, as discussed the pion-Ar cross-section is not well measured and as such the pion interaction length is uncertain. The ProtoDUNE-SP cross-section measurements, developed with the full data-sets for each beam-momentum setting, will be used as input to future simulation of pion transport in LAr.

### 3.4.5 Selection of Stopping Muons

![Figure 3.15](image)

**Figure 3.15:** MC and data histograms of the track length (SCE corrected), continuous-slowing-down-approximation (CSDA) length for candidates under the assumption the particle is a muon and a histogram of the ratio of the two for each event. The final histogram shows the stopping region in detail. The cut to select the stopping muons is indicated. The histograms are normalised by the number of entries.

The well-separated track lengths of the selected beam particles can be used to isolate a sample of the stopping muons from the interacting pions. The stopping range of each particle under the assumption it is a muon can be approximated using the measured beam momentum as an input to the continuous-slowing-down-approximation (CSDA) range. Figure 3.15 shows distributions containing the reconstructed length, CSDA muon assumption length and the ratio of the two for...
each selected track. The criteria,

\[ 0.9 < \frac{\text{Track Length}}{\text{CSDA Stopping Range}} < 1.1, \]  

selects a subsample of stopping particles, predominantly muons. The selection placed on the MC sample uses the simulated momentum for the true beam particle in each event as input to the ratio calculation. The purity of the selected muon sample in MC is 76%.

### 3.4.6 Calorimetric Energy Reconstruction

Calorimetric energy reconstruction is an important feature of LArTPCs. The calorimetric response is used both to reconstruct the energy of particles and to utilise the \(dE/dx\) distributions to distinguish stopping particles species. The beam particle samples in ProtoDUNE-SP can be used to assess and understand the calorimetric response of the detector and the performance of the calibration.

![Calorimetric Energy Reconstruction](image)

Figure 3.16: Pion (a) and stopping muon (b) \(dE/dx\) distributions for the ProtoDUNE-SP beam data after applying the calibration derived using cosmic-ray muons. The distribution for the beam Monte Carlo sample is also shown. The histograms are normalized such that the maximum frequency is one.

A charge signal calibration is applied to the selected tracks in both the pion and muon selections in order to calculate the true deposited energy of the particles as a function of distance \((dE/dx)\) along their trajectory. The charge signal calibration is produced using a sample of stopping cosmic-ray muons collected during the same run period as the beam data shown here. A full description of the calibration procedure
can be found in section 6.3 of Ref. 1.

Figure 3.16(a) shows the distribution of $dE/dx$ values of all hits on the collection plane from the selected beam pion candidates, that is, all candidates that are not selected by the stopping muon selection (eq. (3.5)) described above. The selected particles are MIPs and the distributions follow the expected Landau-Vavilov shape. The MC and Data samples match excellently and the MPVs agree to better than 1%.

Calorimetric energy information of beam stopping muons

Figure 3.16(b) shows the distribution of $dE/dx$ values of all hits on the collection plane from the selected beam muon candidates selected by the stopping particle criteria (eq. (3.5)). As with the pions, the MPVs of the data and MC samples agree to better than 1%.

Figure 3.17: $dE/dx$ vs residual range for selected stopping muons in the 1 GeV/$c$ beam after applying the calibration derived using cosmic-ray muons, in data (a) and MC (b). The expected most probable value of $dE/dx$ is plotted as a function of residual range for both.

Figure 3.16(b) shows the distribution of calibrated $dE/dx$ values of all hits on the collection plane from the beam muon candidates selected by the stopping particle criteria (eq. (3.5)). As with the pions, the MPVs of the data and MC samples agree to better than 1%.

The distribution of the $dE/dx$ vs the residual range for the selected stopping muons is shown for data in fig. 3.17(a) and for MC in fig. 3.17(b). A clear Bragg peak is seen at low residual range, as expected. The measured distribution displays good agreement with the theoretical MPV curve for a stopping muon in argon, in both the minimum ionization region and Bragg peak region of residual range.

The full 1D distribution in Figure 3.16(b) is dominated by hits from the MIP
region of the muon. If instead, the plotted hits are restricted to the last 50cm of the track, where the stopping of the 1 GeV muons first becomes visible in fig. 3.17, the distribution can be seen to broaden from the MIP-like Landau shape significantly. The MC distribution, as seen in fig. 3.18, still matches the data. The agreement demonstrates that the calibration procedure developed using MIP-like particles performs excellently for the stopping region as well.

The results presented in this section will be used as input to predictions of the performance of the first DUNE far detector module. The capabilities of the LArTPC technology in selecting and reconstructing the deposited energy of both muons and charged pions have been demonstrated. The properties discussed will be utilised throughout the search for LLPs decaying to these particles in MicroBooNE.

### 3.5 MicroBooNE

The MicroBooNE detector’s primary physics goal is to investigate the Low Energy Excess (LEE) of electron neutrinos observed by the MiniBooNE experiment [24]. As such it is located in the same beamline, the BNB, at approximately the same distance from the neutrino source. It also receives a highly off-axis flux from the higher energy NuMI beamline.
3.5.1 The MicroBooNE TPC

Figure 3.19: A schematic diagram of the MicroBooNE detector (from Ref. [59]). The cuboid TPC can be seen located inside the cylindrical cryostat.

The MicroBooNE detector [64] is a surface LArTPC with an active volume of 87 tons. The TPC is situated inside a cylindrical cryostat which contains 170 tonnes of LAr. The TPC is made up of a single drift volume with a single APA made up of two induction planes and a collection plane. A diagram of the detector can be seen in fig. 3.19. A summary of the design and key nominal parameters of the TPC can be found in tab. 3.4.

MicroBooNE has operated with a lower drift field (273 V/cm) than its nominal design (500 V/cm) throughout its data taking period. The resultant maximum drift time of $\approx 2.25 \text{ ms}$ is still well below the free electron lifetime throughout MicroBooNE's operation. As a surface detector, MicroBooNE experiences a large cosmic-ray flux and within the drift time approximately 20-30 cosmic rays intersect the detector.
### SECTION 3. LIQUID-ARGON TIME PROJECTION CHAMBER

<table>
<thead>
<tr>
<th>TPC configuration</th>
<th>Cathode-Anode</th>
</tr>
</thead>
<tbody>
<tr>
<td>TPC dimensions</td>
<td>2.32 (height) × 2.56 (width) × 10.36 (length) m³</td>
</tr>
<tr>
<td>Active volume</td>
<td>61 m³</td>
</tr>
<tr>
<td>Instrumented LAr mass</td>
<td>87 t</td>
</tr>
<tr>
<td>LAr Temperature</td>
<td>89 K</td>
</tr>
<tr>
<td>LAr Pressure</td>
<td>1.24 bar</td>
</tr>
<tr>
<td>Number of TPC wire planes</td>
<td>3 (U, V, Y)</td>
</tr>
<tr>
<td>Number of wires (total)</td>
<td>8256 (instrumented)</td>
</tr>
<tr>
<td>U: 1st induction plane</td>
<td>2400</td>
</tr>
<tr>
<td>V: 2nd induction plane</td>
<td>2400</td>
</tr>
<tr>
<td>Y: Collection plane</td>
<td>3456</td>
</tr>
<tr>
<td>Wire orientation (w.r.t. vertical)</td>
<td>U: +60°, V: −60°, Y: 0°</td>
</tr>
<tr>
<td>Wire spacing</td>
<td>3 mm (U, V, Y)</td>
</tr>
<tr>
<td>Gap distance between planes</td>
<td>3 mm</td>
</tr>
<tr>
<td>Wire type</td>
<td>Stainless Steel, diam. 150 µm</td>
</tr>
<tr>
<td>Coating</td>
<td>Copper 2µm, Silver 0.1µm</td>
</tr>
<tr>
<td>E-Field in drift volume</td>
<td>273 V/cm</td>
</tr>
<tr>
<td>Cathode plane voltage</td>
<td>−70 kV</td>
</tr>
<tr>
<td>Anode plane bias voltages</td>
<td>U: −110 V, V: 0 V, Y: +230 V</td>
</tr>
<tr>
<td>Max. drift length</td>
<td>2560 mm</td>
</tr>
<tr>
<td>Drift velocity</td>
<td>1.14 mm/µs</td>
</tr>
<tr>
<td>Max. drift time</td>
<td>2.25 ms</td>
</tr>
</tbody>
</table>

Table 3.4: MicroBooNE TPC design and nominal parameters.

#### 3.5.2 Detector Coordinate System.

The system is defined to be right-handed with the Y-axis vertical and pointing upwards. The Z-axis is the forward direction, co-linear with the BNB beam direction. The x-direction is parallel with the drift pointing away from the APA. The origin of the system is shown by the red cross, located on the anode, at the front face halfway up the detector vertically. Two angular quantities, the polar (θ) and azimuthal (φ) angle are defined by

\[
\theta = \arctan 2 \left( \frac{\sqrt{A_x^2 + A_y^2}}{A_z} \right),
\]

\[
\phi = \arctan 2 \left( \frac{A_y}{A_x} \right),
\]

where \(A_x, A_y, A_z\) are the x, y, z components of direction vector \(\vec{A}\). The coordinate system used for the MicroBooNE detector is shown in fig. 3.20.
3.5.3 Photo-detection system

The MicroBooNE photo-detection system consists of 32 optical units. They are located inside the LAr cryostat behind the wire planes and are arranged as shown in fig. 3.21. Each optical unit is made up of an 8-inch Hamamatsu R5912-02MO PMT positioned behind an acrylic plate coated with tetraphenyl-butadiene (TPB). A photograph and diagram of the optical units are shown in fig. 3.22.

Figure 3.20: A diagram showing the coordinate system used for the MicroBooNE detector. From Ref. [83]. The green (BNB) and orange (NuMI) arrows show the approximation direction of the respective beams at the detector.

Figure 3.21: A diagram showing the placement of the PMTs inside the MicroBooNE cryostat. The circles labelled as “Optical units” are the location of the PMTs. Light guide paddles, also labelled, are a SiPM based light collections system installed in MicroBooNE for R&D purposes. They are not used in analysis. Figure from Ref. [64].
Section 3.2.3 describe how the scintillation light emitted by LAr is of the wavelength 128 nm in the ultra-violet range (VUV light). PMT’s detect light in the visible range ($300 - 650$ nm) and therefore have effectively zero efficiency for 128 nm wavelength photons. The TPB coated plate in front of PMTs absorbs the VUV light before re-emitting it with a wavelength of $\approx 425$ nm where the PMT quantum efficiency is highest ($\approx 20\%$). The PMT readout is split into two copies, one high-gain channel which is attenuated by a factor of 0.18 and one low-gain channel given an attenuation factor of 0.018. Both channels are recorded by the readout electronics to allow a wide dynamic range for the ADC readout of the PMT pulses [64]. The signal from each PMT channel is digitized at a rate of 64 MHz by ADC converters located outside the cryostat.

### 3.5.4 Cosmic Ray Tagger

As MicroBooNE is located on the surface with no overburden, it experiences a high rate of cosmic-ray particles traversing the detector. These cosmic-ray particles can mimic neutrino interactions or beyond the standard model decays and thus represent an important background for the experiment. The Cosmic Ray Tagger (CRT) is an additional detector subsystem designed to identify and reject cosmic-ray activity. It consists of 73 modules made up of interleaved layers of scintillating strips. The location of the CRT panels in relation to the detector can be seen in fig. 3.23. They
Figure 3.23: A diagram showing the placement of the CRT modules around the MicroBooNE cryostat. The right hand side shows the location of the panels relative to the cryostat. The brown lines show simulated cosmic-ray trajectories that cross the CRT panels. From Ref. [84].

are positioned above and below the cryostat as well as on the two sides parallel to the beam direction. Simulation shows the design achieves coverage of 85% of the cosmic muons which pass through the TPC [84].

When a cosmic-ray muon intersects a CRT module its interactions with the plastic material produces scintillation photons which are detected by SiPMs. The signals from each strip can be used to reconstruct the entry and exit points of cosmic rays, and therefore interpolate the trajectory taken through the detector. Furthermore, the CRT system has excellent time resolution (≈ 100 ns) and this can be paired with the photo-detection system to reject events that are of cosmic-ray origin.

The CRT system was added to the detector after the initial runs of data taking. Installation and commissioning was finished in October 2017 and only data taken after that point has the full CRT information available for use.
3.5.5 Readout and Trigger

The following subsection describes the readout and triggering systems of MicroBooNE. The readout is general to both events from the NuMI and BNB beams. The triggering parameters used for this thesis are specifically tuned for events from the NuMI beamline, but the general triggering method is the same for BNB events.

Readout

The first step in the formation and readout of an event from the detector is the arrival of an external trigger signal. This signal initiates the formation of an event and provides the $t_0$ around which the TPC and photodetection outputs are aligned. This trigger signal is known as the hardware trigger and can either be provided by the Accelerator division to correspond to the arrival of a neutrino beam spill or a pulser to collect samples of any beam-unrelated continuous background activity. Once triggered, three TPC windows of 1.6 ms each are read out, one frame before the expected $t_0$ of the neutrino interaction and two afterwards, for a total readout time of 4.8 ms. This is slightly longer than the maximum drift time of 2.3 ms to ensure the neutrino interaction is fully contained in the frames.

Unlike the TPC, the PMTs are not read out continuously. Instead, short windows are selected from four 1.6 ms wide PMT frames surrounding the trigger time. The first of the windows is the 23.4 $\mu$s period following the trigger, within which the neutrino beam spill is expected to arrive. This is referred to as the unbiased beam gate window and data is collected across all PMTs simultaneously. Waveforms outside this window are saved only if they pass the cosmic discriminator threshold, which is set at 130 ADC counts ($\approx 6.5$ Photo-Electrons (PE)). If above the threshold, 40 samples ($\approx 0.6$ $\mu$s) of the individual PMT waveform are saved. There is a dead-time time of 45 samples after each PMT waveform is saved.
Figure 3.24: The fraction of hardware triggers for which the software trigger is fired for a range of ADC thresholds, measured by applying the software trigger offline on unbiased samples collected in the labelled periods. A clear decline in the firing fraction is seen across the range of possible thresholds between the 2016 (green) and 2018 (red) data sets. Labelled at 14% is the firing fraction of the trigger immediately after commissioning when it was set at 9.5 PE (190) ADC.

**Software Trigger**

The Fermilab Accelerator Division (AD) delivers a signal when a neutrino spill has been formed. This signal initiates the hardware trigger, which begins an event readout and starts the unbiased PMT window. With respect to the start of this window, neutrinos from the NuMI beam arrive in the window between $5.64 \, \mu s$ and $15.44 \, \mu s$.

Approximately only 1 in 50 of the NuMI spills results in a neutrino interaction inside MicroBooNE. To avoid recording empty events a light-based software trigger (SW trigger) is used to determine if an event should be stored. This SW Trigger is run on the DAQ machines and requires a minimum of 190 ADC (9.5 PE) of scintillation light in a window (4.69-16.41 $\mu s$) slightly wider than the neutrino arrival window, for the event to be saved. In MicroBooNE’s early run period the SW trigger passing fraction of hardware trigger was $\approx 14\%$. 
A significant decrease in MicroBooNE’s light yield was seen over time, dropping by approximately $\sim 45\%$ in a period from late 2016 to 2017 before stabilising for the rest of MicroBooNE’s run periods. The reason for this decline remains unknown. Investigations into likely explanations related to impurities in the Argon or the deterioration of the wavelength shifter on the optical units are ongoing. This decline caused a reduction in the firing fraction of the software trigger, shown in fig. 3.24. This led to concerns that neutrino interactions could be passing under the threshold and not being saved. In May 2018 a study was performed of the potential impact of the change and as a result, the NuMI SW trigger threshold was lowered from 190 ADC (9.5 PE) to 115 ADC (5.75 PE). This returned the firing fraction to the original 14%.

External and Unbiased Trigger

Even after the application of the software trigger, the majority of beam events recorded by MicroBooNE do not contain a neutrino interaction and are instead triggered by a cosmic ray passing through the detector in coincidence with the arrival of the neutrino window. To accurately model this background MicroBooNE collects a large sample of events with the same trigger conditions as the beam events but with a hardware trigger delivered by a pulser deliberately where there is no beam. These events are referred to as external or beam-off events throughout this thesis. Additionally, a smaller sample of events are collected with no software trigger requirements at all, referred to as unbiased events.
4 The NuMI Beamline and Neutrino Flux

Originally built to provide neutrinos for the MINOS long-baseline oscillation experiment, the NuMI beam [85] is a medium energy neutrino beam located at Fermilab. Running since 2005 it has since serviced a range of oscillation, neutrino cross-section and R&D experiments such as MINERνA [86], ArgoNeut [87], NOνA [88] and MINOS(+) [89].

In addition to the neutrino flux from the BNB, which it was primarily designed to receive, MicroBooNE also records large numbers of neutrinos from NuMI. MicroBooNE is positioned highly off-axis from the NuMI beam and hence receives an extremely different flux profile to the on-axis or small angle off-axis experiments listed above. MicroBooNE utilises this flux to perform cross-section measurements [90], beyond standard model searches [10] and independent validation of BNB results [91, 92].

This section provides details on the NuMI beam and beamline, including the absorber, where the LLPs searched for in this thesis would be produced. The composition of the flux and the properties of the NuMI neutrino interactions at MicroBooNE will be discussed as these interactions make up one of the primary backgrounds for absorber-produced LLPs.

4.1 Neutrino Beam Design

The NuMI beam produces neutrinos by impinging 120 GeV protons on a graphite target. The protons are produced from $H^{-}$ ions which are accelerated to 400 MeV by the linear accelerator (linac) before being passed through a carbon foil to convert them to protons. The protons are then passed into the booster synchrotron where they are accelerated to 8 GeV. For the BNB, protons from the booster are directed towards a beryllium target. For the NuMI beam, the protons are inserted into
another larger synchrotron called the Main Injector which further accelerates the protons to 120 GeV. The protons are then extracted and bent downwards before travelling the 350m to the NuMI target. The layout of the Fermilab accelerator complex can be seen in fig. 4.1.

Figure 4.2 shows a diagram of the NuMI beamline. The collision of protons with the graphite target produces a secondary beam of hadrons, made up predominantly of pions and kaons. Two magnetic van der Meer horns are then used to focus either positive or negative hadrons and to deflect the oppositely charged particles depending
SECTION 4. THE NUMI BEAMLINE AND NEUTRINO FLUX

on the chosen mode. In forward horn current (FHC) mode, a positive (+200 kA) current is applied to the horns. This focuses positively charged particles in the beam direction. In reverse horn current (RHC) mode, a negative current (-200 kA) is applied which instead focuses negatively charged particles. The focused particles then begin to travel down the 675m decay pipe which is filled with helium, where they decay to neutrinos.

<table>
<thead>
<tr>
<th>Neutrino Production Channels</th>
<th>Branching Ratio (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi^\pm \rightarrow \mu^\pm + \nu_\mu(\bar{\nu}_\mu)$</td>
<td>99.9877</td>
</tr>
<tr>
<td>$\pi^\pm \rightarrow e^\pm + \nu_e(\bar{\nu}_e)$</td>
<td>0.0123</td>
</tr>
<tr>
<td>$K^\pm \rightarrow \mu^\pm + \nu_\mu(\bar{\nu}_\mu)$</td>
<td>63.55</td>
</tr>
<tr>
<td>$K^\pm \rightarrow \pi^0 + e^\pm + \nu_e(\bar{\nu}_e)$</td>
<td>5.07</td>
</tr>
<tr>
<td>$K^\pm \rightarrow \pi^0 + \mu^\pm + \nu_\mu(\bar{\nu}_\mu)$</td>
<td>3.353</td>
</tr>
<tr>
<td>$K^0_L \rightarrow \pi^\pm + e^\pm + \nu_e(\bar{\nu}_e)$</td>
<td>40.55</td>
</tr>
<tr>
<td>$K^0_L \rightarrow \pi^\pm + \mu^\pm + \nu_\mu(\bar{\nu}_\mu)$</td>
<td>27.04</td>
</tr>
<tr>
<td>$\mu^\pm \rightarrow e^\pm \nu_e(\bar{\nu}<em>e) + \bar{\nu}</em>\mu(\nu_\mu)$</td>
<td>100.0</td>
</tr>
</tbody>
</table>

Table 4.1: The main neutrino-producing particles in the NuMI beamline and their respective decays [3].

The key neutrino-producing decays are listed in tab. 4.1. Since $m_\mu \gg m_e$, helicity suppression means meson decays to muon neutrinos are highly favoured over decays to electron neutrinos. Therefore the final neutrino beam is predominately composed of muon neutrinos.

Immediately downstream of the Decay Pipe, a large structure (5.5 m wide, 5.6 m tall, and 8.5 m deep) made of an aluminium core surrounded by steel and then concrete is intended to absorb any remaining hadrons. This is called the absorber. Approximately 1/6th of the beam protons pass through the target without interacting, travelling along the decay pipe before colliding with the absorber 725m downstream from the target. This creates a large number of low-energy mesons at the absorber, which then decay to a significant isotropic flux of low energy neutrinos. It is at this absorber, photographed in fig. 4.3, where the LLPs searched for in this thesis would be produced.

During MicroBooNE data taking the NuMI beam has been running in Medium Energy (ME) mode. The peak energy of the on-axis flux has been increased with
SECTION 4. THE NUMI BEAMLINE AND NEUTRINO FLUX

Figure 4.3: (a) The concrete blocks shielding the downstream end of the decay pipe before the installation of the hadron absorber. (b) The completed hadron absorber with the back wall of concrete blocks, and the steel roof blocks both visible. Photographs from Ref. [85].

respect to the early NuMI beam configuration by moving the target further upstream. In addition, the 2nd magnetic horn was moved further downstream, increasing the spacing between the horns and therefore the efficiency of the focusing. The total flux is approximately 30% higher in ME configuration than the earlier low energy (LE) Mode [94].

4.1.1 Proton Delivery Structure

The Proton beam structure directly determines the intensity and timing structure of the neutrino beam. At 8 GeV the time for protons to circulate the booster is 1.6 µs. This determines the length of the proton batches which are transferred to the main injector. Each batch accommodates 84 RF buckets at a spacing frequency of 53 MHz. Of the 84 available buckets, 81 are filled, creating proton bunches. Each batch is approximately equivalent to $5 \times 10^{12}$ protons impinged on the target (POT). The Main Injector is seven times the circumference of the booster and so can accommodate and accelerate six batches from the booster. One slot of the seven must be kept empty to allow time for the kicker magnets, which deflect the beam for
Figure 4.4: The daily and cumulative POT delivery of the NuMI beam line from 2014 to 2019, covering the MicroBooNE data period of this thesis. The periods in FHC and RHC modes are shown in orange and blue respectively. Figure adapted from Ref. [95].

extraction, to ramp up fully. These six batches together form a spill which is 9.6 $\mu s$ long.

The accelerator division utilises a system known as “slip-stacking” to increase the intensity of the proton beam without changing the timing structure described above. During slip-stacking, two booster batches are combined into a single batch inside the Main Injector doubling the number of protons in that batch. During the run period covered in this thesis, the NuMI beam has been run in both 4+6 and 6+6 configurations, where the first number refers to the amount of the 6 batches which have been stacked. A 4+6 spill corresponds to approximately $5 \times 10^{13}$ POT and a 6+6 spill corresponds to $6 \times 10^{13}$ POT.

4.1.2 Neutrino and Anti-neutrino Modes

The NuMI beam data in this thesis covers two periods from autumn 2015 to summer 2016 and autumn 2017 to summer 2018. That is the majority of the “Run 1” and “Run 3” MicroBooNE data taking periods respectively. Figure 4.4 shows the collected POT over time as well as the beam mode in which the POT was delivered. For the portion of Run 1 data used, the beam was in FHC mode and a predominately neutrino beam was delivered to the on-axis experiments. The Run 3 data was taken during a period of RHC current mode and therefore a predominately anti-neutrino beam was delivered.
4.2 Neutrino Flux

Figure 4.5: A schematic diagram of the MicroBooNE detector location relative to the NuMI beamline. From Ref. [83].

MicroBooNE is extremely off-axis with respect to NuMI, and as such it receives a very different flux to the small angle off-axis and on-axis experiments. The location of MicroBooNE with respect to the NuMI beam can be seen in fig. 4.5. The beam points both below and to the right of MicroBooNE and the decay pipe extends beyond the detector. Neutrinos from the NuMI target approach MicroBooNE at approximately $8^\circ$ from the beamline. The further down the decay pipe a neutrino is produced the larger its angle to MicroBooNE from the beamline. Neutrinos produced at the absorber approach the detector backwards at an angle of $120^\circ$.

4.2.1 Simulation Overview

The simulation of the NuMI neutrino flux at MicroBooNE used in thesis was primarily performed by Krishan Mistry and Katrina Miller. It is described in detail in chapter 5 of Ref. [83]. This section summarises the most relevant elements for the LLP search.

The infrastructure for the simulation of the NuMI beamline is shared by many of the experiments in the NuMI beamline. The most recent simulation package is g4numi [96]. It uses GEANT4 [97] (version geant_4_2.p03) to simulate the collision of the protons on the target and subsequent hadron production, as well as the propagation of the particles through the beamline geometry and their eventual decay.
SECTION 4. THE NUMI BEAMLNE AND NEUTRINO FLUX

to neutrinos. The GEANT4 physics list used is FTFP_BERT. g4numi is used by all recent NuMI experiments, including as the default simulation for this thesis. The final outputs of this simulation are called dk2nu files. These are ntuple-like files that contain the information of the produced neutrinos and their ancestry including the neutrino parent’s particle type and full kinematics. Information of the ancestry of the parent is also included to allow for hadron production constraints to be implemented downstream. These files contain all the information required to calculate the neutrino flux for a specific detector location and size, or as input to a neutrino interaction generator software.

The Package to Predict the fluX (PPFX) is used to constrain the flux using a collection of data from experiments measuring hadron production and propagation. Originally written for the MINERνA collaboration [94], it is now used by NOνA, MINOS+ and MicroBooNE. PPFX takes the neutrino parent information contained in the dk2nu files and uses the relevant hadron measurement data to produce a weight for each decay to create a central value flux prediction. The data sets used include a series of experiments that impinged monochromatic beams on fixed targets and measured the kinematics and number of particles downstream of the target. MicroBooNE uses the “thin target” data sets included in PPFX, which are the experiments that use a target width of a few interaction lengths or less. Studies by the Minerva collaboration found these sets produced a flux prediction in better agreement with an in-situ method of measuring the flux [94]. PPFX also includes capabilities to calculate the impact hadron production uncertainties have on the neutrino flux. More details on the implementation is given in section 8.

4.2.2 Flux at MicroBooNE

Figure 4.6 shows the central value flux prediction at MicroBooNE produced by the g4numi simulation after being constrained with PPFX for both FHC (Fig a) and RHC (fig b). As expected the majority of the neutrino flux is muon and anti-muon neutrinos for both horn polarities and across all energies. MicroBooNE’s highly off-axis position means that the majority of neutrinos that reach it are from decays of mesons not focused by the horns. Therefore the effect of the horn polarity on the
Figure 4.6: The central value flux prediction for MicroBooNE from the NuMI beam, for both FHC (a) and RHC (b) configurations. The integrated proportions of the flux are shown in the legend. From Ref. [83].
SECTION 4. THE NUMI BEAMLINE AND NEUTRINO FLUX

flux is much reduced. Large numbers of unfocused “wrong-signed” meson decays contribute to the flux in both RHC and FHC modes. This results in a similar flux of neutrinos and anti-neutrinos in both current modes with only a slight enhancement of the intentionally favoured type. The off-axis position also leads the average energy of a neutrino to be lower than that of other NuMI experiments. The sharp peaks seen in the $\nu_\mu$ at $E_\nu = 29.8$ MeV and $E_\nu = 236$ MeV are the result of two-body decays at rest of pions and kaons, respectively.

As discussed, the NuMI neutrinos approach MicroBooNE from a wide range of angles ($8 - 120^\circ$). As seen in fig. 4.7, energy and angle are highly correlated, with the vast majority of the high energy neutrinos ($> 250$ MeV) coming at small angles from decays at or just after the target. The majority of the low energy decays ($< 250$ MeV) also come from the target angles but significant numbers arrive from all angles. Muons can travel large distances down the decay pipe before decaying to low energy neutrinos. Another source of low energy neutrinos is the absorber. Proton collisions with the absorber at the end of the decay pipe produce a significant

Figure 4.7: The $\nu_\mu$ flux produced in RHC mode as a function of both energy and angle from beamline direction. From Ref. [83].
number of low energy kaons which decay at rest there. This in turn creates a large isotropic flux of KDAR neutrinos and potential LLPs. The location of the absorber with respect to MicroBooNE can be seen in fig. 4.5. The KDAR events approach the detector from below and behind at an angle of approximately 120° from the NuMI beamline.

There is also a significant time delay (∼0.5 µs) between neutrinos arriving from the target and absorber due to the longer combined proton and neutrino travel distance for the absorber flux. This inherent time delay as well as LLP time delays caused by their mass will be discussed further in section 5.1.

### 4.2.3 Kaon Decay-at-rest Flux from the Absorber

The beamline simulation package used, g4Numi [96] is based on a GEANT4 description of the geometry. By default, the simulation estimates a number of at-rest kaons produced in the absorber that would result in a rate of 0.011 (0.0099) KDAR $\nu_\mu$ per POT in FHC (RHC) mode.

The MiniBooNE experiment performed a measurement of the $\nu_\mu$ flux from KDAR at the NuMI absorber [98]. They used a range of Monte Carlo simulation packages to estimate the KDAR rate at the absorber. Predictions are produced using the MARS [99], FLUKA [100] and GEANT4 [97, 101] packages and find production rates in the range of 0.06–0.12 $\nu_\mu$ per POT. MiniBooNE then takes their GEANT4 prediction of 0.085 KDAR $\nu_\mu$ per POT as their central value, with a 30% uncertainty taken from the range between models.

The g4Numi value is significantly smaller than the central value estimated by MiniBooNE and well outside the range of predicted values reported from the different models. If considered to be the real value, it would result in a final MiniBooNE KDAR cross-section an order of magnitude higher than the theoretical predictions. The reason for this discrepancy is not known and is currently under investigation by the g4Numi authors. We scale our signal prediction to match the MiniBooNE rate by re-weighting signal events up by 8.0 (8.6) in the FHC (RHC) signal simulation, as is done in the previous MicroBooNE HPS search [10].
4.3 Neutrino Interactions in MicroBooNE

Although a neutrino measurement is not the aim of this analysis, neutrino oscillation and cross section measurements make up the main goal of the Fermilab LArTPC program and therefore inform many elements of detector design and operation which influence the strategy of this search. Furthermore, neutrino interactions from the NuMI beam will form one of the primary backgrounds to the LLP search. Therefore this section will layout the different modes of neutrino interaction relevant for the NuMI beam and the signatures they produce in LArTPCs.

In LArTPCs, neutrinos interact with either Argon nucleons or whole Argon nuclei via the weak force. The interactions can either be charged current (CC), mediated by a $W^\pm$ boson or neutral current (NC), mediated by a $Z^0$ boson.

![Figure 4.8](a) ![Figure 4.8](b)

Figure 4.8: The total charged current cross-sections for neutrinos (a) and anti-neutrinos (b). The theoretical predictions and a collection of data points collected from a range of experiments are shown. The components for QE, RES and DIS are shown as dashed, dot-dashed and dotted lines respectively. The figures are taken from Ref. [102] and full details of the prediction and data sources used can be found there.

As illustrated in fig. 4.6 the NuMI flux spans a wide energy range from $\mathcal{O}(10)$ of MeV to several GeV. Across this range, a variety of interaction modes contribute to the overall cross section of the neutrino-nucleus interactions. The individual cross-sections of each of these modes is energy dependent as shown in fig. 4.8. The CC anti-neutrino cross section is significantly lower than the neutrino cross section. The fraction is an exact third in the case of pointlike scattering due to the net spin...
of 1 in the interaction direction reducing the probability of backwards scattering.

Quasi-Elastic Scattering

For the energy region 0.1-1 GeV the neutrino cross section is dominated by the Quasi-Elastic Scattering (QE) contribution. The initial interaction produces a clean topology. For a charge current QE (CCQE) interaction on a free nucleon the process is given by,

\[ \nu_l + n \rightarrow l^- + p \]
\[ \bar{\nu}_l + p \rightarrow l^+ + n, \]

where \( l \) is the lepton flavour \( e, \mu, \tau \).

Neutral current QE interactions are given by

\[ \nu_l + p, n \rightarrow \nu_l + p, n \]
\[ \bar{\nu}_l + p, n \rightarrow \bar{\nu}_l + p, n. \]

The final state of a CCQE event will contain a lepton and nucleon, whereas in neutral current events the neutrino produced will exit the detector without interacting and only the nucleon can be observed.

The large size of argon nuclei complicates the possible quasi-elastic final states somewhat. The effects of correlations between multiple target nucleons and intranucleus interactions of the produced particles can lead to the ejection of one or multiple additional final state particles.

Meson Exchange Current

Correlations between nucleons lead to them to form bound states of two or more particles within the nucleus. Neutrinos can interact with these states. The modification on the neutrino interaction cross section by two-nucleon bound states is referred to as the 2 particle-2 hole (2p-2h) effect. In recent years this effect has been proposed
to explain neutrino scattering results in the $O(1 \text{ GeV})$ region where MicroBooNE is active. In particular, enhancements are seen in the measured CCQE-like cross section at the MiniBooNE experiment. The Meson Exchange Current (MEC), where the nucleon pairs are bound by the exchange of virtual mesons, is the largest contribution to this class of events. As seen in fig. 4.9, MEC events resemble CCQE events but with the emission of an additional nucleon from the interaction.

**Resonant Production**

For higher energy neutrinos, there is enough available energy in the centre-of-mass frame such that a neutrino interaction can excite the target nucleon to produce a baryonic resonance. This resonance then decays quickly to produce additional final state particles. For the lower end of the resonant energy range, the dominant resonances are $\Delta(1232)$ baryons which typically decay to a pion and a single nucleon. For example the CC interaction $\nu_\mu n \rightarrow \mu^- \Delta^+(1232)$ and subsequent decay $\Delta^+(1232) \rightarrow n\pi^+$ leads to a final state with a muon, charged pion and a neutron being produced. As neutrons are neutral and therefore often unreconstructed in LarTPCs this final state could mimic the LLP decay final states ($\mu\pi, \mu\mu$) searched for in this thesis.
Resonances decaying to neutral pions and neutrons are also possible. Of particular interest to MicroBooNE and DUNE is NC resonance interactions leading to $\pi^0$ production as this is commonly one of the largest backgrounds in experiments searching for $\nu_e$ appearance. At higher energies, the resonances produced decay into more complicated final states involving multiple pions and can also produce final states with strange quarks such as kaons.

**Coherent Pion Production**

Neutrinos can also interact coherently with the entire Argon nucleus. In these interactions the energy transfer is very low and the nucleus remains intact with a slight recoil. This results in a forwarded-boosted pion. The interactions are as follows:

\[
\begin{align*}
\nu_l + A &\rightarrow l^- + A + \pi^+ \quad \bar{\nu}_l + A \rightarrow l^+ + A + \pi^- \\
\nu_l + A &\rightarrow \nu_l + A + \pi^0 \quad \bar{\nu}_l + A \rightarrow \bar{\nu}_l + A + \pi^0,
\end{align*}
\]

where $A$ represents the nucleus. At the neutrino energies considered here the process is rare in comparison to standard pion resonant production. The final state particles (pion and lepton) can match exactly the final state particles from HNL decay. Furthermore, the lack of nuclear breakup and low energy transfer means the kinematics share many similarities with a LLP decay. Therefore coherent pion production creates an irreducible background in searches for HNL decays within a neutrino beam.

**Deep Inelastic Scattering**

For neutrino energies of several GeV and above, inelastic scattering begins to occur. At these energies, the neutrinos resolve the internal structure of the nucleon and interact with a quark. The struck quark recombines and produces a hadronic shower resulting in a number of hadrons in the final state. This often includes multiple pions as well as smaller numbers of heavier particles. This process is referred to as deep inelastic scattering (DIS). For energies above 10 GeV, DIS interactions dominate the neutrino cross section.
5 Simulation and Reconstruction

The simulation of MicroBooNE events and subsequent reconstruction of both the simulated and data events are handled within the unified software framework LArSoft [104]. The process is multi-staged and consists of the simulation of both signal LLP decays and background neutrino interactions, described in section 5.1, the propagation of the generated particles, ionisation charge and scintillation light through the detector, described in section 5.2, and the steps involved in both simulating and reconstructing the readout of the detector, covered in sections 5.3 and 5.4. Section 5.5 describes the charge calibration that is applied to both data and simulated events. In section 5.6 specific details for the various main data and Monte Carlo (MC) samples that are used in this analysis are outlined.

5.1 Monte Carlo Generation

The first stage of the event simulation is generation of the neutrino interaction or LLP decay. A MC generator simulates the secondary particles produced in the detector and calculates their kinematics. For this analysis, separate generators are used to produce samples for HNL and HPS decays, as well as a neutrino interaction generator for the background samples.

5.1.1 Higgs Portal Scalar Generator

The generator for HPS signal events was developed for use in the MicroBooNE $e^+e^-$ HPS search [10]. The higher mass HPS decays searched for in this thesis are also implemented in the generator. The generator can be used to simulate HPS production in either the NuMI or BNB beams and their subsequent decays in the MicroBooNE detector. In the standard operating mode, it is configured to a single HPS mass ($m_{\text{HPS}}$) and mixing angle ($\theta$).

For NuMI generation, the input is the $\text{dk2nu}$ files outputted by the neutrino flux
SECTION 5. SIMULATION AND RECONSTRUCTION

The generator selects the neutrino parent kaons, and decays them into HPS ($K \rightarrow \pi S$). As a two-body decay of a pseudo-scalar meson, this is isotropic in the kaon’s rest frame. The generator produces a momentum four-vector for the HPS by selecting a random direction from the unit sphere. The momentum is calculated from the fixed decay kinematics. The HPS four-vector is then boosted to the lab frame using the momentum vector of the parent kaon. For this search, only kaon decays at rest are considered and so no such boosting is required. To generate only HPS produced from kaons decaying at rest at the absorber, two selections are placed on the beamline kaons:

- Total kaon momentum $< 10^{-6}$ GeV
- Kaon decay location longitudinal distance from target $> 700$ m.

The generator next checks if the direction vector of the HPS will intersect with the detector volume. If there is no intersection, the decay is discarded and the process begins again with the next kaon in the input file. If an intersection is found, a decay vertex location is selected along the segment of the HPS direction ray which passes through the detector. The exponential reduction of the flux due to scalars decaying is accounted for when selecting a decay location along the trajectory.

The decay mode of the scalar is selected at random based on the branching fractions of the available decay modes ($S \rightarrow e^+ e^-, \mu^+ \mu^-, \pi^0 \pi^0, \pi^+ \pi^-$) for the chosen HPS mass. All of the modes are two body decays, so in each case the two daughter particles are produced back to back in the HPS rest frame, with the direction again drawn from an isotropic distribution. As discussed in section 6.1, the momentum magnitude of the daughters in each decay mode is fixed and depends solely on the mass of the HPS. Finally, each of the two daughter particles is boosted into the lab frame using the HPS momentum vector. The time of the decay is calculated by using the kaon decay time and the time of flight of the scalar to the decay point. The time is randomly shifted to account for the proton timing structure, which is considered to be a uniform distribution across the NuMI beam window, matching that used in the neutrino simulation.

Once the kinematics of the event have been determined, the normalisation factor
for such an event is calculated as the product of a series of weights,

$$w_{ev} = \text{BR}(K^\pm \rightarrow \pi^\pm S) \times P_{\text{dec}} \times \frac{1}{\text{BR}(K \rightarrow \nu + X)} \times w_{\text{imp}}. \quad (5.1)$$

The four terms which contribute to the overall weight are as follows;

- **BR($K^\pm \rightarrow \pi^\pm S$):** The branching fraction of the scalar-producing kaon decay. Which is calculated using eq. (2.3) and depends on the mixing angle $\theta$ and $m_{\text{HPS}}$.
- **$P_{\text{dec}}$:** The probability that the scalar will decay along the segment of its ray which intersects the detector. This can be expressed as $P_{\text{dec}} = e^{-L_i/\gamma\beta\tau} - e^{-L_f/\gamma\beta\tau}$, where $L_i$ and $L_f$ are the lengths from the scalar production to the detector entrance and exit points of the scalar respectively. The factor $\gamma\beta\tau$ is the decay length of the scalar in the lab frame, calculated as the product of the scalar velocity, Lorentz factor, and lifetime. The lifetime is the inverse of the sum of the possible decay widths, described by eqs. (2.5) and (2.6), and is therefore again dependent on the mixing angle $\theta$ and $m_{\text{HPS}}$.
- **BR($K \rightarrow \nu + X$):** During the original neutrino simulation only kaon decays that lead to neutrinos are stored. Kaons that decay with no neutrino in the final state will not be in the $\text{dk2nu}$ files. Therefore to recover the original number of kaons, events must be weighted by the inverse of the branching fraction of the included kaon decays. For positively charged kaons these branching fractions are, $K^+ \rightarrow \mu^+\nu_\mu$ (0.6339), $K^+ \rightarrow e^+\nu_e\pi^0$ (0.0493) and $K^+ \rightarrow \mu^+\nu_\mu\pi^0$ (0.0330), so each kaon decay is scaled up by a factor of 1.40. The branching ratios are taken from the GEANT4 simulation used to perform the original neutrino simulation.
- **$w_{\text{imp}}$:** A weight derived from the original $\text{dk2nu}$ file, called the importance weight. The importance weight results from the suppression of certain neutrino parents with very similar kinematics in the flux simulation to reduce the output size.

The generator can be run in two modes. In the first, the event kinematics are stored along with their weights. The total number of decay events ($N_{ev}$) in the
detector for a specific number of POT can be calculated as

\[ N_{ev} = \sum_{i=1}^{n} w_{ev}^i \times \frac{\text{POT}}{\text{POT}_{\text{sim}}}, \quad (5.2) \]

where the \( \text{POT}_{\text{sim}} \) is the number of simulated protons recorded in the \text{dk2nu} files used. In the second mode, used for the event generation, an accept-reject sampling method \cite{105} is employed in order to produce a sample of unweighted events representative of the weighted event distribution. The maximum possible weight \( w_{\text{max}} \) is estimated for each sample. Then for each event a number \( x \) is drawn at random from a uniform distribution between 0 and 1. If

\[ x < \frac{w_{ev}}{w_{\text{max}}}, \quad (5.3) \]

the event is stored as an unweighted event. Otherwise the event is rejected. The events can then be scaled to a specific POT by \( \frac{\text{POT}}{\text{POT}_{\text{sim}} \times w_{\text{max}}} \).

### 5.1.2 Heavy Neutral Lepton Generator

In order to produce events containing HNL originating from the absorber, an event generator was developed by adapting the HPS generator described above. The structure of the generator is largely the same but the production and decay modes have been modified to the HNL formula described in section 2.2.

As seen in section 2.4, unlike for HPS, the HNL lifetime is much longer than the distance from the production point to the detector. This allows a simplification to be made to the generator. Decays before reaching the detector are assumed to negligible and that the decay probability distribution along the detector intersection is taken to be uniform.

Currently implemented are the two-body charged kaon production modes \( K \to \mu N \) and \( K \to e N \) and the two body lepton-pion HNL decays \( N \to \mu \pi \) and \( N \to e \pi \). This creates four possible configurations the generator can be run in. Events for each of these modes can then be produced separately and combined with appropriate scaling to account for any values of \( |U_{\mu 4}|^2 \) and \( |U_{e 4}|^2 \). For this thesis \( |U_{e 4}|^2 \) is taken
to be zero so only the $K \to \mu N, N \to \mu \pi$ configuration is used. Events are then generated for a input HNL mass ($m_{\text{HNL}}$).

The angular distribution of the HNL decay is discussed in section 2.2.3. Both conjugations of HNL decay ($\mu^-\pi^+$ and $\mu^+\pi^-$) final states are simulated with isotropic angular distributions. The $\mu^-\pi^+$ decays are re-weighted to obtain the angular distribution for Dirac HNLs.

The generator can also take BNB beam simulation as input. A validation of the generator was performed by reproducing results of the HNL flux simulation and generator developed for use in the previous MicroBooNE search [2]. An example comparison of the simulated flux and decay spectrum can be seen in fig. 5.1. The output of the two generators agrees well across all HNL mass values. A small ($\approx 2\%$) discrepancy in the total number of decays arises due to the different simulation approaches of the generators. The previous generator uses a different method to calculate the HNL flux traversing MicroBooNE. Rather than repeatedly decaying the mesons and checking for an intersection with the detector, an analytic kinematic calculation predicts the probability that each meson decay would produce a HNL intersecting the detector. More details of the analytic method developed can be found in section 5 of Ref. [106].
## 5.2 Particle Propagation and Detector Response

For each sample, the list of output particles from the relevant generator is passed into GEANT4 (version 4.10.1_p03d) to simulate their passage through the detector. The GEANT4 physics list used for this stage is FTFP_BERT. The daughter particles are propagated through a description of the detector geometry until they either exit or stop. This is done by incrementally stepping each particle forward, where the
length of the step depends on the physics processes available to the particle. At each step, the energy deposited is calculated in the form of $dE/dx$. The energy deposits are translated into ionisation electrons and scintillation photons according to the electric field strength. The electrons are then instantly projected to the wire planes in groups of 600. The effects described in section 3.3, namely recombination, diffusion, attenuation and space charge are all accounted for here in calculating the size, timing and wire location of the ionisation deposit.

The charge deposits on each wire calculated in the previous stage must be converted to realistic waveforms accounting for the field and electronics response of the detector [117]. A 2D simulation of the electric field is used to calculate the current induced on each of the wire planes due to moving charge. Next the shaping and amplification of the front end electronics, the ASICs configured to a gain of 14 mV/fc and shaping time of 2 µs, is accounted for. Finally, effects relating to the digitization of the signal such as sampling rate, resolution and baseline distortion are simulated.

A voxel-based approach is used to simulate the passage of the scintillation photons to the PMTs. A full GEANT4 simulation of the passage is incredibly computer processing intensive. Instead of running this simulation for each event, a one-off simulation has been run with 300,000 photons deposited per voxel to generate a library. This library can then be looked-up during the simulation to give the probability of photons in each voxel reaching a specific PMT.

5.3 Cosmic Overlay

As previously discussed, as a surface detector MicroBooNE is subject to a continuous flux of cosmic rays, with tens of such rays intersecting the detector in each event. MicroBooNE has developed and utilised a new technique to avoid the need to simulate these cosmic rays when making MC samples. A large sample of beam-off data containing background cosmics has been collected with the unbiased trigger. Simulated waveforms can be superimposed onto the waveforms from these cosmic data events. This produces a cosmic overlay event where the simulated signal exists within a cosmic-ray background which matches that found in data events. The
overlay process has the additional advantage of avoiding the need for an accurate simulation of the detector noise as the overlay event inherits the detector noise from the cosmic data event.

## 5.4 Signal Processing and Event Reconstruction

At this stage, the output of both MC simulation and collected data is effectively identical in structure, i.e. a collection of digitised waveforms for each channel (wire and PMT) of the detector. As such the following stages proceed the same for each with minor exceptions.

### 5.4.1 Optical Reconstruction

The goal of the optical reconstruction is to use the raw waveforms recorded by individual PMTs to construct “flashes”, which correspond to optical activity occurring in coincidence across several PMTs, and therefore likely to be caused by a single neutrino interaction or cosmic ray.

The first stage of the optical reconstruction is to combine the low and high-gain channels (see section 3.5.3). The low-gain channel waveform is used to attempt to correct any saturated pulses on the high-gain channel to produce a single saturation-corrected waveform.

**Optical Hit Finding**

An algorithm constructs optical hits from pulses in the waveform with ADCs over a specific threshold in comparison to a baseline. The baseline is constructed differently for waveforms from the cosmic or beam discriminators, introduced in section 3.5.5. For the shorter cosmic discriminator window, a constant baseline is assumed, set at the ADC of the first sample in the window. For waveforms from the beam discriminator, the long window allows a more complex algorithm to estimate the baseline. This accounts for possible changes of the baseline over the period of the window.
Figure 5.2: Example of a flash across multiple PMT hits. The PMTs are represented by circles located in the y-z position they are each placed at in the detector. The orange represents the integrated amount of light arriving at each PMT in the flash. Figure from Ref. [118].

**Flash Reconstruction**

Once the optical hits have been constructed for each PMT, an algorithm searches for coincident hits (within 100 ns) and uses these to build *flashes*. When a coincidence is found, the ADC of each PMT involved is integrated over an $8\mu$s window in order to collect the late light. There is also a dead time of $8\mu$s after a flash is formed in which no other flash can be constructed. If two candidate flashes occur within $8\mu$s of each other, only the one with the highest total ADC is saved. An estimation of the location of the flash in the y-z plane is made by calculating the mean position of the PMTs involved in the flash, weighted by the PE collected on each. The width of the flash is similarly estimated in both the y and z directions as the variance of the same distribution. An example flash and its position distribution on the PMTs can be seen in fig. 5.2.

**5.4.2 TPC Signal Processing**

To accurately reconstruct particle interactions in MicroBooNE from the raw waveforms, a number of signal processing stages are required. The signal processing aims to extract the true number of ionising electrons passing through a plane from the digitised raw waveforms. In the first stage, *noise filtering*, a series of mitigation measures are used to reduce noise introduced from known sources such as the voltage regulator in the frontend ASICs and the cathode high voltage.

Next, a deconvolution is applied to the waveforms in order to remove any detector and field-related effects and extract the signal waveform. The deconvolution can be
performed in either 1D or 2D. 1D convolution is applied to each waveform in isolation, whereas a 2D convolution is performed across neighbouring wires simultaneously. This allows contributions to the wire current not only from ionization charge passing directly by the wire but also from charge drifting in nearby wire regions. MicroBooNE

![MicroBooNE figure](image)

Figure 5.3: A neutrino candidate from MicroBooNE data measured on the U plane. The displays show the waveforms on a series of wires over 3 µs. Shown from left to right is the raw waveform, the waveform after noise filtering, and after 2D deconvolution. Figure from Ref. [119].

found that intra-wire effects significantly modify the detector response to charge and as such use the computationally expensive but more accurate 2D deconvolution in the current version of the reconstruction. Figure 5.3 shows an example event undergoing signal processing. The deconvolution creates unipolar signal shapes from the bipolar induction plane signals. The processed signals for each wire now correspond to an estimation of the number of electrons arriving on a wire as a function of time.

### 5.4.3 Hit Finding

An algorithm is used to identify peaks in the deconvolved waveforms. These peaks are fitted with Gaussian functions to construct hits. The mean of each Gaussian gives the time the signal occurred, and the integrated area of the hit is proportional
to the amount of deposited charge. The difference between the hit time and the interaction time $t_0$ can be used to calculate the x-position of the original deposition. When combined with the wire location, this gives a 2D coordinate for the hit. These 2D hits form the basic input to the further 3D object reconstruction.

### 5.4.4 Pandora Reconstruction

This analysis utilises the Pandora multi-algorithm pattern-matching reconstruction framework [120]. The version of Pandora used by MicroBooNE is configured primarily for reconstructing neutrinos. Nevertheless the algorithms have been shown to perform well for identifying and reconstructing LLP decays due to the similarity in detector signature and deliberate topology-generic approach of the reconstruction package.

![Diagram of Pandora data-products](image)

**Figure 5.4**: The various Pandora data-products and the hierarchical relationship between them. Figure from Ref. [120].

**Pandora** first uses the hits created in the hit finding stage for each plane to build three individual 2D images. The hits are combined into *clusters* based on their proximity and the geometric expectations of the shape of showers and tracks. **Pandora** combines the information across the available views to perform 3D reconstruction, ultimately building 3D objects corresponding to particles in the detector. The objects are arranged in a parent-daughter hierarchy based on the topology of the event. The collection of these 3D objects, called Particle Flow Particles (*PFParticle*), and the information about their hierarchy is the final output of *pandora*. As seen in fig. 5.4 each *PFParticle*, has a collection of 3D reconstructed points called *SpacePoints* which carry the charge information of the corresponding 2D hits.
The reconstruction of the 2D hits is carried out in two different chains;

- **Cosmic Hypothesis** Chain: This set of algorithms is designed to identify cosmic rays is therefore focused on track reconstruction. Any clusters not identified with a track-like particle are assumed to belong to delta rays produced by a cosmic ray. These hits are clustered simply based on proximity and are associated as a daughter to a cosmic ray track. The vertex of the 3D cosmic ray objects formed is assumed to be at the highest y coordinate value on the track.

- **Neutrino Hypothesis** Chain: This chain aims to find a neutrino interaction vertex and carefully reconstructs all particles emerging from this vertex. The algorithms here are designed to handle the generally more complex topologies, with a new set of algorithms not used in the cosmic chain designed specifically to construct showers. A `PFParticle` is constructed for the parent neutrino and the reconstructed `PFParticles` are added as daughters to the hierarchy emerging outwards from the vertex, as seen in fig. 5.5.

![Figure 5.5: A display showing a Pandora slice of a simulated CC $\nu_\mu$ event reconstructed under the neutrino hypothesis. Each reconstructed visible particle in the hierarchy is shown in a separate colour and the identification of the particles as track or shower is labelled. The true MC particle corresponding to the reconstructed particle is also labelled in the diagram. Figure from Ref. [120].](image)

The cosmic hypothesis chain is run first over the whole event and any hits
unambiguously of cosmic muon origin, such as tracks that enter and exit the detector or are out of time with the trigger are removed. A fast-version of 3D reconstruction is then run to form 3D-SpacePoints. These 3D hits are then separated into groups of topologically associated objects called slices. Each slice attempts to contain solely hits originating from a single interaction from either a cosmic-ray or neutrino. The display in fig. 5.5 shows an example neutrino slice.

Next each slice is individually reconstructed using both the cosmic and neutrino hypothesis chains such that information from both chains is available when attempting to select slices containing neutrinos. A typical data event in MicroBooNE contains around four of these slices, with the large majority being cosmic rays. The identification of slices containing neutrinos or LLPs from the cosmic background will be discussed in section 6 as part of the event selection.

Based on the topology information, each PfParticles, is assigned a continuous score by Pandora between 0 and 1 to categorise it as track-like or shower-like. In the standard MicroBooNE Pandora workflow, an object is reconstructed as a track if its score is $> 0.5$ and a shower if $< 0.5$. The analysis framework used in this work runs a custom chain that attempts to reconstruct all objects as tracks regardless of the score in addition to the shower-like reconstruction.

### 5.5 Calibration

This analysis utilises the reconstructed energy deposits of tracks and showers to distinguish signal from background. A calibration procedure is applied on an event by event basis in order to determine the true energy loss per unit length ($dE/dx$) from the measured charge per unit length ($dQ/dx$). The full calibration proceeds in two stages. The first, known as the $dQ/dx$ calibration, corrects for the position and time dependence in the detector response to deposited charge. Next, an energy scale calibration is performed to determine the true $dE/dx$ from the calibrated $dQ/dx$. A full description of the MicroBooNE charge calibration procedure can be found in Ref. [121].
5.5.1 Charge Calibration

The dominant effects which cause non-uniformities in $dQ/dx$ detector response are SCE, diffusion and argon purity as described in section 3.3. Additionally, two areas of induction plane wires in MicroBooNE are cross-connected. This causes distortions of the electric field between planes in these areas and therefore a modification of the $dQ/dx$ detector response.

Cosmic-ray muons which cross both the anode and cathode are used to calibrate the $dQ/dx$. These particles typically have a momentum of $4 - 5$ GeV and therefore their energy depositions consistently peak at $dE/dx \approx 1.7$ MeV/cm.

![Correction Factor Maps](image)

Figure 5.6: Examples of the $dQ/dx$ correction factor maps used in the data calibration process. Left: the correction factors in the YZ plane for data collected between February and October in 2016. Right: the X (drift) direction correction factors for February 25, 2016. Figures from Ref. [121].

The calibration is performed first in the YZ plane. The plane is segmented into cells. The median $dQ/dx$ of the depositions in each cell is compared to the global medium and a map of correction factors is produced. This stage uses tracks collected over several months as the YZ variations are not time-dependent. Next, the hits are divided in the x (drift) direction and correction factors are produced for this dimension. As the X correction is affected by the purity which changes throughout data collection, a separate correction is produced for each day. Finally, temporal variation in the daily global median $dQ/dx$ value following the spatial calibration are corrected for.

Examples of the YZ and X correction maps can be seen in fig. 5.6. The diagonal region with large correction factors in the YZ planes corresponds to a region of cross-connected wires.
5.5.2 Energy Calibration

The modified box model for recombination, described in section 3.3.2, is used to determine the absolute energy loss from the calibrated $dQ/dx$. Before utilising the model the calibration constant $C_{\text{cal}}$ which translates the $dQ/dx$ in “ADC/cm” to “(number of electrons)/cm” must be determined. This is done using a sample of stopping muons from neutrino interactions due to their well understood energy loss profile. $C_{\text{cal}}$ is varied and the predicted and measured $dE/dx$ distributions of the muons are compared across a series of energy values between 250 MeV and 450 MeV. The $C_{\text{cal}}$ which gives the best agreement (minimum $\chi^2$) between the expected and measured values is chosen.

5.6 Samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>POT ($\times 10^{20}$)</th>
<th>HW Triggers</th>
<th>Events</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Run 1</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Beam On</td>
<td>2.002</td>
<td>5268051.0</td>
<td>611276</td>
</tr>
<tr>
<td>Beam Off</td>
<td>-</td>
<td>9282594.64</td>
<td>912613</td>
</tr>
<tr>
<td>Dirt Overlay</td>
<td>16.73</td>
<td>-</td>
<td>569416</td>
</tr>
<tr>
<td>Neutrino Overlay</td>
<td>23.27</td>
<td>-</td>
<td>911157</td>
</tr>
<tr>
<td><strong>Run 3</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Beam On</td>
<td>5.009</td>
<td>10363137</td>
<td>1104276</td>
</tr>
<tr>
<td>Beam Off</td>
<td>-</td>
<td>33150115.4</td>
<td>3237058</td>
</tr>
<tr>
<td>Dirt Overlay</td>
<td>10.25</td>
<td>-</td>
<td>386248</td>
</tr>
<tr>
<td>Neutrino Overlay</td>
<td>19.83</td>
<td>-</td>
<td>746098</td>
</tr>
</tbody>
</table>

Table 5.2: The number of POT, HW triggers and recorded events for each of the data and background samples used in the Analysis. The number of events is the number of HW triggers which pass the SW trigger.

This section describes the various samples that are produced and analysed for this work. The currently available processed NuMI data sets are from Run 1 ($2 \times 10^{20}$ POT) and Run 3 ($5.01 \times 10^{20}$ POT). These samples will be used for this iteration of the analysis. As both detector and beam conditions vary between the runs, the two runs are analysed separately and in parallel, each with their own sets of Monte Carlo (MC) overlay signal and background samples. The most significant difference between the runs is the beam horn current mode which was set to FHC for run 1 and RHC for the run 3 data used. The overlays are produced using unbiased trigger
events taken in the corresponding time period for each run. In addition, the CRT was constructed and commissioned in time for run 3 so will be used as part of the selection on that data. The two runs will be combined at the final stage of the analysis when setting the limit on the mixing angles for the two models. A summary of the data and background samples used can be found in tab. 5.2. More details on the various samples is given in the following sections.

### 5.6.1 Beam-On Samples

The Beam-on samples refer to data collected when MicroBooNE was exposed to the NuMI beam and received a neutrino trigger. The samples for each run have a number of POT, hardware triggers (HW) and reconstructed events. A number of beam and detector-related selection criteria are applied to ensure that the data is of a quality suitable for analysis. The beam criteria ensure the intensity, current and beam position were all within the expected values, using information collected by the accelerator division. The detector data quality is checked using a database of detector conditions as well as a series of low-level reconstruction quantities, such as the number and position of optical flashes and the number of vertices and tracks reconstructed with pandora.

### 5.6.2 Background Samples

A full prediction of the beam-on data collected in MicroBooNE requires a combination of MC neutrino overlay samples and beam-off data containing cosmic rays. Their combination is used to form the MicroBooNE standard-model (SM) event prediction and therefore describes the background for this analysis.

#### Beam-Off

The majority of NuMI beam-triggered events do not contain a neutrino interaction. To accurately model beam triggered events that contain only cosmic events a large number of events have been collected with the “external” trigger at times when no neutrino spill is expected. These “beam-off” samples are collected at the same
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Time as the corresponding beam period they are intended to model. The trigger information for the samples used can be seen in tab. 5.2.

MC Neutrino Overlay

To model the neutrino background of the search, generic simulated neutrino samples are used. The samples contain simulated neutrino interactions generated within the MicroBooNE cryostat using GENIE. The neutrino interactions are overlaid with cosmic ray data following the process described in section 5.3. These samples are designed to model the entire range and spectrum of NuMI neutrino interactions received by MicroBooNE. The samples are simulated with an intensity of $5 \times 10^{13}$ POT per spill, with the protons delivered with a uniform time distribution across the spill window. The number of events and corresponding simulated POT for each of the neutrino overlay samples can be found in tab. 5.2.

The events are initially generated using the unconstrained NuMI flux simulation. The PPFX package, described in section 4.2.1, is run on the simulated events to produce associated weights. Applying these weights to each neutrino event reweights the nominal simulation to the constrained central value prediction (“PPFX tune”).

The default GENIE v3.0.6 model has been shown to underpredict the neutrino cross-section measured in the data of experiments including T2K, MiniBooNE and MicroBooNE itself. To mitigate this underprediction, fits to T2K CC pionless cross-section data were performed to tune parameters within the theoretical model [122]. The predominant effects of the fit are an increase in normalisation and a shape modification of the CCMEC component. The CCQE axial mass is also raised. The fit leads to an overall 8% increase of NuMI neutrino interactions in MicroBooNE. Again the new CV is achieved by applying weights to the events produced by the default simulation and referred to as the GENIE tune.
Out-of-Cryostat MC Neutrino Overlay

The standard neutrino sample only contains events where the neutrino interacts directly with the LAr. Another background class of events is produced by neutrinos which interact either upstream of the detector or with the external structure of the detector. Despite occurring outside the detector, these interactions can produce daughter particles which then travel into the detector and trigger an event. As the majority of interactions outside the cryostat produce no activity in the detector, these events are generated as their own sample for efficiency reasons. This sample, referred to as “dirt” or “out-of-cryostat”, is generated to contain only events where the neutrino interacted outside the cryostat and produced a daughter which entered the cryostat. In all other respects the sample is created in an identical fashion to the main neutrino sample. The number of events and corresponding simulated POT for each of the neutrino overlay samples can found in tab. 5.2.

5.6.3 Background Sample Normalisation

Each background sample is scaled to correctly describe their contribution to the total SM event rate in MicroBooNE. The samples are scaled to match the beam-on data. The two MC samples are scaled by the ratio of the collected beam POT and the simulated POT for the sample ($POT_{beam-on} / POT_{MC}$).

The beam-off sample is normalised to data using the number of hardware triggers recorded for each sample ($HW_{beam-on} / HW_{beam-off} \times 0.98$). The assumption inherent in this normalisation method is that approximately all the hardware triggers in the beam-on sample do not contain neutrinos. This is a robust assumption for BNB events but breaks down for the NuMI beam where a larger proportion of beam spills result in a neutrino interaction due to the greater beam intensity. Approximately 2% of NuMI spills result in a neutrino interaction so an additional scaling factor of 0.98 is applied to account for this effect.
Figure 5.7: (a) Distribution of flash times for all Run 1 data events. The stacked prediction combines the Beam-off, neutrino overlay MC, and out of cryostat neutrino samples MC. (b) Shows a single bin containing events with a flash during the beam window. The overall normalisation of the data and prediction can be seen to agree well.

Flash Timing Distribution

The background normalisation procedure outlined above can be validated using the timing distribution of the largest flash time in an event. This distribution can be seen for run 1 in fig. 5.7(a) before any selection other than the software trigger. In the period before and after the beam-gate window, which is $5.64 - 15.44 \mu s$, any flashes are a result of the cosmic ray background and as such can be used to validate the normalisation of beam-off to beam-on events. The slow rise in events in the period before the beam window is caused by flashes that occur before the beam window that produce enough late light during the beam window to activate the software trigger. The closer the flash time is to the window, the more likely the (approximately exponentially decaying) late light will trigger the software trigger. The “shoulder” like effect where the number of beam-off events remains briefly high after the neutrino beam window has passed is due to the software trigger window being slightly longer than the delivered beam spill.

The step down feature midway through the beam spill, which is present in beam
data but not the prediction is due to the beam proton delivery structure during Run 1. The majority (70%) of Run 1 data was taken with the beam in a 4+6 slip-stacking configuration. As discussed in section 4.1.1 this means the first four batches in the spill have a higher proton intensity, and therefore produce more neutrinos than the last two batches. The remaining 30% of data was taken in 6+6 configuration. The simulated neutrinos are generated uniformly over the entire neutrino time window, with a POT per spill comparable to the 4+6 mode. The normalisation of the simulation in the analysis is performed using the total POT delivered rather than per spill. This normalisation is demonstrated in fig. 5.7(b) which shows the data and prediction integrated over the beam window for Run 1. The flash timing within the beam window is not utilised in this analysis, so the uniform timing simulation has no impact on the selection.

Figure 5.8: (a) Distribution of flash times for all Run 3 data events. The stacked prediction combines the Beam-off, neutrino overlay MC, and out of cryostat neutrino samples MC is also shown. (b) Shows a single bin containing events with a flash during the beam window. The overall normalisation of the data and prediction can be seen to agree well.

Figure 5.8 shows the same distributions for Run 3. The entirety of the Run 3 beam data was collected in 6+6 slip-stacking mode so the beam structure is more uniform than Run 1. The single bin at the start of the neutrino spill where the expectation exceeds the data significantly is due to a slight delay and rise time in the data which is not simulated. Again the overall normalisation is not affected.
The change to the NuMI software trigger threshold, described in section 3.5.5, occurred during the Run 3 data period. In the figure, the normalisation is executed by splitting the beam-off and beam-on data into the time periods before and after the change and performing the normalisation of the two periods separately before recombining. Similarly, the neutrino MC is split based on the period the underlying unbiased event was collected and a simulated software trigger applied. The impact of the software trigger change on events that pass the final selection is negligible due to stricter light-based criteria applied downstream.

Out-of-Cryostat Normalisation Correction

As can be seen in figs. 5.7(a) and 5.8(a), the contribution of the Out-of-Cryostat events is significant at the trigger level. After selection, the contribution of these events is small. In order to match the normalisation of the MC to data at both the trigger level and after the early stages of the selection, down scalings must be applied to the normalisation. scalings of 0.75 and 0.35 are calculated for Run 1 and Run 3 respectively. These scalings are the factors required to match the total in-beam MC prediction normalisation to data after the application of the software trigger. Each scaling is derived using only a subset of the respective data set, so the normalisation ratios of the full in-beam data to the total in-beam prediction (shown in figs. 5.7(b) and 5.8(b)) are not exactly equal to 1. While the scalings are large and differ between runs, the contribution of Out-of-Cryostat events to the final selected background is very small. Thus the impact of the scaling on the produced limits is negligible even with a 100% normalisation uncertainty applied.

5.6.4 Signal Samples

The generators described in sections 5.1.1 and 5.1.2 are used to produce samples for both HPS and HNL across a range of targeted mass values. The signal samples generated are listed in tab. 5.3 with the number of events for each decay mode. The mass values are chosen to span the range the search is sensitive to. Additional samples are generated near the kinematic boundaries and for mass values where the sensitivity is expected to change rapidly. Figure 5.9 shows examples of generated
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Figure 5.9: Event Displays of some simulated signal events. In both displays, the LLP approaches from approximately the bottom right of the image. In the left display is a $m_{\text{HNL}}=304$ MeV HNL decaying into a muon (track pointing up and right) and a pion (track pointing left). The right image shows a $m_{\text{HPS}}=275$ MeV HPS decaying into a muon (the long track going left) and an anti-muon (the short track) which quickly decays to a Michel electron.

<table>
<thead>
<tr>
<th>HNL Mass (MeV)</th>
<th>Run 1 Events</th>
<th>Run 3 Events</th>
<th>HPS Mass (MeV)</th>
<th>Run 1 Events</th>
<th>Run 3 Events</th>
</tr>
</thead>
<tbody>
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<td>246</td>
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<td>35801</td>
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<td>275</td>
<td>31720</td>
<td>42038</td>
</tr>
</tbody>
</table>

Table 5.3: Simulated signal samples used in the analysis.

events for two mass values. Again the samples are simulated separately for both Run 1 and Run 3 but here the horn current direction has a limited effect on the signal due to the fact that the signal originates from the absorber. The signal samples are overlaid using unbiased trigger cosmic ray samples that have not already been used in the production of the main neutrino overlay or dirt overlay samples. As with the SM neutrino samples, the beam protons are generated with a uniform distribution in time during the simulated beam spill window.

5.6.5 Signal Sample Normalisation

The goal of this analysis is to set a limit on the mixing parameters ($\theta^2, |U_{\mu 4}|^2$) of the two models. Therefore, as the signal normalisation is dependent on the mixing
parameters, the scaling assigned to the signal during the selection development is somewhat arbitrary. When evaluating the sensitivity of the analysis to the mixing parameters, the relationship between the signal event normalisation and the mixing parameters must be evaluated.

The number of LLP decays occurring in the detector is a function of the model mixing angle and $m_{\text{LLP}}$. It can be expressed as:

$$N_{\text{dec}}(X^2, m_{\text{LLP}}) = N_{\text{POT}} \times N_{\text{KDAR}} \times K_{BR}(X^2, m_{\text{LLP}}) \times P_{\text{SA}} \times P_{\text{dec}}(X^2, m_{\text{LLP}}), \quad (5.4)$$

where $N_{\text{KDAR}}$ is the number of kaons decaying at rest at the absorber per POT, and $P_{\text{SA}}$ the probability that a LLP intersects with the detector. The terms $K_{BR}(X^2, m_{\text{LLP}})$ and $P_{\text{dec}}(X^2, m_{\text{LLP}})$ represent the probability of a kaon decaying to a LLP and the probability of a LLP decaying in the detector, respectively. Both are dependent on the square of the LLP models mixing angle ($\theta^2|U_{\mu 4}|^2$), which is represented generically by $X^2$ here.

The kaon branching ratios for the decays to HPS and HNL are given in section 2 (eqs. (2.3) and (2.10)). In both cases the dependence on the mixing angle can be factorised out and used as proportionality to the total number of kaon decays to LLPs,

$$K_{BR}(X^2, m_{\text{LLP}}) = X^2 \times K_{BR}(m_{\text{LLP}}). \quad (5.5)$$

The probability of the LLP decaying in the detector can be expressed as

$$P_{\text{dec}}(X^2, m_{\text{LLP}}) = \left( e^{-\frac{r_L L_1}{\gamma \beta}} - e^{-\frac{r_L L_2}{\gamma \beta}} \right) \frac{\Gamma_{\text{sig}}}{\Gamma_T}, \quad (5.6)$$

where $L_1$ and $L_2$ are the distance from LLP production of the entrance and exit point of the detector. $\Gamma_{\text{sig}}$ and $\Gamma_T$ are the decay width to the signal channel and total decay width respectively. Here the mixing angle dependence is in the total decay length ($\gamma \beta / \Gamma_T$) of the LLP. As it appears in exponential terms, the $X^2$ dependence can not be simply factorised out. In the case that the decay length is much longer than the
distance to the detector, $\gamma/\Gamma \gg L_1, L_2$, the equation can be approximated as

$$P_{\text{dec}}(X^2, m_{\text{LLP}}) \approx (L_2 - L_1) \left( \frac{\Gamma_T}{\gamma} \right) \left( \frac{\Gamma_{\text{sig}}}{\Gamma_T} \right). \quad (5.7)$$

The $X^2$ dependence can now be factorised out to give,

$$P_{\text{dec}}(X^2, m_{\text{LLP}}) \approx X^2 \times P_{\text{dec}}(m_{\text{LLP}}), \quad (5.8)$$

finally giving an event rate directly proportional to $X^4$,

$$N_{\text{dec}}(X^2, m_{\text{LLP}}) \approx X^4 \times N_{\text{dec}}(m_{\text{LLP}}). \quad (5.9)$$

The decay lengths of the LLPs in the two models are discussed in section 2.4. The approximation that the decay length is much longer than the distance to the detector is valid for all values of HNL parameter space considered. For the HPS this approximation breaks down for higher mass values and the reduction in events due to decays of the HPS before reaching the detector becomes significant. Because of the large difference in decay lengths different approaches are used to perform signal normalisation for the HNL and HPS.

For HNL, the generator (section 5.1.2) is used to calculate the number of events expected at a fixed mixing angle. The events are then scaled to the required normalisation using the $|U_{\mu 4}|^4$ proportionality. For the purpose of illustration in the selection, HNL are normalised to $|U_{\mu 4}|^2 = 10^{-8}$. The HPS events used in the selection are simulated at $\theta^2 = 10^{-12}$, a value for which decays before the detector are negligible. The HPS samples are then scaled up by a factor $10^6$ for the purpose of quantifying the selection, which corresponds to an $\theta_{\text{eff}}^2$ of $10^{-9}$. The use of $\theta_{\text{eff}}$ indicates that decays before reaching the detector have been disregarded. When evaluating the final search sensitivity to $\theta^2$ the HPS normalisation is determined using the generator. As described in section 5.1.1, the generator accounts for decays before the reaching detector and can therefore be used to find the $\theta^2$ values which correspond to the required number of HPS events for exclusion.
6 Signal Selection

This section covers the analysis workflow developed to identify LLP candidates and to discriminate them from both neutrino and cosmic-ray background events. First, the properties of the mono-energetic LLP decay signature across the considered range of LLP masses is outlined in section 6.1 Section 6.2 describes the process used to identify and construct candidate vertices for LLP decays. It details efforts made to maximise selection efficiency of the decay topology while still being able to determine useful kinematic features of the LLP. Section 6.3 covers a pre-selection aimed at rejecting neutrino and cosmic events clearly inconsistent with the LLP signal. Throughout this stage of selection, LLP-mass-dependent variables are used minimally to achieve similar efficiency across the signal samples.

6.1 Decay Kinematics

For both physics scenarios, kaon decays-at-rest (KDAR) in the NuMI absorber are considered as the source of the LLPS. The LLPS are produced via the two-body kaon decays $K^+ \rightarrow S\pi^+$ or $K \rightarrow N\mu^+$. Thus for a given LLP mass, the LLPS produced are mono-energetic and low energy. While the low energy of the KDAR LLPS makes their decays difficult to reconstruct, properties of their signature can be levered to discriminate the signal from the neutrino background. The decays will appear in the detector as two tracks emerging from a single vertex. The decay kinematics are highly dependent on the LLP mass ($m_{\text{LLP}}$). Here the underlying true distributions of the decay features are overviewed for a range of $m_{\text{LLP}}$ values.

The specific energy and therefore momentum of the LLP is determined by the two-body decay dynamics given in eq. (2.14). The momentum that the LLPS are produced with decreases as $m_{\text{LLP}}$ increases, approaching zero as the mass approaches the maximum production threshold. The threshold is $m_K - (m_{\text{LLP}} + m_d)$ where $m_K$ is the kaon mass and $m_d$ is the mass of the accompanying daughter.
The LLP itself decays to two daughters – a HNL decays to $\mu^\pm \pi^\pm$ and a HPS decays to $\mu^+ \mu^-$. The decay products have momenta which again depend solely on the $m_{\text{LLP}}$ via the two-body decay kinematics. The momenta of these two daughters are given by
\begin{align}
  p_1^* &= \sqrt{\left( m_{\text{LLP}}^2 + m_1^2 - m_2^2 \right)^2 - 4m_{\text{LLP}}^2m_1^2} \\
  p_2^* &= \sqrt{\left( m_{\text{LLP}}^2 + m_2^2 - m_1^2 \right)^2 - 4m_{\text{LLP}}^2m_2^2},
\end{align}
(6.1)
where the asterisk indicates that the calculation is in the LLP rest frame and $m_1$ and $m_2$ are the daughter masses.

Due to conservation of momentum, these daughters emerge back-to-back in the LLP rest frame, as shown in fig. 6.1. The first is at some angle $\theta_1^*$ from the LLP direction, and the second is at $\theta_2^* = \pi - \theta_1^*$. In fact, the kinematics of the final state are entirely determined by $m_{\text{LLP}}$ and the angle $\theta_1^*$. The final state momenta are given by boosting $p_1$ and $p_2$ into the lab frame which is also shown in fig. 6.1. The momenta of the daughter particles in the lab frame are
\begin{align}
  p_1 &= \frac{(m_{\text{LLP}}^2 + m_1^2 - m_2^2)p \cos \theta_1^* \pm 2E_{\text{LLP}} \sqrt{m_{\text{LLP}}^2p_1^2 - m_1^2p^2 \sin^2 \theta_1^*}}{2(m_{\text{LLP}}^2 + p^2 \sin^2 \theta_1^*)} \\
  p_2 &= \frac{(m_{\text{LLP}}^2 + m_2^2 - m_1^2)p \cos \theta_2^* \pm 2E_{\text{LLP}} \sqrt{m_{\text{LLP}}^2p_2^2 - m_2^2p^2 \sin^2 \theta_2^*}}{2(m_{\text{LLP}}^2 + p^2 \sin^2 \theta_2^*)},
\end{align}
(6.2)
where $p$ is the momentum of the LLP in the lab frame, which depends solely on $m_{\text{LLP}}$. 

---

**Figure 6.1:** Schematics to show the kinematics of the LLP and its daughters in the LLP rest frame (left) and lab frame (right).
Figure 6.2: Truth distributions of the momentum of the LLP decay products for a range of LLP masses. Left: HPS decaying to $\mu\mu$ pairs. Right: HNL decaying to $\mu\pi$ pairs.

The momenta of the final state particles produced by LLP decays are shown in fig. 6.2 for the range of $m_{\text{LLP}}$. The momentum $p_1$ is anti-correlated to $p_2$. The degree of asymmetry again depends on $m_{\text{LLP}}$ and $\theta_1^*$. The step-like behavior in the HNL distributions is caused by the small mass difference between the muon and pion.

Figure 6.3: Truth distributions of the longest predicted track length of the two LLP decay products for a range of LLP masses. Left: HPS decaying to $\mu\mu$ pairs. Right: HNL decaying to $\mu\pi$ pairs.

The continuous-slowing-down-approximation (CSDA) (see section 3.4.5) is used to estimate the propagation length of the decay products in the liquid argon from their momenta. It can be concluded from figs. 6.3 and 6.4 that, as expected, the tracks are typically short, with the longest track in the event being between 5 cm and 30 cm. For low $m_{\text{LLP}}$, a large fraction of the shortest tracks are not long enough to cross several wires in MicroBooNE and therefore are not reliably reconstructed.
After boosting to the lab frame, the angles of the daughter particles with respect to the LLP direction are $\theta_1$ and $\theta_2$ as shown in figure fig. 6.1. The angles are given by

$$\tan \theta_1 = \frac{\sin \theta_1^*}{\gamma (\beta/\beta_1^* + \cos \theta_1^*)},$$
$$\tan \theta_2 = \frac{\sin \theta_2^*}{\gamma (\beta/\beta_2^* + \cos \theta_2^*)},$$

where $\beta$ is the LLP velocity and $\beta_1^*$ and $\beta_2^*$ are the daughter particle velocities in the LLP rest frame. The opening angle $\alpha$ is defined as the 3D angle between the two tracks in the lab frame $\alpha = \theta_1 + \theta_2$. The $\alpha$ distributions for a range of $m_{\text{LLP}}$ are shown in fig. 6.5. The mono-energetic LLPs produce highly peaked opening angle distributions. The most probable opening angle is highly dependent on $m_{\text{LLP}}$. 

Figure 6.4: Truth distributions of the shortest predicted track length of the two LLP decay products for a range of LLP masses. Left: HPS decaying to $\mu \mu$ pairs. Right: HNL decaying to $\mu \pi$ pairs.

Figure 6.5: Truth distributions of the opening angle between the decay products of the LLP for a range of LLP masses. Left: HNL decaying to $\mu \pi$ pairs. Right: HPS decaying to $\mu \mu$ pairs.
For lower $m_{\text{LLP}}, \beta > \beta_1^*, \beta_2^*$, i.e. the boost from the LLP momentum dominates the momentum of the decay products in the LLP rest frame. Therefore the distribution of $\alpha$ peaks at a small value with a tail towards 0. For large $m_{\text{LLP}}, \beta < \beta_1^*, \beta_2^*$, and the $\alpha$ distributions peak at a wide angle and tail to 180°. The distribution for $m_{\text{HNL}} = 277$ MeV is two-sided. At this point, because of the difference in mass between the muon and pion, $\beta_1^* < \beta < \beta_2^*$. Another key feature used to identify

Figure 6.6: The vertex location and momentum of two hundred simulated target events (red) and KDAR HPS (black) in the YZ plane. The arrow stems start at the vertex location and points in the direction of the momentum and the arrow lengths are proportional to the magnitude of the momentum.

KDAR LLP signals is the incoming direction. As discussed in section 4.2, the absorber-produced LLP would approach the detector at a significantly different angle to the vast majority of NuMI neutrinos that are produced at the target. This is illustrated in fig. 6.6, where the momenta of simulated HNLs and background neutrinos can be seen. In the 2D projection shown, the LLPs approach the detector from below and are traveling slightly backwards with respect to the Z-direction, whereas neutrinos from the NuMI beam arrive in a forward direction. The accurate reconstruction of both decay products is needed to determine the incoming direction of the LLP candidate.
6.2 Signal Candidate Construction

The analysis utilises many of the same reconstruction and selection tools that are used to identify neutrino interaction vertices in MicroBooNE. The tools are generic enough such that they still perform well on the signal topology of LLP two-track decays. The following section details these tools, focusing on the modifications made to optimise for the different signal topology.

6.2.1 Slice Identification and Timing

As discussed in section 5.4.4, the Pandora reconstruction algorithm groups objects into “slices” after removing obvious cosmic-ray related activity, with the intention of splitting the event into separate interactions (neutrino and cosmic). The slice identification (SliceID) process then uses a combination of TPC and light information to attempt to identify which slice, if any, corresponds to a neutrino. The SliceID process, described in Ref. [118], forms the first part of this selection. It can be split into the following stages:

1. Require a flash coincident in time with the NuMI beam window.
2. Require that the charge reconstructed in a slice is consistent with the location and intensity of the selected beam flash.
3. Remove slices that contain anode or cathode piercing tracks with a timing that matches an out-of-beam time flash and thus are highly likely to be of cosmic origin.
4. Remove slices that contain a stopping cosmic muon. A series of algorithms lever the calorimetric information to determine the direction of the tracks, and therefore identify cosmics that enter the detector then stop inside the TPC.

If after the four selection stages an event has no slices that pass all the criteria, the event is rejected. If the SliceID selection leaves \( \geq 2 \) remaining slices, a Support Vector Machine (SVM) is used to select the most “neutrino-like” of the remaining slices. The model takes topological features of the reconstructed slice as input and returns a score between 0 and 1 for each slice, with 0 for “cosmic-like” and 1 for fully “neutrino-like” topologies.
Figure 6.7: The stacked prediction (MC+Beam-off) and beam data topological score distributions for reconstructed events that pass the SliceID requirements with the extended flash window. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility.

The SVM has been trained using BNB neutrino MC samples. It utilises several variables, including the reconstructed direction of the neutrino with respect to the BNB beam direction. An example of the topological score distribution is shown in fig. 6.7. The SVM provides excellent separation between cosmic muons and NuMI neutrino interactions. The discrimination of the LLP signal from cosmic rays is weaker, since the LLP decays originate from a different location than the neutrino interactions and have a low associated energy. The impact of this effect on the efficiency of SliceID for the LLP signal is small since the SVM is only utilised for the $\approx 10\%$ of events that have $\geq 2$ slices at the final selection stage. Furthermore, in the majority of these cases, the true LLP slice has the highest topological score and so is selected preferentially over the background. The performance of the SliceID procedure is discussed in section 6.2.1.
SliceID Event Time

The SliceID selection is optimised for neutrino interactions but performs sufficiently well on the LLP decays. As such it is applied unmodified with one exception: the time window in which flashes are considered to be in time with the beam is extended to account for the fact that absorber KDAR LLPs arrive at the MicroBooNE detector with a delay with respect to the neutrinos.

The standard NuMI beam window is calculated for neutrinos arriving directly from the target. LLPs from the absorber are delayed in two ways with respect to neutrinos. Firstly, the combined distance traversed by the proton and LLP is longer. From the point of proton impingement on the target at \( t_{\text{spill}} \), target-produced neutrinos travel directly to MicroBooNE at a distance of \( d_{\text{targ}} = 679 \text{ m} \). Protons producing an LLP in the absorber must first travel a distance of \( l_{\text{pipe}} = 675 \text{ m} \) through the horns and then a distance of \( l_{\text{pipe}} = 675 \text{ m} \) down the decay pipe before they collide with the absorber. The produced LLP then travels from the absorber to MicroBooNE where it decays, corresponding to a distance of \( d_{\text{abs}} \approx 102 \text{ m} \). This gives a total additional travel distance of 138 m, which results in a delay of \( \approx 0.5 \mu s \) for \( \beta = 1 \). Secondly, while the neutrinos and high energy beam protons travel with a velocity \( \beta \approx 1 \), the LLPs, as low-energy massive particles, travel with a velocity \( \beta << 1 \). The interaction event time for target neutrinos, \( t_\nu \), and for absorber produced LLPs, \( t_{\text{LLP}} \), can therefore be expressed as:

\[
t_\nu \approx t_{\text{spill}} + \frac{d_{\text{targ}}}{c},
\]  

(6.4)

and

\[
t_{\text{LLP}} \approx t_{\text{spill}} + \frac{l_{\text{pipe}}}{c} + \frac{d_{\text{abs}}}{\beta c}.
\]

(6.5)

The expression only serves as an approximation as the time between proton collision and parent decay to neutrino or LLP, as well as any distance traveled by the neutrino parent is neglected. The exact time on an event by event basis is included in the event generation.

The LLP velocity \( \beta \) and therefore the time of interaction depend on \( m_{\text{LLP}} \). For
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Figure 6.8: The timing distribution of HNL decaying in the detector as a function of the HNL mass. The target neutrino arrival band and the SW trigger window are also indicated.

A low $m_{\text{LLP}}$ with $\beta \approx 1$ the additional delay is small. A 215 MeV HPS, for example, is produced with $\beta = 0.65$ leading to a delay of $d_{\text{abs}} \approx 0.19 \mu s$. The delay increases with $m_{\text{LLP}}$, and becomes particularly significant for HNLs approaching the kaon decay production threshold as the HNL are produced with very low momentum. Figure 6.8 shows the time of arrival of HNLs as a function of the HNL mass $m_{\text{HNL}}$.

For example, an HNL with $m_{\text{HNL}} = 385$ MeV is produced with a velocity of $\beta = 0.06$ and therefore an approximate delay over $d_{\text{abs}}$ of 5.52 $\mu$s. Approximately 50% of the HNLs arrive after the end of the software trigger window and are not recorded. For a slightly heavier HNL with a mass of $m_{\text{HNL}} = 388$ MeV, the delay is 75 $\mu$s and therefore none of the events arrive within the software trigger window.

Table 6.1: Beam time windows used for the flash selection Pandora SliceID. Shown is the default NuMI window and the adapted range used for this LLP search. The difference in the times between data and MC is due to a small offset between data and simulation that is corrected for after this stage.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Lower Limit ((\mu s))</th>
<th>Upper Limit ((\mu s))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Standard</td>
<td>New</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>5.64</td>
<td>5.44</td>
</tr>
<tr>
<td>Beam-Off Data</td>
<td>6.0</td>
<td>5.80</td>
</tr>
<tr>
<td>MC Overlay</td>
<td>6.0</td>
<td>5.80</td>
</tr>
</tbody>
</table>

The Software trigger timing window is designed with a loose time selection around
SECTION 6. SIGNAL SELECTION

Figure 6.9: The stacked prediction (MC+Beam-off) and beam data timing distributions of the flashes associated to the reconstructed events that pass the SliceID requirements with the extended flash window. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

the expected NuMI time window. The SliceID time window is extended to the end of the software trigger window allowing the selection of LLP events that arrive in the detector after the neutrino spill but inside the software trigger window. The start time of the window is moved forwards by 0.2 µs, in order to provide an additional region to validate the normalisation of the beam-off data to the beam-on data. The original and modified SliceID timing parameters can be found in tab. 6.1.

Figure 6.9 shows the flash timing distributions of events after the modified SliceID selection. The distribution for $m_{\text{HNL}} = 304$ MeV is overlaid on the data and the background predictions. The shift with respect to the neutrino distribution increases the range of flash times in to the region after 15.44 µs where no neutrino background is observed.

SliceID Performance

Figure 6.10 shows the performance of the SliceID on the background and data samples for each run. SliceID rejects a significant number of out-of-cryostat and cosmic-ray events. A neutrino slice is only identified in $\approx 20\%$ of beam-off events and $30\%$ of
Figure 6.10: The stacked prediction (MC+Beam-off) and beam data results of the SliceID pass/fail criteria. Included are all events that pass the software trigger. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

out-of-cryostat events that pass the software trigger.

The efficiency of the SW trigger and the SliceID for the HNL samples is shown in tab. 6.2. The efficiency rises with $m_{\text{LLP}}$ because the amount of deposited energy and length of the decay product tracks are on average longer. For HNL with masses approaching the upper production threshold of $m_{\text{HNL}} = 388$ MeV, the software trigger efficiency declines due to the fraction of events arriving after the end of the software trigger beam window.

<table>
<thead>
<tr>
<th>HNL Masses (MeV)</th>
<th>212</th>
<th>215</th>
<th>230</th>
<th>245</th>
<th>260</th>
<th>269</th>
<th>275</th>
<th>279</th>
</tr>
</thead>
<tbody>
<tr>
<td>SW Trigger Eff</td>
<td>0.96,0.96</td>
<td>0.96,0.96</td>
<td>0.96,0.96</td>
<td>0.97,0.97</td>
<td>0.97,0.97</td>
<td>0.97,0.97</td>
<td>0.99,0.99</td>
<td>0.99,0.99</td>
</tr>
<tr>
<td>SliceID Eff</td>
<td>0.41,0.41</td>
<td>0.44,0.44</td>
<td>0.52,0.52</td>
<td>0.57,0.56</td>
<td>0.60,0.59</td>
<td>0.61,0.61</td>
<td>0.66,0.66</td>
<td>0.66,0.66</td>
</tr>
<tr>
<td>Combined Eff</td>
<td>0.40,0.40</td>
<td>0.42,0.42</td>
<td>0.50,0.50</td>
<td>0.55,0.54</td>
<td>0.58,0.57</td>
<td>0.60,0.59</td>
<td>0.65,0.65</td>
<td>0.66,0.66</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>HPS Masses (MeV)</th>
<th>212</th>
<th>215</th>
<th>230</th>
<th>245</th>
<th>260</th>
<th>269</th>
<th>275</th>
<th>279</th>
</tr>
</thead>
<tbody>
<tr>
<td>SW Trigger Eff</td>
<td>0.97,0.97</td>
<td>0.97,0.97</td>
<td>0.97,0.97</td>
<td>0.98,0.98</td>
<td>0.97,0.97</td>
<td>0.93,0.92</td>
<td>0.54,0.55</td>
<td></td>
</tr>
<tr>
<td>SliceID Eff</td>
<td>0.38,0.39</td>
<td>0.40,0.40</td>
<td>0.51,0.51</td>
<td>0.58,0.58</td>
<td>0.63,0.66</td>
<td>0.68,0.68</td>
<td>0.67,0.66</td>
<td></td>
</tr>
<tr>
<td>Combined Eff</td>
<td>0.37,0.37</td>
<td>0.38,0.39</td>
<td>0.50,0.50</td>
<td>0.57,0.56</td>
<td>0.61,0.61</td>
<td>0.63,0.62</td>
<td>0.36,0.36</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.2: The fractional efficiencies of the software trigger and SliceID processes as well as their combined efficiency for each of the LLP signal samples. Each box contains the Run 1 and Run 3 efficiencies in that order. The statistical uncertainty on the efficiencies is of order 0.001.
6.2.2 Candidate Vertex Building

Once a slice containing an LLP candidate decay has been selected, the tracks that correspond to the two LLP decay products need to be identified. The signal candidates should contain two tracks emerging from a single vertex. The standard Pandora reconstruction frequently misplaces the location of the true decay vertex of the signal events as the signal topology differs from the standard neutrino interactions. To address this effect and to increase efficiency, candidate vertices are constructed considering all possible pairings of reconstructed particles in the slice.

The start and end points of each reconstructed particle are compared, and any objects with start or end points within a distance of 5 cm in 3D space are combined to form an LLP candidate vertex. All objects where a track hypothesis was successfully fitted are considered, as only tracks have a reconstructed end point. If the end point of a track is placed at one of the new candidate vertices, the track direction is reversed. Each position coordinate of the vertex is calculated as the mean of the start positions of the two tracks in that coordinate. Figure 6.11 shows an event display of an example signal event where the Pandora vertex is misplaced at the end.
of the LLP-produced muon. The two-track vertex building algorithm produced a vertex in good agreement with the location of the true vertex.

A single event can have multiple candidate vertices. In this case the only best candidate from each event will be used at the final stages of the selection. Figure 6.12 shows the number of constructed two-track candidate vertices per event for each of the main samples. The majority of background events have no vertices. A single signal mass is shown, but all masses see similar performance with between \( \approx (60 - 70)\% \) of events containing at least one vertex and \( \approx (40 - 50)\% \) containing exactly one vertex.

For the lighter \( m_{\text{LLP}} \) the tracks of the decay product are typically very short, as shown in section 6.1. Therefore the shorter track of the two may often not be reconstructed. In this case either a vertex is not found or the decay products of the shorter or longer track (for example a Michel electron produced by a muon) are identified as the second track. While the ideal candidate has two correctly reconstructed tracks corresponding to each of the direct LLP decay products, misreconstruction occurs frequently. Therefore optimising purely based on this ideal signal would not give the best sensitivity for the search. In addition to the full
### Table 6.3: Number of vertices and events with at least one vertex. All numbers are POT normalised. Percentages are of events passing SliceID. HNL are scaled to $|U_{\mu 4}|^2 = 10^{-8}$, HPS are scaled to $\theta_{\text{eff}}^2 = 10^{-9}$.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1 Events</th>
<th>Vertices</th>
<th>Run 3 Events</th>
<th>Vertices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam-Off</td>
<td>24033 (38.8%)</td>
<td>37313</td>
<td>50068 (38.6%)</td>
<td>77776</td>
</tr>
<tr>
<td>In-Cryo $\nu$ MC</td>
<td>17736 (58.3%)</td>
<td>43226</td>
<td>45582 (59.8%)</td>
<td>119443</td>
</tr>
<tr>
<td>Out-Cryo $\nu$ MC</td>
<td>3620 (30.1%)</td>
<td>4952</td>
<td>4557 (27.8%)</td>
<td>6418</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>45638 (44.1%)</td>
<td>86834</td>
<td>98061 (44.1%)</td>
<td>194260</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>45390 (43.5%)</td>
<td>85490</td>
<td>100207 (45.1%)</td>
<td>203636</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>1.01</td>
<td>1.00</td>
<td>0.98</td>
<td>0.95</td>
</tr>
<tr>
<td>Signal ($m_{\text{HNL}} = 304$ MeV)</td>
<td>10.7 (64.7%)</td>
<td>16.0</td>
<td>26.5 (64.6%)</td>
<td>40.2</td>
</tr>
<tr>
<td>Signal ($m_{\text{HPS}} = 245$ MeV)</td>
<td>8.8 (64.4%)</td>
<td>13.64</td>
<td>22.1 (66.7%)</td>
<td>34.8</td>
</tr>
</tbody>
</table>

Candidate kinematics, the signal selection uses variables that are not reliant on the full reconstruction and identification of both decay products. Examples of such variables include the direction and length of the longest reconstructed track and the total collected energy of the slice. Table 6.3 details the number of events which contain at least one vertex and the total number of vertices for each of the main samples used in this analysis.

### 6.3 Pre-selection

A pre-selection is applied to the events containing candidate vertices. The main purpose of the pre-selection is to reduce the SM neutrino and cosmic-ray background. LLP candidates where cosmic-ray slices are incorrectly reconstructed as signal are also removed. The pre-selection criteria are grouped into two categories, “low-level” selections that are applicable for a generic low-energy event selection, and “high-level” selections that focus on the signatures specific to LLP decays.

In the following plots the bands shown for the combined MC+Beam-off background include both statistic and partial systematic uncertainties on the prediction. The uncertainties cover the neutrino flux, neutrino interaction rate, and the hadron re-interactions with the LAr. There is an additional 100% normalisation uncertainty on the out-of-cryostat interactions. Details of the estimation and propagation of the uncertainties from these effects will be given in section 8.
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6.3.1 Low-level Variables

This group of selection criteria are applied to slice-wide variables as opposed to those specific to a candidate vertex.

Optical Flash Selection

The first stage of the pre-selection applies two further restrictions on the optical flash-based information of the event, beyond that imposed by the SliceID procedure. The optical flash with the largest total collected number of photoelectrons is required to have a reconstructed time in the window of 5.64 to 16.44 µs, which is the same window as used for the extended SliceID. This is more restrictive than the flash requirement in the SliceID as the in-time flash is now required to have the largest number of photoelectrons. Figure 6.9 shows the flash timing distributions for the selected events. The tails of events before and after the beam window are removed by this selection.

Figure 6.13: The stacked prediction (MC+Beam-off) and beam data flash match score distributions for reconstructed events that contain at least one candidate vertex. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

For every selected slice, a flash hypothesis is built using the reconstructed charge information. The collected charge is translated into an estimated scintillation light
deposition that would have accompanied the charge inside the detector. These estimated depositions are then propagated to the PMTs to calculate the amount of light that would have been collected by each PMT. This flash hypothesis is compared to the reconstructed beam flash. The consistency between the hypothesis and the measured flash is quantified by a $\chi^2$ metric referred to as the flash match score. Lower scores indicate a better agreement and hence greater likelihood that the reconstructed slice is of beam origin. Figure 6.13 shows that agreement in this variable is poor. A loose requirement on the flash match score to $< 20$ is therefore applied. This selection is effective at removing background cosmic rays. The total number of events and vertices for each of the main samples after the flash selection requirements are applied is listed in tab. 6.4.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1</th>
<th>Run 2</th>
<th>Run 3</th>
<th>Run 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Events</td>
<td>Vertices</td>
<td>Events</td>
<td>Vertices</td>
</tr>
<tr>
<td>Beam-Off</td>
<td>17815 (74.1%)</td>
<td>26528 (71.1%)</td>
<td>35674 (71.3%)</td>
<td>53387 (68.6%)</td>
</tr>
<tr>
<td>In-Cryo $\nu$ MC</td>
<td>13943 (78.6%)</td>
<td>33122 (76.6%)</td>
<td>32648 (71.6%)</td>
<td>80255 (67.2%)</td>
</tr>
<tr>
<td>Out-Cryo $\nu$ MC</td>
<td>2383 (65.8%)</td>
<td>3146 (63.5%)</td>
<td>2646 (58.1%)</td>
<td>3565 (55.6%)</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>35127 (77.0%)</td>
<td>65077 (74.9%)</td>
<td>71492 (72.9%)</td>
<td>134565 (69.3%)</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>34141 (75.2%)</td>
<td>62796 (73.5%)</td>
<td>70968 (70.8%)</td>
<td>137207 (67.4%)</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>1.03</td>
<td>1.04</td>
<td>1.01</td>
<td>0.98</td>
</tr>
<tr>
<td>Signal ($m_{\text{HNL}} = 304$ MeV)</td>
<td>9.8 (92.0%)</td>
<td>14.7 (92.0%)</td>
<td>24.2 (91.6%)</td>
<td>36.7 (91.4%)</td>
</tr>
<tr>
<td>Signal ($m_{\text{HPS}} = 245$ MeV)</td>
<td>8.2 (92.8%)</td>
<td>12.7 (93.0%)</td>
<td>20.5 (92.6%)</td>
<td>32.3 (92.7%)</td>
</tr>
</tbody>
</table>

Table 6.4: Number of vertices and events with at least one vertex passing the optical flash selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to $|U_{\mu4}|^2 = 10^{-8}$, HPS to $\theta_{\text{eff}}^2 = 10^{-9}$.

**Reconstructed Object Multiplicity**

The low-energy signal decays typically result in few reconstructed objects in the slice, where certain categories of neutrino events can be more complex and thus contain many objects. As these events have more objects, they therefore often contain multiple candidate vertices. This amplifies the effect of these events on the vertex distributions and drives a small disagreement seen in the normalisation prediction for the number of vertices seen in the earlier stages of the selection. Events are required to have $\leq 4$ reconstructed $\text{PFParticles}$ in the slice. Of those objects no more than three can be track like ($\text{Track Score} > 0.5$) and no more than two can be shower like...
Figure 6.14: The stacked prediction (MC+Beam-off) and beam data distributions of the number of total particles, tracks and showers reconstructed in the slice for events that pass the flash based selection requirement. The HNL distribution shown overlaid is for an example mass of $m_{HNL} = 304$ MeV. Its normalisation has been scaled up for visibility. The three distributions are shown for Run 1 (left) and Run 3 (right).
Table 6.5: Number of vertices and events with at least one vertex passing the reconstructed object multiplicity selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to $|U_{\mu 4}|^2 = 10^{-8}$, HPS to $\theta_{\text{eff}}^2 = 10^{-9}$.

(Track Score < 0.5). As shown in fig. 6.14, this selection removes neutrino events while having little impact on signal.

The total number of events and vertices for each of the main samples after the object multiplicity requirements are applied is listed in tab. 6.5. The selection on these variables significantly improves the data-MC agreement in later stages of the analysis.

**Containment**

Background from cosmic rays and out-of-cryostat neutrinos often comprises charged particles that enter the detector. Charged-current $\nu_\mu$ CC interactions typically produce long muon tracks that have a high probability to exit the detector, while the low-energy LLP decay signature produces two short tracks that rarely exit the detector. Events are therefore required to be contained, i.e., the maximum and minimum location in each dimension of all the objects in the slice must be entirely within a volume defined inside the TPC’s active volume. The maximum and minimum points of the slice in each dimension are found by considering the start and end points of each object in the slice. For each dimension, the smallest of these in the slice is taken as the minimum extent, and the largest the maximum.
Figure 6.15: The stacked prediction (MC+Beam-off) and beam data distributions for the maximum and minimum slice points in each dimension for events that pass the object multiplicity selection requirement. The HNL distribution shown overlaid for the maximum and minimum slice points in each dimension for events that pass.
The restrictions on the maximum and minimum of the slice are,

\[ 9 \text{ cm} < \min(x), \max(x) < 253 \text{ cm} \]
\[ -112 \text{ cm} < \min(y), \max(y) < 112 \text{ cm} \]
\[ 14 \text{ cm} < \min(z), \max(z) < 1020 \text{ cm}. \]

The distributions of \( \max(i), \min(i) \) with \( i = x, y, z \) are shown in fig. 6.15, together with the containment requirement boundary. Peaks are observed in all dimensions for exiting cosmic-ray and neutrino backgrounds. In particular, the large beam-off background with high maximum \( y \)-values is due to cosmic rays that enter the detector from above. The neutrino background peaks in the maximum \( z \) and maximum \( x \) distributions are due to exiting tracks and correspond to the direction of neutrinos from the NuMI target. The dip around \( z = 750 \text{ cm} \) in the both the Z dimension distributions is caused by a region of unresponsive wires in the collection plane, which significantly reduces the reconstruction efficiency in that region. The total number of events and vertices for each of the main samples after the containment selection requirements are applied is listed in tab. 6.6.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1 Events</th>
<th>Vertices</th>
<th>Run 3 Events</th>
<th>Vertices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam-Off</td>
<td>3086 (12.8%)</td>
<td>4232 (11.3%)</td>
<td>7054 (14.1%)</td>
<td>9749 (12.5%)</td>
</tr>
<tr>
<td>In-Cryo ν MC</td>
<td>3597 (20.3%)</td>
<td>5664 (13.1%)</td>
<td>7885 (17.3%)</td>
<td>12493 (10.5%)</td>
</tr>
<tr>
<td>Out-Cryo ν MC</td>
<td>347 (9.6%)</td>
<td>487 (9.8%)</td>
<td>461 (10.1%)</td>
<td>655 (10.2%)</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>6949 (15.2%)</td>
<td>10239 (11.8%)</td>
<td>15264 (15.6%)</td>
<td>22227 (11.4%)</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>7030 (15.5%)</td>
<td>10383 (12.1%)</td>
<td>15400 (15.4%)</td>
<td>22897 (11.2%)</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>0.97</td>
</tr>
<tr>
<td>Signal ( m_{\text{HNL}}=304 \text{ MeV} )</td>
<td>7.8 (73.4%)</td>
<td>11.4 (71.2%)</td>
<td>19.6 (73.9%)</td>
<td>28.8 (71.7%)</td>
</tr>
<tr>
<td>Signal ( m_{\text{HPS}}=245 \text{ MeV} )</td>
<td>6.5 (73.9%)</td>
<td>9.7 (71.2%)</td>
<td>16.5 (74.6%)</td>
<td>25.0 (72.0%)</td>
</tr>
</tbody>
</table>

Table 6.6: Number of vertices and events with at least one vertex passing the containment selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to \(|U_{\mu 4}|^2 = 10^{-8}\), HPS to \(\theta_{\text{eff}}^2 = 10^{-9}\).

### 6.3.2 High-level Variables

This group of selection criteria are applied to both slice-wide variables and those specific to a candidate vertex. Unlike the previous set, the variables included here display significant signal-mass dependency. The criteria imposed are kept loose
with the intention that they only remove areas of phase space where there is almost no signal of any mass value or are highly background dominated. Some of these variables also feature later in the BDT selection (see section 7). Earlier iterations of the analysis found using the full (before selection) distributions of the variables in the BDT produced very similar final sensitivities but removing these obviously non-signal like events simplifies the eventual BDT output.

**Opening Angle**

Figure 6.16: The stacked prediction (MC+Beam-off) and beam data distributions for the opening angle of each candidate vertex that passes the containment selection requirement. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

The reconstructed direction at the start of each of the tracks in the candidate vertices can be used to calculate the opening angle $\alpha$ of the candidate decay tracks. As can be seen in section 6.1, the true $\alpha$ of the LLP decay in signal is highly mass dependent, with higher masses leading to wider opening angles. A large contribution of cosmic-ray backgrounds to the two-track candidates is due to single tracks being split into two during reconstruction. When a cosmic-ray track is broken into two tracks, they can be combined to form a LLP candidate vertex. These candidates appear to have tracks emerging back-to-back from the vertex and thus can be identified by their very large ($\alpha \approx \pi$) opening angle. This effect is visible in fig. 6.16.
where cosmic rays are present at very wide opening angles \((\cos \alpha \approx -1)\). Candidate vertices with \(\cos \alpha < -0.94\) are removed from the selection. The total number of events and vertices for each of the main samples after the opening angle selection requirements are applied is listed in tab. 6.7.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1</th>
<th></th>
<th>Run 3</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Events</td>
<td>Vertices</td>
<td>Events</td>
<td>Vertices</td>
</tr>
<tr>
<td>Beam-Off</td>
<td>2535 (10.5%)</td>
<td>3480 (9.3%)</td>
<td>5895 (11.8%)</td>
<td>8114 (10.4%)</td>
</tr>
<tr>
<td>In-Cryo (\nu) MC</td>
<td>3300 (18.6%)</td>
<td>5163 (11.9%)</td>
<td>7308 (16.0%)</td>
<td>11491 (9.6%)</td>
</tr>
<tr>
<td>Out-Cryo (\nu) MC</td>
<td>289 (8.0%)</td>
<td>405 (8.2%)</td>
<td>397 (8.7%)</td>
<td>562 (8.8%)</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>6061 (13.3%)</td>
<td>8920 (10.3%)</td>
<td>13317 (13.6%)</td>
<td>19390 (10.0%)</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>6124 (13.5%)</td>
<td>9048 (10.6%)</td>
<td>13599 (13.6%)</td>
<td>20167 (9.9%)</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>0.99</td>
<td>0.99</td>
<td>0.98</td>
<td>0.96</td>
</tr>
<tr>
<td>Signal ((m_{\text{HNL}} = 304 \text{ MeV}))</td>
<td>7.6 (71.3%)</td>
<td>10.8 (67.9%)</td>
<td>19.0 (71.7%)</td>
<td>27.5 (68.4%)</td>
</tr>
<tr>
<td>Signal ((m_{\text{HPS}} = 245 \text{ MeV}))</td>
<td>6.3 (71.5%)</td>
<td>9.3 (68.0%)</td>
<td>16.0 (72.5%)</td>
<td>23.9 (68.7%)</td>
</tr>
</tbody>
</table>

Table 6.7: Number of vertices and events with at least one vertex passing the opening angle selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to \(|U_{\mu 4}|^2 = 10^{-8}\), HPS to \(\theta_{\text{eff}}^2 = 10^{-9}\).

### Proton Likelihood

Neutrino interactions often produce protons in the final state. The calorimetric information of the detector can be used to separate these events from the signal decays which contain only MIP-like tracks. The log-likelihood particle identification score (LLR PID score) is a powerful variable specifically designed to utilise the calorimetric information collected to separate proton and muon (MIP) tracks. The variable is described in Ref. [123].

The variable combines charge information from each of the wire planes to determine if tracks are proton or MIP-like. The expected \(dE/dx\) distributions of each of the two species as they stop are used to create probability density functions (PDFs). Separate PDFs are formed for each of the three wire planes binned in \(dE/dx\), residual range and pitch, where the pitch describes the angle between the track and the vector that connects adjacent wires in the plane. For a reconstructed track, the \(dE/dx\) information on each plane is compared to the expectation for the two particle types and a likelihood is calculated for both hypothesis. The likelihoods from each
Figure 6.17: The stacked prediction (MC+Beam-off) and beam data distributions for the LLR PID score of the longest (top) and shortest (bottom) track in each candidate vertex that passes the opening angle selection requirement. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

of the three planes are then combined multiplicatively. The LLR PID score is then constructed as a ratio of the likelihoods for each particle hypothesis. Finally, the score is mapped onto the range $[-1, 1]$ where a score of $-1$ indicates a completely proton-like track and $1$ a completely muon-like track.

Figure 6.17 shows the PID score for the longest and shortest tracks in each candidate vertex. There is a population of neutrino events containing highly-proton like tracks for both the longer and shorter tracks. For the longer tracks the majority of both signal and cosmic rays are identified as MIP like as would be expected.
The signal does not peak at 1 as the typical track length is short and the score is constructed in such a way that the LLR score increases with the number of deposits. The shorter tracks peak at 0, where the track was too short to make any discrimination between the hypotheses.

To remove neutrino events containing a proton, vertices where one or both of the tracks have a LLR PID score < −0.5 are removed. The total number of events and vertices for each of the main samples after the proton rejection selection requirements are applied is listed in tab. 6.8.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1</th>
<th>Run 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Events</td>
<td>Vertices</td>
</tr>
<tr>
<td>Beam-Off</td>
<td>2453 (10.2%)</td>
<td>3348 (9.0%)</td>
</tr>
<tr>
<td>In-Cryo ν MC</td>
<td>2622 (14.8%)</td>
<td>3816 (8.8%)</td>
</tr>
<tr>
<td>Out-Cryo ν MC</td>
<td>273 (7.6%)</td>
<td>380 (7.7%)</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>5400 (11.8%)</td>
<td>7591 (8.7%)</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>5349 (11.8%)</td>
<td>7543 (8.8%)</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>1.01</td>
<td>1.01</td>
</tr>
<tr>
<td>Signal ((m_{\text{HNL}} = 304,\text{MeV}))</td>
<td>7.6 (71.1%)</td>
<td>10.8 (67.7%)</td>
</tr>
<tr>
<td>Signal ((m_{\text{HPS}} = 245,\text{MeV}))</td>
<td>6.3 (71.4%)</td>
<td>9.3 (67.9%)</td>
</tr>
</tbody>
</table>

Table 6.8: Number of vertices and events with at least one vertex passing the proton rejection selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to \(|U_{\mu 4}|^2 = 10^{-8}\), HPS to \(\theta_{\text{eff}}^2 = 10^{-9}\).

**Reconstructed Energy**

Figure 6.18 shows the distribution of the combined reconstructed energy of all the objects of the slice \((E_{\text{sl}})\) using charge deposited on the collection plane. For the mono-energetic signal decays this \(E_{\text{sl}}\) will peak at \(E_{\text{LLP}} - (m_{d1} + m_{d2})\), where \(E_{\text{LLP}}\) is the energy of the LLP and \(m_{d1}\) and \(m_{d2}\) are the masses of the two decay products. This corresponds to the combined kinetic energy of the two decay daughters. The reconstructed value will skew to higher values if the daughters of the decay products, for example \((\pi \rightarrow \mu \rightarrow e)\), are reconstructed and included in the slice.

There is a tail of neutrino events with deposited energies much higher than possible for any mass value of LLP. These events are removed by requiring the
SECTION 6. SIGNAL SELECTION

Figure 6.18: The stacked prediction (MC+Beam-off) and beam data distributions for the total slice calorimetric energy for each event which contains a candidate vertex that passes the proton rejection requirement. The HNL distribution shown overlaid is for an example mass of \( m_{\text{HNL}} = 304 \) MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

\( E_{\text{el}} < 500 \) MeV. The total number of events and vertices for each of the main samples after the slice energy selection requirement are applied is listed in tab. 6.9.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1 Events</th>
<th>Vertices</th>
<th>Run 3 Events</th>
<th>Vertices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam-Off</td>
<td>2322 (9.7%)</td>
<td>3157 (8.5%)</td>
<td>5422 (10.8%)</td>
<td>7410 (9.5%)</td>
</tr>
<tr>
<td>In-Cryo ( \nu ) MC</td>
<td>1921 (10.8%)</td>
<td>2718 (6.3%)</td>
<td>4269 (9.4%)</td>
<td>6093 (5.1%)</td>
</tr>
<tr>
<td>Out-Cryo ( \nu ) MC</td>
<td>266 (7.3%)</td>
<td>371 (7.5%)</td>
<td>364 (8.0%)</td>
<td>518 (8.1%)</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>4513 (9.9%)</td>
<td>6253 (7.2%)</td>
<td>10198 (10.4%)</td>
<td>14116 (7.3%)</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>4509 (9.9%)</td>
<td>6246 (7.3%)</td>
<td>10056 (10.0%)</td>
<td>14021 (6.9%)</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>1.00</td>
<td>1.00</td>
<td>1.01</td>
<td>1.01</td>
</tr>
<tr>
<td>Signal ( m_{\text{HNL}} = 304 ) MeV</td>
<td>7.6 (71.0%)</td>
<td>10.8 (67.6%)</td>
<td>18.9 (71.4%)</td>
<td>27.4 (68.2%)</td>
</tr>
<tr>
<td>Signal ( m_{\text{HPS}} = 245 ) MeV</td>
<td>6.3 (71.4%)</td>
<td>9.3 (67.9%)</td>
<td>16.0 (72.4%)</td>
<td>23.9 (68.6%)</td>
</tr>
</tbody>
</table>

Table 6.9: Number of vertices and events with at least one vertex passing the slice energy selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to \(|U_{\mu 4}|^2 = 10^{-8}\), HPS to \(\theta_{\text{eff}}^2 = 10^{-9}\).

Longest Track Length

As discussed in section 6.1 the LLP decay products form short tracks for all the LLP masses considered. The longest possible true track length considered is less than
Figure 6.19: The stacked prediction (MC+Beam-off) and beam data distributions for the length of the longest track in each candidate vertex that passes the slice calorimetric energy requirement. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).

The CRT veto utilises the fast timing of the CRT system to reject events of non-beam origin. It searches for a time coincidence between a recorded CRT hit and...
Table 6.10: Number of vertices and events with at least one vertex passing the track length selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to $|U_{\mu 4}|^2 = 10^{-8}$, HPS to $\theta_{\text{eff}}^2 = 10^{-9}$.

Figure 6.20: The stacked prediction (MC+Beam-off) and beam data distributions for the CRT Veto output (left) and closest CRT cosmic distance (right) for each event that contains a candidate vertex that passes the track length requirement. The HNL distribution shown overlaid is for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are only applicable for Run 3.
The CRT can be used to tag TPC reconstructed tracks of cosmic origin. Each TPC track is projected to the CRT panels, and if the projected point of intersection with the panel is within 15 cm of a CRT hit, the track is assumed to be of cosmic origin. The track projection is performed for each CRT hit using the hit time as the time $t_0$ needed to locate the track in the $x$-dimension.

The closest cosmic distance $d_{CRT}$ is the distance in 3D space between the reconstructed neutrino vertex and the closest point on a track that has been tagged with a CRT hit. If $d_{CRT}$ is small it is likely the event is created by a cosmic ray. As $d_{CRT}$ is calculated at the reconstruction stage, the default Pandora vertex location is used in the calculation rather than the two-track candidate vertex constructed at the analysis stage. Section 6.3.2 shows the $d_{CRT}$ distribution. The peak close to zero, made up predominately of cosmic events, is removed by requiring $d_{CRT} > 20$ cm. The total number of events and vertices for each of the main samples after the CRT selection has been applied is listed in tab. 6.11.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Event</th>
<th>Vertices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam-Off</td>
<td>1234 (2.5%)</td>
<td>1737 (2.2%)</td>
</tr>
<tr>
<td>In-Cryo $\nu$ MC</td>
<td>2132 (4.7%)</td>
<td>2970 (2.5%)</td>
</tr>
<tr>
<td>Out-Cryo $\nu$ MC</td>
<td>129 (2.8%)</td>
<td>181 (2.8%)</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>3410 (3.5%)</td>
<td>4706 (2.4%)</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>3495 (3.5%)</td>
<td>4888 (2.4%)</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>0.98</td>
<td>0.96</td>
</tr>
<tr>
<td>Signal ($m_{HNL} = 304$ MeV)</td>
<td>17.7 (66.7%)</td>
<td>25.7 (63.9%)</td>
</tr>
<tr>
<td>Signal ($m_{HPS} = 245$ MeV)</td>
<td>15.1 (68.3%)</td>
<td>22.5 (64.8%)</td>
</tr>
</tbody>
</table>

Table 6.11: Number of vertices and events with at least one vertex passing the CRT selection. All numbers are POT normalised. The efficiency percentages in brackets are with respect to the output of the candidate vertex building. HNL candidates are scaled to $|U_{\mu 4}|^2 = 10^{-8}$, HPS to $\theta^2_{\text{eff}} = 10^{-9}$.

### 6.3.3 Pre-selection Efficiency Summary

Table 6.12 shows the final number of events with a candidate vertex passing the pre-selection for each sample and the combined prediction. The rejection efficiency of the pre-selection on the beam-off, In-Cryo $\nu$ MC and Out-Cryo $\nu$ MC backgrounds is also shown.
### Table 6.12: Number of events with at least one candidate vertex that pass in each sample after the full event selection. All numbers are POT normalised. HNL candidates are scaled to $|U_{\mu d}|^2 = 10^{-8}$, HPS to $\theta_{\text{eff}}^2 = 10^{-9}$. The efficiencies are given with respect to the number of events that pass the Pandora SliceID procedure.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Run 1 Events</th>
<th>Run 1 Efficiency</th>
<th>Run 3 Events</th>
<th>Run 3 Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam-Off</td>
<td>1552</td>
<td>2.5%</td>
<td>1234</td>
<td>0.9%</td>
</tr>
<tr>
<td>In-Cryo ν MC</td>
<td>1188</td>
<td>3.9%</td>
<td>2132</td>
<td>2.7%</td>
</tr>
<tr>
<td>Out-Cryo ν MC</td>
<td>208</td>
<td>1.7%</td>
<td>129</td>
<td>0.8%</td>
</tr>
<tr>
<td>Beam-On Data</td>
<td>2950</td>
<td>2.8%</td>
<td>3410</td>
<td>1.5%</td>
</tr>
<tr>
<td>Total MC+Beam-Off</td>
<td>2948</td>
<td>2.8%</td>
<td>3495</td>
<td>1.6%</td>
</tr>
<tr>
<td>Data/Pred</td>
<td>1.00</td>
<td>-</td>
<td>0.99</td>
<td>-</td>
</tr>
<tr>
<td>Signal ($m_{\text{HNL}} = 304$ MeV)</td>
<td>7.5</td>
<td>45.2%</td>
<td>17.6</td>
<td>43.1%</td>
</tr>
<tr>
<td>Signal ($m_{\text{HPS}} = 245$ MeV)</td>
<td>6.2</td>
<td>45.9%</td>
<td>15.1</td>
<td>45.6%</td>
</tr>
</tbody>
</table>

When considered together, the total background rejection factor is $\approx 40$ (60) for Run 1 (Run 3). The additional rejection in Run 3 is due to the application of the CRT selection.

![Image](image_url)

**Figure 6.21:** The cumulative selection efficiencies for each stage of the selection. The efficiencies are calculated per event and as a fraction of the number of events that pass the SliceID process. Left: The efficiencies for the beam data and each of the main background samples. The red band indicates the full range of efficiencies for the LLP signal samples. Right: The individual signal sample efficiencies are shown.

*Figure 6.21* shows the cumulative selection efficiency for each sample throughout the selection flow. The efficiency of the pre-selection on the signal varies slightly
depending on the mass and type of LLP but falls in the range of 35% to 50% for all signal samples with the efficiency increasing with LLP mass for both models.

**Figure 6.22**: The relative selection efficiencies for each stage of the selection. The efficiencies are calculated per event and as a fraction of the number of events that pass the previous selection stage. Left: The efficiencies for the beam data and each of the main background samples. The red band indicates the full range of efficiencies for the LLP signal samples. Right: The individual signal sample efficiencies are shown.

Figure 6.22 shows the efficiency of each stage of the selection with respect to the previous stage in order to better indicate the relative rejection power of each criteria with respect to the different background samples. The biggest difference between the signal sample efficiencies is caused by the larger fraction of events where no candidate vertices are found for the low mass HNL.
7 Boosted Decision Trees

After the pre-selection, signal candidates are further discriminated from background using boosted decision trees (BDTs). BDTs are a well established multivariate machine learning technique, which combines input variables to build a classifier to separate signal from background. BDTs have two advantages over a “rectangular” selection for a search with an inherently low signal to background ratio. Firstly, the structure of the decision tree allows correlations between variables to be exploited. Secondly, the iterative training in the boosting process gives events that are initially mis-classified additional weighting in order to maximise background rejection. As some of the variables with the best separation between signal and background have a strong dependence on the LLP mass, a separate BDT is trained for each LLP mass sample. Section 7.1 briefly lays out the principles of BDT operation. The specific configuration of the BDTs and an overview of the BDT training process are described in section 7.2. The construction and description of the input variables used in the BDT are described in section 7.3 and section 7.4 respectively. Section 7.5 shows the evaluation of the performance the BDTs achieve in separating the LLP signal from the backgrounds.

7.1 Boosted Decision Trees

A decision tree takes a set of input features and splits input data recursively using a series of binary criteria on the variables. Decision trees are developed on training samples and are built iteratively in a process described by the following steps [124]. For each input variable, the value which gives the best separation between signal and background is found. Next, the variable which gives the best separation is selected and the samples are split into two nodes based on whether they pass or fail the given criteria. The process is then repeated from the first step for each node in succession, creating a tree-like structure. The growth of the tree terminates when a stopping criterion is reached. These are commonly a restriction on the depth of the node
structure of the tree or on the minimum number of events allowed in a node. Nodes that satisfy the stopping criteria are referred to as *leaves*. Each leaf is given a score according to the signal purity of the events in that leaf. This score then represents the probability of an event that reaches that leaf, when passed through the tree, being signal or background. More details on decision trees and their use in high energy physics can be found in Ref. [124].

In general, due to the way decision trees are constructed they are insensitive to one-to-one mappings of the input variables. Therefore the performance is unaffected by, for example, exchanging a particle’s momentum for its energy or changing the scale of the input variables. Furthermore, due to the ranking of variable sensitivity, the inclusion of variables with little separation power does not degrade the performance of the tree. If a variable offers no separation, it will never be selected for use in the tree.

BDTs refer to the application of boosting algorithms to combine an assemble of decision trees into a single strong classifier. Each tree is created iteratively, using information from the previous tree to improve the training. The training events are re-weighted for each subsequent training iteration using the output of the classifier in the previous step. Events that were previously misclassified are assigned larger weights, such that they are considered with greater importance in subsequent trees. At each training step, a score is given to each of the trees based on the accuracy of its output, and the final BDT classifier score for an event is given by a weighted sum of the scores from each tree after training. To prevent over-fitting on the training samples, each tree is kept to a depth of only a few splitting nodes. Therefore, the final BDT classifier is an ensemble of individual weak classifiers. The final combined classifier should then be stable against fluctuations in the sample and provide an enhanced performance compared to using a single tree.

Gradient boosting is a particular method of boosting which is carried out as an optimisation algorithm of a loss function. This function combines the accuracy of the tree output and a regularisation penalty term for the model complexity. A method similar to a gradient descent algorithm is used to find the minimum of the loss function.
7.2 Training Configuration

The XGBoost gradient boosting library [125] is used to develop the BDTs in this analysis. The non-default hyper-parameters, which control the development and training of the trees, can be found in tab. [7.1]. In order to maximise the separation between the LLP signal and background, the parameters are tuned through repeated evaluation on test simulation data-sets.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Booster</td>
<td>dart</td>
</tr>
<tr>
<td>max_depth</td>
<td>6</td>
</tr>
<tr>
<td>eta</td>
<td>0.3</td>
</tr>
<tr>
<td>objective</td>
<td>binary:logistic</td>
</tr>
<tr>
<td>tree_method</td>
<td>hist</td>
</tr>
<tr>
<td>rate_drop</td>
<td>0.1</td>
</tr>
<tr>
<td>skip_drop</td>
<td>0.5</td>
</tr>
<tr>
<td>Training iterations</td>
<td>50</td>
</tr>
</tbody>
</table>

Table 7.1: XGBoost hyper-parameters used for training the BDTs.

As stated, a separate BDT is trained for each LLP signal mass value. Each of the BDTs are trained with the same background sample made up of a random sample of 30% of the events in the in-cryostat neutrino sample. The signal training sample for each BDT is a random sample of 50% of the corresponding signal sample. Events must pass the pre-selection to be included in the training. There is a further restriction on signal training events that 90% or greater of the hits which make up the slice must be created by either the LLP decay daughters or their subsequent daughters. This ensures mis-reconstructed events within the signal samples, where the candidate slice is of cosmic origin, are not trained on. The training samples are then removed from the samples, which are then scaled up accordingly to once again match the correct POT.

The choice not to train on Beam-Off events is due to the small number of available events passing the pre-selection criteria. The neutrino overlay sample will contain events where cosmic activity from the overlay event has been reconstructed as the candidate vertex. So cosmic events can still be rejected by the BDT even without explicitly training on the Beam-Off sample. Utilising an additional second BDT
trained on beam-off events was explored, but was found not to significantly improve sensitivity.

The BDT ultimately produces a prediction score for all beam-data, background sample, and signal sample events, with a score of 0 representing an entirely background-like event and a score of 1 representing a signal-like event.

### 7.3 Kinetic Variable Construction

Once the two-track candidate vertices are constructed, variables corresponding to the expected KDAR decay kinematics for each vertex can be determined and used as input to the BDT. The key kinematic variables of the decays used in the selection are the 3D opening angle of the two tracks, the invariant mass of the decay, the momentum of the decay products and the reconstructed incoming direction of the LLP. While the opening angle can be determined unambiguously from the direction of each of the tracks in the vertex, the other variables require a reconstruction of the particle’s momentum and therefore an estimation of the mass of the particle.

As the events in this analysis are fully contained, the momentum hypothesis for each track can be estimated using the continuous-slowing-down-approximation (CSDA) range method. If a particle stops through ionisation loss, as described in section 3.2.1, its track length \( R \) can be used to determine its initial momentum. The LLP daughter particles considered in this analysis are all either muons or pions. For muons, the momentum \( p \) is estimated using an interpolation created from the data in Ref. [82] to create a function of the form,

\[
    f \left( \frac{R}{m_\mu} \right) = \beta \gamma m_\mu = p. \tag{7.1}
\]

To apply the same function to estimate the momentum from the range of charged pions, the range \( R \) is scaled by \( m_\mu/m_\pi \), and then the momentum by \( m_\pi/m_\mu \),

\[
    f \left( \frac{R}{m_\mu} \right) = \beta \gamma m_\mu = p \quad \rightarrow \quad f \left( \frac{R}{m_\mu} \cdot \frac{m_\mu}{m_\pi} \right) = \beta \gamma m_\mu \cdot \frac{m_\pi}{m_\mu} = p \cdot \frac{m_\pi}{m_\mu}. \tag{7.2}
\]

Figure 7.1 shows the relationship between the true momentum and reconstructed
momentum for both muons and pions. The sample shown is the decay products of a simulated HNL with $m_{\text{HNL}} = 304$ MeV. Since $m_\mu \approx m_\pi$, there is no method currently available to perform particle identification that reliably separates charged pions and muons in LArTPCs. For the HPS signal, the kinematic quantities are reconstructed by assigning $m_\mu$ to both particles. For HNL decays to $\mu \pi$, the longer track assigned to the vertex is assumed to be the muon and the shorter track is assumed to be the pion. Since $m_\mu < m_\pi$ and since pions have higher probability of re-interacting with the argon, this scenario is most often the correct one, for all HNL mass values. For $m_{\text{HNL}} = 246$ MeV, the muon is the longer track in 55% of decays and for $m_{\text{HNL}} = 385$ MeV in 90% of the decays.

7.4 Input Variables

Variables that give strong and complementary separation between the signal decays and the two classes of background are chosen as input to the BDT. The input variables used were selected by training trees with a large selection of variables and using metrics within XGBoost to determine the importance of each variable. The importance of a variable is calculated from the number of times it is used in the tree to create a selection, and the average separation gain of each time the variable is used. These metrics, combined with iterative development to maximise the separation
power of the BDT, were used to select the final input variables for the trees.

The variables chosen are;

- the calorimetric energy of the slice ($E_{\text{sl}}$),
- the topological score of the slice,
- the maximum and minimum extent of the slice,
- the number of track and shower objects in the slice,
- the angle of the candidate momentum from the absorber direction ($\beta$),
- the opening angle of tracks in the vertex ($\alpha$),
- the reconstructed invariant mass of the vertex ($m_{\text{inv}}$),
- the $\theta$ and $\phi$ angles of the longest track, and
- the length, LLR PID score and track score of both the tracks in the vertex.

The input variables which are newly introduced, or offer a particular strong separation between signal and the background, are shown in figs. 7.2 and 7.3 and are described in this subsection. Descriptions of the remaining variables can be found in section 6.3. After pre-selection, the shape of the Run 1 and Run 3 BDT input variable distributions are largely similar, with the only significant difference being the lower number of cosmic backgrounds in Run 3 due to the additional CRT selection. Therefore only the figures for Run 3, where the majority of the sensitivity of the analysis is derived, are shown. All input variables are shown for an example HNL with $m_{\text{HNL}} = 304$ MeV.

For the majority of the simulated LLP mass values, the highest-ranked contribution to the BDT separation is the total calorimetric energy of the slice $E_{\text{sl}}$, shown in fig. 7.2(a). The decay daughters of mono-energetic LLPs deposit a fixed amount of energy in the detector. The expected value of $E_{\text{sl}}$ for $m_{\text{LLP}} = 304$ MeV is indicated by the blue line. The variable is described in more detail in section 6.3.2. The separation power of $E_{\text{sl}}$ is not dependent on the inclusion of both decay products in the candidate vertex. Instead, as long as their charge deposits are reconstructed as part of the slice, the energy is reconstructed. The deposits can either be included as part of separate objects or, as is often the case, combined into one.

The topological score (fig. 7.2(b)), which is discussed in the context of the beam
Figure 7.2: The stacked prediction (MC+Beam-off) and beam data distributions for (a) the total reconstructed slice energy and (b) the topological score for each event containing a candidate vertex that passes the pre-selection requirements. The HNL distributions shown overlaid are for an example mass of 304 MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run3.

slice selection in section 6.2.1 offers separation between neutrino events and the LLP signal. Despite being designed to separate slices containing neutrinos and cosmic-ray events, the strong identification of certain neutrino topologies gives good separation of those events from the LLP, which are generally identified as “cosmic”-like by the SVM.

Figure 7.3 shows BDT variables that are calculated for each candidate vertex. A criterion is used to define “complete” signal sample candidates where both decay daughters have been correctly identified. Each of the two reconstructed tracks that form the vertex must correspond to a unique true LLP daughter. This “complete” criterion is used only in plotting to show the underlying distributions. Due to the separation power of variables such as $E_{sd}$ that do not require the inclusion of both true decay daughters in the vertex, restricting the BDT selection to target only “complete” vertices would reduce the sensitivity of the analysis.

The momentum estimates of the two tracks in the candidate vertex are summed to obtain the estimated momentum vector of the candidate vertex, and therefore the reconstructed incoming direction of the LLP. The angle $\beta$ is defined between the momentum vector of the candidate and the expected direction of an LLP from
Figure 7.3: The stacked prediction (MC+Beam-off) and beam data distributions for a selection of BDT input variables. The HNL distributions shown overlaid are for an example mass of $m_{\text{HNL}} = 304$ MeV. Its normalisation has been scaled up for visibility. The distributions are shown for Run 3.
the absorber. The expected direction is calculated as the vector from the absorber, where the LLP signal originates from, to the candidate decay vertex location. For a vertex in the centre of the detector, the expected incoming vector would be $[0.323, 0.738, -0.591]$, in the MicroBooNE detector coordinates. Figure 7.3(a) shows the BDT input variable $\cos \beta$, where as expected $\cos \beta \approx 1$ for a large fraction of the HNL signal candidates.

As shown in the truth level distributions in section 6.1, the decay product track lengths are short and spread over a small range for each mass value. Figures 7.3(c) and 7.3(d) show the track length distributions for the shorter and longer tracks in each vertex respectively. The shorter track length offers less individual separation but is included so that the full kinematics of the candidate vertices are provided to the BDT. As the track length variables contain identical information to the CSDA estimated momentum, the estimated momentum of the tracks is omitted from the input to the BDT.

The invariant mass of the LLP decay vertex ($m_{\text{inv}}$) is calculated from the reconstructed momenta of the two candidate tracks, their assumed masses and the opening angle $\alpha$. For HNLs, it is again assumed that of the two tracks in the vertex, the longer is the muon and the shorter the pion. Figure 7.3(b) shows the invariant mass distribution for the example signal mass $m_{\text{HNL}} = 304$ MeV. The expected value of $m_{\text{inv}} = m_{\text{HNL}}$ is indicated by the blue line.

The direction of the longer track is included in the BDT as the angles $\theta$ and $\phi$ of the track in the detector coordinates (see section 3.5.2). The distributions are shown in figs. 7.3(e) and 7.3(f). The signal distributions peak broadly at the expected direction from the absorber, which is approximately $\theta = 2.20$ and $\phi = 1.15$, in this coordinate system. The $\phi$ variable, in particular, offers additional cosmic rejection. Cosmic-ray events, which are generally downwards-going, create tracks that are aligned with $\phi = \pm \frac{\pi}{2}$.

The resolution of the kinematic BDT variables, while similar across the simulated signal samples, is dependent on $m_{\text{LLP}}$. Of note is the HNL sample with $m_{\text{HNL}} = 385$ MeV, near the production threshold. For this mass value decay products are
produced with a very large opening angles, $\alpha \approx \pi$ (see section 7.3). Therefore the incoming angle ($\beta$) of the HNL for this mass value is impossible to determine. The near back-to-back tracks also lead to the two decay products frequently being reconstructed as a single track, where the second track of the vertex is a daughter of one of the true LLP decay particles such as a Michel electron. Therefore for this mass value, the longest track length distribution peaks at a length equivalent to the combined momentum of the two daughters, which is fixed for each HNL decay.

7.5 BDT Performance

The performance of the BDTs on the test samples is shown in the BDT score distributions in Figure 7.4 for a selection of HNL and HPS masses. The BDTs offer strong rejection against beam-off events despite not being explicitly trained upon. Higher LLP masses produce a more distinct signal identification, due to the additional energy, and therefore better kinematic reconstruction of the events.

A figure of merit used to assess the performance of BDTs is the Receiving Operator Characteristic (ROC) curve. The curve describes the relationship between the signal efficiency (the fraction of signal correctly identified as signal) versus background rejection power (fraction of events correctly identified as background), across the range of thresholds on the BDT score. Figure 7.5 shows these curves for each of the BDTs trained. The BDT performs similarly well for all the signal samples trained on. The Area Under Curve (AUC) is defined as the integral of the area to the left and below each ROC curve, and can be used as a metric for the quality of a BDTs separation. The further from the diagonal (which is equivalent to categorising events at random) the better the performance of the BDT. As signal events can then be selected with high efficiency with a BDT score selection which rejects sufficient amounts of background for the search to be sensitive.
Figure 7.4: The BDT performance on the signal and two main background samples. Shown is the Run1 and Run3 output for a selection of representative HPS and HNL mass points.
Section 7. Boosted Decision Trees

Figure 7.5: The ROC curves for each trained BDT. The background rejection is quantified using all three background samples, each weighted to POT. The HPS samples are shown with dashed lines and the HNL with solid lines.

7.6 Signal Region

The structure of the BDT score distributions in the signal rich region is best evaluated by performing a logit transformation,

$$\text{logit}(s) = \ln \left( \frac{s}{1-s} \right) \quad \text{for} \quad s \in (0, 1) \quad (7.3)$$

to the output scores of the BDT (s). This transformation is the inverse of the logistic transformation that is performed by xgboost when outputting the classification score.

Figure 7.6 shows the predicted BDT score distribution after the logit transformation for a BDT trained on HNL events generated for $m_{\text{HNL}} = 304$ MeV. If, at this stage, multiple candidates still remain for an event, only the candidate with the highest BDT score is kept. The binning used in the calculation of the exclusion limits is shown. For each mass point the BDT score is binned between 0 ($= \text{logit}(0.5)$) and the maximum score assigned to an event in the run. Ten evenly spaced bins are used. Due to lack of statistics in the background samples, downward fluctuations produce bins at high BDT score with zero background prediction where the true
expected background value is non-zero. To mitigate this, these bins are merged with the previous bin.

The BDTs are then evaluated on the NuMI beam data samples and the score distributions are compared to the predicted background distribution to investigate the existence of an excess in the signal regions. In the absence of any significant excess, it is these BDT distributions which are used as input to the confidence limit setting on the HPS and HNL mixing parameters, discussed in section 9.
8 Systematic Uncertainties

To calculate the impact of systematic uncertainties on the mixing parameter limits, a full range of uncertainty sources is considered for the background samples and signal samples. The cosmic beam-off sample is taken from data and therefore has no associated systematic uncertainties other than the statistical fluctuations in the sample. For the neutrino MC background the following sources are considered: flux simulation, cross-section modelling, hadron interactions with argon, and detector variations. For signal, uncertainties related to the kaon production at the absorber, detector variations and final state hadron re-interactions are accounted for. As a decay rather than an interaction, there are no cross-section uncertainties associated with the signal.

8.1 Methods

Two simulation methods are used to calculate the uncertainties on the MC predictions used in the analysis.

- **Sample Re-simulation**: For this method, a MC simulation is carried out with a single simulation parameter changed. To reduce the impact of the statistical variations, the underlying true events are kept the same. Usually, a parameter is varied from its central value (CV) to the upper and lower limits of its assigned ±1σ uncertainty. In the case of on-off effects in the simulation, a one-sided variation is applied with the relevant parameter switched. The modified simulations are then compared to the CV simulation to determine the impact of the uncertainty on the analysis quantities. This method is used for the assessment of the detector uncertainties.

- **Event Re-weighting**: Alternatively, uncertainties can be assessed by re-weighting events. Events are assigned weights derived from the ratio between the CV truth distribution and modified distributions, produced with the altered
parameters, as a function of one or more variables of interest. The applied weights modify the underlying truth distributions of the CV to the “universe” with the modified parameters. This approach is not applicable where the phase space of the modified parameter is not fully covered by the CV phase space, as event weighting cannot account for event properties not present in the original simulation. This method is used for the assessment of the flux, cross-section and hadron re-interaction uncertainties.

While weights can be used for single parameter shifts, their key advantage is enabling the use of the “multi-sim” method in a computationally efficient way. In the multi-sim method, instead of shifting a parameter by $\pm 1\sigma$, multiple parameters are randomly sampled within their uncertainty range simultaneously. The sampling is repeated many times, and each iteration produces a new “universe”, represented by a set of event weights. The multi-sim method gives a better description of the effect of a parameter on the physics distributions. In addition, correlations between parameters can be taken into account.

For a given analysis parameter, the uncertainty is then estimated by comparing the CV and the sample variation(s). A covariance matrix is constructed as

$$E_{ij} = \frac{1}{N_{\text{uni}}} \sum_{s=0}^{N_{\text{uni}}} (x_{si} - x_{ci}^{\text{CV}})(x_{sj} - x_{cj}^{\text{CV}}), \quad (8.1)$$

where $x_{si}$ is the value of the $i$-th bin in the universe $s$ and $x_{ci}^{\text{CV}}$ is the central value of the corresponding bin. Here, $N_{\text{uni}}$ is the number of universes. In the case of a unisim variation, $N_{\text{uni}} = 1$ and $x_{si}$ is the bin value in the varied sample. For both methods, the uncertainty distributions are assumed to be Gaussian. Therefore, the systematic uncertainty for each bin is given by,

$$\sigma_i = \sqrt{E_{ii}}, \quad (8.2)$$

which is equivalent to the standard deviation of the differences between each universe and the CV.
8.2 Background Uncertainties

The background uncertainties are presented here for the binned BDT score distributions, as shown in section 7.6. The same single example signal point is used ($m_{\text{HNL}} = 304$ MeV) but the uncertainties are of similar magnitude and shape across all LLP mass values. In the final limit setting, the uncertainties are calculated for each signal mass point individually.

8.2.1 Neutrino Flux

Uncertainties on the neutrino flux arise primarily from uncertainties on the rates and kinematics of hadron production in the beamline. The PPFX package used to produce the constrained flux prediction is used to estimate these uncertainties. Each of the parameters in the constrained prediction are simultaneously sampled within their estimated uncertainties. Repeated re-sampling is used to produce 600 alternative flux predictions. The varied channels are summarised in tab. 8.1.

<table>
<thead>
<tr>
<th>Type</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thin target</td>
<td>$pC \rightarrow \pi X$</td>
<td>Constraints on pion production from $pC$ collisions.</td>
</tr>
<tr>
<td></td>
<td>$pC \rightarrow K X$</td>
<td>Constraints on kaon production from $pC$ collisions.</td>
</tr>
<tr>
<td></td>
<td>$pC \rightarrow \text{nucleon}X$</td>
<td>Constraints on proton/neutron production from $pC$ interactions.</td>
</tr>
<tr>
<td></td>
<td>$nC \rightarrow \pi X$</td>
<td>Constraints on pion production from $nC$ collisions.</td>
</tr>
<tr>
<td></td>
<td>nucleon-A</td>
<td>Nucleons interacting in a material that is not Carbon.</td>
</tr>
<tr>
<td></td>
<td>Meson Incident</td>
<td>Mesons that interact on any material in the beamline.</td>
</tr>
<tr>
<td>Attenuation</td>
<td>Others</td>
<td>Interactions not covered by thin target data.</td>
</tr>
<tr>
<td>Absorption</td>
<td>Absorption</td>
<td>Corrections to the absorption cross sections.</td>
</tr>
</tbody>
</table>

Table 8.1: The categories of constraints and parameters which determine the PPFX flux prediction, from Ref. [83].

Figure 8.1 shows the fractional uncertainty on the RHC $\nu_{\mu}$ flux prediction binned in neutrino energy. The uncertainties are of similar magnitude across both neutrino flavour and horn current mode [83]. The largest contributions to the uncertainty is from nucleons interacting with materials that are not carbon (“nucleon-A”) and secondary mesons re-interacting with the material in the beamline (“Meson Incident”) as these channels are the least constrained by the hadron production experiment data used in the prediction.

The 600 alternative flux predictions are binned in neutrino flavour, energy and
Figure 8.1: The fractional uncertainties on the RHC (Run 3) $\nu_\mu$ neutrino flux binned by neutrino energy. The uncertainty contribution from each hadron production constraint is shown. From Ref. [83].

Figure 8.2: The distributions of the BDT scores for the PPFX flux variations on the neutrino background sample. The central value is shown in red and the colour scale represents the number of universes. The calculated percentage uncertainty for each bin is shown in the lower panel. The distributions are shown for Run 1 (left) and Run 3 (right).
angle relative to the beamline. These distributions are used to generate weights for each analysis event. The event weight sets produced are then applied in turn to assess the impact of the flux variations on the BDT score. Figure 8.2 shows the spread of the BDT score distributions across all universes as well as the calculated fractional uncertainty on each bin. The uncertainty is ≈ 15% across the BDT scores for both runs. The single high BDT score bin in the Run 1 distribution with an uncertainty > 30% contains only four MC events so the variation is likely due to the low statistics.

A full consideration of the flux uncertainties also includes variations in the beamline conditions, for example, changes in horn current, horn position and beam spot location. These uncertainties have been shown in other NuMI MicroBooNE analyses [90, 126] to be small and subdominant in comparison to the hadron uncertainties and therefore are not re-assessed here.

### 8.2.2 Neutrino Cross Section

![Figure 8.3: The distributions of the BDT scores for the GENIE cross-section variations on the neutrino background sample. The central value is shown in red and the colour scale represents the number of universes. The calculated percentage uncertainty for each bin is shown in the lower panel. The distributions are shown for both Run 1 (left) and Run 3 (right).](image)

The neutrino cross-section uncertainties are assessed by varying the parameters within GENIE, the generator used to perform the neutrino interaction simulation.
Events are weighted based on the generated properties of the interaction, including the interaction mode, neutrino energy, momentum transfer, and final state particles. In total, 44 model parameters are considered. The publication covering the use of GENIE v3.0.6 in MicroBooNE [122] contains details of the parameters, their central values and assigned one sigma uncertainties.

The parameters are simultaneously sampled within their uncertainties to generate event weight sets corresponding to 600 alternative universes. Figure 8.3 shows the spread of the BDT score distributions across all universes as well as the calculated fractional uncertainty on each bin. The percent uncertainty is \( \approx 15\% \) across the BDT scores for both runs. As with flux uncertainty, the high BDT score bin in the Run 1 distribution containing only four MC events has an uncertainty \( > 30\% \).

### 8.2.3 Hadron-argon Interactions

The hadrons produced in neutrino interactions can interact strongly with the argon atoms in the detector. These interactions affect the hadrons propagation through the argon and therefore impacts the reconstruction of events. Uncertainties on the cross-sections of hadron-argon processes will therefore impact the selection of neutrino background. They are assessed using the GEANT4Reweight framework [127]. The framework, as used by MicroBooNE, considers variations in the GEANT4 cross-section model for positive pions, negative pions and protons. For pions, the cross-sections for the possible interaction modes, listed in tab. 8.2, are individually varied. For protons, only the elastic and total inelastic cross-sections are treated separately.

<table>
<thead>
<tr>
<th>Channel</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic</td>
<td>( \pi^\pm + N \rightarrow \pi^\pm + N' )</td>
</tr>
<tr>
<td>Inelastic/Quasielastic</td>
<td>( \pi^\pm + N \rightarrow \pi'^\pm + N' )</td>
</tr>
<tr>
<td>Absorption</td>
<td>( \pi^\pm + N \rightarrow N' )</td>
</tr>
<tr>
<td>Single Charge Exchange</td>
<td>( \pi^\pm + N \rightarrow \pi^0 + N' )</td>
</tr>
<tr>
<td>Double Charge Exchange</td>
<td>( \pi^\pm + N \rightarrow \pi^\mp + N' )</td>
</tr>
<tr>
<td>Pion Production</td>
<td>( \pi^\pm + N \rightarrow n\pi + N' )</td>
</tr>
</tbody>
</table>

Table 8.2: The reaction modes of the pion-nucleus interactions considered, where \( N \) represents an Argon nucleus.

The cross sections are simultaneously varied to produce 1000 alternative universe weight sets. Figure 8.4 shows the spread of the BDT score distributions across
all universes as well as the calculated fractional uncertainty on each bin. The bin uncertainties are all on the order of (2-10)% and hence subdominant in the analysis.

### 8.2.4 Detector Variations

The re-simulation method is used to assess the impact of detector-related uncertainties on the predicted neutrino background. A selection of modified detector simulation parameters which cover the range of expected variation are chosen. For each variation a new sample is produced from the same underlying events, which can then be compared to the central value simulation. The list of variations can be found in tab. 8.3.

The first category, wire modifications, describes changes made to the amplitudes and widths of simulated TPC wire waveforms. Full details of the procedure can be found in Ref. 128. The modifications are made as a function of 5 variables which cover the full range of detector responses to an energy deposition. They are the location \((x,y,z)\) positions and the angular orientation of the depositing particle’s trajectory with respect to the drift \((\theta_{xz})\) and wire \((\theta_{yz})\) direction. The modifications
The size of the MC samples available to assess the detector variations is limited by the available computing resources. The Run 1 variation samples used here each contain approximately 300,000 events. The Run 3 samples available are smaller, with 100,000 events each. This constitutes a third and a seventh of the statistics in the main Run 1 and Run 3 neutrino samples, respectively. The limited sample sizes lead to large statistical fluctuations when attempting to estimate the impact of the detector variations on the BDT score distributions. Figure 8.5 shows the BDT score prediction for each of the detector variation samples as well the fractional changes on each bin. The statistical fluctuations are particularly large for high (signal-like) BDT scores where the vast majority of background events are rejected. Often no
events from the variation samples occur in the final BDT score bin for a particular mass. In particular, for the BDT mass point shown here \( m_{\text{HNL}} = 304 \text{ MeV} \), the Run 3 CV sample, used to compare against the variations, contains no events in the final bin so no uncertainty prediction can be made.

In the absence of a reliable bin by bin prediction method, the detector-related uncertainty is estimated to be 30% on all bins. Different values for the uncertainty between (0-70)% were evaluated in the final limit setting. The expected sensitivity of the search is largely insensitive to the value chosen. This is due in part to the large uncertainties from sample statistics (discussed in the next section 8.2.5) dominating the total uncertainty in the bins with the most sensitivity to the signal. The background fitting procedure used in the extraction of the final limits (described in section 9.2) further reduces the impact of the uncertainty value on the final result.

**8.2.5 Sample Statistics**

The predicted distributions are subject to statistical uncertainties due to finite statistics in the samples used to form the prediction. These uncertainties apply to both the cosmic beam-off and MC neutrino background samples. The statistical
uncertainty in each bin is calculated as

$$\sigma_{\text{pred stat}} = \sqrt{\sum_i w_i^2},$$

(8.3)

where the sum is over all the events in the bin and $w_i$ is the weight of each event.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Weight Run 1</th>
<th>Weight Run 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam-Off</td>
<td>0.56</td>
<td>0.31</td>
</tr>
<tr>
<td>In-Cryo $\nu$ MC</td>
<td>0.11</td>
<td>0.33</td>
</tr>
<tr>
<td>Out-Cryo $\nu$ MC</td>
<td>0.08</td>
<td>0.16</td>
</tr>
</tbody>
</table>

Table 8.4: The average weight applied to each of the background samples when scaling to the data POT to obtain the background prediction.

Table 8.4 contains the average value of weights that are applied to the background samples for each run. For the beam-off sample, the weights are solely the normalisation factor from the POT-HW Trigger scaling (see section 5.6.3), which are the same for each event in a run. The weights on the neutrino background sample are a convolution of the sample normalisation and the GENIE and PPFX tune weights which are applied on an event by event basis. The rate of external triggering was increased after Run 1 and the beam-off weight for Run 3 is therefore smaller due to the increased ratio of available beam-off events to beam-on events. The MC samples are of similar sizes for each run. Therefore after scaling to the POT values for each run ($2.00 \times 10^{20}$ and $5.01 \times 10^{20}$) the Run 3 events obtain larger weights. The weights for the in-cryo neutrino MC simulation incorporate the up-scaling due to the removal of the 30% of events that were used for BDT training.

### 8.2.6 Summary of Background Uncertainties

The percentage uncertainty on each bin for the example BDT score distribution are shown in Figure 8.6. Here the percentages are calculated from the total background prediction, the combination of neutrino MC and cosmic-ray beam-off samples. For both runs, the errors arising from the sample statistics dominate in the high BDT score bins. The contributions from uncertainties on the neutrino background to the total uncertainties are larger in Run 3 than for Run 1 due to the additional rejection of cosmic-ray events by the CRT selection (section 6.3.2).
Figure 8.6: The percentage uncertainty on each BDT score bin, broken down by the source of uncertainty. The distributions are shown for Run 1 (left) and Run 3 (right).

### 8.3 Signal Uncertainties

The dominant contribution to the systematic errors on the signal sample arises from uncertainties on the rate of at-rest kaon (KDAR) production in the NuMI absorber. As discussed in section 4.2.3, the normalisation error is estimated to be 30%, symmetric around the central value, which is the same as used in the previous absorber HPS search [10]. The error was originally estimated by the MiniBooNE collaboration from the range of KDAR rates predicted in simulation [98].

The same multi-sim method described in section 8.2.3 is used to assess the impact of pion-argon interactions on the signal selection of the $\mu\pi$ HNL final state. It is found to be of order $\sim 2\%$ which is negligible in comparison to the kaon normalisation error. The detector related variations considered for background in section 8.2.4 are also estimated for the signal samples using the re-simulation method.

#### 8.3.1 Detector Variations

For each of the signal mass point samples, a fraction of the events ($\approx 20\%$) is re-simulated with each of the detector parameters modified. The BDTs trained with the corresponding CV sample events, is applied to the variation samples. The variation samples are then compared to the CV signal sample. The majority of signal events fall in the BDT bins most significant to the analysis. Therefore the error estimate is less affected by statistical variations than for the background.
Figure 8.7: The fractional change of the number of LLP events that fall into the primary signal region (BDT score > 2.95) for each detector variation of the signal samples. The Run 3 HNL samples are shown on the left and the Run 3 HPS samples on the right. The quadrature sum of the variations is shown for each signal sample.

Figure 8.7 shows the fractional variation on a defined “signal-like” BDT region for each of the main signal samples considered in the analysis. Only the Run 3 samples are shown here. The Run 1 variations are of similar magnitude. The variations still experience statistical variations due to the sample size, but are in general < 10% and the largest quadrature sum is 15%. The detector effects are therefore sub-dominant compared to the 30% normalisation uncertainty arising from the kaon production. The quadrature sum for each mass point is included as a normalisation uncertainty in the final limit setting.

### 8.4 Sample Normalisation Uncertainties

In addition to the modeling and statistical errors on the background and signal predictions, two sources of uncertainty on the normalisation of the analysis samples are considered:

- A correlated normalisation uncertainty arising from the POT counting is applied
to all samples used in the analysis. A 2% error on the number of POT delivered is estimated from the uncertainty on the beamline toroidal monitor measurement [94].

- The out-of-cryostat sample normalisation is discussed in section 5.6.3. The sample is not constrained by an external PPFX prediction and significant scalings are made to the out-of-cryostat samples for each run. As the contribution of out-of-cryostat events to the final selection is small, the impact of the scalings on the result is negligible. The sample normalisation is set as an unconstrained parameter in the final fits performed to extract the limits.
9 Limit Setting

In this section, the predicted BDT distributions for the SM background will be compared to the distributions produced when the BDTs are applied to the beam data. The statistical methods used to set upper limits on the mixing angles ($|U_{\mu 4}|^2$, $\theta^2$) are detailed, and the upper limits on HPS and HNL production are shown.

9.1 BDT Application to Beam Data

The trained BDTs are applied to the beam-on data. The resulting distributions are compared to the background prediction. Figures 9.1 to 9.5 shows the BDT distributions for each of the HPS and HNL mass points. The data and background predictions are found to be in good agreement across both of the run periods studied. No significant excess consistent with LLP decay is observed in any of the LLP BDT score distributions and therefore limits on the on HPS and HNL mixing angles are derived.

9.2 Hypothesis Testing and Limit Setting

In the search for a LLP signal appearance, the compatibility of the data with two different hypotheses is tested:

- The NULL (background-only) hypothesis where there is no signal present and therefore represents the SM neutrino plus cosmic background.
- The TEST (signal+background) hypothesis where the observed distribution is given by the sum of the SM background prediction and the signal decay contribution.

The level of signal contribution in the TEST hypothesis depends on the mixing parameters. Therefore the hypothesis for each LLP mass is constructed from a reference signal normalisation, which is then multiplied by a signal strength parameter $\mu$. 
Figure 9.1: The stacked prediction (MC+Beam-off) and beam data of the BDT score distributions for HPS with $m_{HPS} = 212, 215$ and 230 MeV. The corresponding HPS distributions are shown added to the background prediction. They are normalised to the minimum number of events which can be excluded at 90% CL, and then scaled by a further factor of 5 for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).
Figure 9.2: The stacked prediction (MC+Beam-off) and beam data of the BDT score distributions for HPS with $m_{\text{HPS}} = 245, 260$ and 269 MeV. The corresponding HPS distributions are shown added to the background prediction. They are normalised to the minimum number of events which can be excluded at the 90% CL, and then scaled by a further factor of 5 for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).
Figure 9.3: The stacked prediction (MC+Beam-off) and beam data of the BDT score distributions for HPS with $m_{\text{HPS}} = 275, 279$ and HNL with $m_{\text{HNL}} = 230$ MeV. The corresponding LLP distributions are shown added to the background prediction. They are normalised to the minimum number of events which can be excluded at 90% CL, and then scaled by a further factor of 5 for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).
Figure 9.4: The stacked prediction (MC+Beam-off) and beam data of the BDT score distributions for HNL with $m_{\text{HPS}} = 250$, 277 and 304 MeV. The corresponding HNL distributions are shown added to the background prediction. They are normalised to the minimum number of events which can be excluded at 90% CL, and then scaled by a further factor of 5 for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).
Figure 9.5: The stacked prediction (MC+Beam-off) and beam data of the BDT score distributions for HNL with \( m_{\text{HPS}} = 331, 358 \) and 385 MeV. The corresponding HNL distributions are shown added to the background prediction. They are normalised to the minimum number of events which can be excluded at 90\% CL, and then scaled by a further of factor of 5 for visibility. The distributions are shown for Run 1 (left) and Run 3 (right).
The reference value and scaling parameter can be translated into the relevant mixing angle ($|U_{\mu 4}|^2, \theta^2$) using the procedure outlined in section 5.6.5.

In order to calculate confidence limits, the probability distribution functions (PDFs) of a test statistic for both the NULL and TEST hypotheses are derived. The PDFs are estimated using an ensemble method where large sets of pseudo-experiments are generated via MC methods. Pseudo-experiments simulate the results of repeated data-collection processes. For each hypothesis, the pseudo-experiments are generated by sampling from a Poisson distribution with a mean value given by the expected number of events for the hypothesis. The effects of systematic uncertainties are incorporated as shifts to the nominal predictions before each Poisson sampling. The mean of the Poisson distribution for each pseudo-experiment is itself varied by randomly sampling within the defined uncertainty distributions.

9.2.1 Profile Likelihood

The test statistic with the most separation power when comparing two simple hypotheses is a ratio of likelihoods [129]. A test statistic is therefore constructed as the ratio of likelihoods of the TEST and NULL hypotheses. The likelihood gives the probability of the observed data for a given hypothesis. For each bin, the likelihoods $L^{\text{NULL}}$ and $L^{\text{TEST}}$ are given as the Poisson probabilities [130],

\[
L^{\text{NULL}} = e^{-b} b^d / d!,
\]

\[
L^{\text{TEST}}(\mu) = e^{-(b+\mu s)} (b + \mu s)^d / d!,
\]

(9.1)

where $b$ is the predicted number of background events, $s$ the reference number of signal events and $d$ the number of observed events. For a signal strength parameter $\mu = 0$, $L^{\text{TEST}}(\mu)$ reduces to $L^{\text{NULL}}$.

The effects of systematic errors on the predictions can be considered as a set of nuisance parameters ($\theta$). The background and signal predictions for a bin then become functions of these nuisance parameters ($b(\theta), s(\theta)$). For a binned distribution
the likelihoods can be combined multiplicatively across $n$ bins to give

$$L(\mu, \theta) = \prod_{i=1}^{n} \left( \frac{(\mu s_i(\theta) + b_i(\theta))^{d_i}}{d_i!} e^{-\left(\mu s_i(\theta) + b_i(\theta)\right)} \prod_{\theta_j \in \theta} f(\theta_j) \right)$$

where the index $i$ indicates the bin number. The newly-introduced penalty terms $(f(\theta_j))$ represent constraints for each of the nuisance parameters $\theta_j$. The constraint terms are usually Gaussian in form [131].

The introduction of systematic uncertainties broadens the PDFs and therefore degrades the hypothesis separation power of the simple likelihood ratio. The data can be used to find “best-fit” models to reduce the impact of the systematic uncertainties on the sensitivity. A common technique used is the profile likelihood ratio described in full in Ref. [132]. In this method, the likelihood, parameterised as a function of $\theta$, is maximised for each hypothesis. The profile likelihood can be expressed as

$$Q(\mu) = \frac{L(\text{data} | \text{TEST}, \mu, \hat{\theta}_\mu)}{L(\text{data} | \text{NULL}, \hat{\theta}_0)},$$

(9.3)

where $\hat{\theta}_\mu$ and $\hat{\theta}_0$ are maximum likelihood estimators for the TEST hypothesis (with the signal strength factor $\mu > 0$) and for the NULL hypothesis ($\mu = 0$) [131]. Here, “data” may refer to the actual experimental observation or a pseudo-experiment data-set. For mathematical convenience, the profile distribution is usually expressed as the negative log-likelihood ratio (NLLR),

$$\text{NLLR} = -2 \ln Q(\mu).$$

(9.4)

The NLLR is calculated for both the observed data and each pseudo-experiment to find both the median expected and observed limits on the signal.

### 9.2.2 $\text{CL}_s$ Method

Figure 9.6 shows an example of the NLLR PDF distributions for the NULL and TEST hypotheses generated by calculating the profile likelihood for repeated pseudo-experiments. The separation between the NULL and TEST distributions indicates the sensitivity of the test. The NLLR value observed in data is also shown. A high
value indicates the data is more consistent with the NULL hypothesis, whereas a low value indicates the data is more compatible with the TEST hypothesis. The test statistic distributions can be used to calculate confidence level (CL) values, which quantify the probability of each hypothesis producing an outcome that is less signal-like than observed in data. In extracting the final sensitivity, two CL quantities are used:

- $\text{CL}_{sb}$ is the probability for the TEST hypothesis to produce an outcome more background-like than that observed in the data.
- $\text{CL}_b$ is the probability for the NULL hypothesis to produce an outcome more background-like than that observed in the data.

The region corresponding to each value is labeled in fig. 9.6. The modified frequentist $\text{CL}_s$ method [133] is commonly used in particle physics for setting exclusion limits. It is constructed as,

$$\text{CL}_s = \frac{\text{CL}_{sb}}{\text{CL}_b}. \quad (9.5)$$

The division by $\text{CL}_b$ protects against false exclusions where the analysis has no sensitivity. If the data fluctuates significantly below the background prediction, small values of $\text{CL}_{sb}$ can arise despite little or no separation between the TEST and NULL hypothesis distributions.
To calculate the exclusion limits, $\text{CL}_s$ is repeatedly calculated as the signal strength ($\mu$) is altered. The exclusion limit is set at the signal strength which gives $1 - \text{CL}_s < \alpha$, where $\alpha$ is a fraction determining the desired confidence level. For this analysis, $\alpha = 0.1$, corresponding to exclusion at the 90% CL.

### 9.3 Limits on the Mixing Parameters

**COLLIE**, a CL$_s$ method software toolkit for confidence level limit evaluation [?], [133], [134], is used to set the final limits on the signal strength parameters. For each mass point, the corresponding BDT score distribution for the measured data, the signal expectation, and each component of the background prediction are given as inputs to the software. The associated systematic errors on each distribution are provided, as described in section 8. The normalisation of the out-of-cryo neutrino sample is entered as an unconstrained nuisance parameter. The largest impact of the systematic errors on the observed sensitivities is found to be the $\approx 33\%$ uncertainty on the signal prediction normalisation. This is due to two factors. Firstly, in the most signal-like BDT region, the estimated systematic errors on the background prediction are dominated by the statistical variations. Secondly, the profile likelihood ratio technique constrains the background systematic uncertainties using the observed data.

At this stage the two runs are combined. The distributions for each run are entered into the limit setting as separate channels and their likelihoods are combined. The background predictions and associated systematic uncertainties are fitted as separate components for the two runs. The limits are also calculated assuming each of the background predictions and associated uncertainties are fully correlated between runs. The addition of these correlations is found to make no significant difference to the final observed sensitivity.

The minimum excluded signal strength determined by **COLLIE** is translated into limits on the mixing parameters following the procedures described in section 5.6.5. The final limits are presented and discussed in the following sections, first for the HNL model (section 9.3.1), and then for the HPS model (section 9.3.2).
9.3.1 HNL Limits

| $m_{\text{HNL}}$ [MeV] | MicroBooNE Limits on $|U_{\mu 4}|^2$ ($\times10^{-8}$) |
|-------------------------|----------------------------------|
|                         | Observed | Median Expected | Exp. 1$\sigma$ | Exp. 2$\sigma$ |
| 246                     | 12.91    | 13.74           | 11.33-17.02    | 9.65-20.81     |
| 250                     | 8.57     | 7.89            | 6.46-9.83      | 5.44-12.00     |
| 277                     | 3.05     | 2.55            | 2.10-3.11      | 1.84-3.84      |
| 304                     | 1.46     | 1.52            | 1.24-1.85      | 1.05-2.28      |
| 331                     | 0.85     | 0.94            | 0.77-1.15      | 0.67-1.42      |
| 358                     | 0.54     | 0.65            | 0.53-0.80      | 0.46-1.00      |
| 385                     | 0.92     | 0.67            | 0.55-0.83      | 0.46-1.03      |

Table 9.1: The 90% CL observed and expected limits on $|U_{\mu 4}|^2$ obtained by this analysis. The limits are produced using NuMI beam data corresponding to $7.01 \times 10^{20}$ POT. The observed, median expected, 1$\sigma$ and 2$\sigma$ limits are all multiplied by a factor of $10^8$.

Figure 9.7: The 90% CL observed and median expected limits on the HNL mixing parameter $|U_{\mu 4}|^2$. The 1$\sigma$ (68%) and 2$\sigma$ (95%) interval bands on the expected limit are also shown.

The observed and expected 90% CL limits on $|U_{\mu 4}|^2$ are shown for each HNL mass point in tab. 9.1 and in fig. 9.7. The median expected limit represents the limit value in the case that the measured data distribution matches the background prediction. The expected 1$\sigma$ and 2$\sigma$ intervals cover the range of expected limits produced by 68% and 95% of background prediction outcomes, respectively. The observed limits are contained in the 1$\sigma$ interval for all mass points, with the exception of $m_{\text{HNL}} = 385$ MeV. For this mass point the observed limit is within the 2$\sigma$ interval.
Figure 9.8: The experimental limits on the $m_{\text{HNL}} - |U_{\mu 4}|^2$ parameter space. The observed limits produced by this analysis are shown in dark blue. The solid line indicates the limit for Majorana HNL. The dot-dashed line shows the same result scaled by a factor of $\sqrt{2}$ for Dirac HNLs.

The limits have been produced under the assumption that the HNLs are Majorana particles. For a Dirac HNL, only decays to the charge conjugated final state $\mu^{-} \pi^{+}$ are allowed (see section 2.2.3) and the expected rate of decay is therefore halved for the same $|U_{\mu 4}|^2$ value. Weighting the events to the angular decay distribution for Dirac HNLs does not significantly affect the BDT selection. Therefore the limits for Dirac HNL are calculated from the Majorana limit by applying a factor $\sqrt{2}$ to account for the reduced decay rate.

Figure 9.8 shows the observed limit in comparison to the existing experimental limits in similar regions of parameter space (see section 2.3 for details regarding each of the existing limits). The results extend MicroBooNE’s sensitivity to $|U_{\mu 4}|^2$ by approximately an order of magnitude compared to the previous MicroBooNE HNL result [2]. In the range $300 < m_{\text{HNL}} < 385$ MeV, the results produced by this search are of similar sensitivity as the limits published by the NA62 collaboration [37]. The E949 [38], PS191 [34] and T2K [33] collaborations set stronger limits across the range $300 < m_{\text{HNL}} < 385$ MeV. The T2K measurement provides no limit point for masses above 380 MeV. Here, the MicroBooNE limit is of equal or greater sensitivity than
the NA62 result.

### 9.3.2 HPS Limits

<table>
<thead>
<tr>
<th>$m_{\text{HPS}}$ [MeV]</th>
<th>MicroBooNE Limits on $\theta^2_{\text{eff}} \times 10^{-9}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Observed</td>
</tr>
<tr>
<td>212</td>
<td>30.83</td>
</tr>
<tr>
<td>215</td>
<td>12.10</td>
</tr>
<tr>
<td>230</td>
<td>2.83</td>
</tr>
<tr>
<td>245</td>
<td>1.36</td>
</tr>
<tr>
<td>260</td>
<td>1.18</td>
</tr>
<tr>
<td>269</td>
<td>0.85</td>
</tr>
<tr>
<td>275</td>
<td>0.82</td>
</tr>
<tr>
<td>279</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Table 9.2: The 90% CL observed and expected limits on $\theta^2_{\text{eff}}$ obtained by this analysis. The limits are produced using NuMI beam data corresponding to an exposure of $7.01 \times 10^{20}$ POT. The observed, median expected, 1σ and 2σ limits are all multiplied by a factor of $10^9$.

![Figure 9.9](image)

Figure 9.9: The 90% observed and median expected limits on the HPS mixing parameter $\theta^2$. The 1σ (68%) and 2σ (95%) interval bands on the expected limit are also shown.

The observed and expected 90% CL limits on $\theta^2_{\text{eff}}$ are shown for each HPS mass point in tab. 9.2 and in fig. 9.9. The observed limits are contained in the 1σ interval for all mass points with the exception of $m_{\text{LLP}} = 215$ MeV which is within the 2σ interval.

The limits on $\theta^2_{\text{eff}}$ shown here do not account for the reduction of the HPS flux
due to decays before reaching the detector. These effects are significant for the HPS model (see section 2.4). Therefore, the final excluded region of $\theta^2$ values is determined using the HPS signal generator (see section 5.1.1), which fully accounts for the HPS decay length effects. The upper and lower values of the excluded regions are found as the $\theta^2$ values which correspond to the required number of events for exclusion. More details can be found in section 5.6.5.

Table 9.3: The limit values of $\theta^2_{\text{eff}}$ and the corresponding values of $\theta^2$ which produce the number of events for exclusion. The $\theta^2$ values therefore represent the upper and lower bounds of the excluded region.

<table>
<thead>
<tr>
<th>$m_{\text{HPS}}$ [MeV]</th>
<th>$\theta^2_{\text{eff}}$</th>
<th>Lower $\theta^2$</th>
<th>Upper $\theta^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>212</td>
<td>$3.08 \times 10^{-8}$</td>
<td>$3.13 \times 10^{-8}$</td>
<td>$2.50 \times 10^{-5}$</td>
</tr>
<tr>
<td>215</td>
<td>$1.21 \times 10^{-8}$</td>
<td>$1.25 \times 10^{-8}$</td>
<td>$1.49 \times 10^{-6}$</td>
</tr>
<tr>
<td>230</td>
<td>$2.83 \times 10^{-9}$</td>
<td>$3.14 \times 10^{-9}$</td>
<td>$9.00 \times 10^{-8}$</td>
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<tr>
<td>245</td>
<td>$1.36 \times 10^{-9}$</td>
<td>$1.63 \times 10^{-9}$</td>
<td>$3.20 \times 10^{-8}$</td>
</tr>
<tr>
<td>260</td>
<td>$1.18 \times 10^{-9}$</td>
<td>$1.55 \times 10^{-9}$</td>
<td>$1.32 \times 10^{-8}$</td>
</tr>
<tr>
<td>269</td>
<td>$0.85 \times 10^{-9}$</td>
<td>$1.14 \times 10^{-9}$</td>
<td>$1.02 \times 10^{-8}$</td>
</tr>
<tr>
<td>275</td>
<td>$0.82 \times 10^{-9}$</td>
<td>$1.09 \times 10^{-9}$</td>
<td>$5.05 \times 10^{-9}$</td>
</tr>
<tr>
<td>279</td>
<td>$0.99 \times 10^{-9}$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 9.3 shows the values of $\theta^2$ which correspond to the lower and upper bounds of the excluded region for each $m_{\text{HPS}}$. For $m_{\text{HPS}} = 279$ MeV, the observed limit of $\theta^2_{\text{eff}} = 0.99 \times 10^{-9}$ is higher than the median expected result ($\theta^2_{\text{eff}} = 0.80 \times 10^{-9}$), at the boundary of the 1$\sigma$ interval. For the observed limit level, no values of $\theta^2$ produce sufficient events in the detector to be excluded. Therefore the region this analysis excludes ends at $m_{\text{HPS}} = 275$ MeV.

The region of $m_{\text{HPS}} - \theta^2$ parameter space corresponding to the observed exclusion is shown in Figure 9.10. The existing experimental limits and limit reinterpretations in similar regions of parameter space are also shown. The results constrain a region of parameter space for $212 < m_{\text{HPS}} < 275$ MeV not previously excluded by any dedicated experimental HPS search. The existing limits in this region are reinterpretations of decades old CHARM, LSND, and PS191 measurements, preformed recently by authors outside the respective collaborations [50, 52, 55]. Discussed in detail in section 2.3, these reinterpretations are performed without access to the original experimental data or MC simulation.
Figure 9.10: The experimental limits on the $m_{\text{HPS}} - \theta^2$ parameter space. The observed limit produced by this analysis is shown in dark blue. Dedicated HPS searches are indicated with solid lines. Reinterpretations of historical data are shown with dashed lines.

The lower boundary of the region excluded by this analysis is comparable to that of the LSND reinterpretation limit. The lower limit of the exclusion region from the reinterpretation of PS191 data extends further than the one given by this analysis, but the upper limit does not extend as high. The CHARM experiment excludes a region that is almost entirely disjoint from the one produced here. It is not possible to reach the majority of this region of parameter space with our experimental approach since all HPS would decay before reaching MicroBooNE.
10 Conclusions

This thesis presents a search using the MicroBooNE LArTPC for two hidden-sector long-lived particle (LLP) models, predicting the production of Heavy Neutral Leptons (HNL) and Higgs Portal Scalars (HPS). The search targets mono-energetic LLPs, produced by kaons decaying at rest (KDAR) at the NuMI absorber. NuMI beam data taken across two MicroBooNE run periods (Run 1 and Run 3), combining FHC and RHC NuMI beam modes corresponding to $7.01 \times 10^{20}$ POTs, are used. A shared detector signature of the two models, comprising decays to two track-like objects, is studied. This decay signature is produced by HNL decaying to $\mu \pi$ pairs and HPS decaying to $\mu \mu$ pairs, which are the dominant decay channels for HNL with masses above 245 MeV and HPS with masses in the range 212–279 MeV, respectively.

The performance and capabilities of the LArTPC technology are demonstrated using an analysis performed with ProtoDUNE-SP test beam data. A sample of beam pions and muons is selected using a combination of beamline and TPC information. A subsample of stopping muons with $\approx 76\%$ purity is isolated from the pions using the measured beamline momentum and length of the TPC track. The performance of the calorimetric energy reconstruction is excellent for both the pion and stopping muon samples. The measured resolutions of the calibrated TPC data and simulation response to energy depositions are similar, with the most probable values agreeing to better than 1%.

LLP decays in MicroBooNE are studied by producing MC simulation samples for 15 benchmark masses of the LLP ($m_{\text{LLP}}$). Eight HPS samples are generated for $m_{\text{HPS}}$ in the range [212–279] MeV and seven HNL samples are generated for $m_{\text{HNL}}$ in the range [246-385] MeV. The efficiency of the neutrino software trigger on the low energy LLP events is found to be $> 95\%$ across all masses for events arriving in time with the neutrino beam.

The LLP decays are reconstructed using the pandora framework. The SliceID
process originally designed to identify and isolate neutrino interaction candidates from the large cosmic-ray background is shown to perform well on the LLP decays, with an efficiency between 37% and 66% which rises with $m_{\text{LLP}}$. The difference in topology between KDAR LLP decays and target-produced neutrino interactions results in frequent mis-reconstruction of the location of the decay vertex. Therefore LLP vertices are constructed using a dedicated algorithm that identifies all candidates where two reconstructed objects emerge from a potential vertex.

A pre-selection is applied to the candidate vertices which achieves a reduction factor of $\approx 40$ (Run 1) and $\approx 60$ (Run 3) for the cosmic-ray and neutrino background. The additional background rejection in Run 3 is due to the use of the cosmic ray tagger. This stage of selection uses only variables with minimal dependence on $m_{\text{LLP}}$. The efficiency of the pre-selection on the signal is within the range of 35% to 50% for all $m_{\text{LLP}}$.

A boosted decision tree (BDT) is trained for each simulated mass point to utilise $m_{\text{LLP}}$ dependent kinematics to further discriminate the signal from the background. The BDT algorithm performs well for all $m_{\text{LLP}}$, with AUC metrics in the range 0.91–0.93.

The systematic uncertainties on the background and signal predictions are estimated using both re-simulation and event-weighting methods. The total systematic uncertainty on each of the signal predictions is found to be $\approx 33\%$. The dominant contribution is from the 30% uncertainty on the rate of kaon production at the absorber. The systematic uncertainties on the neutrino background prediction arising from the modelling of the detector, the flux, cross sections, and hadron-argon interactions are considered.

The cosmic-ray background prediction is derived from data events so has no associated modelling errors. For the most signal-like BDT region, the statistical uncertainties arising from the limited sample size for the background estimation are the largest contributions to the total uncertainty, at the level of (20–50)%. 

No significant excess is observed for either model in the signal-like region of the BDT distributions. In the absence of signal, the modified frequentist CLs method is
employed to produce limits on the model mixing parameters ($|U_{\mu 4}|^2, \theta^2$). All limits are given at the 90% CL.

For the Majorana HNL model, upper limits are set on the mass-mixing parameter $|U_{\mu 4}|^2$ in the range $[1.3 \times 10^{-7}, 5 \times 10^{-9}]$ for masses in the range 246–385 MeV. The limits are of similar sensitivity to those produced by the NA62 collaboration [37]. This represents approximately an order of magnitude increase in sensitivity to the previous MicroBooNE HNL result [2].

The limits on the scalar-Higgs mixing angle $\theta^2$ in the HPS model exclude a region with a lower boundary between $[3.1 \times 10^{-8}, 1.1 \times 10^{-9}]$ and an upper boundary between $[2.5 \times 10^{-5}, 5 \times 10^{-9}]$ for scalars with a mass of $m_{\text{HPS}} = 212–275$ MeV. This result sets the first constraint in this region of parameter space from a dedicated experimental search for such a Higgs Portal scalar and it is also the first search in this mass range using a LArTPC.

MicroBooNE has collected an additional $1.5 \times 10^{21}$ POTs of NuMI beam data not processed for use in this thesis. As the search is statistically limited, the inclusion of this data will improve the sensitivity to both models. The event reconstruction used in this analysis is developed for beam neutrino events. As such it is not fully optimised for the identification of the specific absorber KDAR decay signature. Targeted improvements to the reconstruction algorithms could therefore improve background discrimination.

This search sets the most sensitive limits produced by a LArTPC in the regions of parameter space considered for both the HNL and HPS models. The simulation and analysis methods used in this work could be employed in future LLP searches in the LArTPCs of the SBN and DUNE programmes to further extend the sensitivity to both models. In particular, the ICARUS detector, which serves as the far detector for the SBN programme, is also located close to the NuMI absorber allowing it to perform LLP searches with a strategy similar to that pursued in this thesis.
References


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