MEASUREMENT OF π^+ – ARGON ABSORPTION AND CHARGE EXCHANGE INTERACTIONS USING PROTODUNE-SP

By

Jacob Calcutt

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ABSTRACT

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ProtoDUNE-SP is a prototype detector for the upcoming Deep Underground Neutrino Experiment (DUNE). It's a Liquid Argon Time Projection Chamber (LArTPC) with a similar configuration to DUNE's detector, and is designed to provide a test-bed for the future experiment. In addition to serving as a prototype, its 0.3 - 7 GeV/c charged particle beam line provided the ability to perform physics measurements of pions, protons, kaons, muons, and electrons. Importantly, the LArTPC allowed for the measurement of hadronic interactions on argon nuclei.

Pions are often present in the final state of neutrino interactions in the energy range of DUNE's neutrino beam. These particles can undergo various types of interactions with argon nuclei in the detector, and this can interfere with the characterization of neutrino interactions in DUNE's far detector. The rate of these so-called secondary interactions will be accounted for using Monte Carlo simulation of neutrino interactions. Measurements of secondary interaction rates provide necessary data which can be used to estimate and propagate uncertainties or provide tunes of the secondary interaction model used within DUNE's experimental simulation.

This analysis provides a simultaneous measurement of the π^+ -Ar absorption and charge exchange cross sections using 1 GeV/ $c \pi^+$ data taken by ProtoDUNE-SP during its initial run period in Fall 2018. This is one of the first hadronic interaction measurements provided by ProtoDUNE-SP. It is also the first π^+ -Ar absorption measurement in 20 years and the first ever π^+ -Ar charge exchange measurement.

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CHAPTER 1

EXECUTIVE SUMMARY

The field of study of neutrino oscillation has entered the precision era. Next-generation experiments – the Deep Underground Neutrino Experiment (DUNE) and Hyper-Kamiokande (Hyper-K) – will collect a large rate of accelerator-based neutrino-interaction events. This will provide researchers with the ability to answer remaining key questions within oscillation physics. DUNE, the physics program on which this thesis will focus, will attempt to answer the following questions:

What are the precise values of the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix
 mixing angles (θ₁₂, θ₂₃, θ₁₃)? Specifically, is θ₂₃ lower than, greater than, or even
 equal to 45° (known as maximal mixing)?

11 2. Does neutrino oscillation violate Charge-Parity symmetry (is δ_{CP} of the PMNS matrix 12 non-zero)?

13 3. What is the ordering of the neutrino masses (what is the sign of Δm_{31}^2)?

Great effort must be taken to reduce systematic uncertainty to a suitable level to achieve 14 precise measurements related to the questions stated above. Necessary for this is the proto-15 typing of DUNE's far detector with ProtoDUNE-SP. ProtoDUNE-SP serves as a test-bed for 16 DUNE's detector components and event reconstruction, a first-attempt at calibration which 17 will be employed at DUNE, and a source of physics measurements using its charged particle 18 beam line which will serve as necessary inputs to DUNE's simulation. One of the particles 19 provided by the beam line $-\pi^+$ – is important to study, as it is often found in the final state 20 of neutrino interactions. As such, it has the ability to interfere with the reconstruction of 21 the incident neutrino's energy or its flavor. For example, if a π^+ is absorbed by an argon 22 nucleus nearby the primary neutrino interaction, the pion's energy could be missed in recon-23

1

struction of the neutrino's energy. Additionally, if a π^+ is produced in a neutral current ν_{μ} 24 interaction it could instead undergo a charge exchange interaction, where it is converted into 25 a π^0 , nearby. The π^0 will promptly decay into two photons, which will produce showers in 26 the detector. These showers could mimic an electron shower and could cause the ν_{μ} neutral 27 current interaction to be misidentified as a ν_e charged current interaction. These errors will 28 be accounted for in DUNE's oscillation analyses using Monte Carlo simulation of events in 29 DUNE's far detector. However, if the rate of pion interactions are misestimated, DUNE's 30 measurements could be biased. This thesis presents a measurement of the π^+ -Ar absorption 31 and charge exchange in order to reduce these systematic effects in DUNE's analyses. 32

33 This thesis will be organized as follows. Chapter 2 will describe the Standard Model of particle physics and how neutrinos fit (or rather do not fit) within this theory. It will also 34 provide an overview of interactions of both neutrinos and charged pions on nucleons and 35 nuclei. Chapter 3 will describe DUNE's physics program and detector design and provide 36 motivation for this measurement. In Chapter 4, the ProtoDUNE-SP detector – the detector 37 used for this measurement – will be discussed. Specifically, this chapter will focus on the 38 design and components of the detector, the software used for reconstructing particle trajec-39 tories and interactions, and calibration of the detector. Chapter 5 will discuss the beam 40 line which supplies the ProtoDUNE-SP detector with its test beam particles. Chapter 6 will 41 describe the event selection used to characterize Monte Carlo events and data sets. Chapter 42 7 will discuss the strategy used to conduct this measurement including the strategy used to 43 extract the cross section and the statistical fit used in the analysis. Chapter 8 will discuss 44 the systematic uncertainties within the analysis. Chapter 9 will discuss validations of the 45 statistical fit using fake data generated from Monte Carlo simulation. Finally, Chapter 10 46 will present the results of the measurement on real data. 47

CHAPTER 2

THEORY

As DUNE's physics program centers around neutrinos, this chapter will provide a description of our current understanding of these particles as part of the Standard Model of Particle Physics. Within this, an overview of the theory of neutrino-nucleus interactions will be given. The physics of charged pions will also be discussed, as these are often produced within neutrino-nucleus interactions.

54 2.1 The Standard Model

The Standard Model of Particle Physics represents the most up-to-date understanding of the universe at the subatomic level. It has provided immensely accurate descriptions of particle interactions (manifested as the electromagnetic and strong and weak nuclear forces) and successfully predicted the presence of multiple elementary particles. The Standard Model is rooted in the local symmetry group

$$SU(3) \times SU(2)_L \times U(1)$$
 (2.1)

where the first term encompasses the strong interaction and the second and third terms give rise to the electroweak interaction. Here, the L subscript denotes this describes a "lefthanded" chiral theory.

From the symmetry groups denoted in Equation 2.1, the interactions between matter and forces arise. In the development of the theory, a Lagrangian is constructed which describes a free fermion field and invariance under some local gauge transformation is enforced. If the fermion field is not invariant under that gauge transformation, an interaction with some vector field is introduced. Depending on the field and the gauge under consideration, these vector fields may also interact amongst themselves to ensure gauge invariance. The quanta of these vector fields are known as gauge bosons, and are modeled as being exchanged between

interacting fermions. At this point, all gauge bosons and fermions have zero mass. However, 70 this is wrong as known from experiment: three of the bosons and all fermions have mass. 71 With the possible exception of neutrinos, these particles all gain mass due to the presence of 72 the so-called Higgs field (the quantum of which is the scalar Higgs Boson, famously discovered 73 in 2012 [1][2]). The bosons gain mass as the result of spontaneous symmetry breaking, and 74 the fermions gain mass through coupling to the Higgs fields via Yukawa interactions [3]. 75 The following sections describe the gauge bosons and the elementary fermions (quarks and 76 leptons), as well as composite particles formed from quarks (hadrons). 77

78 2.1.1 Gauge Bosons

The most familiar of the gauge bosons is the photon, which is a massless, neutral particle that couples to electric charge and thus mediates the electromagnetic force. Figure 2.1a shows a Feynman diagram representing an elementary electromagnetic interaction vertex, where f is some charged fermion and the boson γ is the photon in the interaction.



Figure 2.1: Elementary interaction vertices of the electroweak interactions.

The photon arises within the Standard Model as one of the vector fields necessary to achieve $SU(2) \times U(1)$ gauge invariance (which describes the electroweak interaction). The other fields introduced by requiring this invariance are the Z^0 and W^{\pm} bosons which mediate the neutral and charged current weak interactions respectively. Elementary weak interactions are also shown in Figure 2.1, where the neutral current interaction is represented in Figure



Figure 2.2: Electroweak self-interaction vertices.

2.1a with the Z^0 as the boson in the interaction and f is some fermion, and the charged current interaction is in Figure 2.1b. The W^{\pm} and Z^0 bosons are the three gauge bosons mentioned above which gain their mass through the Higgs mechanism. Within electroweak theory, interactions between the W, Z, and photon also occur. These elementary interaction vertices are shown in Figure 2.2.

Finally, SU(3) invariance introduces eight gluons to facilitate the strong nuclear force. 93 This force couples to a property known as color, which, like electric charge for the elec-94 tromagnetic interaction, is common to all particles that experience the strong interaction 95 (quarks and gluons themselves). Color differs from electric charge in that there are 3 colors 96 (red, green, and blue) plus 3 anti-colors (anti-red, anti-green, and anti-blue) rather than just 97 positive or negative electric charge. The gluons themselves carry color, and thus, due to 98 color conservation, annihilate quarks of one color and create quarks of another color during 99 interactions. In Figure 2.3a, the quarks entering and exiting the vertex are implied to have 100 different colors. Similar to the electroweak bosons, interactions between the gluons arise as 101 part of SU(3) invariance, giving rise to vertices such as Figures 2.3b and 2.3c. 102

103 2.1.2 Quarks

The elementary components of matter are a group of 12 fermions (and their antiparticle partners) separated into 6 quarks and 6 leptons. The quarks engage in all three forces



Figure 2.3: Interaction vertices of the strong force.

described previously, while the leptons feel only the electromagnetic and weak forces (andwithin the leptons, the neutrinos only engage in the weak forces as they are neutral).

The quarks come in six flavors: up, down, charm, strange, top, and bottom, which are 108 separated into three generations as shown in Table 2.1. Each generation contains one quark 109 with electric charge equal to $\frac{2}{3}e$ and the other with charge of $-\frac{1}{3}e$ (where e is the basic unit 110 of electric charge). The first group includes u, c, and t quarks and are collectively known 111 as "up-type" quarks, while the second group includes d, s, and b quarks and are known as 112 the "down-type" quarks. As mentioned earlier, the quarks carry a property known as color 113 which is similar to electric charge. In an analogy to primary colors of visible light, this 114 comes in the form of three charges – (anti-)red, (anti-)green, or (anti-)blue. The analogy to 115 the primary colors of light comes from the fact that the three color charges (or a color and 116 its anticolor) add together to a net-0 or "white" color charge. A special property of color – 117 color confinement – is that no isolated free particle can exist in a colored state. This leads 118 to quarks forming bound states known as hadrons. Most often, these come in the form of 119 mesons (bound states of a quark and an antiquark with one type of color and its anticolor) 120 and baryons (bound states of three quarks each with one of the colors). Baryons and mesons 121 will be discussed further in the next section. 122

In addition to the strong interaction, the quarks also take part in the weak interaction. In charged current weak interaction, the quarks transition between up-type and down-type flavors. Within the Standard Model Lagrangian, the quarks are described as two-component

Generation	Quark	Charge (e)	Mass (MeV/c^2)
т	u	2/3	2.4
L	d	-1/3	4.8
ТТ	c	2/3	1270
11	s	-1/3	104
III	t	2/3	$1.712 \ge 10^5$
	b	-1/3	4200

TABLE 2.1: The quark generations along with the charge and mass of the individual quarks.

states, comprised of the up-type and down-type of each generation, as shown in Equation2.2, which are operated upon in the weak interaction.

$$\Psi^{q} = \begin{pmatrix} \psi^{u} \\ \psi^{d} \end{pmatrix}, \begin{pmatrix} \psi^{c} \\ \psi^{s} \end{pmatrix}, \begin{pmatrix} \psi^{t} \\ \psi^{b} \end{pmatrix}$$
(2.2)

If these were eigenstates of the weak interaction, one would expect this process to transition between quarks only *within* generations (i.e. u would only transition to d, c to s, and t to b). This is not the case, and cross-generation transitions are allowed. This can represented by a set of quark states (d', s', b') that are linear combinations of the normal down-type quarks. The Cabibbo-Kobayashi-Maskawa (CKM) matrix mixes the normal down-type quarks into the special weak-eigenstate quarks as seen in Equation 2.3.

$$\begin{pmatrix} d'\\s'\\b' \end{pmatrix} = \begin{pmatrix} U_{ud} & U_{us} & U_{ub}\\U_{cd} & U_{cs} & U_{cb}\\U_{td} & U_{ts} & U_{tb} \end{pmatrix} \begin{pmatrix} d\\s\\b \end{pmatrix}$$
(2.3)

134 2.1.3 Hadrons

As stated above, quarks cannot be observed in isolated states¹, and reside in composite particles known as hadrons. Most commonly, these are combinations of a quark and an antiquark

¹That is, at energy scales relevant to this thesis. At high enough energies, a phase transition to a state known the quark-gluon-plasma occurs wherein quarks and gluons are not confined to hadrons [4]

Generation	Lepton	Charge (e)	Mass (MeV/c^2)
т	е	-1	.511
L	$ u_e $	0	_
ТТ	μ	-1	105.7
11	$ u_{\mu}$	0	_
III	τ	-1	1777
111	$ u_{ au}$	0	_

TABLE 2.2: The lepton generations along with the charge and mass of the individual leptons. Note that the neutrinos are assumed to be massless within the Standard Model and so no masses are stated for these particles here.

(mesons) or combinations of three quarks/antiquarks (baryons). More exotic combinations
such as tetraquarks (two quarks and two antiquarks) and pentaquarks (four quarks and one
antiquark) have recently been discovered at the Large Hadron Collider [5].

The baryons include familiar particles like protons and neutrons (made of *uud* quarks and udd quarks respectively); higher energy resonances of the same sets of quarks such as Δ^+ and Δ^0 ; and particles including second or third generation quarks such as Λ^0 , Λ_c^+ , and Λ_b^0 (uds, udc, udb respectively). Many other combinations of quark flavors exist, as do similar combinations of quark flavors but with differing quantum numbers. For example, the Δ^+ and proton have the same flavors of quarks, but have total angular momentum of 3/2 and 1/2 respectively.

The mesons are similarly characterized by properties of their constituent quarks (flavor, angular momentum, etc.). The mesons include the charged and neutral pions (whose quark content is $u\overline{d}$, $d\overline{u}$, and $(u\overline{u} - d\overline{d})/\sqrt{2}$ for π^+ , π^- , π^0 respectively), kaons (which include a strange quark), and various other combinations of quark flavors and angular momenta.

The pions are of particular interest within neutrino physics. They play an important role in nuclear dynamics, as they are the long-range mediator of the nuclear force according to Yukawa theory [4], and are discussed further in Section 2.4.

154 2.1.4 Leptons

Similar to the quarks, the 6 leptons are separated into 3 generations, each containing 1 155 charged lepton and its neutral partner. The charged leptons are the electron (e), muon (μ), 156 and tau (τ) , which each have a charge of -1e and masses as seen in Table 2.2. In each 157 generation is also the neutral partner to the charged lepton: the electron neutrino (ν_e) , 158 muon neutrino (ν_{μ}) , and tau neutrino (ν_{τ}) . The leptons are all colorless particles, and thus 159 do not feel the strong force. However, all left-handed leptons and right-handed antileptons 160 engage in the weak interaction. To represent this, the leptons are given Lepton numbers: 161 L_e, L_{μ} , and L_{τ} , which are equal to 1 (-1) for (anti-)leptons in the generation denoted by the 162 subscript. These lepton numbers are absolutely conserved in the weak interaction. 163

¹⁶⁴ 2.2 Neutrinos: Not-so-standard Particles

165 2.2.1 Neutrino Oscillations

This overview of the Standard Model particles seems tidy, but there are some subtle peculiar-166 ities, especially with the neutrinos. This is hinted at in Table 2.2, where no masses are stated 167 for the neutrinos. Within the Standard Model, the neutrinos are predicted to have no mass. 168 However, it is now understood that at least two neutrinos in fact do have mass, as indicated 169 by the presence of the process known as *neutrino oscillation*. This process was first theo-170 rized by Bruno Pontecorvo in an attempt to explain a deficit of observed electron neutrinos 171 produced from nuclear reactions in the sun. In 1968, the Davis experiment [6] measured only 172 about 1/3 of expected solar electron neutrinos. Pontecorvo suggested this deficit could be 173 explained if electron neutrinos produced in the Sun transformed into muon or tau neutrinos 174 (which the Davis experiment was unable to detect) before reaching Earth [7]. Takaaki Kajita 175 from Super Kamiokande and Arthur B. McDonald from the Sudbury Neutrino Observatory 176 were awarded the 2015 Nobel Prize in Physics for the discovery of oscillations [8][9]. 177

178 2.2.2 Neutrino Mixing

Neutrino oscillations arise from the facts that a) neutrinos have nonzero mass and b) the flavor eigenstates are not equivalent to the mass-energy eigenstates. Similar to quark mixing and the CKM matrix, neutrino mixing is described by the unitary Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix as shown in Equation 2.4, where $\nu_{1,2,3}$ are the mass-energy eigenstates.

$$\begin{pmatrix} \nu_{e} \\ \nu_{\mu} \\ \nu_{\tau} \end{pmatrix} = U_{PMNS} \begin{pmatrix} \nu_{1} \\ \nu_{2} \\ \nu_{3} \end{pmatrix} = \begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{pmatrix} \begin{pmatrix} \nu_{1} \\ \nu_{2} \\ \nu_{3} \end{pmatrix}$$
(2.4)

When neutrinos are produced via the weak interaction, they are produced as definite flavor states. However, the propagation of the neutrinos is described by the time-evolution operator (equivalently the Hamiltonian operator). As such, the neutrinos travel as eigenstates of the Hamiltonian: the mass-energy states.

188 2.2.3 Oscillation Probability

The derivation of the oscillation probability is shown in the following example. Consider a neutrino that evolves in time, $|\nu(t)\rangle$. Suppose it begins as a muon neutrino, such that $|\nu(0)\rangle = |\nu_{\mu}\rangle$. In a vacuum, its evolution is described by the time-evolution operator (e^{-iHt}) as such:

$$|\nu(t)\rangle = e^{-iHt} |\nu(0)\rangle = e^{-iHt} |\nu_{\mu}\rangle$$
(2.5)

Because $|\nu_{\mu}\rangle$ is not an eigenstate of the Hamiltonian, this is expanded to the following:

$$|\nu(t)\rangle = e^{-iHt} \left(U_{\mu 1} |\nu_1\rangle + U_{\mu 2} |\nu_2\rangle + U_{\mu 3} |\nu_3\rangle \right)$$

= $U_{\mu 1} e^{-iE_1 t} |\nu_1\rangle + U_{\mu 2} e^{-iE_2 t} |\nu_2\rangle + U_{\mu 3} e^{-iE_3 t} |\nu_3\rangle$

¹⁹³ Suppose an experiment is attempting to measure the rate at which ν_{μ} oscillate to ν_e by ¹⁹⁴ detecting the ν_e^2 . The probability to detect the neutrino as ν_e at some point in time is ¹⁹⁵ related to the following matrix element

$$\langle \nu_e | \nu(t) \rangle = \sum_j U_{ej}^* U_{\mu j} e^{-iE_j t}$$
(2.6)

where the sum over j runs over the mass-energy states. The probability is then given by

$$P(\nu_{\mu} \to \nu_{e}) = |\langle \nu_{e} | \nu(t) \rangle|^{2} = \sum_{j,k} U_{ej}^{*} U_{\mu j} U_{ek} U_{\mu k}^{*} e^{-i(E_{j} - E_{k})t}$$
(2.7)

197 For a general pair of states a, b this probability is

$$P(\nu_a \to \nu_b) = \sum_{j,k} U_{bj}^* U_{aj} U_{bk} U_{ak}^* e^{-i(E_j - E_k)t}$$
(2.8)

Assuming the neutrino is ultrarelativistic, the energy can be expanded as such:

$$E_{j} = \sqrt{|\vec{p}|^{2} + m_{j}^{2}} = |\vec{p}| \sqrt{1 + \frac{m_{j}^{2}}{|\vec{p}|^{2}}}$$
$$\approx |\vec{p}| \left(1 + \frac{m_{j}^{2}}{2|\vec{p}|^{2}}\right) = |\vec{p}| + \frac{m_{j}^{2}}{2|\vec{p}|}$$
$$\approx E + \frac{m_{j}^{2}}{2E}$$

Where the approximation $E \approx |\vec{p}|$ was used in the final step. The difference in the exponential term becomes

$$E_j - E_k \approx \frac{\Delta m_{jk}^2}{2E} \tag{2.9}$$

where $\Delta m_{jk}^2 = m_j^2 - m_k^2$. There are three mass splittings, Δm_{21}^2 , Δm_{32}^2 , and Δm_{31}^2 , two of which are independent³. Δm_{21}^2 is known to be positive (this is discussed later), while the sign of Δm_{32}^2 – also known as the *neutrino mass hierarchy* – is an open question in neutrino physics. This is highlighted in Figure 2.4, which shows the two possible orderings of the neutrino mass states.

²This is commonly known as an electron neutrino appearance analysis. ${}^{3}\Delta m_{31}^{2} = \Delta m_{32}^{2} + \Delta m_{21}^{2}.$



Figure 2.4: Representation of the two possible neutrino mass hierarchies. The left is the normal hierarchy with $m_3 > m_2 > m_1$. The right is the inverted hierarchy with $m_2 > m_1 > m_3$ [10].

The probability stated in 2.8 is often rewritten by splitting the real and imaginary components of the unitary PMNS matrix and approximating $t \approx L$ where L is the distance the neutrino has traveled:

$$P(\nu_{a} \rightarrow \nu_{b}) = \delta_{ab}$$

$$-4\sum_{j>k} \Re \left[U_{bj}^{*} U_{aj} U_{bk} U_{ak}^{*} \right] \sin^{2} \left(\frac{\Delta m_{jk}^{2} L}{4E} \right)$$

$$\pm 2\sum_{j>k} \Im \left[U_{bj}^{*} U_{aj} U_{bk} U_{ak}^{*} \right] \sin \left(\frac{\Delta m_{jk}^{2} L}{2E} \right)$$
(2.10)

205 Here, the third term is positive (negative) for (anti-)neutrinos.

The PMNS matrix is parameterized by 3 mixing angles $-\theta_{12}$, θ_{13} , and θ_{23} – and a phase factor $-\delta_{CP}$ – and is commonly factored into a product of three rotation matrices as such:

$$U_{PMNS} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta_{CP}} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta_{CP}} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
(2.11)

where c_{ij} and s_{ij} are $\cos \theta_{ij}$ and $\sin \theta_{ij}$. δ_{CP} is a phase factor that determines whether neutrino oscillations violate charge-parity (CP) symmetry. This symmetry and its violation are described in the next subsection, and the presence of CP symmetry violation within oscillations is one of the most important unanswered questions in neutrino physics.

212 2.2.4 CP Symmetry Violation

The violation of parity symmetry in the weak interaction was discovered in observations of 213 cobalt 60 decays [7]. Under this symmetry, the weak interaction should behave the same 214 under the complete reversal of coordinate system used to describe the system $((\hat{x}, \hat{y}, \hat{z}) \rightarrow$ 215 $(-\hat{x},-\hat{y},-\hat{z})$. However, it was observed that, when the spins of cobalt atoms in a sample 216 were aligned in a particular direction, the electrons resulting from neutron decays within 217 the cobalt atoms (shown in Figure 2.5) came out opposite the cobalt spins. Under a parity 218 transformation, the spin would not flip, but the direction of emission would. The electrons 219 would then be emitted in the direction of the spins, thus violating the symmetry [7]. The 220 parity symmetry violation in weak interactions is in fact maximal [7], leading to it being 221 described by a left-handed chiral theory (hence the L in the subscript of 2.1). A result 222 of the parity violation is that there are no interacting right-handed (left-handed) neutrinos 223 (antineutrinos). 224

In addition to violating parity symmetry, the weak interaction also violates charge symmetry. For example, a left-handed neutrino would be transformed into a left-handed antineutrino under charge conjugation and undergo weak interactions under charge symmetry. This is not the case, however, and thus the weak interaction violates charge symmetry as well. The weak interaction in the lepton sector *does not* violate CP symmetry⁴ under a simultaneous charge conjugation and parity transformation, left-handed neutrinos turn into right-handed antineutrinos which both undergo weak interactions.

Returning to the subject of neutrino oscillations, the CP-violating phase-factor δ_{CP} in the PMNS matrix (Equation 2.11) has the ability to introduce CP violation in the neutrino sector by producing an asymmetry between neutrinos and antineutrinos in the oscillation

⁴The weak interaction in the quark sector, however, does violate CP symmetry [7].

probability. If present (i.e. $\delta_{CP} \neq 0, \pi$), this oscillation asymmetry could be responsible the matter-antimatter asymmetry we observe in the universe [11]. The presence of a CPviolating value of δ_{CP} is one of the key unanswered questions in neutrino physics and is one focus of the upcoming oscillation experiments DUNE [12] and HyperK [13].



Figure 2.5: Feynman diagram of a neutron decaying to a proton.

239 2.2.5 MSW Effect

In matter, the oscillation probability is modified due to the presence of coherent forward 240 elastic scattering of neutrinos by the surrounding matter. Specifically, the Charged Current 241 process is available for ν_e , but not for $\bar{\nu}_e$, since only electrons and not positrons are present in 242 normal matter (for example, the surrounding earth). A potential created by these processes is 243 added to the Hamiltonian in Equation 2.5. This modifies the time evolution of the neutrino 244 flavors, resulting in a modified oscillation probability and effective oscillation parameters 245 in matter. This results in what is known as the MSW effect, wherein resonant behavior 246 is exhibited in the effective mixing angles⁵. The resonance can only be present for either 247 neutrinos or antineutrinos, depending on the ordering of the neutrino masses [14]. Thus, by 248 measuring the asymmetry between neutrino and antineutrino oscillations, the MSW effect 249

⁵This is named after Mikheyev, Smirnov, and Wolfenstein. Wolfenstein first discovered that neutrinos were affected by the potential created by the surrounding matter. Mikheev and Smirnov discovered the resonant behavior.

can be exploited to determine the ordering of the neutrino masses. The sign of Δm_{21}^2 was 250 determined by analyzing solar neutrinos which are subject to the matter effect as they travel 251 through the Sun [15]. The same principle can be used to determine the mass hierarchy (the 252 sign of Δm_{32}^2) using accelerator-based neutrino experiments. Similar to the question of CP 253 violation, this is an important, unanswered question in neutrino physics and will be explored 254 by future experiments such as DUNE. A discussion of DUNE and its physics potential will 255 be given in Chapter 3. In order to give context to that chapter, the following to sections 256 discuss interactions of both neutrinos and pions with nucleons and nuclei. 257

258 2.3 Neutrino Interactions

Neutrino oscillation experiments rely on detecting neutrinos through identifying the par-259 ticles produced by interactions on target nuclei. Through reconstructing these products, the 260 flavor, sign (neutrino vs. antineutrino), and energy of the incident neutrino are inferred. This 261 section provides a description of neutrino-nucleus interactions. In most types of neutrino-262 nucleus interactions⁶, the neutrino interacts primarily with a constituent nucleon. These 263 broadly fall into two categories: Charged Current (CC) and Neutral Current (NC). The CC 264 interaction occurs with the exchange of a W^{\pm} as shown by the vertex in Figure 2.1b while 265 the NC interaction occurs with the exchange of a Z^0 shown in Figure 2.1a. 266

267 2.3.1 Quasielastic Scattering

The first major CC interaction is CC Quasielastic (CCQE). This interaction occurs in the forms given in Equation 2.12, and is represented by the Feynman diagrams shown in Figures 2.6 and 2.7 for neutrinos and antineutrinos respectively.

$$\nu_l + n \to l^- + p \tag{2.12}$$
$$\bar{\nu}_l + p \to l^+ + n$$



Figure 2.6: Feynman diagram for the neutrino CCQE interaction.



Figure 2.7: Feynman diagram for the antineutrino CCQE interaction.

The cross section for these processes depend on the vector form factors $(F_1 \text{ and } F_2)$ and 271 axial form factors $(F_A \text{ and } F_P)$ of the CC interaction, which themselves depend only on the 272 four-momentum transfer Q^2 between the neutrino and nucleon in the interaction [16]. F_1 273 and F_2 are related to the electromagnetic form factors of the nucleons, which are extracted 274 from electron scattering data [14]. The pseudoscalar form factor F_P can either be neglected 275 through approximation [14] or related to F_A [16], such that F_A is the only unknown portion 276 of the CCQE cross section. The exact shape of the axial form factor is not described by 277 theory, and a dipole approximation is generally used as shown in Equation 2.13. 278

$$F_A(Q^2) = \frac{g_A}{\left(1 + \frac{Q^2}{M_A}\right)^2} \tag{2.13}$$

Here, g_A is the axial-vector coupling constant of the weak charged current, which is obtained from neutron decay data, and M_A is the axial mass, which can be obtained from fitting to neutrino scattering data.

⁶Other than coherent neutrino–nucleus scattering.

282 2.3.2 Resonant Pion Production

The next set of major neutrino-nucleon interactions are resonant pion production. These 283 interactions occur through both CC and NC channels, and result in a pion exiting the inter-284 action along with the nucleon and final state lepton. In these interactions, the neutrino inter-285 acts inelastically with a nucleon and excites it into some resonance (i.e. a nucleon resonance 286 or Δ resonance). The forms of the CC interactions (without specifying the intermediate res-287 onance) are given in 2.14, while the NC interactions are given in 2.15. Multiple resonances 288 contribute to the amplitudes of these processes, but at lower energies, the $\Delta(1232)$ resonance 289 dominates [17]. The most commonly used model to describe the Δ resonance interaction 290 is the Rein-Sehgal model [16][17]. The NC interaction resulting in a π^0 is important as a 291 background to CCQE ν_e events, where the γ showers from the π^0 decay can be mistaken 292 as an e shower during event reconstruction, and the rate of this background is important to 293 constrain in ν_e appearance measurements. 294

$$\nu_{l} + p \to l^{-} + p + \pi^{+}, \qquad \bar{\nu}_{l} + p \to l^{+} + p + \pi^{-} \qquad (2.14)$$

$$\nu_{l} + n \to l^{-} + p + \pi^{0}, \qquad \bar{\nu}_{l} + p \to l^{+} + n + \pi^{0}$$

$$\nu_l + n \to l^- + n + \pi^+, \qquad \bar{\nu}_l + n \to l^+ + n + \pi^-$$

$$\begin{aligned}
\nu_l + p \to \nu_l + p + \pi^0, & \bar{\nu}_l + p \to \bar{\nu}_l + p + \pi^0 & (2.15) \\
\nu_l + p \to \nu_l + n + \pi^+, & \bar{\nu}_l + p \to \bar{\nu}_l + n + \pi^+ \\
\nu_l + n \to \nu_l + n + \pi^0, & \bar{\nu}_l + n \to \bar{\nu}_l + n + \pi^0 \\
\nu_l + n \to \nu_l + p + \pi^-, & \bar{\nu}_l + n \to \bar{\nu}_l + n + \pi^-
\end{aligned}$$

295 2.3.3 Deep Inelastic Scattering

Another important set of processes in oscillation experiments are the CC and NC Deep Inelastic Scattering (DIS) processes. In these, the neutrino and the intermediary gauge boson it exchanges with the nucleon are energetic enough to resolve the individual quark constituents of the nucleon. The nucleon is broken apart and a hadron shower is produced as a result of quark confinement. The form of these interactions is given in 2.16. Here, N is either nucleon and X is a set of hadrons.

$$\nu_l + N \to l^- + X, \qquad \bar{\nu}_l + N \to l^+ + X \qquad (2.16)$$

$$\nu_l + N \to \nu_l + X, \qquad \bar{\nu}_l + N \to \bar{\nu}_l + X$$

These processes dominate the total cross section at high energies $(E_{\nu} \gtrsim 20 \text{ GeV})$ [16]. The inclusive DIS cross section⁷ is described by functions representing the structure of the nucleons known as parton distribution functions (PDFs) [16][17][14].

There exists a transition region between the resonance and DIS regimes called the Shallow Inelastic Scattering (SIS) region [16][18]. This region is not as well understood as the DISdominated region [16][18], and different simulation frameworks take a variety of approach to modeling this transition [16][18].

303 2.3.4 Neutrino–Nucleus Scattering

Neutrino oscillation experiments use nuclear targets for their detection medium. This complicates the relatively simple picture of neutrino-nucleon scatter in a few key ways. Firstly, coherent scattering become possible, wherein each component of the nucleus contributes to the interaction amplitude *coherently* and the nucleus is left in its ground state. An important type of coherent scattering is coherent pion production as shown in 2.17 (top: CC, bottom: NC). The NC process is an important background for ν_e appearance channels as the γ showers from the π^0 decay can mimic an *e* shower.

$$\nu_l + A \to l^- + \pi^+ + A, \qquad \bar{\nu}_l + A \to l^+ + \pi^- + A \qquad (2.17)$$
 $\nu_l + A \to \nu_l + \pi^0 + A, \qquad \bar{\nu}_l + A \to \bar{\nu}_l + \pi^0 + A$

⁷Full expressions found in [16][17][14]

Additionally, the presence of the nuclear medium complicates the behavior of both the 311 initial and final state. For CCQE interactions most models assume the Impulse Approxi-312 mation, in which the neutrino scatters elastically off nucleons in the nuclear ground state, 313 followed by quasifree ejection of the nucleons from the nucleus. The nuclear state (i.e. the 314 kinematic distribution of nucleons within the nucleus) is commonly described by a Rela-315 tivistic Fermi Gas model, where the nucleons are free particles subject to Fermi motion and 316 populate states according the Pauli exclusion principle. Despite the fact it is commonly used, 317 it poorly describes electron scattering data. Other models and approximations for the initial 318 nuclear state have been utilized in recent years to overcome this limitation. An important 319 development toward improved modeling of the initial nuclear state comes in the form of the 320 inclusion of nucleon–nucleon correlations and meson exchange currents (MEC). These con-321 tribute to multinucleon excitation, and raise the cross section of events that produce no final 322 state pion. In addition to these initial state effects, DIS interactions are further complicated 323 through modifications of the nucleon PDFs by the nuclear medium [17][18]. 324

Finally, the presence of Final State Interactions (FSI) can modify the observable products 325 of the primary interaction as they attempt to exit the nucleus. The hadronic products of 326 each interaction (including pions in resonance interactions and hadron showers from DIS) 327 can possibly reinteract as they travel through the nucleus. A common model for this is an 328 intranuclear cascade, wherein the interaction products step through the medium and can 329 undergo an interaction with the surrounding nucleons. These resulting particles are then 330 added into the cascade process and can then go on to interact again. This goes on until 331 all active particles exit the nucleus or are absorbed back into the nucleus. This results in a 332 modified set of observable particles (i.e. with missing or additional particles, and/or with 333 smeared kinematics). For resonance interactions, further complications arise from the fact 334 that the surrounding nuclear medium modifies the properties of the intermittent Δ resonance. 335 Processes such as those listed in 2.18 increase the width of the Δ within the nucleus [18]. 336

$$\Delta + N \to N + N \tag{2.18}$$
$$\Delta + N + N \to N + N + N$$
$$\Delta + N \to \pi + N + N$$

337 2.4 Pions

The last section illustrated the complexities in neutrino scattering created by the nuclear environment. The pion is often produced in neutrino interactions, and as will be seen in Chapter 3, must be accounted for in neutrino oscillation analyses at DUNE. This section serves to describe the pion's role within the nucleus, and its interactions with nuclei.

The pion is the lightest meson, and is a spin-0, isospin-1 boson. It has three charge states 342 (as evident by its isospin). These are described in Table 2.3. Yukawa predicted that a point-343 particle similar to the pion mediated the force between point-like nucleons within nuclei [7][4]. 344 In fact, at ranges greater than 0.7 fm, intranuclear interactions are well described by this 345 pion exchange picture [19]. At greater than 2 fm, one-pion exchange dominates, while two-346 pion exchange contributions become equal or greater than one-pion exchanges between 0.8 347 and 2 fm [20]. Below this, the point-like approximation of the pion and nucleons breaks 348 down, and the quark-gluon degrees of freedom become important [4][20]. In the point-like 349 approximation, the nucleon acts as a source of the pion field, resulting in a field of the form 350 given by Equation 2.19. Here, τ_3 and σ are Pauli isospin and spin operators and f is a 351 coupling constant. This has a striking similarity to the potential from a magnetic dipole, as 352 shown in Equation 2.20 [20]. 353

$$\phi_N(\vec{x}) = -\frac{f}{m_\pi} \tau_3 \sigma \cdot \nabla_x \frac{e^{-m_\pi |\vec{x} - \vec{r}|}}{4\pi |\vec{x} - \vec{r}|}$$
(2.19)

$$\phi_M(\vec{x}) = -\mu \cdot \nabla_x \frac{1}{4\pi |\vec{x} - \vec{r}|}$$
(2.20)

Pion	Quark Content	Charge (e)	${\rm Mass}\;({\rm MeV/c^2})$	I_3
π^+	$u ar{d}$	+1	139.57	+1
π^0	$\frac{u\bar{u}+d\bar{d}}{\sqrt{2}}$	0	134.98	0
π^{-}	$dar{u}$	-1	139.57	-1

TABLE 2.3: The pion along with their quark coontent, charge, mass, and the third component of its isospin.

354 2.4.1 Pion–Nucleon Scattering

It is important to consider pion-nucleon scattering as a basis for pion-nucleus scattering. 355 This interaction is purely elastic up to the threshold for the $\pi + N \rightarrow \pi + \pi + N$ process 356 at $T_{\pi} \approx 170$ MeV [20]. When viewed in a partial wave analysis, the s- and p-wave (angular 357 momentum l = 0, 1 respectively) contributions to the interaction dominate when compared 358 to the d- and f-waves (l = 2, 3) [20]. Furthermore, the s-wave interactions are small compared 359 to the p-wave interactions [21]. The dominant effect in the p-wave component, and thus the 360 overall interaction, is the resonance appearing around pion kinetic energy $T_{\pi} \approx 180$ MeV. 361 This is due to the coupling to the $\Delta(1232)$ spin 3/2, isospin 3/2 resonance [20][19][21]. This 362 resonance can be seen in Figure 2.8. 363

Two processes are of particular interest for this thesis: single charge exchange and absorption. For absorption, additional particles must be involved in the process in order to conserve energy and momentum. As such, the absorption of pions by singular free nucleons is forbidden⁸. This will be discussed in Sections 2.4.2 and 2.4.3. Single charge exchange is free from this requirement and, for incident π^{\pm} , takes the forms in Equation 2.21. It too will be discussed in Section 2.4.3.

⁸This is approximately true for bound nucleons as well, as the interaction is suppressed due to the momentum that must be supplied by the nucleon, which is much larger than the Fermi momentum [21].



Figure 2.8: $\pi^{\pm} - p$ cross sections as functions of pion lab momentum k_{lab} and center-of-mass energy W [20].

$$\pi^{+} + n \to \pi^{0} + p \tag{2.21}$$
$$\pi^{-} + p \to \pi^{0} + n$$

370 2.4.2 Pion–Deuteron Scattering

The scattering of pions by deuterons (a proton-neutron bound state) is the simplest extension of pion-nucleon scattering to multiple-body systems. The total cross section is comprised of contributions from elastic scattering, inelastic scattering (wherein the deuteron is broken up), absorption, and pion production at higher energies. The interaction can be well approximated by the sum of the $\pi - p$ and $\pi - n$ cross sections, as shown in Figure 2.9. However, the observed cross section is lower in the resonance region due to a broadening of the resonance caused by the motion of the nucleons within the deuteron as well as a shadowing effect of one nucleon by the other [20]. These effects are indicative of the complications that arise in the nuclear environment.



Figure 2.9: The $\pi - d$ total cross section. Black points are data, the dashed line is the sum of the $\pi - p$ and $\pi - n$ cross sections, and the solid line includes effects from nucleon motion and shadowing as described in the text [20].

As mentioned before, pion absorption on singular nucleons is forbidden, and multiple 380 nucleons must contribute to the absorption process. As such, the $\pi - d$ absorption process 381 is prototypical of this interaction in nuclei. It has been determined experimentally that 382 two-nucleon absorption in nuclei is dominated by absorption on deuteron-like pairs in the 383 $\Delta(1232)$ resonance region [19]. The "rescattering" model is an elementary model that gives a 384 qualitative understanding of the physics of $\pi - d$ absorption. In this, a scatter on one nucleon 385 is followed by absorption on the other. The leading terms in this theory are again the s- and 386 p-wave contributions. The so-called s-wave rescattering consists of a the pion undergoing an 387 s-wave scatter by the first nucleon, followed by p-wave absorption on the second nucleon. 388 In p-wave rescattering, the pion strikes the first nucleon creating an intermediate Δ state. 389 This Δ then interacts with the second nucleon creating the final dual-nucleon state [20]. 390

Quantitatively, however, this description falls short, and a full three-body framework that treats $\pi - d$ absorption on equal footing with other $\pi - d$ scattering processes has been more successful in predicting experimental results [20].

394 2.4.3 Pion–Nucleus Scattering

Similar to the extension of pion scattering from single-nucleon targets to the deuteron, the 395 extension to the nucleus is complicated by the influence of additional nucleons on the inter-396 action. The same basic processes (elastic and quasielastic scattering, single charge exchange, 397 absorption on more than one nucleon) are present, and the $\Delta(1232)$ resonance still plays an 398 important role. However, the dynamics are enriched by the nuclear environment. Recalling 399 the dipole-like interaction of the pion with the nucleon, the nuclear environment acts as a 400 polarizable and refractive medium for the pion, in analogy with the scattering of light by 401 electromagnetic dipoles [20]. The Δ resonance is also influenced by the medium; its peak 402 shifts lower and its width broadens as the nuclear mass increases [20][19]. 403

404 2.4.3.1 Elastic Scattering

The analogy to light propagation is evident in elastic scattering off nuclei, whereby the nucleons diffract the incoming pion wave similar to light by atoms in an optically diffractive medium [20][19]. Within the resonance region, the imaginary part of the $\pi - N$ scattering amplitude becomes large, producing deep minima in the angular distribution of the scatters. These minima are still present, but become more shallow outside of the resonance region where the real part of the scattering amplitude becomes larger [20]. This can be seen in Figure 2.10.

412 2.4.3.2 Inelastic Scattering

As with elastic scattering, inelastic scattering is an extension of the $\pi - N$ interaction to the nuclear environment. The difference lies in the transition of the nucleus to excited states.



Figure 2.10: Elastic pion scattering cross sections. a) Diffractive patterns are present within the resonance region. b) Diffractive patterns are suppressed outside of the resonance region [20].

Two broad regimes exist for this: 1) a low energy transfer region wherein the nucleus is excited to discrete states 2) a high energy transfer region in which the quasifree $\pi - N$ interaction dominates [20] and the struck nucleon is knocked out to continuum states [19]. This quasifree process is the leading contribution to the inelastic cross section [20], and is subject to in-medium effects that shift the location of the quasifree peak as seen in Figure 2.11.

421 2.4.3.3 Absorption

422 As previously stated, $\pi - d$ absorption is prototypical of absorption within nuclei, due to 423 the suppression of single nucleon absorption by energy and momentum conservation. For 424 nuclei with A > 2, absorption quasideuteron pairs (I = 0, pn pairs) remains the leading



Figure 2.11: A collection of data representing spectra of pions relative to outgoing kinetic energy T_{π} and lab angles θ_L for inclusive inelastic scattering on various nuclei. The arrows represent quasifree peaks assuming no in-medium effects applied to the $\pi - N$ scattering amplitude [19].

contribution to 2-nucleon absorption [19]. However, the presence of more nucleons influences 425 the interaction in a few ways. Firstly, direct interactions on multi-nucleon (N > 2) groups 426 contribute to the cross section. The absorption of π by 3 nucleons becomes significant even 427 for 3 He targets [19]. These direct absorption processes provide insight into correlations 428 between nucleons, and experiments such as LADS have detailed measurements of π -nuclear 429 absorption relative to outgoing nucleon multiplicities and kinematics [22]. Additionally, 430 multiple nucleons become involved in the absorption via Initial State Interactions (ISI – 431 wherein the pion undergoes a quasifree scatter off a single nucleon and is absorbed later) 432 and Final State Interactions (FSI – wherein the pion is absorbed by a set of nucleons and 433 these nucleons go on to interact with other nucleons within the nucleus). Data has shown 434 that the average number of nucleons substantially involved in the absorption process appears 435 to be considerable and at least somewhat A-dependent [19]. The contribution of ISI to 436 multinucleon absorption of pions in nuclei appears constant relative to A [19], while FSI 437 contributes more as A increases [20]. Additionally, the energy spectra of exiting nucleons is 438
439 similar to multistep, cascade processes [20].

440 2.4.3.4 Single and Double Charge Exchange

 π -nuclear single charge exchange (the processes shown in Equation 2.21) is an extension of 441 the quasifree inelastic interaction discussed above, but with a $\Delta I_3 = \pm 1$ transition of the 442 nuclear isospin [20]. Charge exchange makes up roughly 10% of the π -nuclear reaction⁹ 443 in the resonance region [20]. Like the other interactions described so far, the process is 444 complicated by the nuclear medium. Mainly, double charge exchange $(\pi^{\pm} + A \rightarrow \pi^{\mp} + A')$ 445 can occur. Here, two subsequent single charge exchange interactions occur. The outgoing π^0 446 from the initial interaction exchanges charge with another nucleon, resulting in a $\Delta I_3 = \pm 2$ 447 isospin transition and a flip of the pion's charge. Double charge exchange is a relatively rare 448 process, with a cross section roughly 10% of the single charge exchange cross section [20]. 449

450 2.4.4 Outlook

As highlighted by this section, pion-nucleus interactions contain complex dynamics. Particularly in heavy nuclear environments, these interactions become quite complicated. DUNE's nuclear target, argon, is no exception to this, and so care must be taken to model these processes within DUNE's experimental simulation. Currently, limited data exists for pion-Ar interactions, especially the exclusive interactions like absorption (a single measurement [22]) and charge exchange (no measurements). This thesis provides data for these interactions that can be used to validate and improve the pion interaction model used by DUNE.

CHAPTER 3

458

THE DEEP UNDERGROUND NEUTRINO EXPERIMENT

As discussed in the previous chapter, there are a few questions in neutrino physics that 459 remain unanswered. The Deep Underground Neutrino Experiment (DUNE) seeks to an-460 swer these questions once it begins to take data later this decade. Many experiments have 461 already made enormous progress in getting us to the point where the answers to these ques-462 tions are in reach. These experiments focused on neutrinos produced from several sources: 463 neutrinos produced in nuclear reactors, neutrinos produced by cosmic ray interactions in 464 the atmosphere, neutrinos produced within the Sun, and neutrinos produced from particle 465 accelerators. A global fit to the data from these experiments has been performed to provide 466 current estimates of the oscillation parameters [23]. These are presented in Table 3.1. Note 467 that only the normal mass ordering is given here, as the analysis found the inverted ordering 468 was disfavored at $\Delta \chi^2 = 4.7$ [23]. 469

Though systematic uncertainties in previous-generation experiments have required great effort to overcome, the experiments were limited primarily by statistical uncertainty. DUNE

Parameter	Best-Fit $\pm 1\sigma$	3σ Range
$\sin^2 \theta_{12}$	$0.310\substack{+0.013\\-0.012}$	0.275 - 0.350
$\theta_{12}[^{\circ}]$	$33.82^{+0.78}_{-0.76}$	31.61 - 36.27
$\sin^2 \theta_{23}$	$0.582\substack{+0.015\\-0.019}$	0.428 - 0.624
$\theta_{23}[^{\circ}]$	$49.7^{+0.9}_{-1.1}$	40.9 - 52.2
$\sin^2 \theta_{13}$	$0.022240^{+6.5\times10^{-4}}_{-6.6\times10^{-4}}$	0.02044 - 0.02437
$ heta_{13}[^\circ]$	$8.61^{+0.12}_{-0.13}$	8.22 - 8.98
$\delta_{CP}[^{\circ}]$	217^{+40}_{-28}	135 - 366
$\Delta m_{21}^2 [10^{-5} \text{eV}^2]$	$7.39_{-0.20}^{+0.21}$	6.79 - 8.01
$\Delta m_{31}^2 [10^{-3} \text{eV}^2]$	$2.525_{-0.031}^{+0.033}$	2.431 - 2.622

TABLE 3.1: Oscillation parameters as determined by the fit to global data in Reference [23]. Only the normal ordering of the mass hierarchy is shown here.

472 is a next-generation long baseline accelerator-based neutrino oscillation experiment, and
473 will collect enough neutrino events to become limited primarily by systematic uncertainties.
474 This chapter provides the motivation for the results of this thesis which will be used to meet
475 DUNE's stringent systematic uncertainty requirement.

476 3.1 DUNE's Physics Program

The goals of DUNE's accelerator-based oscillation analyses will be to determine whether 477 neutrino oscillations violate CP-symmetry, determine the neutrino mass hierarchy, and to 478 determine precise values of the oscillation parameters. The DUNE Far Detector Technical 479 Design Report [24] presents sensitivity studies which show DUNE's ability to achieve these 480 goals. In these studies, simultaneous fits to $\nu_{\mu} \rightarrow \nu_{\mu}$, $\bar{\nu}_{\mu} \rightarrow \bar{\nu}_{\mu}$, $\nu_{\mu} \rightarrow \nu_{e}$, and $\bar{\nu}_{\mu} \rightarrow \nu_{e}$ 481 $\bar{\nu}_e$ far detector samples were performed, with near detector samples included in order to 482 introduce flux and cross section constraints. $\sin^2 2\theta_{13}$, θ_{12} , and Δm_{12}^2 were all constrained 483 with uncertainties derived from those shown in Table 3.1, while $\sin^2 \theta_{23}$, Δm_{32}^2 , and δ_{CP} 484 were freely varied. More details on the fits can be found in [24]. 485

The sensitivity studies show promise in DUNE's physics program. For 50% of true 486 δ_{CP} values, DUNE can determine the presence of CP violation at the 5σ level after 10 487 years of its nominal run plan. If $\delta_{CP} = -\pi/2$ (which provides a maximal CP-violating 488 effect), CP violation can be discovered after only seven years. For any value of δ_{CP} , the 489 mass hierarchy can be determined after only two to three years. This reduces to only 490 about one year if $\delta_{CP} = -\pi/2$. After about fifteen years of the nominal run plan, the 491 resolution on the measurement of δ_{CP} approaches 5° for CP-conserving values and 15° 492 for CP-violating values. After high exposure, the measurement of $\sin^2 2\theta_{13}$ approaches the 493 precision of reactor experiments (which currently provide the main constraints on that angle), 494 and the simultaneous measurement of all oscillation parameters without external constraint 495 becomes possible. 496

497 3.2 The DUNE Detectors

DUNE seeks to achieve these goals as a long-baseline oscillation experiment, and, as such, is comprised of two sets of detectors: its far detector (FD) and near detector (ND) complexes. This is shown in Figure 3.1, which gives an overview of DUNE's facilities including the neutrino beam facility and the near detector complex located at Fermilab (Batavia, IL) and the far detector complex at Sanford Underground Research Facility (Lead, SD).



Figure 3.1: Overview of the future DUNE experiment. Toward the right is the neutrino beam facility and the near detector complex at Fermilab in Batavia, IL. Toward the left is far detector complex 1300km away at Sanfurd Underground Research Facility in Lead, SD [25].

The FD complex seeks to measure the number and flavor of neutrinos after they have had a chance to oscillate after traveling some distance. By measuring the rates at the FD, the oscillation probabilities (and more specifically, the parameters describing these probabilities) are probed directly. The ND, on the other hand, provides constraints on flux and neutrino cross section uncertainties within the models used for the oscillation analyses.

The planned DUNE FD will be comprised of four modules. Two of the modules (including the first to be installed) will be 10kt active volume single-phase (SP) Liquid Argon Time Projection Chambers (LArTPCs). This detector technology is the same as ProtoDUNE-SP and will be explained in detail in Chapter 4. One other module will be a dual-phase LArTPC (which is slightly different to the SP technology, but will not be explored here), while the final module's design is still to be determined. One common trait between all four modules
is that their sensitive volumes will be 10kt of liquid argon. This argon will serve as both the
target and detection medium for DUNE's neutrino beam.

The DUNE ND complex will be comprised of multiple detector subsystems. Included in 516 these subsystems is a set of small, modular LArTPCs known as ArgonCube. It is necessary to 517 have a portion of the near detector's target be argon in order to cancel neutrino interaction 518 model uncertainties between the near and far detectors. This part of the detector will 519 also be allowed to move lateral to the incident neutrino beam. Because the far detector 520 is located at an angle of 0° with respect to the beam direction (it is "on-axis"), gathering 521 data "off-axis" provides independent measurements of the neutrino beam. This off-axis data 522 reduces systematic uncertainties surrounding the neutrino beam model. Other subsystems 523 in the ND complex include a gaseous argon TPC downstream of the LArTPC portion (to 524 help measure muons which punch through the back of the LArTPC), a fine-grained plastic 525 scintillator detector (which remains on-axis to monitor the stability of the beam), and an 526 electromagnetic calorimeter surrounding the previous two subsystems (which will assist in 527 measuring all of the final state energy within the neutrino interactions). 528

529 3.3 The Role of Pion Interaction Systematic Uncertainties

To precisely measure the oscillation parameters, DUNE will attempt to discern the flavor and energy of the neutrinos interacting within the detector. Equation 2.10 (repeated here), shows the importance of successfully determining these quantities. Misidentification of the flavor will of course change the overall interaction rates of the various neutrino flavors, thus the extracted oscillation probability. Misestimation of the energy will change where in the energy distribution of interactions an event lies, thus distorting the energy spectrum of events, and further distorting the apparent oscillation probability.

$$P(\nu_{a} \rightarrow \nu_{b}) = \delta_{ab}$$

$$-4\sum_{j>k} \Re \left[U_{bj}^{*} U_{aj} U_{bk} U_{ak}^{*} \right] \sin^{2} \left(\frac{\Delta m_{jk}^{2} L}{4E} \right) \qquad (2.10)$$

$$\pm 2\sum_{j>k} \Im \left[U_{bj}^{*} U_{aj} U_{bk} U_{ak}^{*} \right] \sin \left(\frac{\Delta m_{jk}^{2} L}{2E} \right)$$

Both of these quantities are inferred from the final state particles resulting from the interaction. Figure 3.2 shows an example ν_{μ} interaction with multiple hadrons in the final state highlighting how complicated the final state of the interaction can be.



Figure 3.2: Cartoon of a ν_{μ} interaction with multiple hadrons in the final state [26].

532

For determining the flavor, reconstruction software attempts to identify the outgoing 533 leptons from CC interactions (μ^{\pm} and e^{\pm} from muon and electron neutrinos respectively). 534 Specifically for ν_e CC events, the e^- will produce an electromagnetic shower at the interaction 535 vertex. A background to this interaction is a ν_{μ} NC interaction with a π^+ in the final state. 536 This π^+ can potentially strike a nearby Ar nucleus and create a π^0 in a charge exchange 537 interaction. This π^0 will promptly decay into two photons which will shower similarly to the 538 e^- . This could cause this event to be wrongly selected as a ν_e CC event. Corrections for 539 this type of background is taken from simulation, and any uncertainty on the rate of π^+ -Ar 540

charge exchange interactions will translate to an uncertainty on the true number of ν_e events (and thus limit the precision of the oscillation measurements).

Similarly, smearing between true and reconstructed neutrino energy will be influenced on 543 the modeling of π^+ interactions. In DUNE, the neutrino energy is estimated by the energy 544 of the final state particles using a calorimetric energy reconstruction given in Equation 3.1. 545 Here, E^l is the energy of the outgoing lepton, T_i^{Nucleon} is the kinetic energy of any final 546 state protons or neutrons, and E_i^{π} is the total energy of pions in the final state¹. The rest 547 mass of any pion must be included since some of the incident neutrino energy must be used 548 to produce the pion. A π^+ in the final state could undergo an absorption interaction on a 549 nearby nucleus and produce a proton. The reconstruction software could fail to identify that 550 there was a pion in the final state and the rest mass of the pion could be lost in Equation 3.1. 551 Again, simulation is used to account for this type of effect (and similar other effects), and any 552 uncertainty in the rate of π^+ -Ar absorption limits the resolution of oscillation measurements. 553

$$E_{\text{Reco}}^{\nu} = E^{l} + \sum_{i} T_{i}^{\text{Nucleon}} + \sum_{i} E_{i}^{\pi}$$
(3.1)

These two examples are not an exhaustive list of regions where uncertainty on the rates 554 of these interactions will add to DUNE's total systematic uncertainty. Rather, they are 555 illustrative of the goal of the analysis presented in this thesis. Measurements of these inter-556 action cross sections will provide constraints within DUNE's oscillation analyses, and will 557 reduce DUNE's systematic uncertainty. This is an important task, as DUNE's systematic 558 uncertainty budget is limited to 2% in order to achieve the physics goals laid out in this 559 chapter [24]. An example of how pion scattering data can be used for the benefit of neutrino 560 experiments is given by T2K's use of world π^+ scattering data to constrain the nuclear model 561 used within their neutrino interaction simulation [27]. 562

¹Other particles such as kaons have been ignored for this example, but, in general, could be present in the final state.

CHAPTER 4

563

THE PROTODUNE-SP DETECTOR

Currently, the single-phase ProtoDUNE detector (ProtoDUNE-SP) is the world's largest 564 active Liquid Argon Time Projection Chamber (LArTPC). This detector is designed to be 565 a prototype of DUNE's single phase far detector, located in CERN's North Area. Detector 566 installation and integration began in 2017 and finished Summer 2018. This was followed by 567 a commissioning phase (including its charged particle beam line commissioning) in the late 568 Summer & early Fall of 2018. After commissioning, cosmic ray data and beam line data 569 was taken up to the CERN long shut down¹. Since then, cosmic ray data taking has been 570 ongoing. 571

Section 4.1 describes the general operation principles of LArTPCs. Section 4.2 describes the specific design of ProtoDUNE-SP. Section 4.3 provides a description of the characterization of data taken by the TPC. Section 4.4 describes the reconstruction of events in the TPC. Section 4.5 highlights the calibration of the detector. Finally, Section 4.6 describes the Monte Carlo simulation of events within the detector. The beam line will be described separately in Chapter 5.

578 4.1 LArTPC Principles

The detection principles of LArTPCs are based on the detection of ionization electrons and scintillation light produced by charged particles passing through the liquid argon (LAr). The argon sits between a set of anode wires and a cathode, which create a (nominally) uniform electric field. The ionization electrons drift along the electric field toward the anode wires. These wires are instrumented with electronics and detect signals produced by the drifting ionization. A configuration can be achieved such that several planes of wires can

¹During this time, the Super Proton Synchrotron, from which the ProtoDUNE-SP beam line originates, was shut down to allow for upgrades.

measure the ionization. In such a configuration, two wire planes sit in front of a third. The 585 electric field lines terminate on the third plane, meaning the drifting electrons ultimately 586 deposit onto this wire. Thus this plane is called the "collection plane." Before collection, 587 the electrons drift past the two other "induction planes." Bipolar signals are induced on 588 these planes as the electrons drift first toward and then away from these wires on their way 589 toward the collection plane. If these are oriented in different directions to the collection 590 591 plane, the combination of signals provide a 2D projection of the charged particle's position as it traversed the LAr. The third dimension is given by the time which the ionization took 592 to finish drifting. As the drift velocity is constant and known from the electric field, one can 593 measure the initial position as: 594

$$x = t_{\text{drift}} * v_{\text{drift}} = (t_f - t_0) * v_{\text{drift}}$$

$$\tag{4.1}$$

where x is the lateral position of the track, t_f is the readout time, t_0 is the time at the start of charge drift, and v_{drift} is the known drift velocity. These principles are shown in Figure 4.1. This shows a neutrino interaction producing two charged particles. These go on to ionize the LAr, and the ionization electrons drift against the electric field created by the anode wires and cathode plane. Signals are produced on the wires: the plane labeled 'V' shows bipolar signals created by induction; the plane labeled 'Y' shows unipolar collection signals.

By ionizing the LAr as it travels through the TPC, the charged particle loses energy. 602 603 Thus, by measuring the amount of ionization (the size of the signals produced on the wires), one can measure the energy lost by the particle during its traversal of the LAr. This allows 604 LATTPCs to provide calorimetric energy measurements of the particles it detects. The 605 ProtoDUNE-SP event display shown in Figure 4.2 highlights this capability. In this, a beam 606 particle enters the TPC from the left of the figure. It travels through the LAr until it 607 undergoes an interaction with an Ar nucleus, producing two visible particle tracks. The 608 strength of the signals is shown by the color of the tracks. The incident beam particle 609



Figure 4.1: Design and operating principles of a LArTPC[28].

610 is a beam π^+ candidate, and deposits considerably less energy per unit distance than the 611 products of its interaction.

Detecting the deposited energy provides Particle Identification (PID) of the charged particles because the mean rate of energy loss is well described by the Bethe formula[29] shown in Equation 4.2.

$$\left\langle -\frac{dE}{dx}\right\rangle = Kz^2 \frac{Z}{A} \frac{1}{\beta^2} \left(\frac{1}{2} \ln \frac{2m_e c^2 \beta^2 \gamma^2 W_{max}}{I^2} - \beta^2 - \frac{\delta(\beta\gamma)}{2}\right)$$
(4.2)

Here, z is the charge number of the incident particle, Z and A are the atomic number and mass of the material through which the particle is traveling, and I is the mean excitation of the material. $K = 4\pi N_A r_e^2 m_e c^2$ where N_A is Avogadro's number, and m_e and r_e are the mass and classical radius of the electron. W_{max} is the maximum energy transfer to an



Figure 4.2: ProtoDUNE-SP event display showing a candidate beam π^+ entering from the left and undergoing an interaction with an Ar nucleus.

atomic electron for a single collision by a particle of mass M and is given by Equation 4.3.

$$W_{max} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + 2\gamma m_e/M + (m_e/M)^2}$$
(4.3)

The main dependence on the incident particles comes from the factor $1/\beta^2$ [29]. For particles at the same energy, heavier particles will have a smaller β and thus will deposit a larger amount of energy per unit length. PID can be performed on particles by observing how much energy they deposited along their travel through the LAr. Thus, the products of the interaction in Figure 4.2 appear to be protons, making this event a candidate for π^+ absorption. The exact technique used in this analysis to separate π^{\pm} from protons will be described in Chapter 7.

In addition to ionization, the charged particles create scintillation light by the excitation and subsequent radiative decay of argon excimers. Scintillation light from LAr is produced isotropically in a narrow band around 128 nm and has a large yield of 24,000 photons per MeV deposited at a drift field of 500 V/cm (ProtoDUNE-SP's operating drift field value)[30]. It is produced in both a fast (~5ns) and slow (~ $1.3 - 1.4 \mu$ s) component at a ratio of 1:3[30]. The LAr is transparent to its own scintillation light[28], allowing photon detectors within the LAr to collect the light produced by the charged particles. This provides important timing and triggering capabilities for neutrino experiments.

This section provided an overview of LArTPC detection principles. However, certain complications arise in normal operating situations. The next subsections will provide overviews of the following effects in LArTPCs which modify this simple interpretation of tracking: recombination of ionization electrons(4.1.1); attenuation of ionization electrons due to LAr impurities (4.1.2); the Space Charge Effect created by the accumulation of positive Ar in the bulk of the LAr(4.1.3).

641 4.1.1 Recombination

Recombination is the effect by which ionized electrons thermalize with the Ar and then 642 quickly attach to the positive Ar^{1+} ions created by the charged particle. This modifies 643 the charge observed by the wires and must be accounted for in calibration in order to 644 accurately measure the energy deposited by charged particles. There has been limitation 645 in theoretical treatments of recombination to provide a global description of data [31]. The 646 preferred models for LArTPCs with similar electric fields to ProtoDUNE-SP are the Birks 647 and Box models. Both models are based off of the principle recombination effect arising from 648 ionization electrons attaching to other Ar^{1+} ions created by the charged particle (as opposed 649 to reattaching to its original atom) and both depend on the electric field. These models differ 650 in that the Box model neglects electron diffusion and ion mobility during recombination and 651 uses "Box model" boundary conditions rather than Birks' cylindrical assumptions [31]. The 652 ICARUS experiment found good agreement to fits of the Birks model [32], while ArgoNeuT 653 achieved good agreement with a "modified Box model" [31] which enabled another parameter 654 to vary in order to achieve agreement to the Birks model at low dE/dx [31]. ProtoDUNE-SP 655

also adopted this modified Box model.

657 4.1.2 Ionization Attenuation

Impurities in the LAr, such as water and O_2 , can capture ionization electrons as they drift toward the anode plane. This reduces the final amount of collected charge, and is simply modeled as an exponential decay as in Equation 4.4. Here, Q_C is the collected charge, Q_0 is the initial charge deposited, t_d is the drift time, and τ is the "drift electron lifetime." This lifetime is lowered by the presence of impurities.

$$Q_C = Q_0 e^{-t} d^{/\tau} \tag{4.4}$$

663 4.1.3 Space Charge Effect

The Ar^{1+} ions created by the charged particles drift toward the cathode, but at a much 664 slower velocity. As such, if enough positive ions are created, positive charge can build up 665 in the bulk of the LATTPC. This accumulated charge can distort the electric fields, causing 666 the so-called Space Charge Effect (SCE). This is especially the case for LArTPCs on Earth's 667 surface such as ProtoDUNE-SP. These surface detectors are subject to a large cosmic ray 668 flux, which constantly replenishes the positive charge. This large accumulation of charge 669 causes the field lines to be bend toward the center of the TPC, resulting in distorted particle 670 tracks. Through modifying the electric field, the SCE also changes recombination. The 671 specifics of SCE in ProtoDUNE-SP will be discussed in Section 4.5.1. 672

673 4.2 The ProtoDUNE-SP Detector

With a total of 770 tonnes of LAr (420 tonnes are within the instrumented volume), ProtoDUNE-SP is the largest LArTPC ever constructed [30]. It provided a test bed for many components and engineering challenges of the single phase technology that will comprise the first DUNE far detector. It was designed to satisfy stringent requirements and achieve

improved levels of LArTPC performance required by DUNE, and it surpassed these in many 678 cases [30]. This section describes the design of the ProtoDUNE-SP components including 679 the following: the cryostat surrounding the TPC and the LAr purification system (4.2.1); the 680 TPC components (4.2.2); the Cold Electronics (CE) used to readout the TPC signals (4.2.3); 681 the photon detector system used to readout scintillation light (4.2.4); the cosmic ray tagger 682 (4.2.5); the Data Acquisition (DAQ), timing, and triggering systems (4.2.6). The detector 683 will be described in terms of a right-handed coordinate system with y as the vertical axis 684 pointing up, z horizontal and pointing approximately along the beam axis, and x horizontal 685 and pointing along the electric field. 686

687 4.2.1 Cryostat and Purification

The cryostat, cryogenics, and purification system serve the role of keeping the argon in 688 a liquid state with as little impurities as possible in order to avoid signal attenuation as 689 described in Section 4.1.2. The TPC is encased in a membrane cryostat, which is formed of a 690 corrugated membrane that holds the liquid and gaseous (from boil-off) argon with insulation, 691 fireproofing, and supports outside of this [33]. The internal dimensions are 8.5m x 7.9m x 692 8.5m, making this the largest LAr cryostat ever constructed [30]. The membrane contains 693 several openings to allow installation of detector elements, electrical/signal feedthroughs, the 694 support structure for the TPC (which is suspended within the membrane), and cryogenic 695 systems [34]. 696

Due to ProtoDUNE-SP's larger drift distance (3.6m), a higher purity of LAr had to be achieved in order to limit the attenuation of ionization during drift. The purification systems used for ProtoDUNE-SP were built off those developed for ICARUS, MicroBooNE (another LArTPC neutrino experiment at Fermilab), and a LAr purity demonstrator based at Fermilab [30]. This purification system is the largest to date, and, along with the rate of recirculation and avoidance of leaks in the cryostat, reached an equivalent oxygen contamination of a few parts per trillion (ppt) [30]. This is in line with DUNE's requirement for 704 < 100 ppt contamination in its single phase far detector [35].

705 4.2.2 TPC

The TPC of ProtoDUNE-SP is an active volume of 7.2m x 6.0m x 6.9m separated by a 706 cathode at x = 0 into two drift volumes each of drift distance 3.6m and a drift field of 707 500 V/cm. The cathode is formed of six Cathode Plane Assemblies (CPAs) biased at -180 708 kV. Each side contains three Anode Plane Assemblies (APAs) opposite the cathode which 709 contain the instrumentation wires and CE used to readout the wires. Surrounding the top 710 and bottom and sides parallel to the drift field is the Field Cage (FC) that provides (in 711 addition to the APAs and CPAs) electrostatic boundary conditions to achieve the intended 712 drift field. Penetrating into the x < 0 drift volume (henceforth called the "beam side") is the 713 Beam Plug which minimizes the energy loss and interactions of beam particles with inactive 714 material. This layout is shown in Figure 4.3. 715



Figure 4.3: Diagram of the ProtoDUNE-SP TPC components [34].

The CPAs are 1.15m wide and 6.1m and consist of three vertically stacked cathode panels.

In order to avoid an electrical breakdown of the TPC which could destroy the CE, the CPAs
are constructed of heavily resistive materials which give them a very long discharge time. The
panels are constructed from a fire-retardant fiberglass-epoxy composite and are laminated
on both sides with a Kapton film [30].

The APAs are formed of a rectangular stainless steel frame 6.1m high, 2.3m wide, and 721 76mm thick. Bonded directly over each side of the frame is a bronze wire mesh with 85%722 723 optical transparency that provides a grounded shield plane for four sets of wires on each side of the frame. Each successive wire plane is 4.75mm above the previous, with the inner most 724 plane also 4.75mm above the mesh. The inner most plane is the X plane and is oriented 725 vertically. Above the X plane is the V layer oriented at -35.7° from vertical, proceeded 726 by the U plane oriented at $+35.7^{\circ}$ from vertical. Finally, the Grid (G) plane lies above 727 the U plane and is oriented vertically. The G plane serves as a protective shield against 728 electrostatic discharge and is not read out. The rest of the wires are connected to front-end 729 CE and serve as the main instrumentation wires. The voltages of the wire planes ($V_{\rm G=-665}$ 730 V, $V_{\rm U=-370}$ V, $V_{\rm V=0}$ V, $V_{\rm X=+820}$ V) are chosen such that the field lines terminate on the 731 X plane, thus designating the X plane as the collection plane. The V and U planes are 732 thus the induction planes. The X and G planes both have a wire pitch of 4.79mm, but 733 are staggered from each other by half a wire pitch (meaning the G plane wires sit above 734 and between two X plane wires). The V and U planes both have a wire pitch of 4.67mm. 735 Each side has separate X and G planes, while the V and U planes are wrapped once around 736 the APA. The angle of the V and U planes is such that 1) each wire crosses only a given 737 collection wire on each side only once and 2) an integral number of CE boards reads out 738 one APA. The first point serves to reduce ambiguities in track reconstruction. A diagram 739 of an APA with a limited number of wires displayed is shown in Figure 4.4. Additionally, 740 electron diverters were installed between the APAs on the beam. These were formed of two 741 vertical electrode strips mounted on insulating board that, with voltages applied between 742 the electrodes, modified the local drift field such that electrons drifted away from the gaps 743

and toward the active area. During operation, high currents were drawn from the diverters'
power supplies due electrical shorts in the cold volume. They were therefore left unpowered
during operation, and, due to a resistive path to ground, the outer electrode was grounded.
This was not the intended voltage, as it then collected charge near the gaps between APAs
and distorted tracks crossing between APAs [30].



Figure 4.4: Diagram of an APA with its wire planes labeled. The bronze wire mesh is not shown. As it is shown, it is oriented on its side. The right side of the figure is the top of the APA when it is oriented vertically. The connections to the front-end CE boxes can be seen on the right side [34].

The Field Cage covers the remaining four sides of the drift volumes not covered by the 749 APAs or cathode plane. It provides the remaining electrostatic boundary conditions to 750 create uniform electric fields in the drift volumes. The top and bottom are comprised of six 751 FC assemblies each, while four end wall panels each consisting of four assemblies oriented 752 parallel to the x direction (the nominal drift direction). The assemblies are made of parallel 753 metal profiles connected to each other by a resistive divider chain to provide the voltage 754 gradient, I-beams that form an insulating support structure, and ground planes for the top 755 and bottom assemblies. The ground planes prevent (at the top) a high electric field entering 756 the gaseous argon and (at the bottom) a high electric field reaching the cryostat floor and 757 cryogenic services [34]. 758

On the beam side FC wall closest to the beam $(z \approx 0)$, a beam plug is installed. This plug displaces the LAr and reduces the mass through which the beam particles must travel before reaching the TPC. This then reduces the energy loss and interactions upstream of the active volume. It is formed of a series of alternating fiberglass and stainless steel rings, forming a cylinder capped by low mass fiberglass plates. It extends about 5 cm inside the field cage boundary. A printed circuit board acting as a mini field cage covers the inside face of the plug in order to reduce drift field distortions. It is filled with nitrogen at a pressure of 1.3 bar to balance against the hydrostatic pressure of LAr at its positioned height. The beam plug can be seen on the right side of Figure 4.3. In addition to the beam plug, the cryostat warm structure and insulation are modified to further reduce upstream interactions [30].

769 4.2.3 Cold Electronics

Each APA has a total of 2560 sense wires, resulting in a total of 15,360 channels to be read out. 20 Front End Mother Boards (FEMBs) are located directly on top of each APA and within the LAr to read out the sense wires. By being placed close to the wires, the capacitance of each channel is reduced, thus reducing the noise recorded by the electronics. The CE collect the signals from the APA wires, then amplify, shape, and digitize them before transmitting them to Warm Interface Boards (WIBs). These interface electronics then handle transmitting these signals to the DAQ.

The FEMBs consist of an analog motherboard containing eight 16-channel analog Front-End (FE) ASICs that provide the amplification and shaping of the signals, and eight 16channel Analog to Digital Converter (ADC) ASICs. These ASICs are both custom circuits designed by Brookhaven National Laboratory (BNL) [36]. In addition to the analog motherboard is a mezzanine card containing a commercial Altera Cyclone IV FPGA which provides clock and control signals to the two sets of ASICs. The FEMB layout can be seen in Figure 4.5.

The FE ASICs provided amplification with a programmable gain of 4.7, 7.8, 14, and 25 mV/fC and a 5th-order anti-aliasing shaper with programmable peaking time of 0.5, 1, 2, and 3μ s. It also included options for enabling AC coupling, selectable baseline adjustment for operating at 200 mV for unipolar pulses on the collection plane or 900mV for bipolar pulses on the induction planes, and a selectable pre-amplified leakage current of either 100, 500, 1000,



Figure 4.5: Diagram of the Cold Electronics in ProtoDUNE-SP [36].

or 5000 pA [36]. These ASICs also contained an internal, programmable pulse generator for electronics calibration. At normal running conditions, the FE ASIC gain is set to 14 mV/fC and the peaking time is set to 2 μ s for all channels [30]. At cryogenic temperature, the FE ASIC packaging puts stress on the ASIC chip causing a channel dependent non-uniform lowering by up to 150 mV of the 200 mV collection mode baseline [36]. In addition to this, large input charge caused the FE ASICs to saturate. Due to this, the baselines for both collection and induction plane channels were set to 900 mV [30].

The ADC ASICs have 16 12-bit digitizers operating at speeds up to 2 MHz and an 8:1 796 multiplexing stage resulting in a pair of parallel serial readout lines that send output signals 797 to the FPGA. At cryogenic temperature, the ADC ASIC suffered from an issue caused by 798 failures in transistor matching. This effect is hard to simulate at LAr temperatures and is 799 not present at room temperature. The mismatch between transistors effected the transition 800 between the six most significant bits and six least significant bits in the ADC's "domino" 801 architecture, causing the ADC output to prefer 0 and multiples of 63 in the dynamic range 802 of the ADC [36]. This issue, referred to as "sticky codes," was corrected for after data-taking 803 and will be further discussed in Section 4.3. 804

The signals from the ADC ASICs are collected by the FEMB's FPGA, which further

serializes the 16 pairs of data streams into four 1.25 Gbps links to the WIBs. The FPGA also 806 provides a calibration pulse to the FE ASICs as a cross-check for electronics calibration [36]. 807 The WIBs serve as the interface between the CE and DAQ, and are each controlled by 808 an Altera Arria V GT FPGA. Data cables from all FEMBs on a given APA feed through 809 a signal flange to a Warm Interface Electronics Crate (WIEC). The WIECs each contain 810 one Power and Timing Card (PTC) which is connected to both a 48 V power supply and 811 the detector timing system via a bidirectional fiber optical link. The PTC is connected 812 to a Power and Timing Backplane (PTB) also housed in the WIEC. The PTB steps down 813 the power and then fans out the power and clock signals from the PTC to five WIBs also 814 contained in the WIEC. Each WIB distributes power to and controls up to 4 FEMBs. The 815 WIB FPGA reorganizes and transmits FEMB data over fiber optical links to the DAQ. It 816 also includes a real-time digital diagnostic readout on a Gb Ethernet link and an on-board 817 component that can provide independent clocking to the FEMBs. These two components 818 allowed for installation and checkout tests to be performed on the FEMBs before they were 819 connected to the timing system and DAQ [36]. 820

821 4.2.4 Photon Detectors

To collect scintillation light produced by charged particles in the LAr, 10 bar-shaped photon detectors 8.6 cm in height, 2.2 m in length, and 0.6 cm thick were embedded in each APA frame. Three different designs of photon detection technology were used in order to test options for use in DUNE's far detector modules. In each, the \sim 128 nm scintillation photons were converted into visible light using wavelength shifters. This visible light is trapped within the photon detectors and eventually collected by an array of silicon photomultipliers [30].

828 4.2.5 Cosmic Ray Tagger

Located upstream and downstream (relative to z/beam direction) of the ProtoDUNE-SP cryostat is a cosmic ray tagger (CRT) used to provide triggers from cosmogenic muons. The CRT is formed of scintillation counters recycled from the outer veto of the Double Chooz experiment that coarsely measure the x and y position of cosmic muons which pass through it. Coincidence hits registered upstream and downstream of the detector can be used to form tracks that can then be matched to reconstructed tracks in the TPC and provide calibration [30].

836 4.2.6 Data Acquisition, Timing, Triggering

The DAQ reads in data from the TPC, photon detectors, and CRT. Two readout solutions were employed for the TPC as tests for the DUNE far detector readout: RCE [37] and FELIX [38]. During the beam run, one APA (located on the x > 0 side) used FELIX, while the other 5 APAs used RCE. artDAQ [39] was used as the software framework that controlled the data-flow including event building, configuration, and writing of data to disk [30].

The timing system provides a 50 MHz clock to all subsystems of the detector. It also 842 serves to distribute triggers created by the Central Trigger Board (CTB). The CTB is a hard-843 ware triggering system that forms trigger words based on the status of individual subsystems 844 (CRT, photon detectors, beam instrumentation). These words are sent to the timing system 845 which ultimately makes the readout decisions. Various trigger conditions can be created by 846 creating requirements of subsystem statuses (active vs. inactive). When these requirements 847 are met, the CTB sends off its trigger words to the timing system, which then determines if 848 an event should be formed. If so, it issues the trigger to the DAQ and the various readout 849 systems [30]. Importantly, the CTB can create beam-on and beam-off triggers based on if 850 the beam instrumentation recorded a particle passing through the beam line. This way, TPC 851 events containing a beam particle can be easily identified and used for analysis. 852

Each triggered readout of the detector, also known as an "event," consists of 3ms of data taking: 6000 consecutive samples taken at a rate of 2MHz from each ADC. The event is built from data taken in by the DAQ starting 250 μ s before the trigger time. This collects signals from charge deposited in the detector before the trigger, but that arrive within the time of the event. Coinciding data from the photon detectors and CRT are saved in the output stream as well, and matching to beam instrumentation (which will be described in Chapter 5) is done after data taking.

4.3 TPC Characterization

Before performing analysis, several data preparation steps are required to convert the 861 waveforms in units of ADC to units of charge, as well as to mitigate readout issues. The first 862 step is to determine the pedestal of each channel, as voltage offsets are introduced at the 863 input of the front end amplifiers and these vary on a channel-by-channel basis. Additionally, 864 for a given channel, the pedestal varies from one TPC event to the next. As such, the 865 pedestal is evaluated separately for each channel and each event [30]. The pedestals are 866 determined by finding the mean of all (typically) 6000 samples in an event for each channel. 867 For each channel in the event, its pedestal is subtracted from all ADC samples in the 868 waveform. This difference is then multiplied by the channel's gain. This gain q is determined 869 by using the 6-bit DAC included in the FE ASIC to inject a known amount of charge Q. 870 For the collection plane, the integral of the ADC signal over the pulse A is related to the 871 input charge as Q = gA. Special runs were taken where the DAC injected known amounts 872 of charge. For each charge setting, the mean of the ADC integral of the resulting waveforms 873 were determined. A line constrained to pass through 0 was fit to a set of these mean 874 values near charge inputs typical to operation (up to several overlapping Minimum Ionizing 875 Particles). The slope of this line is proportional to g for that channel [30]. Figure 4.6 shows 876 an example of this. 877

In addition to the gain calibration, readout issues are identified and mitigated. The first readout issue is the aforementioned sticky codes issue. ADC values subject to sticking as well as the channels which exhibit the issue were initially identified by scanning a few waveforms and the pedestal histograms for every channel. The channels with particularly prevalent sticky codes are identified, and the list of known sticky codes is used to mitigate the



Figure 4.6: Example of gain determination for one channel in PDSP. The slope of the line divided by the charge level of each DAC step ($Q_s = 3.43$ fC = .4 ke) gives the gain of the channel [30].

issue in less problematic channels. The mitigation works on these channels known to exhibit
sticky code issues by replacing any ADC sample at a sticky code with a value taken from
interpolation between the nearest non-sticky neighbors [30]. An example of this is shown in
Figure 4.7.



Figure 4.7: Example of ADC waveform before (top) and after (bottom) pedestal subtraction and sticky code mitigation. The spikes are samples which have stuck to the code represented by the upper horizontal dashed line. They are removed and replaced by interpolating to the nearest non-sticky neighbors [30].

In addition to the sticky code mitigation, preparations to remove tails resulting from AC coupling in the CE and correlated noise are also performed [30].

889 4.4 Event Reconstruction

After events are recorded, and an amount of data preparation is performed (described previously in Section 4.3), reconstruction software builds up a description of what happened during the event. This is done in a two step process: 1) hit finding which identifies localized charge deposits on wires and 2) pattern recognition which separates collections of hits into objects representing particle tracks and showers, and which also attempts to associate particles together in a hierarchy representing series of interactions.

Ideally, charge depositions on the wires should form (possibly overlapping) Gaussianshaped signals when read out by the electronics. Thus, a hit-finding algorithm attempts to identify these separate depositions of charge by fitting Gaussian peaks to the waveform in a given wire. Each Gaussian peak thus represents one reconstructed hit or, in other terms, a localized deposition of charge in the detector. An example of this is given in Figure 4.8, where three hits have been reconstructed to the shown waveform.



Figure 4.8: Example of three hits reconstructed to a single wire's waveform [30].

Because induction wires are wrapped around the APA, charge on either side of the APA can create a signal on a given wire. Thus, a disambiguation must be performed to determine which side of the APA the signal came from. Collections one wire from each plane are formed by identifying signals that arrived within a narrow time window. Sometimes, multiple pairs of induction wires can be matched to the collection plain. To determine which ones were truly paired, the algorithm attempts to minimize the difference in charge between that on the collection plane wire and on the induction plane wires. Simulation shows that this assigns >99% of hits to correct wire segments [30].

The second part of reconstruction is pattern recognition, which is performed by the Pan-910 dora framework [40]. This software has been successfully used in other LATTPC experiments 911 such as MicroBooNE [41]. The first step in the pattern recognition is to preform two dimen-912 sional clustering of the reconstructed hits in each view. It then attempts to match sets of 913 914 2D clusters between the views, with care taken to resolve ambiguities. Afterwards, 3D hits are created. Then, in order to provide a detailed description of events, particle interaction 915 hierarchies are created. Pandora then attempts to pick out particles originating from the 916 beam line. All clusters are reconstructed first under a cosmic ray hypothesis. Clear cosmic 917 ray candidates are then identified and removed. After these cosmic particles are removed, 918 Pandora attempts to divide the detector into 3D regions containing all hits produced by a 919 given particle interaction. These regions could contain cosmic rays that were not previously 920 identified as such or particles that originated from the beam. Parallel reconstruction chains 921 (one for cosmic rays and the other for test-beam particles) are then performed on these 922 detector regions. The reconstruction for the beam particles is intended to resolve intricate 923 hierarchies of particles such as from hadronic interactions. After the dual reconstruction is 924 performed, a boosted-decision-tree algorithm tries to identify which region (if any) originated 925 from the incoming beam [30]. The full reconstructed hierarchy (links between parent and 926 child particles) in the beam region are made available for analysis. Further pattern recog-927 nition tries to identify whether the reconstructed particles were track-like (such as pions, 928 protons, muons) or shower-like (electromagnetic showers from electrons or photons). Recon-929 structed track and shower objects are created for the corresponding particles. These provide 930 information such as track length or shower direction (depending on the object) to users. 931

932 4.4.1 Hit Classification Using Machine Learning

In addition to the track/shower discrimination from Pandora, a machine learning-based clas-933 sification was developed. A convolutional neural network (CNN) was trained to classify hits 934 into track-like, shower-like, empty, or Michel-like categories. The track-like category repre-935 sents hits coming from particles like pions and muons, the shower-like category represents 936 hits from electron or photon showers, and the empty category represents hits resulting from 937 noise. The Michel-like category represents electrons which originate from the decay of muons 938 in the LAr, which appear different to electron showers. The output of the network is a set of 939 scores representing how similar to each category the hit appears. The Michel-like category 940 can overlap with the track-like and shower-like categories, and was not used for this analy-941 sis. The other three category scores are constrained to sum to one such that the hit can be 942 classified as only one of these categories (that with the highest score). 943

The network uses as input 48×48 pixel² images created from wire readout data with the 944 hit in question at the center. Each pixel is filled with the ADC value from the readout 945 data. One axis of the image represents the wire which recorded the hit, while the other 946 axis is the time coordinate (which has been downsampled by taking an average over time 947 samples). The readout data used as input has been prepared according to the procedure 948 described in 4.3. MC simulation was used to train the network by identifying whether the 949 hit was due to charge deposited by a particle (or was created by noise) and what type of 950 particle created the hit. Further information on network architecture and training can be 951 found in Reference [42]. The analysis presented in this thesis utilized the CNN scores as an 952 alternate track/shower discrimination technique. Scores for the full reconstructed particle 953 were calculated by averaging over all hits in the particle. Cuts can be placed on these average 954 scores to categorize full particles as tracks or showers. The use of this within this analysis is 955 described further in Chapter 6 956

957 4.5 Detector Calibration

In order to conduct useful physics analyses such as the measurement presented here, the relationship between deposited energy in the detector and the response of the detector must be determined. Several effects that must be taken into account have already been described in Sections 4.1.3, 4.1.1, and 4.1.2. This section serves to describe the procedures taken to calibrate for these effects.

963 4.5.1 Space Charge Effect in ProtoDUNE-SP

As previously described, the steady flux of cosmic rays produces a buildup of charge from the slowly drifting Ar^{1+} ions produced by ionization. This so-called Space Charge Effect leads to a persistent distortions of the drift field. These alter the drift paths of ionization electrons and also affect the amount of prompt charge recombination, resulting in spacial distortions of reconstructed tracks and modified reconstructed dE/dx of tracks. The spatial distortions of reconstructed tracks is evident in Figure 4.9, where the end points of cathode-crossing cosmic rays are pulled inward from the edges of the detector (the dashed lines).



Figure 4.9: Projection of reconstructed track end points from cathode-crossing cosmic ray muons. The presence of SCE causes the end points to deviate from the boundaries of the TPC volumes represented by the dashed lines [30].

Figure 4.10 shows the distortions normal to four of the detector faces for events piercing
the respective face within data events. These provide the magnitude of spatial distortions
at these points of the detector in data events. A simulation of SCE was developed for
ProtoDUNE-SP. This is shown in Figure 4.11, which is analogous to Figure 4.10. Data-MC
discrepancies can be seen here that possibly stem from incorrect values of the Ar¹⁺ drift
velocity (amounting to a different amount of accumulated charge) and/or unsimulated flow of the liquid argon.



Figure 4.10: Spatial distortions normal to four detector faces from data events. Top: upstream & downstream relative to the z-direction. Bottom: Upper & lower faces relative to the y-direction. The reconstructed location of the end points of cathode-crossing tracks that pierce through the respective face show the distortions perpendicular to that face at the reconstructed 2D location [30].

977

In order to overcome the inability of the simulation to reproduce the SCE seen in data, a data-driven simulation of space charge was implemented. This consisted of creating a set of both spatial and electric field distortion maps to modify the nominal simulated distortions. These maps can also be used to correct for SCE in both data and MC by recovering the original positions and also accounting for the modified electric field. These are created as follows:

1. The ratio of the data to simulation map are taken for each of the relevant faces of the



Figure 4.11: Spatial distortions normal to four detector faces from MC events. Top: upstream & downstream relative to the z-direction. Bottom: Upper & lower faces relative to the y-direction. The reconstructed location of the end points of cathode-crossing tracks that pierce through the respective face show the distortions perpendicular to that face at the reconstructed 2D location [30].

detector. This produces a 2D map of scale factors at each of these faces.

2. Spatial distortions in the y-direction are calculated by linearly interpolating the scale factor maps between the top and bottom faces. The same is done for z-direction distortions by interpolating the scale factor maps between the upstream and downstream faces. The x-direction distortions are then taken as the average between the distortions in y and z. This creates a 3D map with scale factors in all three directions. These are used to rescale the magnitudes of the spatial distortions maps.

3. The resulting distortions in each 3D map are then reversed in order to form maps that
can be used to correct for the spatial distortions in both data and MC. The correction
repositions the reconstructed ionization charge depositions to their original locations.

4. The gradient of the spatial distortion along the local drift direction (determined from
the reversed maps) and the known drift velocity are used to form 3D electric field
distortion maps.

⁹⁹⁸ These data-driven maps are used to modify the reconstructed position of ionization charge ⁹⁹⁹ in simulation as well as to improve the prediction of prompt recombination effects [30].

1000 4.5.2 Electron Lifetime

As discussed in Section 4.1.2, impurities in the liquid argon can capture drifting electrons before they reach the instrumentation wires. This reduces the amount of charge reaching the collection plane wires and is measured as an exponential decay as a function of drift time as in Equation 4.4, where τ is the drift electron lifetime. A larger τ corresponds to a higher liquid argon purity.

1006 The electron lifetime can be measured by fitting the dQ/dx of cosmic ray collection plane hits as a function of drift time. To do this, cosmic rays that pass through the CRT and the 1007 front and back faces of the TPC were selected. The CRT was used to measure the initial 1008 time t_0 at which the track traveled through the TPC. The difference between the time the 1009 hit collected on the wire and t_0 was used as the drift time. The most probable value of 1010 dQ/dx for hits in slices of 100 μ s drift times was fit according to Equation 4.5 to extract the 1011 lifetime. Two example fits, taken at the beginning and end of the beam data run are shown 1012 in Figure 4.12. The later data shows a higher lifetime resulting from higher purity [30]. 1013

$$\frac{dQ(t)_{\rm MPV}}{dx} = \frac{dQ_{0,\rm MPV}}{dx} \exp(-(t_{hit} - t_0)/\tau)$$

$$\tag{4.5}$$

1014 4.5.3 Energy Calibration

Reconstructed dQ/dx is affected by electronics gain variations, SCE, and attenuation. Previous sections describe the calibrations for these. Additional effects have also been calibrated out via a two-step process laid out here: first to equalize the detector response (using a sample of throughgoing cosmic rays), then with a determination of the absolute energy scale (using a sample of stopping cosmic rays).



Figure 4.12: Fits to the drift electron lifetime τ for data collected at two different periods of time. Left is an earlier period with a lower period and shows a lower lifetime (10.39 \pm 0.2586 ms) compared to the right (88.95 \pm 14.32 ms) [30]

The equalization step accounts for nonuniformities from various effects that depend sep-1020 arately on x and y - z positions of the hit. Effects that depend on y - z position include 1021 non-uniform wire response from nearby dead channels, detector features such as the electron 1022 diverters, and transverse diffusion. This portion of the equalization step is done separately 1023 for each half of the detector on either side of the central cathode and as a function of y and 1024 z. The median dQ/dx value of hits in a given y-z bin is determined and compared to the 1025 median dQ/dx value of the half of the detector wherein the hit lies (x > 0 or x < 0) to 1026 obtain a correction factor defined as such: 1027

$$C(y,z) = \frac{(dQ/dx)_{\rm YZ}^{\rm G}}{(dQ/dx)_{\rm YZ}^{\rm L}}$$
(4.6)

where the numerator is the global median dQ/dx value on that side of the detector and the denominator is the median value on that y - z bin.

Following this, effects that depend on x position such as longitudinal diffusion are equalized. Similar to the corrections in the y - z plane, the median dQ/dx value of hits in an xbin are compared to the median value of all hits in the detector. This produces a correction factor that depends on x position as such defined in Equation 4.7.

$$C(y,z) = \frac{(dQ/dx)_{\rm YZ}^{\rm G}}{(dQ/dx)_{\rm YZ}^{\rm L}}$$
(4.7)

Finally, the dQ/dx values are normalized to the average value at the two anodes using the following factor:

$$N_Q = \frac{(dQ/dx)^{\rm A}}{(dQ/dx)^{\rm G}} \tag{4.8}$$

where the numerator is the average of the mean values at either anode, and the denominator is the mean value over the whole TPC. Thus, the dQ/dx of every hit in an event is equalized according to Equation 4.9.

$$(dQ/dx)_{\rm C} = N_Q C(y, z) C(x) (dQ/dx)$$
(4.9)

Next the measured dQ/dx must be translated to the energy loss of the particle per unit length dE/dx using a sample of cosmic muons that stop in the detector. dQ/dx values in the minimum ionizing region (120 to 200 cm from the end of the track) are converted to dE/dx using Equation 4.10 from the modified Box model [31] and fit to values predicted by Landau-Vavilon theory [43] as a function of residual range (the distance along the track from the hit to the end of the track).

$$\frac{dE}{dx} = \left(\exp\left(\frac{(dQ/dx)_{\rm C}}{C_{\rm cal}}\frac{\beta'W_{\rm ion}}{\rho\mathcal{E}} - \alpha\right)\right) \left(\frac{\rho\mathcal{E}}{\beta'}\right) \tag{4.10}$$

In Equation 4.10, W_{ion} is the amount of energy required to ionize an Argon atom (equal to 23.6 x 10⁻⁶ MeV/electron), ρ is the density of liquid argon at ProtoDUNE-SP operating temperature (equal to 1.38 g/cm³), \mathcal{E} is the local electric field at the location of the hit, α and β' are modified Box model parameters and were measured by ArgoNeuT with values of 0.93 and 0.212 (kV/cm)(g/cm²)/MeV) respectively [31]. Finally, C_{cal} is a calibration constant that accounts for electronics gain and ADC conversion, and corrects for any residual effects not explicitly calibrated previously and is the parameter of interest in the fit [30].

The normalization factor N_Q , equalization maps C(y, z) and C(x), and calibration constant C_{cal} are measured separately for MC and each run of data, and are applied during analysis when extracting the values of dE/dx for each hit considered.

1055 4.6 Monte Carlo Simulation

The simulation of test beam events in the TPC begins with the simulation of test beam 1056 particles generated within the beam line. A dedicated Geant4 [44] simulation of the beam 1057 line transports particles from their production point toward the face of the ProtoDUNE-SP 1058 TPC. More details can be found in Reference [45]. The rest of the PDSP simulation chain is 1059 based in the analysis framework LArSoft [46]. The beam line simulation results are passed 1060 to an event generator module that creates particles to be simulated by Geant4. The events 1061 are created when a "primary" particle (such as a π^+) travels through two triggering planes 1062 and reaches the outside of the PDSP cryostat structure. Additionally, checks are performed 1063 for when particles interact or decay (if applicable) in the beam line such that events are 1064 also created if some downstream particle (for example a μ^+ from a π^+ decay) reaches the 1065 cryostat. Without this check, the rate of test beam muons was severely underpredicted 1066 by the event generator in early simulation productions. The set of simulation used in this 1067 analysis included this hierarchy check. Each event created by this event generator is assigned 1068 a primary particle: either the original particle or the last-extant particle which reached the 1069 cryostat structure (i.e. the μ^+ described above). These primary particles serve as the main 1070 particles considered in the analysis. Other particles originating from the beam line which are 1071 "in time" with the beam are passed on to the next stage of the simulation. These additional 1072 particles are added in if they are within 4.5ms of the primary particle, similar to what can 1073 occur in events in data. Cosmic-ray particles as simulated by CORSIKA [47] are overlaid on 1074 the event and passed on to the Geant4 step as well. 1075

All particles generated by the beam-based event generator and the overlaid cosmics are then passed to Geant4 to simulate their transport through the detector. It also facilitates the interaction of hadrons with the detector material (via the Bertini Cascade Model [48]), thus serving as the signal interaction model of the analysis. The full geometry of the detector is considered, allowing for particles to interact and lose energy within the uninstrumented portion of the detector geometry (i.e. the steel cryostat structure, insulation, etc.). As 1082 charged particles travel through the LAr portion of the detector, ionization is created which1083 is then passed on to the drift simulation step of the simulation.

The drift simulation transports the ionization electrons produced during the Geant4 simulation stage along field lines toward the wire planes. The nominal electric field map used within the simulation is distorted according to the data-driven SCE maps discussed earlier in Section 4.5.1. The full electronics response to the ionization drift and collection onto the wires is simulated, creating waveforms which are then passed to the reconstruction chain described earlier.

CHAPTER 5

PROTODUNE-SP BEAM LINE

Test beam particles are delivered to ProtoDUNE-SP from an extension of the existing H4 1091 beam line in the CERN North Area. This beam line is known as the H4-VLE (very low 1092 energy) beam line as it supplies particles $(\pi^+, \mu^+, e^+, K^+, \text{ and } p)$ in the momentum range 1093 0.3 - 7 GeV/c. Within the North Area Secondary Beam facility, protons form the CERN 1094 Super Proton Synchrotron (SPS) impinge on a beryllium target to create a beam of secondary 1095 particles. These particles are transported through the H4 beam line before impinging on a 1096 secondary target to create the test beam for ProtoDUNE-SP. These test beam particles are 1097 momentum-selected¹ and transported through the H4-VLE beam line toward ProtoDUNE-1098 SP. 1099

1100 5.1 Beam Line Instrumentation

The H4-VLE beam line is instrumented with a set of various devices to aid in particle identification (PID), momentum reconstruction, and tracking the beam. The layout of the beam line is shown in Figure 5.1. The instrumentation consists of scintillating planes (XBTF) for triggering and time of flight (TOF) measurements; scintillating fiber monitors (XBPF) for profiling, tracking, and momentum reconstruction; and Cherenkov detectors (XCET) as part of the PID process. Throughout the beam line are bending magnets which direct the beam toward ProtoDUNE-SP – with one also being used as part of a momentum spectrometer.

1108 5.1.1 Fiber Monitors

The XBPF profile monitors [49] are comprised of a set of 192 square scintillating fibers of width 1 mm set side-by-side to provide a measurement of a beam particle's position in one direction. Two can be placed in perpendicular orientations to provide a 2D measurement of

¹Nominal momentum settings consist of 0.3, 0.5, 1, 2, 3, 6, and 7 GeV/c



Figure 5.1: Diagram of the H4-VLE beam line instrumentation layout. XBTF (orange lines) are scintillating planes used for triggering and TOF measurement; XBPF (blue lines) are scintillating fiber monitors used for tracking and momentum reconstruction; XCET (orange circles) are Cherenkov detectors used for PID (sometimes in conjunction with the TOF); the green triangles are bending magnets throughout the beam line.

the particle's position. Each fiber is connected to an individual Hammamatsu S13360-130 silicon photomultiplier (SiPM) on one end². Figure 5.2 shows a photograph of a prototype XBPF module taken from [49]. Further discussions of these devices and their readout are found in this reference as well as Reference [45]. The XBPF data was packaged such that, for each trigger in the beam line, the statuses (on/off) of the 192 fibers were separated into six 32-bit words. Two examples of this decoding is given in Figure 5.3.



Figure 5.2: XBPF module. Taken from Reference [49].

 $^{^{2}}$ On the other end of the set of fibers is an aluminized mylar mirror.


Figure 5.3: Two examples of XBPF data decoding. The most significant bit (MSB) and least significant bit (LSB) are labeled at the top of each example. a) The 0th fiber in the fourth 32-bit word is active. Thus the active fiber is (0 + 3 * 32) = 96. b) Two fibers are active: the 30th and 29th fibers in the third 32-bit word. Thus fibers (30 + 2 * 32) = 94 and (29 + 2 * 32) = 93 are active.

The last two sets of XBPF devices (shown immediately before the XCET devices and after the last XBTF plane in Figure 5.1) were used for tracking the particle as it entered into the TPC. 2D positions were reconstructed in both sets of XBPFs and used to create a trajectory between these points along the beam direction. This trajectory was further projected to the face of the active TPC to give the reconstructed position at the beam window.

These projected trajectories were used within analysis to cut out events considered as background to our pion sample. The difference in position between this reconstructed beam point and the start of the reconstructed TPC track, as well as the angle between the reconstructed beam trajectory and the starting angle of the reconstructed TPC track, were used to exclude various backgrounds (i.e. cosmics or particles from "upstream" interactions before the start of the active TPC volume).

1130 5.1.1.1 Issues with XBPFs

In Winter 2019, two issues were identified within the data obtained by the XBPF during the 1131 initial beam run. In the first, the rate of fiber activations for the upper half of the fibers in 1132 the first XBPF was higher than the lower half. This can be seen in Figure 5.4 where the 1133 number of activations for each fiber for each selected event in the first XBPF are plotted. In 1134 talks with the device experts, this was determined to be caused by a configuration issue in 1135 the ASICs controlling the readout of this XBPF. This amounted to a higher efficiency in the 1136 upper half of fibers in this device. However, this was not an issue in ProtoDUNE-SP data 1137 analysis as this effect was suppressed by the lower trigger rate of the ProtoDUNE-SP detector 1138 compared to the trigger rate of the beam line (a subset of beam line particles triggered the 1139 detector). 1140



Figure 5.4: Active fibers in the first XBPF device from every event from a 1 GeV/c run. Note, multiple fibers can be active in any one event. The jump in rate at fiber 96 is due to a configuration problem in the readout electronics.

The second issue identified was due to a bug in the software controlling the data acquisition for the XBPFs, and occurred in all XBPF devices. In this issue, systematically repeated hits were being recorded in the last 64 fibers of each XBPF. This can be seen in Figure 5.5, where a bump is present starting near fiber 128 of the second XBPF device. Figure 5.6 highlights this issue, as it shows the number of times a fiber was activated in two subsequent

events. A large spike in this rate can be seen starting at fiber 128. In discussions with the 1146 device expert, this was determined to be due to a software bug, in which the data in the 1147 last two words was not being cleared between events in the XBPF devices. This caused a 1148 "hangover" in the apparent activation of fibers in these two words. This resulted in extra 1149 reconstructed hits seen during analysis, which led to ambiguity in the reconstructed momen-1150 tum and incident tracks. An attempt to mitigate this was implemented by simply scanning 1151 the last two words of each event for repeated fibers, and then masking the repeated fibers 1152 (in the second event). The results for this are shown in Figure 5.7 1153



Figure 5.5: Active fibers in the second XBPF device from every event from a 1 GeV/c run. Note, multiple fibers can be active in any one event. A small bump can be seen starting around fiber 128.

1154 5.1.2 Momentum Reconstruction Using XBPFs

Within Figure 5.1, three XBPFs are labeled as "Momentum Spectrometer." Coincident signals in these three monitors were used to measure the deflection of the test beam particle by the bending magnet which the monitors surround. The angle of deflection is then used, along with the known magnetic field, to reconstruct the particle's momentum. A diagram of this measurement technique is shown in Figure 5.8. The lateral position (χ_1 , χ_2 , χ_3) of the particle – given by the activated fiber in each of the three XBPFs – is used with the known



Figure 5.6: Rate of repeated fiber activations in the second XBPF device from every event from a 1 GeV/c run. The large jump at fiber 128 highlights the issue.



Figure 5.7: Active fibers in the second XBPF device from every event from a 1 GeV/c run before (black) and after (blue) the mitigation procedure.

distances between each monitor (L_1, L_2, L_3) in Equations 5.1 and 5.2 to reconstruct the momentum. In these, $M \equiv \alpha + \chi_1$, $\alpha = \frac{\chi_3 L_2 - \chi_2 L_3}{L_3 - L_2} \cos \theta_0$, $\Delta L \equiv L_3 - L_2$, and $\Delta \chi \equiv \chi_2 - \chi_3$. θ_0 is the nominal bending angle of the beam and is equal to 120.003 mrad [45]. This measurement has a nominal 2% resolution according to Monte Carlo studies [45].

$$\cos\theta = \frac{M[\Delta L \tan\theta_0 + \Delta\chi\cos\theta_0] + L_1\Delta L}{\sqrt{[M^2 + L_1^2][(\Delta L \tan\theta_0 + \Delta\chi\cos\theta_0)^2 + \Delta L^2]}}$$
(5.1)



Figure 5.8: Momentum Spectrometer technique

Shortly after commissioning, a 5% offset in the reconstructed momentum was observed, and this was determined to originate from a bulk shift of the fibers in the third profiler of the spectrometer. Monte Carlo studies determined the fiber shift to be 1.45 ± 0.18 mm in the plane perpendicular to the beam. This was used as a systematic uncertainty within this analysis and will be discussed further in Chapter 8.

1170 5.1.3 Scintillating Planes

The XBTF scintillating planes are of similar design to the XBPF – sets of 192 fibers arranged side-by-side and set perpendicular to the beam direction – but without individual readout of the fibers. Instead, the fibers are bundled into two groups, which are read out by two separate Hammamatsu H11934-200 photomultiplier tubes (PMTs). Figure 5.9 shows the bundled nature of the XBTF fibers.

The first and third (last) XBTFs – as shown in Figure 5.1 – are used for measure the TOF of the test beam particle over a distance of 28.575 m. The second (middle) and last XBTFs are used as a trigger for the rest of the beam line instrumentation as well as a prerequisite for triggering beam-type events within the ProtoDUNE-SP detector.



Figure 5.9: XBTF module. The bundling of the two sets of fibers can be seen on the left [49].

1180 5.1.3.1 Issue with XBTFs

1181 A ~ 4 ns "jitter" can be seen in the left plot of Figure 5.11b where a small bump in the TOF 1182 distribution exists around 100 ns. The cause for the issue was never identified. Furthermore, 1183 it has little effect on the analysis, due to the cuts used for PID (see below).

1184 5.1.4 Cherenkov Devices

The two Cherenkov devices each consist of a 1.9 m long tube filled with the radiator gas (CO2) 1185 followed by a stainless steel enclosure. This enclosure houses a PMT at the bottom to collect 1186 the Cherenkov light and a curved mirror to guide Cherenkov light toward the PMT. The fill-1187 pressure of the two devices were set to two different values to allow for discrimination between 1188 certain particle types. Figure 5.10 [45] shows the Cherenkov threshold pressure of CO2 at 1189 various momenta for different particle types, as well as the maximum possible pressure value 1190 for the two XCET devices. Consider an example setup at 3 GeV/c momentum. One device 1191 can be set above the electron threshold but below the μ/π thresholds, while the other can be 1192 set above the μ/π threshold but below the K/p threshold in order to distinguish positrons, 1193 muons/pions, and kaons/protons. Further discussion of Cherenkov devices within the beam 1194

1195 line PID algorithm will be given in the following section.



Figure 5.10: CO2 Cherenkov threshold pressures across ProtoDUNE's beam momentum range for the various particles present in the beam line. The dashed red lines show the maximum pressures for the two Cherenkov devices present in the beam line. Taken from Reference [45].

1196 5.2 Beam Line PID

As mentioned above, the Cherenkov devices and TOF as measured by the XBTFs were 1197 used for PID of the beam line particles. Table 5.1 shows the conditions of the Cherenkov 1198 devices and TOF value used for the PID algorithm across the various nominal momentum 1199 settings. As shown in this table, for nominal momenta below 3 GeV/c, one Cherenkov device 1200 is used to distinguish e from the other particles, and the TOF is then used to distinguish 1201 μ/π from p. At 3 GeV/c, both Cherenkov devices are used to separate e, μ/π , and K/p. 1202 Finally, at 6 – 7 GeV/c, the two Cherenkov devices are used to separate $e/\mu/\pi$, K, and p. 1203 Figure 5.11 demonstrates this for the various beam momentum settings. 1204

		$\rm Momentum ~(GeV/{\it c})$			
		1	2	3	6 - 7
e	TOF (ns)	0, 105	0, 105	_	_
	Low-p Status	1	1	1	1
	High-p Status	_	_	1	1
μ / π	TOF (ns)	0, 110	0, 103	_	_
	Low-p Status	0	0	0	1
	High-p Status	_	_	1	1
K	TOF (ns)	_	_	_	_
	Low-p Status	_	_	0	0
	High-p Status	_	_	0	1
p	TOF (ns)	110, 160	103, 160	_	_
	Low-p Status	0	0	0	0
	High-p Status	—	_	0	0

TABLE 5.1: A summary of beam line instrumentation logic used in the identification of particle types. Each cell reflects how a particular type of instrumentation is used at a given reference momentum. When time of flight is used, the values of the lower and upper cuts are given in nanoseconds. In the case of the high-pressure Cherenkov ("High-p Status") and the low-pressure Cherenkov ("Low-p Status"), zero and one represent the absence and presence of a signal respectively. When a given piece of instrumentation is not involved in a logic decision at a given momenta, a dash is used.



(a) Nominal beam momentum = 1 GeV/c. Vertical lines represent the time of flight cuts used for electrons (blue), and muons/pions (red).



(c) Nominal beam momentum = 3 GeV/c.

Figure 5.11: Time of flight distributions for different reference momenta, separated by particle using the PID techniques listed in table 5.1. The distributions are normalized such that the maximum height is equal to 1. Taken from Reference [30].



(b) Nominal beam momentum = 2 GeV/c. Vertical lines represent the time of flight cuts used for electrons (blue), and muons/pions (red).



(d) Nominal beam momentum = 6 GeV/c.

CHAPTER 6

EVENT SELECTION

This section describes the characterization of reconstructed data and MC events. Included is a set of data-MC comparisons detailing the cuts used in the selection. The data shown here is from Run 5387 of the initial ProtoDUNE-SP running period in the Fall of 2018.

1209 For data, an event is included in the set if it passes the following criteria:

- 1210 1. It is an event that was triggered by the beam line
- 1211 2. It follows the π/μ beam line selection.

1205

3. It has singular hits in each beam profile monitor. This is to eliminate ambiguity in thebeam line momentum and tracking reconstruction.

For MC, due to the lack of fully simulated beam line instrumentation, the only require-1214 ment is that the simulated event was generated from a (primary) π^+ or μ^+ in the beam 1215 line simulation. Only μ^+ and π^+ are considered because at 1 GeV/c (the beam momentum 1216 used for this analysis), the beam line PID can distinguish π^+ and μ^+ from e^+ and p, but 1217 not from each other. The criteria for the beam line PID can seen in Table 5.1. Figure 5.11a 1218 shows that the protons are well separated by the TOF cut used to select μ^+/π^+ . The MC 1219 events have been normalized to the number of data events that pass the aforementioned data 1220 criteria. 1221

1222 6.1 Truth Definitions

1223 The MC events which pass the above criteria are separated into the following categories 1224 based on truth information of the primary beam particle:

1225 1. Muons: The primary beam particle was a μ^+ .

1226 2. Upstream Interaction: The primary beam π^+ did not reach the TPC Fiducial Volume 1227 (FV).

1228 3. Past FV: The primary beam π^+ extended past the FV in the z-direction¹.

4. Background Interaction: The primary beam π^+ interacted within the FV, and that interaction was a background (not Absorption or Charge Exchange) inelastic interaction. This includes any inelastic interaction between the primary π^+ and an Ar nucleus with an outgoing π^{\pm} above a momentum threshold of 150 MeV/c. Note: this threshold is discussed further below.

5. Absorption: The primary beam π^+ interacted within the FV in an Absorption interaction. This is the first type of signal event and is defined as a π^+ which interacted with an Ar nucleus and resulted in no outgoing π^{\pm} (above threshold) or π^0 .

1237 6. Charge Exchange: The primary beam π^+ interacted within the FV in a Charge Ex-1238 change interaction. This is the second type of signal event and is defined similarly to 1239 Absorption, but with any number of π^0 present.

1240 7. Other: The primary beam π^+ ended within the FV, and did not interact inelastically 1241 (i.e. it decayed in flight or came to a stop and then decayed at rest).

The signal categories have been defined to occur within the FV (defined for primary particles ending before z = 222 cm). This is due to the fact that the grounded electron diverters created electric field distortions (as described in Section 4.2.2) which caused reconstructed tracks to break in their vicinity. A data-driven simulation of the electric field distortions was implemented, which attempted to account for this effect in MC. The track-breaking effect can be seen in the Figure 6.1, which shows the reconstructed endpoint of beam tracks in the

¹Reminder: using a right-handed coordinate system, the z-direction is horizontal and follows the beam direction, the x-direction is horizontal and points away from the wires on the beam side TPCs, and the y-direction is vertical and points up.

1248 TPC in the z direction. The legend shows the truth categories described in the previous section. Note that the exact effect is not perfectly modeled by the simulation, and a systematic



Figure 6.1: Reconstructed endpoint of beam tracks within the TPC. The vertical line represents the FV cut at 222 cm. The spike immediately after the FV cut is the track-breaking effect from the grounded electron diverters.

1249

1250 uncertainty on the strength of this effect in MC was implemented. This will be discussed

1251 further in Section 8.3.

Additionally, as mentioned above, the signal definitions are defined to have no charged pi-

- 1253 ons above a momentum threshold of 150 MeV/c. This is due to the inefficiency to reconstruct
- 1254 charged pions exiting the primary interactions which are below this threshold.

1255 6.2 Event Selection

The events that pass the previously stated criteria are then categorized according to the results of the TPC reconstruction. Ultimately, attempts are made to distinguish π^+ from μ^+ and then to distinguish absorption and charge exchange interactions from other π^+ interactions and stopping π^+ . Every event is accounted for and characterized into one of the following categories:

1261 1. The event contained no Pandora-reconstructed beam track *or* it did not leave enough 1262 hits on the collection plane wires. If, after the Pandora reconstruction described in 1263 Section 4.4 is performed, either no beam object was found or the beam object was 1264 reconstructed as a shower, the event is placed in this category. Also, events are placed 1265 here if there are not enough hits on the collection plane wires, as these are used in later 1266 cuts and in binning the events.

2. The event contained a reconstructed beam track, but it was not considered consistent
with coming from the beam. This is done in order to pick out events in which the pion
interacted upstream of the TPC FV or if Pandora erroneously reconstructed a cosmic
particle as the beam track. This is described in Section 6.3.

- 1271 3. The event was consistent with the incident track, but it extended past the FV cut in
 1272 the z-dimension (222 cm).
- 4. The event remained in the FV, but it was rejected by the combined absorption and
 charge exchange selection. The selection criteria for this and the following two categories is presented in Section 6.4.
- 5. The event passed the combined absorption/charge exchange selection, and was distin-guished as an absorption interaction.

1278 6. The event passed the combined absorption/charge exchange selection, and was distin-1279 guished as a charge exchange interaction.

75

1280 6.3 Beam Cuts

1281 Sometimes, the wrong particle is identified as the beam particle by the Pandora reconstruction. As mentioned above, these could come from a cosmic muon or particle resulting 1282 from an interaction before the active volume of the detector. Information about the starting 1283 position and direction of the reconstructed track identified as beam is used to separate these 1284 out and place them in their own category. For the cuts in position, the mean (μ) and width 1285 (σ) of the beam track distribution in x, y, and z is found (using SCE-corrected informa-1286 tion). Any track that is at least 3σ away from the mean in any direction is categorized as 1287 inconsistent with the beam. Additionally, the direction of the track is taken from the vector 1288 connecting the SCE-corrected start and end points of the track. The means of the angles 1289 relative to the Cartesian planes $(\bar{\theta}_x, \bar{\theta}_y, \bar{\theta}_z)$ are found. Then, for each beam track, the cosine 1290 of the angle between its direction and the mean direction (defined by the mean angles) is 1291 found. This is defined in Equation 6.1. Any track which has $\cos(\theta) < 0.95$ is considered 1292 inconsistent with the beam. 1293

$$\cos(\theta) = \cos(\theta_x) * \cos(\bar{\theta}_x) + \cos(\theta_y) * \cos(\bar{\theta}_y) + \cos(\theta_z) * \cos(\bar{\theta}_z)$$
(6.1)

Figure 6.2 shows the distributions of the position (relative to the μ and σ) of the beam in each direction, as well as two views of the $\cos(\theta)$ distribution. The 3σ cuts in position and the $\cos(\theta) < 0.95$ cut in direction are shown as the vertical black lines. As can be seen in these plots, the cosmic particles and upstream interactions tend to have extreme angles and positions.

1299 6.4 Absorption and Charge Exchange Selection

By analyzing reconstructed particles that have been associated to the TPC beam track as daughter particles, the tracks ending within the FV are separated between two categories: 1) absorption or charge exchange 2) other events. Because both absorption and charge exchange events contain no charged pion (above threshold) in the final state, the selection strategy is



(a) SCE-corrected start x position reconstructed TPC track relative to mean and width of all beam tracks.



(c) SCE-corrected start y position reconstructed TPC track relative to mean and width of all beam tracks.



(b) SCE-corrected start y position reconstructed TPC track relative to mean and width of all beam tracks. Note that a bump in the distribution exists towards the right of the plot. This was recently identified as caused by a known detector effect present in data. Further investigation and possible treatments in MC simulation is ongoing.



(d) Cosine of the angle between reconstructed beam track and the mean track.



(e) Cosine of the angle between reconstructed beam track and the mean track. Zoomed-in to highlight cut region.

Figure 6.2: Distributions used to determine consistency with the beam line. The vertical black lines represent the cut values used.

1304 to identify events with a charged pion daughter.

The daughter particles are separated between track-like (ideally from μ , π , p, etc.) and 1305 shower-like (ideally from e, γ) objects using the results of the CNN described in Section 1306 4.4.1. For daughter particles of beam tracks, the CNN-based track/shower discrimination 1307 performed better than Pandora's native track/shower discrimination, and so was used for this 1308 analysis. Each hit in an event receives a set of scores produced by the CNN that encodes the 1309 degree to which it appears to be produced by a track-like particle or a shower-like particle. For 1310 each associated daughter, the scores from all of its hits are averaged to produce aggregated 1311 scores for the reconstructed particle. The Pandora reconstruction software was configured to 1312 1313 reconstruct both a track-like and shower-like object for each reconstructed particle cluster in an event, so that analyzers could use alternate track/shower discrimination (such as the 1314 CNN method described here) and access the information accordingly. 1315

At time of writing, only the calibration for collection plane hits was at a suitable state, 1316 and so only these hits were used to calculate the aggregated scores. A cut on the track-1317 like score of the daughter particle at 0.3 (shown in Figure 6.3) was used to separate the 1318 daughters into shower-like and track-like. Here, the track score of every reconstructed particle 1319 associated as a daughter particle to the primary reconstructed TPC particle. The MC has 1320 been categorized by the true particle that created the reconstructed particle object. The 1321 fields "Daughter+" and "Daughter++" represent particles that are products of reinteractions 1322 of final state particles and so on. The field "Self" refers to segments of the true primary 1323 particle that were associated as a daughter (i.e. the track ended early). Finally, the field 1324 " γ " represents photons emitted by the nucleus following a primary interaction (i.e. from 1325 nuclear de-excitation), while " $\pi^0 \gamma$ " represents photons truly originating from the decay of a 1326 π^0 created within a primary interaction. 1327

If the daughter is considered track-like, an attempt is made to identify charged pions by identifying particles that appear to be a Minimum Ionizing Particle (MIP). This MIPlike determination is done first by looking at the energy deposited per unit length by the



Figure 6.3: CNN Track scores of all reconstructed particles associated as daughters to the primary beam.

reconstructed track. For this, the truncated-mean dE/dx (defined to be the total energy 1331 deposited by a reconstructed hit divided by the track pitch of that hit) is used in order to 1332 exclude the large energy deposits from stopping particles. In its calculation, the lowest 16%1333 and highest 16% of hits in a track are ignored. The distribution of the truncated mean 1334 dE/dx for all daughter tracks is shown in Figure 6.4a. Particles are immediately considered 1335 MIP-like if they fall between 0.5 and 2.8 MeV/cm, and are considered not MIP-like if they 1336 are above 3.4 MeV/cm. For other particles (those that fall below .5 MeV/cm or between 1337 2.8 and 3.4 MeV/cm), another step is done in the selection. This step consists of comparing 1338 the dE/dx of each hit in the track to the expectation value for protons and producing a χ^2 1339 value. Ideally, protons should have a low χ^2 and pions should have a high χ^2 . This is shown 1340 in Figure 6.4b. These particles are considered MIP-like if they have a χ^2 above 70. 1341



(a) Truncated mean dE/dX of all reconstructed tracks associated as daughters to the primary beam.



(b) PID χ^2 value of all reconstructed tracks associated as daughters to the primary beam.

Figure 6.4: Distributions used for combined absorption and charge and exchange selection. Vertical black lines represent the cuts used. Note that the events were separated into multiple regions of truncated mean dE/dX, as indicated by the multiple black lines on the left plot.

If any of the daughter particles appears MIP-like, it is considered to be a charged pion originating from the primary interaction, and the event is rejected from the absorption and charge exchange selection.

Following the combined absorption and charge exchange selection, these interactions are separated by attempting to identify showers originating from the decay of π^0 daughters. A daughter shower is considered as coming from a π^0 decay if it is at least 5 cm away from the end of the primary track and has at least 80 MeV of energy. These cuts are chosen to exclude any activity around the interaction vertex which originated from lower-energy pions and protons or nuclear de-excitation photons from both the primary and downstream interactions. This can be seen in Figure 6.5.



(a) Distance between the end of the reconstructed beam track and start of showers associated as daughters to the primary track.



(b) Total deposited energy of all showers associated as daughters to the primary track.

Figure 6.5: Distributions used to separate absorption from charge exchange. The black vertical lines represent the cuts used.

Channel	Efficiency	Purity
Absorption	0.53	0.52
Charge Exchange	0.23	0.80

TABLE 6.1: Effiency and purity of the signal categories.

1352 6.5 Binning

The bin variables used for the event selection categories described in the previous sec-1353 tion are as follows. Events that fall in the first two categories (no beam track and events 1354 that fail the beam cuts) are each placed in single, unitless bins. Events that end past the 1355 FV cut are binned according to their SCE-uncorrected ending position in z. Finally, the 1356 three "interaction" categories (absorption, charge exchange, and other) are binned according 1357 to their ending kinetic energy. This is determined by first calculating their reconstructed 1358 kinetic energy using the reconstructed beam line momentum, assuming they are pions, and 1359 then subtracting the energy of each collection plane hit up to but not including the last. 1360 Occasionally, large hits from large amounts of vertex activity or from crossing cosmic tracks 1361 saturate the cold electronics, resulting in seemingly enormous reconstructed energy deposits 1362 on the order of a few hundred to a thousand MeV. Thus, any hit above 80 MeV is ignored in 1363 the calculation. This value was chosen such that the saturated electronics hits are skipped, 1364 but truly large energy deposits like from overlapping hits are kept. 1365

This binning is shown in Figure 6.6, where the reconstructed distributions from the 1366 nominal MC are shown. Additionally, these distributions are broken down by their true 1367 category (i.e. a signal interaction in a given energy bin or a muon). These are displayed as 1368 the stacked histograms, where the different colors represent the specific true category. The 1369 bin edges for the interaction distributions were chosen based on the smearing between true 1370 and reconstructed kinetic energy shown as the spread in the different colored portions of the 1371 stacks. The purity and efficiency for the absorption and charge exchange selections is also 1372 shown in Table 6.1. 1373



(g)

Figure 6.6: Reconstructed distributions of events from the nominal MC. The distributions are broken down by true categories, shown in 6.6g.

1374 6.6 Selected MC Event Displays

This section provides some examples of successes and failures in the event selection within the MC sample used in the analysis. Shown in the following figures are reconstructed event displays in the view of the collection plane near the beam entrance. The x-axis is the wire number which is equivalent to the position in z. The y-axis is the time (or tick) at which the charge reached the wire plane. This is equivalent to the horizontal position away from the wire plane.

The first example, shown in Figure 6.7, is a true absorption interaction correctly selected as absorption. The pion is shown as the yellow track entering from the left, and it interacts with a nucleus. The interaction produces two protons. These are correctly identified as proton-like tracks by the event selection and are shown as the light blue and pink tracks in the display.



Figure 6.7: MC absorption event correctly identified as absorption.

Next, Figure 6.8 shows a true charge exchange event incorrectly identified as an absorption event. Again, the beam enters from the left shown as the tan track, and interacts with a nucleus. A very energetic proton exits the interaction and travels toward the lower right of the display shown as the green track. This proton is correctly identified as a proton. However, a π^0 also exits the interaction. Near the vertex, one of the γ s produced by the decay of this is identified as a small shower (represented by the black rectangles near the vertex). Its reconstructed energy is too low to be identified as resulting from a π^0 . The other



1393 γ is not identified. The pink track extending from the top to bottom of the plot is a cosmic muon

Figure 6.8: MC charge exchange event incorrectly identified as absorption.

1394

The third example in Figure 6.9 is a background inelastic event (one a charged pion in the final state) selected as absorption. The beam pion enters from the left (shown as the red track), and strikes a nucleus. Both a π^+ and π^0 exit the interaction. The π^0 promptly decays, and the resulting showers are not associated to this event as daughters. The π^+ is reconstructed as the tan track exiting the interaction, but it does not appear to be a pion when its calorimetry information is checked in the event selection procedure. The light blue track extending from the top right to the bottom left is a cosmic muon.



Figure 6.9: MC background inelastic event incorrectly identified as absorption.

The next example in Figure 6.10 shows the pion as a tan track entering from the top left before interacting with a nucleus. A resulting proton is reconstructed as the light blue track heading toward the bottom of the figure. A π^0 exits the interaction and promptly decays. 1405 The resulting photons are reconstructed as the red and yellow showers, and identified as1406 such.



Figure 6.10: MC charge exchange event correctly identified as charge exchange.

Figure 6.11 shows an absorption event misidentified as charge exchange. The beam pion is reconstructed as the pink track and interacts with a nucleus. A neutron exits the interaction before itself interacting and resulting in a proton track (the tan track toward the right). A proton also exits the interaction, but was reconstructed as a shower (represented by the black boxes at the end of the track). This proton appears as a π^0 shower and so the event is selected as charge exchange.



Figure 6.11: MC absorption event incorrectly identified as charge exchange.

Figure 6.12 shows a background inelastic misidentified as charge exchange. The pion, reconstructed as the tan track, enters from the left and ends in an inelastic interaction. A high energy π^+ exits the interaction and reinteracts nearby the primary interaction, resulting in a charge exchange event. The π^0 from the secondary interaction decays, and a shower is reconstructed and associated to the primary interaction.



Figure 6.12: MC background inelastic event incorrectly identified as charge exchange.

Finally, Figure 6.13 shows a muon that is misidentified as a background inelastic interaction. The muon, reconstructed as the yellow track, enters from the top left of the plot and its track is ended prematurely. The remainder of the muon is reconstructed as a MIP-like track (the red track) and associated as a daughter to the primary track. The blue and yellow tracks toward the left of the figure extending from top to bottom are cosmic muons.



Figure 6.13: MC muon incorrectly identified as a background inelastic interaction.

1423 6.7 Selected Data Event Displays

This section provides example events in 5 of the 6 selection categories (all but the category in-track" category) used in the fit to data. The dataset containing these events, Run 5809, is different from the one used to display the event selection cuts. The first example in Figure 6.14 is a selected absorption event. The pion candidate enters from the left, and appears to interact with a nucleus. The reconstruction does not associate any tracks as daughters to this primary particle. Despite this, there appear to be a pair of heavily-ionizing protons exiting the interaction. A cosmic muon crosses the primary track in a nearly-vertical trajectory, and a pair of cosmic muons appear toward the right.



Figure 6.14: Selected absorption event.

1431

The second example shown in Figure 6.15 is a selected charge exchange event. The pion candidate enters from the left, and appears to interact with a nucleus. Clearly seen after the interaction is an apparent shower structure resulting from the decay of a π^0 .



Figure 6.15: Selected charge exchange event.

1434

The third example in Figure 6.16 is a selected background inelastic interaction. The pion candidate enters from the left, and results in an interaction with multiple particles exiting. A daughter pion candidate travels from the interaction toward the top right of the plot.



Figure 6.16: Selected background inelastic interaction event.

The fourth example in Figure 6.17 is a π⁺/μ⁺ candidate extending past the fiducial
volume. The primary particle appears to come to a stop near wire number 700. A break in
the particle's ionization track is seen near wire number 500. This is the dead region caused
by the grounded electron diverters. Additionally, a cosmic muon is seen crossing the primary track.



Figure 6.17: Event selected as extending past the fiducial volume.

1442

Finally, in Figure 6.18 is another π^+/μ^+ candidate that extends past the fiducial volume. This time, however, the reconstruction (not shown) ends near the grounded electron diverters. The remainder of the primary particle's ionization to the right of the grounded electron diverters is reconstructed as a separate track, and is associated as a daughter to the primary track.



Figure 6.18: Event selected as extending past the fiducial volume, and specifically ending near the electron diverter region.

CHAPTER 7

1448

CROSS SECTION MEASUREMENT TECHNIQUE

This analysis measures π^+ - Ar absorption and charge exchange cross sections using beam-1449 triggered events in ProtoDUNE-SP. The measurement employs a fit which extracts the 1450 number of signal (absorption and charge exchange) interactions as well as the number of 1451 background events (incident muons, non-signal interactions, stopping pions) from this data. 1452 Truth-level information (information representing the exact results of the simulation, rather 1453 than reconstructed information taken from a simulated detector response) is then used to 1454 extract the cross section according to a technique derived from the Liquid Argon in A Test 1455 Beam experiment (LArIAT) [50]. That technique, known as the "Thin Slice Method" (de-1456 scribed in Section 7.2) was used to measure hadron cross sections using a LArTPC wherein 1457 the detection medium (LAr) also serves as the target. This method is distinct from mea-1458 surements using thin targets. This chapter first describes these thin target cross section 1459 measurements, as well as the Thin Slice Method. It then specifies how the Thin Slice 1460 1461 Method is used on truth information to extract the cross section from simulation. It then describes the statistical fit used to interpret the data. 1462

1463 7.1 Thin Target Cross Section Experiment

Historically, hadron scattering experiments have been performed by firing a beam of 1464 particles onto a thin piece of material as a target. By counting the number of interactions, 1465 the cross section for an interaction can be measured as a function of the incident energy 1466 (since the target is thin, a negligible amount of energy is lost before an interaction, and the 1467 1468 cross section is measured at the incident beam energy). A simple cartoon of the experimental setup can be seen in Figure 7.1. Here, a beam of pions of width A and flux Φ impinges on a 1469 target of thickness t. After passing through the target, N_{Inter} pions have interacted, while 1470 N_{Surv} have passed through without interacting. The cross section can be extracted from 1471

1472 Equation 7.1.

$$\frac{N_{Inter}}{\Phi A} = \frac{N_{Inter}}{N_{Inc}} = 1 - e^{-nt\sigma} \tag{7.1}$$

Here, σ is the cross section for the relevant interaction, n is the number density of atoms in the target material, and N_{Inc} is the number of incident pions as given by $\Phi \times A$. This can be slightly simplified by expanding the exponential term around t as such:

$$\frac{N_{Inter}}{\Phi A} = \frac{N_{Inter}}{N_{Inc}} \approx 1 - (1 - nt\sigma + \mathcal{O}(t^2)) = nt\sigma$$
(7.2)



Figure 7.1: Cartoon of a thin target scattering experiment.

1476 7.2 The Thin Slice Method

By virtue of being a LArTPC, ProtoDUNE-SP is not thin, and thus cannot be used for the simple thin target experiment as described above. However, LArIAT [50] used a method they called the Thin Slice Method to mock-up a series of multiple thin target experiments in an extended volume of LAr in order to measure hadronic cross sections in an extended LAr volume. The segmentation created by the collection plane wires allows analyzers to treat an extended volume of LAr as if it were multiple thin targets stacked in front of one another.

This can be seen in Figure 7.2, where a cartoon of a pion track in a LATTPC is shown. The 1483 vertical dashed lines represent the collection wires of the TPC, and the red dot represents the 1484 point at which the pion interacts. One can treat every slice the pion passes through (up to 1485 and including the slice which contains the interaction) as a separate thin target experiment. 1486 In each of these, the pion enters the slice and either interacts, or decays. From this, one can 1487 count the number of incident pions $(N_{Inc}$ as described above) by counting the number of 1488 times a pion enters a slice (it passes by a new wire) and the number of interactions (N_{Inter}) 1489 to extract the cross section. 1490



Figure 7.2: Cartoon of the thin slice method applied to a pion track within a LArTPC. The red point represents a hadronic interaction.

If the energy of the pion is known as it enters each slice, then energy-dependence is added to Equation 7.2, as reflected in Equation 7.3. Here, the thickness t is the width of the wire spacings.

$$\frac{N_{Inter}(E)}{N_{Inc}(E)} = nt\sigma(E) \tag{7.3}$$

Mechanically, this calculation is achieved by using two histograms thus called "Incident" and "Interacting" which respectively represent the denominator and numerator of Equation

7.3. As the pion enters into a new slice, the Incident histogram is filled at the corresponding 1496 energy. This is done for the entire pion track up to the end, meaning a track can contribute 1497 multiple entries in the histogram. For example, in Figure 7.2, the pion track will contribute 1498 an entry for every section of Ar up to and including the interaction point (represented by 1499 the red dot). If the pion undergoes an interaction of interest, the Interacting histogram is 1500 filled according to the energy of the pion as it entered the final slice (this will be the same 1501 energy for the final entry into the Incident histogram). A demonstration of this is shown in 1502 Figure 7.3. 1503



Figure 7.3: Demonstration of the cross section calculation using Equation 7.3.

1504 7.3 Thin Slice Method on Truth Information

The previous section described how the Thin Slice Method could be used on reconstructed 1505 information to determine hadronic cross sections. The measurement presented in this thesis 1506 is slightly different, but is generally based on this method. Rather than using reconstructed 1507 information to determine the Incident histogram, it is taken directly from truth information 1508 from ProtoDUNE-SP Monte Carlo simulation. This simulation will be modified by perform-1509 ing a fit to collected data. This fit, known as a "template fit" which is described later in 1510 Section 7.4, will vary the number of signal and background interactions (binned in true end-1511 ing kinetic energy) within the MC. This will of course change any true Interacting histogram 1512 created from this information. It will, in turn, also change the true Incident histogram, as 1513 the number of slices (equivalently, the distance traveled by the pion) depend on the pion's 1514 starting and ending energy. In this way, the varied MC which best describes the data can be 1515 used to extract a varied cross section. This section describes the procedure used to extract 1516 the cross section from truth information. 1517

The ProtoDUNE-SP MC simulation contains a set of π^+ and μ^+ created by the beam 1518 impinging on the detector. Pions that interact before the start of the LAr are ignored and 1519 do not contribute to the Incident distribution. For all other pions (those that enter into 1520 the TPC), their energy at the initial TPC point (E_0) is used as an entry in the Incident 1521 distribution. Using a uniform spacing¹, the energy deposited by the pion as it was simulated 1522 by Geant4 is separated into "slices". The energy at each slice boundary crossed by the pion 1523 is calculated by summing the energy deposited in the previous slice and subtracting that 1524 from the previous incident energy. Thus, the energy as the pion crosses slice boundary i is 1525 equal to $E_{i-1} - \delta E_{i-1,i}$ where $\delta E_{i-1,i}$ is the energy deposited between slice boundaries i-11526 and i. This is demonstrated in Figure 7.4, where the labels E_i represent the energy of the 1527 pion as it crosses each slice boundary. All of the energies after E_0 are then given an entry 1528

¹Note, the width of the spacing to extract the cross section from truth info is arbitrary. For this analysis, the wire spacing (.47974cm) was used.

in the Incident distribution as well. This occurs for every pion that reaches the TPC, and
along each pion up to some fiducial volume edge. Then, for each pion ending in a signal
interaction within the fiducial volume, the energy of the pion at its interaction point is used
as an entry in the Interacting histogram. The resulting Interacting and Incident histograms
are used as in Equation 7.3 and Figure 7.3 to compute the cross section.



Figure 7.4: Cartoon diagram showing a pion track split up into multiple slices and the energy denoted at each slice boundary.

1533

It is instructive to consider this measurement technique under a varied cross section 1534 model. If the cross section is higher over the momentum range of the simulated pions, more 1535 interactions will occur (N_{Inter} will be higher). The pions will (on average) travel through 1536 less slices before they interact, and thus contribute less events to the Incident histogram. For 1537 an overall lower cross section, the inverse is true: less interactions occur, and the pions travel 1538 further on average (creating more entries in the Incident histogram). This line of thought can 1539 be extended to more complicated variations in shape as well. The number of interactions at a 1540 given energy will change, and so too will the entries in the Incident distribution. This serves 1541 as the guiding principle used in this measurement: if one is able to measure the number 1542 of interacting pions at a given energy (and equally importantly, the number of pions that 1543

do not interact), the Thin Slice Method can extract cross sections using truth information from a varied Monte Carlo simulation that best describes the data. The following section describes the fit strategy used to interpret the data in terms of a varied Monte Carlo sample in order to extract the absorption and charge exchange cross sections in this manner.

1548 7.4 Fit Strategy

This analysis uses a binned maximum likelihood fit to 1 GeV/c momentum ProtoDUNE-1549 SP beam line events to estimate the number of signal and background interactions in the 1550 data set. The fit results in a set of varied MC which best matches this data and from which 1551 the signal cross sections are extracted. A set of signal parameters $(\vec{\theta})$ and nuisance (also 1552 called systematic) parameters (\vec{p}) controlled by the fit vary simulated π^+ and μ^+ events. 1553 The fit attempts to find the set of parameters that best describe the data by maximizing 1554 the likelihood $L(\vec{\theta}, \vec{p}; \vec{n})$ to observe a set of events \vec{n} given the model parameters $\vec{\theta}$ and \vec{p} . 1555 Additionally, we include constraints to the nuisance parameters represented by predictions of 1556 their central values \vec{q} and the uncertainties on these predictions represented by a covariance 1557 matrix V_{Cov} . As such, the likelihood L is made of two components: a statistical term and a 1558 systematic term: 1559

$$L(\vec{\theta}, \vec{p}; \vec{n}) = L_{\text{Stat}}(\vec{\theta}, \vec{p}; \vec{n}) L_{Syst}(\vec{p}; \vec{q}, V_{\text{Cov}})$$
(7.4)

For compatibility with the fitting routines (discussed later) in finding the best fit parameters and their uncertainties, the minimum of twice the negative log-likelihood $(-2 \ln L)$ is found instead of the maximum likelihood². Additionally, minimizing this value is equivalent to minimizing twice the negative of the natural logarithm of the likelihood ratio λ [29]. The likelihood ratio is defined as

$$\lambda = L(\vec{\theta}, \vec{p}; \vec{n}) / L(\vec{\theta_T}, \vec{p_T}; \vec{n})$$
(7.5)

²The fitting routines implemented in ROOT work by minimizing rather than maximizing some value.

where $\vec{\theta_T}, \vec{p_T}$ represents the true, unknown underlying model. Plugging Equation 7.4 into this results in the following.

$$\lambda = L_{\text{Stat}}(\vec{\theta}, \vec{p}; \vec{n}) L_{\text{Syst}}(\vec{p}; \vec{q}, V_{\text{Cov}}) / L_{\text{Stat}}(\vec{\theta_T}, \vec{p_T}; \vec{n})$$
(7.6)

¹⁵⁶⁷ Where there is no true value of L_{Syst} shown in the denominator, as it is trivially equal to ¹⁵⁶⁸ one. $-2 \ln \lambda$ is thus defined as

$$-2\ln\lambda = -2\ln\left(L_{\rm Stat}(\vec{\theta}, \vec{p}; \vec{n})/L_{\rm Stat}(\vec{\theta_T}; \vec{n})\right) - 2\ln L_{\rm Syst}(\vec{p}; \vec{q}, V_{\rm Cov}).$$
(7.7)

In this fit, we are seeking to categorize a fixed number of events (a set of beam linetriggered events) based on the results of ProtoDUNE-SP reconstruction described in Section 4.4. As such, the likelihood L_{Stat} is the multinomial likelihood as defined in Equation 7.8.

$$L_{\text{Stat}}(\vec{\theta}, \vec{p}; \vec{n}) = N! N^N \prod_j y_j (\vec{\theta}, \vec{p})^{n_j} / n_j!$$
(7.8)

Here, $y_j(\vec{\theta}, \vec{p})$ and n_j are the number of predicted and measured events in reconstructed bin 1574 j, and $N = \sum_j n_j = \sum_j y_j(\vec{\theta}, \vec{p})$ is the total number of beam line events. As stated before, 1575 $L_{\text{Stat}}(\vec{\theta_T}, \vec{p_T}; \vec{n})$ depends on some true underlying model denoted by $\vec{\theta_T}, \vec{p_T}$. This model is 1576 unknown, but $L_{\text{Stat}}(\vec{\theta_T}, \vec{p_T}; \vec{n})$ is estimated using the measured events as shown in Equation 1577 7.9.

$$L_{\text{Stat}}(\vec{\theta_T}, \vec{p_T}; \vec{n}) = N! N^N \prod_j n_j^{n_j} / n_j!$$
(7.9)

1578 From this, the statistical portion of $-2\ln\lambda$ is defined as follows.

$$-2\ln\lambda_{\text{Stat}} = 2\sum_{j} n_j \ln\frac{n_j}{y_j}$$
(7.10)
The systematic term $-2 \ln \lambda_{\text{Syst}}$ is a constraint term that assumes the systematic parameters \vec{p} are Gaussian distributed around their central values \vec{q} and whose uncertainties are described by a covariance V_{Cov} :

$$-2\ln\lambda_{\text{Syst}} = \sum_{i,j} (p_i - q_i)(V_{\text{Cov}}^{-1})_{ij}(p_j - q_j).$$
(7.11)

1582 With this, the full statistic minimized by the fit is given by Equation 7.12.

$$-2\ln\lambda = 2\sum_{j}n_{j}\ln\frac{n_{j}}{y_{j}} + \sum_{i,j}(p_{i} - q_{i})(V_{\text{Cov}}^{-1})_{ij}(p_{j} - q_{j})$$
(7.12)

A crucial step in the analysis is the extraction of true information (the set of true events 1583 from which the number of signal interactions and slices which form the cross section calcula-1584 tion as in Section 7.3) from reconstructed quantities. In general, this is known as "unfolding" 1585 and is a common problem within High Energy Physics [51]. Several unfolding techniques 1586 exist, each with their own benefits and drawbacks (typically, a balance is made between bi-1587 ased results, bin-to-bin correlations, uncertainty, and smoothness) [52]. The fit done within 1588 this analysis, known as a template fit, performs the role of unfolding. Included in the set of 1589 parameters are a set of "template weights" assigned to the MC signal events which vary the 1590 normalization of signal events in a given true energy bin, and which also have a subsequent 1591 effect on the predicted reconstructed distributions. The fit simultaneously varies the tem-1592 plate weights and the other parameters, then compares the resulting predicted reconstructed 1593 distributions to the measured distributions until it converges at a minimum $-2\ln\lambda$ value. 1594

The role of the template parameters is highlighted in Equation 7.13, which shows the relationship between the true and reconstructed events as predicted by MC. \hat{y}_i represents the number of events in true bin *i* for the indicated true category (absorption, charge exchange, muon background, or pion backgrounds). The events have a chance ϵ^k to be selected as some selection category *k* when the reconstructed information is passed through the event selection (described in Section 6). Reconstruction effects smear the events from some true

bin i to some reconstructed bin j in selection category k. This is represented by $t_{i,j}^k$ which 1601 can be thought of as a "smearing matrix." In general, ϵ^k and $t_{i,j}^k$ depend on the true category 1602 they act on. \hat{y}_i , ϵ^k and $t_{i,j}^k$ all depend on some subset of the fit parameters $\vec{\theta}$ and can be 1603 modified at each step in the fit. A parameter f^{μ} is used to vary the normalization of muons 1604 in the sample, as this is uncertain. Lastly, c_i^{Abs} , c_i^{Cex} are the template parameters that 1605 control the normalization of absorption and charge exchange events in true bin i. The sums 1606 extend over the number of true bins n_T for the different true categories. Since the number 1607 of impinging π^+/μ^+ is known and static, the fit is constrained as in Equation 7.14. 1608

$$y_{j}^{k} = \sum_{i}^{n_{T}} c_{i}^{\text{Abs}} \hat{y}_{i}^{\text{Abs}} \epsilon^{k} t_{i,j}^{k} + \sum_{i}^{n_{T}} c_{i}^{\text{Cex}} \hat{y}_{i}^{\text{Cex}} \epsilon^{k} t_{i,j}^{k} + \sum_{i}^{n_{T}} f^{\mu} \hat{y}_{i}^{\mu} \epsilon^{k} t_{i,j}^{k} + \sum_{l}^{n_{\pi} \text{BG}} \sum_{i}^{n_{T}} \hat{y}_{i}^{l} \epsilon^{k} t_{i,j}^{k}$$
(7.13)

$$N = \sum_{j} y_j = \sum_{j} n_j \tag{7.14}$$

In addition to the constraint on the overall number of incident particles, the number of incident particles in bins of true initial momentum (where it was generated by the beam event generator module), is also held constant. This has been omitted from Equation 7.14 for clarity.

Thus, the fit changes $\vec{\theta}$ and \vec{p} until the measured and predicted reconstruction distributions best match. The result of the fit is a set of best-fit parameters $\vec{\theta}_0$ and \vec{p}_0 and their covariance which will be used for error propagation as described in the Section 7.5. The best-fit parameter values produce a set of modified MC events that can be used as in Section 7.3 to extract cross sections.

The fit uses the MIGRAD [53] routine of the Minuit2 [54] minimizer library within ROOT [55] to find the maximum likelihood ratio. The MIGRAD routine estimates the gradient of the likelihood ratio surface at each fit point and follows the gradient until it reaches the best-fit point. After finding the best-fit point, the HESSE routine within Minuit2 is called. This computes the Hessian matrix: the second derivative of the $-2 \ln \lambda$ surface around the best fit point. The Hessian matrix is inverted to create the covariance matrix which describes the post-fit uncertainties and correlations of the fit parameters.

1625 7.5 Error Propagation

The output of the fit – the best-fit parameters ϕ_0^{-3} and their associated covariance matrix Σ – can be used to propagate the post-fit errors to the extracted cross sections. First, the Cholesky decomposition [56] of the post-fit covariance matrix is computed. This representation of the covariance matrix (shown in Equation 7.15) is the product of an upper triangular matrix R with positive diagonal elements and its transpose R^T .

$$\Sigma = R^T R \tag{7.15}$$

1631 A random set of fit parameters $\vec{\phi_t}$ (also known as a "throw") can be generated by multiplying 1632 a random unit Gaussian vector $\vec{r_t}$ by R and adding this to the best-fit parameter values $\vec{\phi_0}$, 1633 as shown in Equation 7.16. $\vec{\theta_t}$ will be randomly distributed with the same covariances of the 1634 post-fit covariance matrix [56].

$$\vec{\theta_t} = \vec{\phi_0} + R\vec{r_t} \tag{7.16}$$

This procedure is repeated on the order of 1000 times to generate an ensemble of throws. Each set of thrown parameters is used to calculate the cross section as described in Section 7.3. The cross section covariance matrix V is computed as in Equation 7.17, where V_{ij} is the covariance between bins i and j, σ_{it} is the cross section in bin i for throw t and σ_{i0} is the best-fit cross section in bin i. Note: the bins i, j include both absorption and charge exchange to account for the covariances between these channels.

$$V_{ij} = \frac{1}{N} \sum_{t}^{N} (\sigma_{it} - \sigma_{i0}) (\sigma_{jt} - \sigma_{j0})$$
(7.17)

³The set of parameters $\vec{\phi}$ includes both the signal parameters $\vec{\theta}$ and systematic parameters \vec{p} .

If any parameter is thrown into an unphysical region (i.e. for the template parameters, below zero), the throw is repeated until all parameters are within their allowed regions. This may results in truncated Gaussian distributions for any parameters that experience this issue. If this truncated area is small, the distribution is considered valid and has a negligible effect on the cross section covariance.

This throwing procedure makes an assumption that the likelihood surface around the best fit point is distributed according to a multivariate Gaussian. If this assumption holds, the covariance matrix from the fit describes a multidimensional contour with constant χ^2 around the best-fit point which represents the probable spread of fit parameters. Additionally, the cross section covariance created by this propagation procedure describes a constant- χ^2 contour centered around the best-fit cross section point [57][58].

CHAPTER 8

1652

SYSTEMATIC UNCERTAINTIES

This chapter describes the systematic uncertainties and their implementation within the analysis. The uncertainties discussed stem from the dE/dx calibration, the reconstructed beam line momentum, the modeling (via Geant4) of the hadrons as they pass through the detector, the effect of the electron diverters on reconstructed track, and differences in the rate of both events without a reconstructed track and those failing the beam cuts. These uncertainties are parameterized within the fit and are constrained by a covariance within the systematic term given in Equation 7.11.

1660 8.1 dE/dX Calibration

Section 4.5.3 describes how the measured charge per unit distance dQ/dx is translated into the energy deposited per unit distance dE/dx (which is used for the energy measurements of particles in this analysis). Part of this dE/dx extraction is the determination of a calibration constant C_{cal} by analyzing stopping muons. There is some uncertainty in what this calibration constant is, and as such, it has been implemented as a systematic parameter in the fit.

As $C_{\rm cal}$ is varied within the fit, it has two large effects. The first is to change the MIP-1667 like separation of daughter tracks during the event selection as described in Section 6.4, and 1668 1669 the second is to migrate events between bins since more apparent energy will be accounted for in the energy reconstruction. This parameter was first implemented within the fit by 1670 rescaling the dE/dx in each step of the fit where the prediction histograms are refilled before 1671 comparing to data. This caused instability within the fit, as events would fail to migrate bins 1672 until the parameter was turned enough. This "threshold" behavior caused discontinuities in 1673 the $-2\ln\lambda$ surface, and so a different approach was opted for. Instead of implementing 1674 this effect directly on the events, a weighting scheme was implemented, where varied MC 1675

1676 samples were created for various values of C_{cal} . In each bin of the prediction histograms, 1677 the ratio to nominal was taken to form a weight for that bin and C_{cal} . These weights were 1678 then interpolated between in order to form a smoothly-varying surface that could be used 1679 within the fit. Each step of the fit, the events are given a weight which depends on the bin 1680 the event falls into and the value of C_{cal} for that fit step.

1681 8.2 Beam Momentum

Section 5.1.2 describes how the beam line instrumentation reconstructs momentum using sets of fiber monitors surrounding a bending magnet in the beam line. This section also mentions a bulk shift to the fibers in one of the monitors that affected the reconstructed momentum. This shift was found to be 1.45 ± 0.18 mm. In addition to the uncertainty in the shift is an estimated 1% uncertainty on the magnetic field. Recalling Equation 5.2 (repeated here), these systematic uncertainties affect the reconstructed momentum as such: the fiber shift varies θ , which can then cancel out a variation in B.

$$p = \frac{299.7924}{\theta} \times \int_0^{L_{\text{mag}}} (Bdl) \tag{5.2}$$

These parameters would then be degenerate within the fit, and so these effects were combined into a single momentum rescaling parameter c_p . The prior uncertainty on c_p is given by the shifts to p due to variations in both parameters added in quadrature. The effect of the variation to B is trivially 1%. For the effect of the fiber shift, the nominal beam line MC simulation was ran with the fibers in the third monitor shifted by its 1 σ uncertainty (0.18mm). This results in an average 0.7% shift in the reconstructed momentum. The uncertainty on c_p is thus given in Equation 8.1.

$$\sigma_{cp} = \sqrt{.007^2 + .01^2} = .012 \tag{8.1}$$

1696 Within the analysis, the effect of this scaling parameter is to change the difference between

1697 true and reconstructed momentum r (defined in Equation 8.2).

$$r = \frac{p_{\text{Reco}} - p_{\text{True}}}{p_{\text{True}}}$$
(8.2)

The beam simulation show this is Gaussian distributed with mean μ and width σ . Some variation to c_p will then result in a distribution with varied μ' and σ' . An event can then be given a weight according to its value of r and the μ' and σ' resulting from the value of c_p within one step of the fit. This weight is given in Equation 8.3, which is the ratio of two Gaussian distributions.

$$w = \frac{\sigma}{\sigma'} \exp\left(\frac{(r-\mu)^2}{2\sigma^2} - \frac{(r-\mu')^2}{2\sigma'^2}\right)$$
(8.3)

The dependences of μ' and σ' on c_p were found from studies of the beam line MC simulation and used within the fit to form the weights as defined in 8.3.

During fit validation, it was found that this beam momentum parameter created instability in the fit due to its tendency to create extremely large weights for certain events at large parameter variations. This made it difficult to properly assess the post-fit error of the other parameters. As such, this parameter was chosen to be fixed during fits. Its pre-fit uncertainty was propagated to the cross section uncertainties by adding it in quadrature to post-fit parameter covariance matrix.

1711 8.3 Electron Diverter Effect

As shown in Figures 6.1 and 8.1, the simulation of the grounded electron diverters (which causes tracks to prematurely break), differs from data. To account for the uncertainty in the strength of the track-breaking effect, a simple weighting scheme was developed to artificially vary the track-breaking strength.

The weighting scheme varies the fraction of tracks ending above 222 cm, which end in the "track-breaking" region of 222–234 cm. This fraction, f, is defined as

$$f = \frac{N_{\text{Break}}}{N_{>222}} = \frac{N_{\text{Break}}}{N_{>234} + N_{\text{Break}}}$$
(8.4)



Figure 8.1: Enhanced view of the reconstructed endpoint of beam tracks within the TPC.

where N_{Break} is the number of broken tracks (ending between 222 and 234 cm), and $N_{>222}$ and $N_{>234}$ are the number of tracks above 222 and 234 cm respectively. The probability for a track ending above 222 cm to break is thus f, while the probability for a track to not break is 1 - f.

1722 Consider some variation as such: $f \to f' = cf$. Each track ending above 222cm is thus 1723 given a weight as follows, depending on if was or was not broken.

$$W_{\text{Break}} = \frac{f'}{f} = \frac{cf}{f} = c \tag{8.5}$$

$$W_{>234} = \frac{1 - f'}{1 - f} = \frac{1 - cf}{1 - f}$$
(8.6)

The nominal value of f, the fraction of events ending in the electron diverter region, in MC is 0.6133. The central value of the scale factor c was set to 0.50 as taken from comparisons ¹⁷²⁶ between MC and data shown here. The uncertainty on this was set naively to 20%.

1727 8.4 Beam Efficiencies

It was found that the Pandora had an apparent difference between data and MC in 1728 the efficiency for identifying beam particles in the TPC. Additionally, shape differences in 1729 the position and direction of reconstructed beam tracks (possibly due to inaccuracies in 1730 mapping SCE as described in Section 4.5.1) created a difference in the fraction of events 1731 passing the beam cuts. These two uncertainties were parameterized as efficiency-like effects 1732 by varying the numbers of events in the following categories: 1) no reconstructed beam 1733 track, 2) reconstructed beam track that fails the beam cuts, 3) reconstructed beam track 1734 that passes the beam cuts. Let the fraction of events categorized as such be represented by 1735 f_1 , f_2 , and f_3 respectively. These fractions sum to one $(f_3 = 1 - f_2 - f_1)$ and can be varied 1736 as follows. 1737

Consider some variation to these fractions (these are, in effect, variations to the two efficiency-like effects):

$$f_1 \to f'_1 = c_1 f_1$$

$$f_2 \to f'_2 = c_2 f_2$$

$$f_3 \to f'_3 = 1 - c_2 f_2 - c_1 f_1$$
(8.7)

Similar to the previous section, the events are given weights according to how they are categorized:

$$W_{1} = \frac{f_{1}'}{f_{1}} = c_{1}$$

$$W_{2} = \frac{f_{2}'}{f_{2}} = c_{2}$$

$$W_{3} = \frac{f_{3}'}{f_{3}} = \frac{1 - c_{2}f_{2} - c_{1}f_{1}}{1 - f_{2} - f_{1}}$$
(8.8)

The nominal values for the fraction of events with no track or failing the beam cuts in MC are 0.164 and 0.2305 respectively. The central value of the no-track parameter was set to 1.62 taken from comparisons to data and MC, and its uncertainty was naively set to 20%.
The central value and uncertainty for the beam cut parameter were naively set to 1.00 and
10% respectively.

1743 8.5 Hadronic Interaction Modelling

In addition to uncertainties in the modeling of the detector systems described in the 1744 previous few sections, there are uncertainties in the hadronic interaction model. While 1745 the π^+ absorption and charge exchange interactions are measured by this analysis, the 1746 rate of background interactions (quasielastic, double charge exchange, production) can differ 1747 between data and MC as well. This can lead to wrongly estimated rates of categorization 1748 errors within the fit, and cause biased results of the signal interactions. The same is true 1749 of the rate of proton interactions as well. Protons are often emitted into the detector as 1750 a result of the primary π^+ -Ar interactions, and can go on to interact in the nearby argon, 1751 producing their own interaction products. These products can influence the event selection 1752 and produce categorization errors. Thus, differing rates of proton-argon interactions within 1753 data and MC can also bias the cross section results. 1754

To facilitate the propagation of hadronic modeling uncertainties related to the Geant4 1755 stage of the MC simulation (as discussed in Section 4.6), the Geant4Reweight [59] framework 1756 was used. This framework is able to create weights for events based on some variation applied 1757 to a cross section model in GEANT4. The weights created from this framework work by 1758 determining how likely the event was to occur given the nominal cross sections and the set 1759 of steps taken by a particle, and then comparing this to how likely the same event was to 1760 occur under some variation. The weights are generated under some flat scale factor applied 1761 over a user-defined region of momentum. The momentum regions and prior uncertainties 1762 for each variation were determined by a crude examination of the spread of models studied 1763 within Reference [27]. The description of the systematic parameters are given in Table 8.1. 1764 Geant4Reweight creates a weight for each parameter by running over each π^+ and proton 1765

Channel	Momentum Range	Prior Uncertainty
π^+ Quasielastic	$0500~\mathrm{MeV/c}$	$\pm 36\%$
π^+ Quasielastic	$5002000~\mathrm{MeV/c}$	$\pm 33\%$
π^+ Pion Production	$0-2000~{ m MeV/c}$	$\pm 33\%$
π^+ Double Charge Exchange	$02000~\mathrm{MeV/c}$	$\pm 33\%$
Proton Reaction	$02000~\mathrm{MeV/c}$	$\pm 33\%$

TABLE 8.1: Description of the Geant4Reweight parameters used within the fit.

created within the event and calculating a weight for that particle. These are all multiplied 1766 together to create full event weights. For each parameter, a weight is created at intervals 1767 of 10% from -90% to +100%. In order to create a smoothly varying effect within the fit, 1768 the variations must be interpolated between. Prior to the fit, sets of MC are produced 1769 at each variation for each parameter (note: only one parameter is varied at a time). For 1770 each truth category and reconstructed bin, the ratio between the varied and nominal MC 1771 are calculated and interpolated between using a spline. Then, when running the fit, each 1772 parameter contributes a weight to the event corresponding to the value of the spline at the 1773 parameter's value. All weights from all Geant4Reweight parameters are multiplied together 1774 when creating the predicted distributions for each step of the fit. 1775

1776 8.6 Systematic Covariance Matrix

Table 8.2 summarizes the size of the prior uncertainties that comprise the systematic covariance matrix. Note that all uncertainties described in this section are treated as uncorrelated before the fit.

Parameter	Nominal Value	Prior Uncertainty
$dE/dX C_{cal}$	1.011×10^{-3}	$\pm 10\%$
Beam Momentum	1.00	$\pm 1.2\%$
Electron Diverter Fraction	0.5	± 0.20
No Track Fraction	1.62	± 0.20
Failed Beam Cuts Fraction	1.00	±0.10
π^+ Quasielastic Low	1.00	$\pm 36\%$
π^+ Quasielastic High	1.00	$\pm 33\%$
π^+ Pion Production	1.00	$\pm 33\%$
π^+ Double Charge Exchange	1.00	$\pm 33\%$
Proton Reaction	1.00	$\pm 33\%$

TABLE 8.2: Description of the Geant4Reweight parameters used within the fit.

CHAPTER 9

FIT VALIDATION

This chapter demonstrates validation of the fit framework described in Section 7.4. It includes the systematic uncertainties detailed in Chapter 8. In all tests, a set of MC simulation produced according to the 1 GeV/c beam setting is fit to various fake data inputs also produced from MC simulation. These inputs could be the nominal MC or a set of varied MC. The specifics of the fake data will be described in each section.

To evaluate how the fit performed, several quantities will be examined including the 1786 post-fit values of the parameters, the extracted cross sections, and a goodness of fit metric. 1787 Particular attention will be paid toward the post-fit values of the systematic parameters 1788 as they compare to their prior uncertainties. The goodness of fit will be investigated by 1789 comparing the minimum $-2 \ln \lambda$ (defined in Section 7.4) found by the fit in question to the 1790 distribution of minimum $-2 \ln \lambda$ found in a set of fits to systematically and statistically varied 1791 fake data. This comparison will take the form of a p-value, defined to be the probability 1792 of a fit resulting in a $-2 \ln \lambda_{\text{Min}}$ at least as extreme as the one in question. This is defined 1793 in Equation 9.1 where $t_{\rm Fit}$ represents the $-2\ln\lambda_{\rm Min}$ of the fit in question, and f(t) is the 1794 distribution of $-2 \ln \lambda_{\text{Min}}$ found from the set of systematically and statistically varied fake 1795 data. 1796

$$p = \int_{t_{\text{Fit}}}^{\infty} f(t)dt \tag{9.1}$$

Figure 9.1 shows the distribution of $-2 \ln \lambda_{\text{Min}}$ from 1000 toy fits to systematically and statistically varied fake data. The systematic variations were created with the systematic parameters chosen according to the input covariance matrix (in a manner similar to the post-fit throws described in Section 7.5). Then, each set of systematically-varied fake data was statistically fluctuated. This distribution will be used throughout the following sections to determine p-values for each fit.

Finally, the cross sections extracted from the post-fit MC will be compared to the cross



Figure 9.1: Post-fit $-2\ln\lambda$ distribution of the toy experiments described above.

sections as produced by the fake data input using the χ^2 defined in Equation 9.2.

$$\chi_{\sigma}^2 = \sum_{i,j} (\sigma_i - \bar{\sigma}_i) (V^{\sigma})_{i,j}^{-1} (\sigma_j - \bar{\sigma}_j)$$

$$(9.2)$$

Here, σ_i represents the measured cross section in bin i, $\bar{\sigma}_i$ represents the cross section from either the nominal MC or fake data input (this will be specified), and $(V^{\sigma})_{i,j}^{-1}$ is the value of bin i, j of the inverted cross section covariance matrix as computed in the error propagation procedure described in Section 7.5. This will be used similar to the minimum fit statistic distribution discussed above to determine a p-value for the cross section results. The distribution of χ^2_{σ} from the set of 1000 toy fits is shown in Figure 9.2.



Figure 9.2: χ^2_{σ} distribution of the toy experiments described above.

1811 9.1 Asimov Fit

The first validation test is a simple "Asimov" fit. In this fit, the input fake data is the same as the nominal MC within the fit. This tests the base functionality of the fit and whether or not the fit can correctly identify the minimum (the starting point of the fit). It also shows the level of sensitivity the fit has for the signal and nuisance parameters. The results are shown in Figures 9.3, 9.4, and 9.5. The first shows that the best-fit parameters are at the starting point, as expected. The parameters in these plots are enumerated as in Table 9.1. This will be the same for the rest of the chapter.

0	Absorption factor 400–500 ${\rm MeV}/c$	10	Beam cut efficiency
1	Absorption factor 500–600 ${\rm MeV}/c$	11	Beam momentum resolution
2	Absorption factor 600–700 ${\rm MeV}/c$	12	dE/dX calibration constant
3	Absorption factor 700–800 ${\rm MeV}/c$	13	Electron diverter effect strength
4	Absorption factor 800–1000 ${\rm MeV}/c$	14	Geant4Reweight Double Charge Exchange
5	Charge Exchange factor 500–600 ${\rm MeV}/c$	15	Geant4Reweight Pion Production
6	Charge Exchange factor 600–700 ${\rm MeV}/c$	16	Geant4Reweight Quasielastic Low
7	Charge Exchange factor 700–800 ${\rm MeV}/c$	17	Geant4Reweight Quasielastic High
8	Charge Exchange factor 800–900 ${\rm MeV}/c$	18	Geant4Reweight Proton
9	Muon factor	19	No-track efficiency

TABLE 9.1: The parameters used within the fit. The numbers correspond to the bins shown in the figures throughout the chapter.

1818

The post-fit and nominal MC reconstructed distributions in Figure 9.4 are identical to the Asimov fake data, and both distributions have a $-2\ln\lambda$ of 0 with respect to the fake data as expected from this closure test.



(a) Pre-fit and post-fit parameters.



(b) Post-fit correlation matrix of the fit parameters.

Figure 9.3: A	simov fit	results.
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1821

Pre-fit $-2\ln\lambda_{\text{Stat}}$	0.00
Post-fit $-2\ln\lambda_{\text{Stat}}$	0.00
Post-fit $-2\ln\lambda_{Syst}$	0.00
Fit p-value	1.00
Nominal χ^2_{σ}	0.00
Fake Data χ^2_σ	0.00
Nominal σ p-value	1.00
Fake Data σ p-value	1.00

TABLE 9.2: Numerical results of the fit to Asimov fake data.



Figure 9.4: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the Asimov fit.



Figure 9.5: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and Asimov Fake Data (red points). 9.5c is the correlation between the cross sections. The first five rows are the absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

1822 9.2 Statistically Independent Nominal MC

This test is similar to the previous Asimov fit where the input fake data is the nominal 1823 MC. However, half of the nominal MC was used as the input fake data, and the other half was 1824 used as the input MC. This is to test the performance of the fit to a statistically-independent 1825 set of nominal MC. The input fake data is expected to deviate from the input MC by a normal 1826 statistical fluctuation. This can be seen in Figure 9.7, where the fake data points no longer 1827 lay directly on top of the input MC. As can also be seen in Table 9.3, the post-fit $-2\ln\lambda$ 1828 between the post-fit and fake data reconstructed distributions is less than that between the 1829 pre-fit and fake data distributions, as expected. In Figure 9.6b, the systematic parameters 1830 can be seen to vary from nominal, but within the set of prior uncertainties presented within 1831 the plot (as the blue bands). Finally, the χ^2_{σ} between the measured and fake data cross 1832 sections as shown in Figure 9.8 shows the measured cross section is statistically consistent 1833 with the cross section extracted from the fake data set. 1834





(c) Post-fit correlation matrix of the fit parameters.

(d)

Figure 9.6: Fit results for the statistically independent nominal MC fit.



Figure 9.7: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the statistically independent nominal MC fit.



Figure 9.8: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and Fake Data produced from statistically independent nominal MC (red points). 9.8c is the correlation between the cross sections. The first five rows are absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

Pre-fit $-2\ln\lambda_{\text{Stat}}$	14.72
Post-fit $-2\ln\lambda_{\text{Stat}}$	7.54
Post-fit $-2\ln\lambda_{Syst}$	0.21
Fit p-value	0.97
Nominal χ^2_{σ}	0.21
Fake Data χ^2_σ	0.27
Nominal σ p-value	1.00
Fake Data σ p-value	1.00

TABLE 9.3: Numerical results of the fit to statistically independent fake data.

1835 9.3 Systematic Variation

1836 In this test, the fake data has been generated by using a statistically independent set of MC produced with varied systematic parameters. This is generated by first creating a 1837 random set of systematic parameter values. To create these values, a vector of random, unit-1838 Gaussian distributed values is produced and then multiplied by the lower triangle of the 1839 Cholesky decomposition of the prior covariance matrix of the systematic parameters. This 1840 produces a set of values for the parameters with all correlations encoded. These systematic 1841 parameter values are then applied to half of the MC sample. Both the fake data reconstructed 1842 distributions and the cross sections are extracted from this varied MC sample. The other 1843 half of the MC is used as the input MC to be varied within the fit. The results are shown in 1844 Figures 9.9, 9.10, and 9.11. Figure 9.9a now includes the input systematic parameters used 1845 to create the variation (labeled "Toy Values"). As can be seen in this figure, the post-fit 1846 systematic parameters approach the input values. Shown in Table 9.4, the $-2\ln\lambda$ between 1847 MC and fake data show a large reduction as a result of the fit. Finally, in Figure 9.11 one 1848 can see that the χ^2_σ between the measured and fake data cross sections shows a consistent 1849 fit result.



(a) Pre-fit and post-fit parameters.



(b) Post-fit correlation matrix of the fit parameters.

Figure 9.9: Fit results for the systematically varied fit.

1850



(a) Reconstructed distribution of events selected as Absorption.



(c) Reconstructed distribution of events selected as neither Absorption or Charge Exchange.



(b) Reconstructed distribution of events selected as Charge Exchange.



(d) Reconstructed distribution of events which extend past the Fiducial Volume



(e) The number of events which fail beam cuts (left bin) or lack a reconstructed beam track (right bin).

Figure 9.10: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the systematically varied fit.



Figure 9.11: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and systematically varied Fake Data (red points). 9.11c is the correlation between the cross sections. The first five rows are absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

Pre-fit $-2\ln\lambda_{\text{Stat}}$	155.87
Post-fit $-2\ln\lambda_{\text{Stat}}$	12.69
Post-fit $-2\ln\lambda_{Syst}$	2.84
Fit p-value	0.69
Nominal χ^2_{σ}	0.07
Fake Data χ^2_σ	0.19
Nominal σ p-value	1.00
Fake Data σ p-value	1.00

TABLE 9.4: Numerical results of the fit to systematically and statistically varied fake data.

1851 9.4 Geant4Reweight Fake Data

For this test, fake data is produced by reweighting¹ half of the nominal MC according 1852 to some set of π^+ -Ar and p-Ar cross section variations using Geant4Reweight. Three sets of 1853 fake data were created. The first set was created varying the signal cross sections by some 1854 "reasonable" amount (i.e. similar to the level of the prior uncertainties of the Geant4Reweight 1855 parameters). The second set was created by varying the signal cross sections by an amount 1856 larger than the prior uncertainties on the Geant4Reweight parameters. The final set was 1857 created by varying both the signal and background cross sections. The background cross 1858 sections were varied in a different parameterization than those used in the fit: the bins of the 1859 Geant4Reweight variations in the fake data did not align with the bins in the fit parameters. 1860

1861 9.4.1 Reasonable Variations

The first set of fake data was created with the absorption cross section increased by 30% and the charge exchange cross section reduced by 10% across the full MC momentum range. Shown in Figure 9.12a, the systematic parameters are kept within their prior uncertainties. The reconstructed distributions in Figure 9.13 shows the fit ends in good agreement with the fake data distributions as can be seen in the post-fit $-2\ln\lambda$. Finally, the cross section extracted from the fit agree quite well with the cross sections extracted from the fake data set as can be seen in the "Fake Data χ^2 " in Figure 9.14.

 $^{1^{1}}$ A process to produce varied Monte Carlo samples assuming alternate cross section models, described in Section 8.5.



Figure 9.12: Fit results for the reasonable-variation Geant4Reweight fake data fit.

Pre-fit $-2\ln\lambda_{\text{Stat}}$	30.34
Post-fit $-2\ln\lambda_{\text{Stat}}$	7.65
Post-fit $-2\ln\lambda_{Syst}$	0.54
Fit p-value	0.97
Nominal χ^2_{σ}	3.58
Fake Data χ^2_σ	0.45
Nominal σ p-value	0.94
Fake Data σ p-value	1.00

TABLE 9.5: Numerical results of the fit to reasonable-variation Geant4Reweight fake data.



Figure 9.13: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the reasonable Geant4Reweight fake data fit.



Figure 9.14: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and less extreme Geant4Reweight Fake Data (red points). 9.14c is the correlation between the cross sections. The first five rows are absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

1869 9.4.2 Plausible Variations

The second set of fake data created with Geant4Reweight contained an increase to the absorption cross section by 80% and a reduction of the charge exchange cross section across the full momentum range by 60%. Shown in Table 9.6, the fit ends with a consistent $-2 \ln \lambda$ the post-fit nuisance parameters are within their prior uncertainties showing a successful fit to the fake data. In Figure 9.17, a drastic reduction in χ^2_{σ} is shown, indicating the fit can successfully pick out a variation to the signal cross sections at this level.



Figure 9.15: Fit results for the plausible-variation Geant4Reweight fake data fit.

Pre-fit $-2\ln\lambda_{\text{Stat}}$	151.75
Post-fit $-2\ln\lambda_{\text{Stat}}$	8.01
Post-fit $-2\ln\lambda_{Syst}$	1.33
Fit p-value	0.94
Nominal χ^2_{σ}	20.60
Fake Data χ^2_σ	0.92
Nominal σ p-value	0.29
Fake Data σ p-value	1.00

TABLE 9.6: Numerical results of the fit to plausible-variation Geant4Reweight fake data.



Figure 9.16: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the plausible-variation Geant4Reweight fake data fit.



Figure 9.17: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and plausible-variation Geant4Reweight Fake Data (red points). 9.17c is the correlation between the cross sections. The first five rows are absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

1876 9.4.3 Extreme Variations

The final set of fake data created with Geant4Reweight weights was intended to represent 1877 "extreme" variations. The variations applied to the MC are to increase the total inelastic 1878 cross section by 80% up to 800 MeV/c momentum and to reduce the total inelastic cross 1879 section by 60% above 800 MeV/c. As can be seen in the Figures 9.18 - 9.20, the fit finds a 1880 minimum, but the results indicate a poor result. A few of the systematic parameters shown 1881 in Figure 9.18a are pulled outside of their prior uncertainties. The post-fit $-2\ln\lambda$ in Table 1882 9.7 is large, indicating a bad goodness-of-fit. Similarly, the χ^2 between the measured cross 1883 sections and those extracted from fake data is actually *higher* than that to the nominal MC. 1884 This suggests that the parameterization used within the fit is not suitable for this fake data. 1885 As described in Section 8.5, the systematic parameter for pion production is a single bin from 1886 0 to 2 GeV/c, whereas the variation used to create the fake data has a more complicated 1887 shape to it. This is an example of where the fit on data could fail to find a useful result. If this 1888 was seen in a fit to data, we would reconsider the parameterization of the Geant4Reweight 1889 parameters (i.e. the coarseness of the variation bins). 1890



(a) Pre-fit and post-fit parameters.



(b) Post-fit correlation matrix of the fit parameters.

Figure 9.18: Fit results for the extreme Geant4Reweight fake data fit.



Figure 9.19: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the extreme Geant4Reweight fake data fit.



(c) Cross Section Correlations

Figure 9.20: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and extreme Geant4Reweight Fake Data (red points). 9.20c is the correlation between the cross sections. The first five rows are absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

Pre-fit $-2\ln\lambda_{\text{Stat}}$	358.02
Post-fit $-2\ln\lambda_{\text{Stat}}$	31.62
Post-fit $-2\ln\lambda_{Syst}$	5.87
Fit p-value	0.03
Nominal χ^2_{σ}	0.27
Fake Data χ^2_σ	6.04
Nominal σ p-value	1.00
Fake Data σ p-value	0.84

TABLE 9.7: Numerical results of the fit to unreasonable-variation Geant4Reweight fake data.

1891 9.5 Pion Angle Variation

The next set of fake data used to validate the fit considers a variation to the outgoing 1892 direction of pions produced in quasielastic (QE) events. Note that this is defined according 1893 to the signal definition, and the outgoing pion is required to have above 150 MeV/c for the 1894 event to be considered QE. This is done to test whether the fit is resilient to mismodeling of 1895 outgoing pion kinematics in the Geant4 model used. The angular distribution of outgoing 1896 pions in QE events was modified by-hand to create a varied MC sample. This is done in bins 1897 of true momentum at interaction in order to prevent some variation to be imparted on the 1898 distribution of pion momentum at interaction. The bin edges for these are (0, 400, 600, 800,1899 1000, 2000) MeV/c. In each final momentum bin, the ratio of the varied distribution to the 1900 nominal distribution is used as an event weight to create a set of fake data. Cross sections 1901 from the set of varied MC used to create the fake data are extracted and compared to the 1902 post-fit MC. 1903

1904 9.5.1 Flat Distribution

In this set of fake data, the angular distribution of final state pions is flattened. The nominal distribution, varied distribution, and ratio used for weighting from the 600-800 MeV/c bin are shown in Figure 9.21.



(a) Outgoing pion angular distributions.

(b) Ratio used for weighting QE events.

Figure 9.21: Inputs for this fake data test.

As can be seen in Figure 9.23, small variations occur throughout the distributions. The

most interesting bin is the lowest bin in Figure 9.23d, as it can be explained from the 1909 variation applied. This bin contains QE events with a forward-going pion. Since these 1910 forward-going events have been suppressed in the fake data, this bin has been lowered. Still, 1911 the results of this fit are promising. The post-fit $-2\ln\lambda$ in Table 9.8 shows that the fit is 1912 insensitive to variation, indicating a robustness against data-MC disagreements of this type. 1913 The small variations in the bins mentioned previously show low sensitivity to this type of 1914 physical variation. Furthermore, the χ^2 between the Measured and Nominal & Fake Data 1915 cross sections in Figure 9.24 show a consistent measurement. 1916



(a) Pre-fit and post-fit parameters.



(b) Post-fit correlation matrix of the fit parameters.

Figure 9.22:	Fit	results	for	the	flat	pion	fit.
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Pre-fit $-2\ln\lambda_{\rm Stat}$	18.56
Post-fit $-2\ln\lambda_{\text{Stat}}$	6.61
Post-fit $-2\ln\lambda_{Syst}$	0.33
Fit p-value	0.98
Nominal χ^2_{σ}	0.31
Fake Data χ^2_σ	0.55
Nominal σ p-value	1.00
Fake Data σ p-value	1.00

TABLE 9.8: Numerical results of the fit to varied pion angular distribution fake data.


Figure 9.23: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the flat pion fit.



Figure 9.24: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points), Nominal (blue points), and flat pion Fake Data (red points). 9.24c is the correlation between the cross sections. The first five rows are absorption, and the last four rows are charge exchange. Note that the correlations between the two cross section types are included.

CHAPTER 10

RESULTS

This chapter shows the results of the fit to ProtoDUNE-SP beam data from Run 5809 taken 1918 during its initial running period in the Fall of 2018. The data is comprised of beam-triggered 1919 events with a PID corresponding to π/μ (as defined in Section 5.2). The pre-fit and post-fit 1920 parameters and their corresponding uncertainties are shown in Figure 10.1a along with their 1921 post-fit correlation matrix. The pre-fit (referred to as "Nominal") MC, post-fit MC, and data 1922 event distributions are shown in Figure 10.2. Lastly, the cross sections extracted from the 1923 fit to data are shown in Figure 10.3. This figure contains the correlation matrix and 1-D 1924 error bars (taken from the diagonal of the covariance matrix) as computed from the error 1925 propagation procedure described in Section 7.5. 1926

Figure 10.1a shows the effect on the systematic parameters as a result of the fit. The dE/dX calibration and beam cut efficiency parameters are tightly constrained within the fit, but remain within their prior uncertainties. The Geant4Reweight parameters remain unconstrained by the fit.

The event distributions shown in Figure 10.2 show good agreement between the post-fit MC and data distributions. The resulting p-value of the fit is 0.998, pointing to a successful parameterization of the fit. However, it suggests that the fit could be "too good". This could be due to the choice of parameterization of the fit (perhaps the effects of the efficiencylike systematic parameters are too strong), or it could be due to the size of the post-fit uncertainties being too large.

Finally, the extracted cross sections shown in Figure 10.3 remain consistent with the nominal-MC cross section, as indicated by the χ^2_{σ} of 6.70 shown in these plots. The σ pvalue of this is 0.81, indicating the post-fit cross sections remain consistent with the nominal cross sections.



Figure 10.1: Fit results for the fit to ProtoDUNE-SP data.

Pre-fit $-2\ln\lambda_{\text{Stat}}$	874.37
Post-fit $-2\ln\lambda_{\text{Stat}}$	4.14
Post-fit $-2\ln\lambda_{Syst}$	0.31
Fit p-value	0.998
Nominal χ^2_{σ}	6.70
Nominal σ p-value	0.81

TABLE 10.1: Numerical results of the fit to ProtoDUNE-SP run 5809 data.



Figure 10.2: Reconstructed distributions of events in data (black points), Nominal MC (blue histogram), and post-fit results (red histogram) for the fit to real data.



Figure 10.3: Cross sections extracted from truth information taken from the post-fit MC ("Measured", black points) and Nominal (blue points). 10.3c is the correlation between the cross sections. The first four rows are the absorption, and the last three rows are charge exchange. Note that the correlations between the two cross section types are included.

1941 10.1 Future Work

Some shortcomings within the analysis are worth addressing here. The cross sections 1942 shown in this chapter have relatively large error bars, and remain compatible with the nomi-1943 nal MC at this level of uncertainty. Though this compatibility is not an issue, a reduction in 1944 the measurement's uncertainty would allow us to determine if there is a significant difference 1945 to the cross section models used in DUNE's simulation. A larger data set (such as more 1946 runs taken during Fall 2018) would of course reduce the statistical uncertainties, while a 1947 better understanding of the underlying cause of the Pandora reconstruction efficiency would 1948 improve the systematic uncertainties. The improved understanding of what is causing the 1949 data-MC discrepancies regarding the reconstruction efficiency could provide a more suitable 1950 uncertainty parameterization than the ad-hoc efficiency factors currently used in the fits. 1951 We also chose to neglect SCE uncertainties in this analysis, though these are in development 1952 and will be added in the future. Following the implementation of the SCE uncertainties, the 1953 other runs taken in Fall 2018 will be added. This will increase the size of the data set in 1954 the fit by a factor of 9. These issues will all be iterated upon in future work as this analysis 1955 moves toward publication by the DUNE collaboration. Additionally, a planned second run 1956 of ProtoDUNE-SP will provide even more data for this and future measurements. 1957

1958 10.2 Conclusion

Presented in this thesis is one of the first measurements of π^+ interactions on Argon using 1959 ProtoDUNE-SP data. This measurement would have been impossible without the large 1960 amount of work undertaken within the DUNE collaboration to construct and commission 1961 this detector, currently the largest single-phase LATTPC to have operated. The rapid data-1962 taking in the Fall of 2018 was followed by an immense effort to carefully categorize and 1963 calibrate the data and also to produce an accurate simulation of the detector. An exciting 1964 future awaits ProtoDUNE-SP, as additional configurations of the detector and more beam 1965 data are planned in the coming years. 1966

This analysis shows the first ever measurement of π^+ -Ar charge exchange and the 1967 first measurement of π^+ -Ar absorption in this energy range. The LADS collaboration 1968 measured [22] π^+ -Ar absorption at an energy range below that shown in this thesis. The 1969 LADS measurement is compared to the measurement from this analysis as well as to the 1970 prediction from $Geant4^1$ in Figure 10.4a, while the this measurement of charge exchange is 1971 compared to Geant4 in Figure 10.4b. Of interest is the disagreement between the Geant4 1972 model and the LADS data in the resonance region. A similar analysis using data from 1973 ProtoDUNE-SP at lower momentum will provide a chance to explore this region further. At 1974 higher momentum, the results of this analysis show close agreement with the Geant4 model 1975 for both channels. 1976



Figure 10.4: The measured π^+ -Ar absorption (left) and charge exchange (right) cross sections compared to the nominal Geant4 model. Additionally, the left plot contains an earlier measurement of absorption from the LADS experiment [22].

The fit used to perform this analysis is based on analyses from the T2K experiment to measure ν_{μ} and $\bar{\nu}_{\mu}$ interactions in their near detector ND280 [60][61][62][63][64]. It includes systematic uncertainties due to the detector and signal model. The benefit of doing such an analysis is that it produces robust estimates of the uncertainties and correlations on the extracted cross sections. This allows the data to be properly compared to interaction models used within detector simulations for upcoming experiments including the Short-Baseline

¹These curves were generated by an application within the Geant4Reweight framework. A 150 MeV/c pion momentum threshold was applied in order to match the signal definition for these measurements. The LADS data does not include this threshold.

Neutrino Program at Fermilab and, ultimately, DUNE. By doing this, important systematic
uncertainties regarding the rate of secondary interactions of neutrino interaction products
can be constrained, and will help allow DUNE to achieve the experimental precision required
for its physics goals.

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