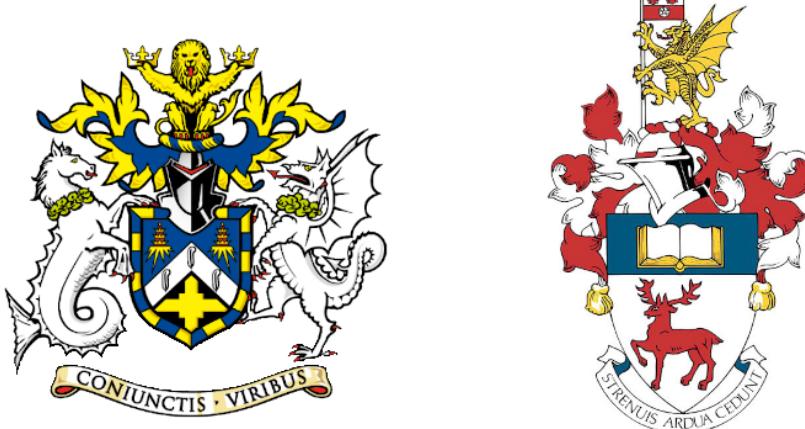


¹ EXPANDING THE PHYSICS REACH
² OF DUNE IN THE NEAR AND
³ FAR DETECTORS



⁴

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⁷ of the Degree of Doctor of Philosophy

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¹² December 2024

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Abstract

31

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¡Oh memoria, enemiga mortal de mi descanso!

El ingenioso hidalgo don Quijote de la Mancha

MIGUEL DE CERVANTES SAAVEDRA

Acknowledgements

34 Work in progress ...

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List of Abbreviations

ADC	Analog to Digital Converter	LBNF	Long Baseline Neutrino Facility
ALEPH	Apparatus for LEP Physics	MEC	Meson-Exchange Current
ALICE	A Large Ion Collider Experiment	MuID	Muon IDentification system
BDT	Boosted Decision Tree	NC	Neutral Current
CAF	Common Analysis File	ND	Near Detector
CC	Charged Current	ND-GAr	Near Detector Gaseous Argon
DIS	Deep Inelastic Scattering	ND-LAr	Near Detector Liquid Argon
DM	Dark Matter	PDG	Particle Data Group
DUNE	Deep Underground Neutrino Experiment	POT	Protons On Target
ECal	Electromagnetic Calorimeter	QE	QuasiElastic
FD	Far Detector	RES	RESonant
FHC	Forward Horn Current	RHC	Reverse Horn Current
GAr	Gaseous Argon	SIS	Shallow Inelastic Scattering
HPgTPC	High Pressure gaseous Time Projection Chamber	SM	Standard Model
LAr	Liquid Argon	SNB	Supernova Neutrino Burst
LBL	Long BaseLine	TP	Trigger Primitive
		WIMP	Weakly Interacting Massive Particle

Introduction

37 *The beginning is the most important part of any work.*

38 – Plato, *The Republic*

39 The Standard Model (SM) of particle physics [1–3] has provided a deep understanding
40 of the electromagnetic, weak and strong interactions, and over the past decades it has
41 passed all kind of precision tests [4]. However, the SM by itself can not explain certain
42 observed phenomena, such as the baryon asymmetry of the universe [5], the existence of
43 Dark Matter (DM) [6], or the origin of neutrino masses [7].

44 One of the biggest puzzles in physics nowadays is how the universe came to be
45 matter-dominated. Following the Big Bang, matter and antimatter were created in equal
46 amounts. A. D. Sakharov described what are the necessary conditions to generate a
47 matter-antimatter asymmetry in the early universe [8]. One of them is the existence
48 of interactions that violate the CP symmetry. It has already been established that
49 the amount of CP violation in the quark sector is not enough to generate the baryon
50 asymmetry [9]. Leptons could contribute to the CP violation through the neutrino
51 oscillation mechanism [10]. However, there is no experimental evidence for this so far.

52 Another yet to be solved mystery of modern physics concerns the nature of DM.
53 From astrophysical observations (see Ref. [6] and references therein), we are aware of
54 the existence of some unknown matter which only interacts gravitationally with other
55 particles. Usually, extensions of the SM include feasible DM candidates. These are usually
56 very stable, heavy particles with small interactions (if any) with SM particles. These

CHAPTER 1. INTRODUCTION

57 states are known as weakly interacting massive particles (WIMPs) [11, 12]. Experiments
58 looking for DM have set the interaction cross section between DM and SM particles to
59 be very small for DM masses below 1 TeV [13].

60 Among other next generation particle experiments, the Deep Underground Neutrino
61 Experiment (DUNE) stands out. Conceived as a neutrino oscillation experiment, it will
62 provide definitive answers to different open questions in the neutrino sector. Its main
63 goals are the discovery of CP violation in the leptonic sector and the determination
64 of the neutrino mass ordering [14]. It will also provide precision measurements of the
65 oscillation parameters within the three-flavour picture.

66 The DUNE far detector (FD) will also search for baryon-number violation and
67 neutrinos originated from supernova explosions. Moreover, its near detector (ND)
68 complex will sit next to the most powerful neutrino beam to date, allowing for a
69 rich neutrino cross section programme. This broad physics range requires a superb
70 performance from the detectors, which can also be used to look for other BSM phenomena.

71 In this thesis, I explore three different aspects of DUNE. Focusing on the data
72 acquisition system of the far detector, I start by proposing a method to enhance the
73 sensitivity of the online processing to low energy events. The idea is to modify the
74 processing chain in order to have more information available to form trigger decisions.
75 I motivate this new approach using both ProtoDUNE data and Monte Carlo (MC)
76 samples, as well as with the results from a test in a real detector setup.

77 Then, I investigate the potential of detecting neutrino fluxes from DM annihilations
78 inside the Sun with DUNE. Although this is the territory of the large volume neutrino
79 telescopes, a detector with the high resolution and pointing capabilities of the DUNE
80 FD can provide complementary information in certain regimes. I present here the results
81 of a preliminary analysis, showing the projected sensitivities for the general case and
82 two particular DM scenarios.

83 Finally, I discuss my work on the reconstruction of ND-GAr, the gaseous argon
84 component of the DUNE ND. These efforts were focused towards the development of
85 the particle identification strategy in the detector. Following a series of additions and

86 upgrades in the reconstruction, I make use of that to perform the first event selection
87 studies with fully reconstructed events in this detector.

88 This thesis opens with an overview of the status of neutrino physics in Chapter
89 2. I start summarising the role that neutrinos play in the SM, to then focus on the
90 developments that lead to the discovery of neutrino oscillations and how to accommodate
91 massive neutrinos in the model. I then discuss the phenomenology of the neutrino
92 oscillations, as well as the current experimental landscape and open questions. In the
93 final section, I review the basics of the neutrino-nucleus interaction modelling, which is
94 of great importance for DUNE.

95 Chapter 3 introduces DUNE, its physics programme and various components. I give
96 detail descriptions of the LBNF beamline, the near detector and the far detector designs.
97 I also discuss the current staging plans for DUNE. This leads to the of ND-GAr, the
98 more capable near detector planned for DUNE Phase II.

99 In Chapter 4 I start by reviewing how the trigger primitives (TPs), the basic building
100 blocks of the DUNE far detector trigger chain, are formed. I then motivate how to
101 use the filtering to enhance the TP generation in the induction channels. I describe
102 the concept of matched filter, and how to optimise it using ProtoDUNE-SP data. I
103 use different MC samples to study its performance, and assess how it improves the hit
104 finding. Finally, I present the results of the tests we performed at the VD ColdBox setup
105 at CERN, were for the first time we collected TP data with a matched filter.

106 The solar DM analysis is presented in Chapter 5. After reviewing the theoretical
107 basis for the solar DM capture and how capture and annihilation rates are related,
108 I introduce the analysis framework used. I then focus on the event selection studies
109 based on two topologies: high-energy DIS events and low-energy $1\mu 1p$ QE events. I
110 use these to extract the projected sensitivities for the DM-nucleon scattering cross
111 section, and compare them to the current status of other direct and indirect DM searches.
112 Additionally, I discuss the potential of DUNE in two specific DM models. I end with a
113 discussion of the systematic uncertainties relevant for this analysis.

114 Chapter 6 starts with a description of GArSoft, the simulation and reconstruction

CHAPTER 1. INTRODUCTION

software of ND-GAr. Then, I describe the charge calibration procedure I implemented using a MC sample of stopping protons. I use this to compute the mean ionisation loss per unit length of the tracks, and show how this procedure can be used for particle separation. Next, I summarise my investigations on the muon and pion separation using the information from the calorimeter. I outline the strategy I followed for the training and testing of the classifiers, commenting on the achieved performance using a neutrino interaction sample. Following this, I introduce the possibility of using the fast timing of the calorimeter to perform a time-of-flight measurement. It will allow to separate pions and protons in a momentum range not accessible to other methods. Additionally, I present a method to identify the decays of charged pions in the TPC, when the decay angle is too small and the pion and muon get merged into a single track. I construct a collection of variables from the track fit that allow to locate the position of the decay. Lastly, I propose a new clustering algorithm optimised for our calorimeter. I then demonstrate its impact in the context of the neutral pion reconstruction. The Chapter finishes with an overview of the integration of these reconstruction items in GArSoft.

The event selection studies are covered in Chapter 7. I start by describing the MC neutrino interaction sample I use for the studies. Then, I focus on the ν_μ CC selection, which includes an optimisation of the fiducial volume. I also explore the kinematics of the selected primary muon and the location of the neutrino vertex. Next, I study the performance of the selections based on the reconstructed charged pion multiplicity, paying special attention to the $1\pi^\pm$ selection. I briefly discuss the possibility of adding the neutral pions in the analysis. Following that, I present the results on the energy reconstruction for the selected charged-current events. I finish with a detailed discussion of the different sources of systematic error relevant for ND-GAr. These include flux and neutrino interaction modelling uncertainties, as well as detector effects.

Eventually, the thesis concludes with Chapter 8. There, I summarise the main results presented in this work, and discuss future plans for the different projects.

2

143

144

Neutrino physics

145 *Little particles of inspiration sleet through the universe all the time traveling
146 through the densest matter in the same way that a neutrino passes through a
147 candyfloss haystack, and most of them miss.*

148

– Terry Pratchett, *Sourcery*

149 Ever since they were postulated in 1930 by Wolfgang Pauli to explain the continuous
150 β decay spectrum [15] and later found by F. Reines and C. Cowan at the Savannah
151 River reactor in 1953 [16], neutrinos have had a special place among all other elementary
152 particles. They provide a unique way to probe a wide range of quite different physics,
153 from nuclear physics to cosmology, from astrophysics to colliders. Moreover, there is
154 compelling evidence to believe that the study of neutrinos may be key to unveil different
155 aspects of physics beyond the SM, difficult to test elsewhere.

156 In this Chapter, I will review the basics of neutrino physics, from its role within the
157 SM to the main open questions related to the neutrino sector, paying special attention
158 to the phenomenology of neutrino oscillations.

159 2.1 Neutrinos in the SM

160 The SM of fundamental interactions was initially proposed in 1967 by S. Glashow,
161 S. Weinberg and A. Salam[1–3]. This theoretical framework describes the dynamics
162 of leptons and quarks, by introducing a collection of mediating gauge vector bosons
163 and one scalar particle, known as the Higgs boson. It assumes that the local $SU(3) \times$

CHAPTER 2. NEUTRINO PHYSICS

164 $SU(2)_L \times U(1)_Y$ gauge symmetry is an internal symmetry of the system, with $SU(3)$
165 describing quantum chromodynamics, and $SU(2)_L \times U(1)_Y$ being the gauge groups of
166 the electroweak sector. For a detailed overview of the SM of electroweak interactions,
167 see Ref. [17].

168 In the SM, neutrinos appear in three flavours, namely ν_e , ν_μ , and ν_τ . These are
169 associated with the corresponding charged leptons, e , μ , and τ . Neutrinos exist only
170 as left-handed particles, grouped in doublets with the charged leptons, while the later
171 come in both chirality states:

$$\begin{pmatrix} \nu_e \\ e_L^- \end{pmatrix}, \quad \begin{pmatrix} \nu_\mu \\ \mu_L^- \end{pmatrix}, \quad \begin{pmatrix} \nu_\tau \\ \tau_L^- \end{pmatrix}, \quad e_R^-, \quad \mu_R^-, \quad \tau_R^-. \quad (2.1)$$

172 Similarly, quarks also exist in both chirality states, and are grouped as:

$$\begin{pmatrix} u_L \\ d_L \end{pmatrix}, \quad \begin{pmatrix} s_L \\ c_L \end{pmatrix}, \quad \begin{pmatrix} t_L \\ b_L \end{pmatrix}, \quad u_R, \quad d_R, \quad s_R, \quad c_R, \quad t_R, \quad b_R. \quad (2.2)$$

173 The fact that there are no right-handed neutrino fields implies that neutrinos are
174 strictly massless within the SM. This restriction follows from the experimental observation
175 that all neutrinos produced via weak interactions are pure left-handed helicity states
176 (and similarly antineutrinos are pure right-handed states). The hypothetical existence
177 of right-handed neutrinos could be indirectly inferred from the observation of non-zero
178 neutrino masses, nevertheless the existence of neutrino masses is not a sufficient condition
179 for the existence of such fields.

180 Left and right-handed fermions transform differently under $SU(2)_L \times U(1)_Y$ rotations,
181 as the right-handed particles are singlets under $SU(2)_L$. Applying a local transformation,
182 they change as:

$$\begin{aligned} \psi_L &\longrightarrow e^{-iY\beta(x)/2} e^{-iT_a\alpha_a(x)} \psi_L, \\ \psi_R &\longrightarrow e^{-iY\beta(x)/2} \psi_R, \end{aligned} \quad (2.3)$$

183 where $Y/2$ and T_a are the generators of $SU(2)_L$ and $U(1)_Y$, respectively, and $\beta(x)$ and

2.1. NEUTRINOS IN THE SM

Table 2.1: Values of T_3 and $Y/2$ assigned to the first generation of fermions.

	e_L	ν_e	e_R	u_L	d_L	u_R	d_R
T_3	-1/2	1/2	0	1/2	-1/2	0	0
$Y/2$	-1/2	-1/2	-1	1/6	1/6	2/3	-1/3

184 $\alpha_a(x)$ are the parameters of the rotation.

185 The values of the quantum numbers $Y/2$ and T_3 , the third component of the weak
186 isospin, have to be assigned to the different particles. The values of T_3 follow from the
187 commutation relations of the generators of $SU(2)$. After the spontaneous symmetry
188 breaking $SU(2)_L \times U(1)_Y \rightarrow U(1)_{EM}$, one finds the relation which determines the electric
189 charge:

$$Q = T_3 + \frac{Y}{2}, \quad (2.4)$$

190 Setting the electric charge to -1 for electrons, we can find the values of the hypercharge
191 for the rest of the fermions. The resulting values for the first generation of leptons and
192 quarks are shown in Tab. 2.1.

193 It is clear that the free Lagrangian of the theory is not be invariant under the gauge
194 transformations, as the kinetic terms contain derivatives. Therefore, to make it invariant,
195 one needs to introduce a set of gauge bosons. They appear in the so-called covariant
196 derivative, which replaces the common derivative and transforms in the same way as the
197 fermion fields under local rotations. This constrain fixes completely the transformations
198 of the spin-1 fields. For left and right-handed particles, the covariant derivatives are
199 given by:

$$\begin{aligned} D_\mu \psi_L &= \left(\partial_\mu + ig' \frac{Y}{2} B_\mu + ig T_a W_\mu^a \right) \psi_L, \\ D_\mu \psi_R &= \left(\partial_\mu + ig' \frac{Y}{2} B_\mu \right) \psi_R, \end{aligned} \quad (2.5)$$

200 where W_μ^i , $i = 1, 2, 3$ and B_μ are the gauge bosons for the $SU(2)_L$ and $U(1)_Y$ factors,
201 respectively, and g and g' are the corresponding gauge couplings. It can be shown that
202 these fields transform in the adjoint representation of the gauge group.

CHAPTER 2. NEUTRINO PHYSICS

Table 2.2: Neutral current couplings.

	u	d	ν_e	e
$2v_f$	$1 - \frac{8}{3}\sin^2\theta_W$	$-1 + \frac{4}{3}\sin^2\theta_W$	1	$-1 + 4\sin^2\theta_W$
$2a_f$	1	-1	1	-1

So far, the theory only contains massless particles, as adding bare mass terms to the Lagrangian would spoil the gauge symmetry. Therefore, the mass terms need to be induced by a spontaneous violation of the symmetries. In the SM, the responsible for this is the Higgs mechanism. The Higgs doublet is coupled to the gauge bosons through the covariant derivative, and to the fermions through the Yukawa couplings. Upon spontaneous symmetry breaking, the vacuum expectation value of the Higgs field generate the mass terms of the particles.

In order to obtain the physical intermediate vector boson states, we need to perform the following redefinitions:

$$\begin{aligned} A_\mu &= \sin \theta_W W_\mu^3 + \cos \theta_W B_\mu, \\ Z_\mu &= \cos \theta_W W_\mu^3 - \sin \theta_W B_\mu, \\ W_\mu^\pm &= \frac{1}{\sqrt{2}} (W_\mu^1 \mp iW_\mu^2), \end{aligned} \tag{2.6}$$

where A_μ is the photon field, and Z_μ and W_μ^\pm are the neutral and the charged weak boson fields, respectively. The Weinberg angle, θ_W , relates the weak coupling constants and the electric charge:

$$e = g' \cos \theta_W = g \sin \theta_W. \tag{2.7}$$

At this point, the interacting part of the electroweak Lagrangian can be re-written as the sum of three contributions: the electromagnetic (EM), charged-current (CC) and neutral-current (NC) components:

$$\begin{aligned} \mathcal{L}_{\text{EW}}^{\text{int}} &= \mathcal{L}_{\text{EM}} + \mathcal{L}_{\text{CC}} + \mathcal{L}_{\text{NC}} \\ &= -eA_\mu J_{\text{EM}}^\mu - \frac{g}{2\sqrt{2}} (W_\mu^+ J_{\text{CC}}^\mu + \text{h.c.}) - \frac{g}{2\cos\theta_W} Z_\mu J_{\text{NC}}^\mu, \end{aligned} \tag{2.8}$$

2.2. TROUBLE IN THE NEUTRINO SECTOR

218 with the currents defined as:

$$\begin{aligned} J_{\text{EM}}^\mu &= \sum_f Q_f \bar{f} \gamma^\mu f, \\ J_{\text{CC}}^\mu &= \sum_\ell \bar{\nu}_\ell \gamma^\mu (1 - \gamma_5) \ell + \sum_f \bar{u}_f \gamma^\mu (1 - \gamma_5) d_f, \\ J_{\text{NC}}^\mu &= \sum_f \bar{f} \gamma^\mu (v_f - a_f \gamma_5) f, \end{aligned} \quad (2.9)$$

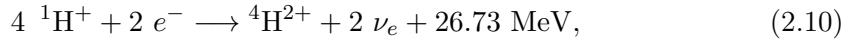
219 where f denotes any SM fermion, ℓ and ν_ℓ a charged lepton and a neutrino of any flavour,
220 and u_f and d_f an up-like and a down-like quarks of any flavour. For the NC case, the
221 values of the v_f and a_f couplings are given in Tab. 2.2.

222 As seen in Eq. (5.8), in the electroweak theory neutrinos are coupled to the Z boson
223 in a universal way. Therefore, by measuring the so-called invisible decay width of the Z
224 boson we have an estimate of the number of light (i.e. lighter than the Z boson) neutrino
225 flavours. This number was measured by LEP in a combined analysis of $e^+ e^- \rightarrow \mu^+ \mu^-$
226 and $e^+ e^- \rightarrow \text{hadrons}$ to be $N_\nu = 2.9840 \pm 0.0082$ [18].

227 2.2 Trouble in the neutrino sector

228 2.2.1 The solar neutrino problem

229 Neutrinos are produced everywhere in vast amounts. One of the most prominent sources
230 of neutrinos in our vicinity is our Sun. The Sun is powered mainly by two nuclear fusion
231 reactions, the p – p chain and the CNO cycle. In both cases, the overall reaction is:



232 where part of the released energy is lost to the neutrinos. The electron neutrinos
233 produced are often labelled after the processes that generate them. Figure 2.1 shows the
234 solar neutrino flux as a function of the neutrino energy, broken down by the production
235 process.

CHAPTER 2. NEUTRINO PHYSICS

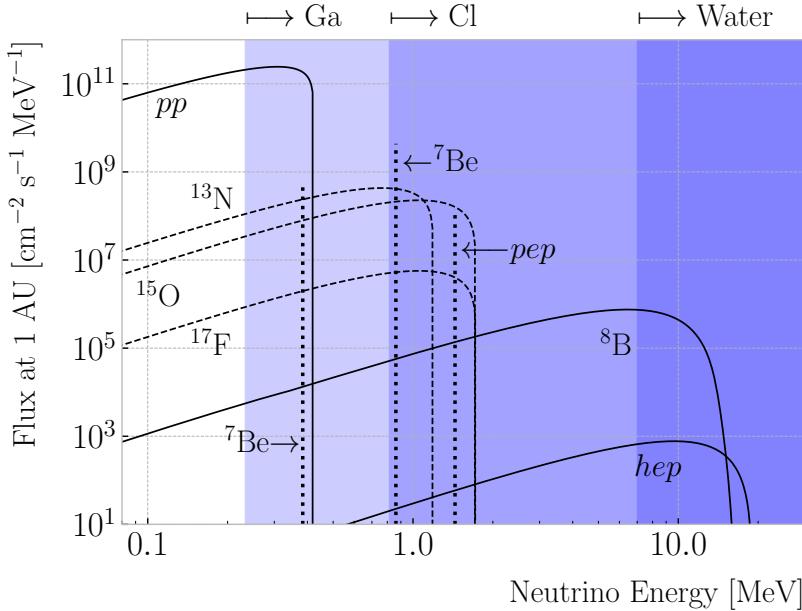


Figure 2.1: Solar neutrino fluxes for the solar model BS05(OP). The detection thresholds for Gallium, Chlorine and water-based experiments are also shown. Figure adapted from Ref. [20].

In the late 1960s, the Brookhaven Solar Neutrino Experiment, led by R. Davis, started

data taking with the goal of measuring the solar neutrino flux [19]. The experiment

used a tank containing 380 m^3 of tetrachloroethene (C_2Cl_4), a liquid commonly used

in dry-cleaning, located 1.5 km underground in the Homestake mine, in Lead, South

Dakota. The incoming neutrinos would get captured following the reaction:



therefore allowing to measure the neutrino flux by counting the ${}^{37}\text{Ar}$ isotopes. The

threshold for this reaction is 0.814 MeV, just below the 0.862 MeV line from the ${}^7\text{Be}$

ground state transition.

The results of the experiment were compared to the theoretical predictions made by

J. Bahcall [21]. During its operation from 1968 to 2002, the experiment observed a solar

ν_e flux that was approximately a third of the total prediction [22].

In the early 1990s, the SAGE [23] and GALLEX [24] experiments started operations.

2.2. TROUBLE IN THE NEUTRINO SECTOR

248 The detection principle used for both experiments was similar to that of the Homestake
 249 experiment, but using ^{71}Ga instead of C_2Cl_4 . With a detection threshold of 0.233 MeV,
 250 the Gallium-based experiments were able to observe the pp neutrino flux. Both
 251 experiments measured a solar electron neutrino flux that was a factor of two lower
 252 than the predictions, demonstrating that this deficit was energy-dependent.

253 In the early 2000s, the SNO experiment put an end to the solar neutrino puzzle
 254 [25, 26]. Thanks to its directionality capabilities, being a Cherenkov light detector, as
 255 well as to its heavy water target, SNO measured the total solar neutrino flux through
 256 the NC process:

$$\nu_\alpha + d \longrightarrow n + p + \nu_\alpha, \quad (2.12)$$

257 where $\alpha = e, \mu, \tau$. This measurement agreed with the solar model predictions. Then,
 258 measuring the CC reaction:

$$\nu_e + d \longrightarrow p + p + e^-, \quad (2.13)$$

259 they were able to establish that the ν_μ and ν_τ solar fluxes are in fact non-zero, revealing
 260 that electron neutrinos were transitioning into different flavours.

261 2.2.2 The atmospheric neutrino problem

262 When cosmic-rays interact with the atoms in the upper atmosphere, a plethora of
 263 hadrons, mainly π and K mesons, are produced. In particular, for the charged pions,
 264 we have the following decay chain dominates:

$$\begin{aligned} \pi^+ &\longrightarrow \mu^+ + \nu_\mu, \\ \mu^+ &\longrightarrow e^+ + \bar{\nu}_\mu + \nu_e, \end{aligned} \quad (2.14)$$

265 and similar for the antiparticles. For neutrino energies < 1 GeV, the ratio:

$$\frac{N(\nu_\mu + \bar{\nu}_\mu)}{N(\nu_e + \bar{\nu}_e)}, \quad (2.15)$$

266 of produced neutrinos and antineutrinos is, in good approximation, equal to two [27].

CHAPTER 2. NEUTRINO PHYSICS

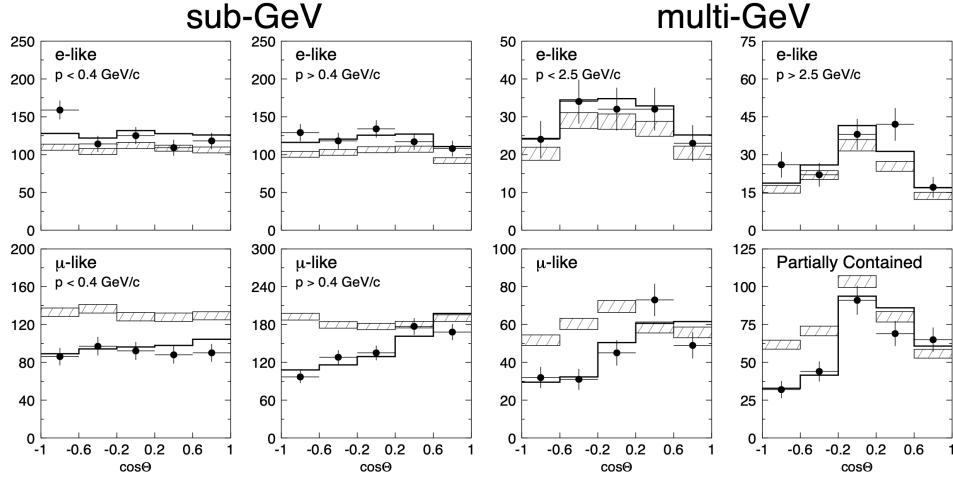


Figure 2.2: Zenith angle distributions for the selected ν_e (top row) and ν_μ (bottom row) events in the SK detector. The hatched region corresponds to the expectation in the case of no oscillations, whereas the solid line indicates the best-fit in the case of $\nu_\mu \rightarrow \nu_\tau$ oscillations. Figure taken from Ref. [32].

267 During the 1980s, several proton decay experiments, like Kamiokande [28], IMB [29],

268 MACRO [30], and Soudan-2 [31], measured the flux of atmospheric neutrinos. This was

269 an important part of their research programme, as the atmospheric neutrinos constitute

270 their main background. All these experiments reported an atmospheric neutrino ratio

271 lower than the predictions.

272 A few years before the SNO discovery, in 1998, Super-Kamiokande (SK) collaboration

273 measured the atmospheric ν_e and ν_μ spectra as a function of the zenith angle [32].

274 Upward-going particles have negative zenith angle, $\cos \Theta < 0$, indicating that they

275 entered from the bottom of the detector. These upward-going neutrinos had to travel

276 through the Earth in order to reach the detector, allowing SK to probe a broad range

277 of baselines. Figure 2.2 shows the reported distributions (black dots), compared to the

278 no oscillations prediction (hatched region). This measurement confirmed that muon

279 neutrinos transition to other flavours, and that this phenomenon depends both on the

280 energy and the path length of the neutrino.

281 The SK and SNO findings provided definitive evidence for the existence of neutrino

282 oscillations, and therefore non-zero neutrino masses. This constitutes one of the

283 groundbreaking discoveries of modern physics and has acted as driving force for beyond

2.3. MASSIVE NEUTRINOS

284 the Standard Model (BSM) physics. The minimal extension of the SM we can do to
 285 address these phenomena is introducing different masses for at least two of the neutrinos.
 286 This way, we are left with three neutrino mass eigenstates ν_1 , ν_2 , and ν_3 , with masses m_1 ,
 287 m_2 , and m_3 respectively, which in general will not coincide with the flavour eigenstates,
 288 ν_e , ν_μ , and ν_τ .

289 2.3 Massive neutrinos

290 The existence of neutrino oscillations imply that neutrinos are massive particles. However,
 291 as we have seen before, within the SM neutrinos are massless, as they do not have a
 292 mass term in the Lagrangian. If one wants to give neutrinos a mass, the particle content
 293 of the SM needs to be expanded.

294 A way of generating massive neutrinos while maintaining gauge invariance is by
 295 introducing an arbitrary number of sterile neutrinos N_i , $i = 1, \dots, m$. These allow for
 296 two different types of neutrino mass terms:

$$-\mathcal{L}_{M_\nu} = \sum_{i=1}^m \sum_{j=1}^3 M_D^{ij} \bar{N}_i \nu_{Lj} + \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m M_N^{ij} \bar{N}_i N_j^c + \text{h.c.}, \quad (2.16)$$

297 where M_D is a complex $m \times 3$ matrix and M_N a complex and symmetric $m \times m$ matrix.
 298 The first term, often referred to as the Dirac mass term, arises from the corresponding
 299 Yukawa interaction after the spontaneous electroweak symmetry breaking, similar to
 300 the other fermions. The second term, called the Majorana mass term, is allowed in the
 301 Lagrangian, as it is a singlet of the gauge group. However, it violates lepton number
 302 conservation by two units.

303 If one imposes lepton number symmetry conservation, the Majorana term must
 304 banish, $M_N = 0$. In this case, if $m = 3$ we can identify the sterile neutrinos as the
 305 right-handed component of the neutrino field. The Dirac mass matrix can be diagonalised
 306 using two unitary matrices, V_R^ν and V_L^ν , as:

$$M_D = V_R^\nu \text{ diag}(m_1, m_2, m_3) V_L^{\nu\dagger}, \quad (2.17)$$

CHAPTER 2. NEUTRINO PHYSICS

307 where m_i , $i = 1, 2, 3$ are the masses of the three neutrino mass eigenstates.

308 The neutrino mass term can be written in term of the resulting eigenstates as:

$$-\mathcal{L}_{M_\nu} = \sum_{i=1}^3 m_i \bar{\nu}_{Di} \nu_{Di}, \quad (2.18)$$

309 with:

$$\nu_{Di} = \left(V_L^{\nu\dagger} \nu_L \right)_i + \left(V_R^{\nu\dagger} N \right)_i. \quad (2.19)$$

310 In this scenario, both the low energy particle budget and the symmetries of the SM
 311 have to be modified. Moreover, the masses of the neutrinos are generated exclusively
 312 through the Higgs mechanism, which does not explain why they are much smaller than
 313 those of the charged leptons.

314 Going back to the general case, we can re-write Eq. (2.16) in matrix form as:

$$-\mathcal{L}_{M_\nu} = \frac{1}{2} \left(\bar{\nu}_L^c, \bar{N} \right) \begin{pmatrix} 0 & M_D^T \\ M_D & M_N \end{pmatrix} \begin{pmatrix} \nu_L \\ N^c \end{pmatrix} + \text{h.c.} = \bar{\nu}^c M_\nu \nu + \text{h.c.}, \quad (2.20)$$

315 with $\nu = (\nu_L, N^c)^T$ being a $(3+m)$ -dimensional vector grouping the active and the
 316 sterile neutrinos. The matrix M_ν , which is a complex $(3+m) \times (3+m)$ symmetric
 317 matrix, can be diagonalised by means of a unitary matrix V^ν , yielding:

$$M_\nu = V^\nu \text{ diag}(m_1, m_2, \dots, m_{3+m}) V^{\nu T}. \quad (2.21)$$

318 Using this eigendecomposition, the neutrino mass term can be expressed as:

$$-\mathcal{L}_{M_\nu} = \frac{1}{2} \sum_{i=1}^{3+m} m_i \bar{\nu}_{Mi} \nu_{Mi}, \quad (2.22)$$

319 where the states ν_{Mi} , commonly referred to as Majorana neutrinos, are defined as:

$$\nu_{Mi} = \left(V^{\nu\dagger} \nu \right)_i + \left(V^{\nu\dagger} \nu \right)_i^c, \quad (2.23)$$

320 in such a way that the Majorana condition, $\nu_M^c = \nu_M$, holds true.

2.4. NEUTRINO OSCILLATION FORMALISM

321 As a consequence of the Majorana condition, the neutrino and the antineutrino states
 322 can be described in terms of a single field. As opposed to the charged leptons, which
 323 need to be represented by a four-component or Dirac spinor, the Majorana neutrino is
 324 described by a two-component or Weyl spinor.

325 If the eigenvalues of the Majorana mass matrix, M_N , are much larger than the
 326 electroweak symmetry breaking scale, the diagonalisation of M_ν leads to 3 light and m
 327 heavy neutrino states:

$$-\mathcal{L}_{M_\nu} = \frac{1}{2}\bar{\nu}_l M_l \nu_l + \frac{1}{2}\bar{\nu}_h M_h \nu_h, \quad (2.24)$$

328 where the two mass matrices are given by:

$$\begin{aligned} M_l &\simeq -V_l^T M_D^T M_N^{-1} M_D V_l, \\ M_h &\simeq V_h^T M_N V_h, \end{aligned} \quad (2.25)$$

329 with V_l and V_h two unitary matrices.

330 This scenario represents the so-called see-saw mechanism [33–37]. The name comes
 331 from the fact that the masses of the heavy states are proportional to M_N , whereas for
 332 the light states they are proportional to M_N^{-1} . While both the heavy and the light
 333 neutrinos are Majorana particles, it can be shown that the heavy states are mainly
 334 right-handed, whereas the light ones are mostly left-handed.

335 2.4 Neutrino oscillation formalism

336 Neutrino oscillations were first proposed in 1958 by B. Pontecorvo [38], inspired by the
 337 neutral kaon oscillation phenomenon [39]. Neutral kaons, K^0 and \bar{K}^0 , have opposite
 338 strangeness (± 1) and are produced in strong processes. It was observed that, when
 339 having a beam initially pure of neutral kaons of one type, these would transition into
 340 their antiparticles while propagating. Because the weak interaction does not conserve
 341 strangeness, neutral kaons can change their identity via the processes shown in Fig. 2.3.

342 The mixing considered initially by Pontecorvo was between the neutrino and the

CHAPTER 2. NEUTRINO PHYSICS

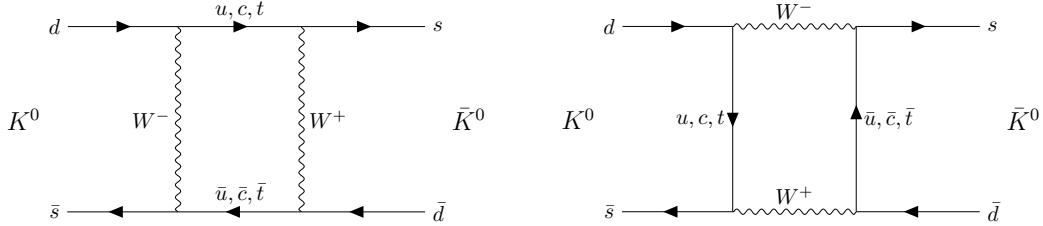


Figure 2.3: $K^0 \rightleftharpoons \bar{K}^0$ mixing through W^\pm exchange.

343 antineutrino states, as only one neutrino flavour was known at the time. After the
344 discovery of the muon neutrino, the mixing between flavours was also explored [40].

345 In the general case, we have 3 active and m sterile neutrinos, resulting in $3 + m$
346 neutrino mass eigenstates. Working in the mass basis, the leptonic charged-current
347 Lagrangian can be written as:

$$-\mathcal{L}_{CC}^{lep} = \frac{g}{\sqrt{2}} (\bar{e}_L, \bar{\mu}_L, \bar{\tau}_L) \gamma^\mu U \begin{pmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_{3+m} \end{pmatrix} W_\mu^+ + \text{h.c.}, \quad (2.26)$$

348 where U is a $3 \times (3 + m)$ matrix which obeys $UU^\dagger = I_{3 \times 3}$, but in general will not be
349 unitary, $U^\dagger U \neq I_{(3+m) \times (3+m)}$.

350 The leptonic mixing matrix, U , establishes how the neutrino mass states couple to
351 the charged leptons. In general, a complex $n \times n$ matrix can be fully specified by $2n^2$ real
352 parameters. If the matrix is unitary, then the number of independent parameters reduces
353 to n^2 , as one has to impose n normalisation and $n(n - 1)$ orthogonality constraints.
354 In our case, we can further reduce the number of parameters by performing a phase
355 redefinition of the charged lepton fields, without affecting the physics. This is not true
356 for the neutrinos. As they may be their own antiparticles, one is not allowed to remove
357 any physically relevant phases. If we consider n generations of leptons, the total number
358 of parameters in the mixing matrix is $n^2 - n$. Out of these, half of them are mixing
359 angles, while the other half are complex phase factors.

360 Considering the extended SM without any additional sterile neutrino states, the
361 resulting 3×3 mixing matrix is unitary. This matrix, often called the Pontecorvo-Maki-

2.4. NEUTRINO OSCILLATION FORMALISM

362 Nakagawa-Sakata (PMNS) matrix [41, 42], relates the set of active neutrinos and the
363 three mass eigenstates as:

$$|\nu_\alpha\rangle = \sum_{i=1}^3 U_{\alpha i}^* |\nu_i\rangle, \quad (2.27)$$

364 where the Greek index α denotes the flavour $\{e, \mu, \tau\}$ and the Latin index i the mass state
365 $\{1, 2, 3\}$. This leptonic mixing matrix may be parametrized in terms of 6 parameters,
366 of which are mixing angles θ_{12} , θ_{13} and θ_{23} , one CP-violating phase δ_{CP} and 2 Majorana
367 phases α and β :

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13} e^{-i\delta_{CP}} \\ 0 & 1 & 0 \\ -s_{13} e^{i\delta_{CP}} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\alpha} & 0 \\ 0 & 0 & e^{i\beta} \end{pmatrix}, \quad (2.28)$$

368 where $c_{ij} \equiv \cos \theta_{ij}$ and $s_{ij} \equiv \sin \theta_{ij}$. This matrix is analogous to the Cabibbo-Kobayashi-
369 Maskawa (CKM) matrix in the quark sector. If neutrinos are Dirac fermions, we can
370 drop the Majorana phases in the PMNS matrix, as in this case we can perform the
371 phase redefinitions. However, these phases play no role on the neutrino oscillation
372 phenomenology.

373 In the case that additional sterile neutrinos states are present, the full leptonic mixing
374 matrix would not be unitary in general. For instance, in the see-saw scenario, the 3×3
375 submatrix for the three light Majorana neutrinos is not unitary. However, the deviations
376 from unitarity are of the order $\mathcal{O}(M_D/M_N)$, and therefore expected to be negligible.

377 2.4.1 Oscillations in vacuum

378 Consider the case where a neutrino of flavour α is produced at $t = 0$, and then it
379 propagates through vacuum. Such a state will evolve in time according to the relation:

$$|\nu_\alpha(\vec{x}, t)\rangle = \sum_{i=1}^3 U_{\alpha i}^* e^{-i(E_i t - \vec{p}_i \cdot \vec{x})} |\nu_i(\vec{x} = \vec{0}, t = 0)\rangle, \quad (2.29)$$

380 in the plane wave approximation, as the mass eigenstates are also eigenstates of the free
381 Hamiltonian.

CHAPTER 2. NEUTRINO PHYSICS

This way, the probability for the neutrino to transition from flavour α to flavour β

will be given by:

$$P(\nu_\alpha \rightarrow \nu_\beta) = |\langle \nu_\beta | \nu_\alpha(\vec{x}, t) \rangle|^2 = \left| \sum_{i=1}^3 \sum_{j=1}^3 U_{\alpha i}^* U_{\beta j} e^{-i(E_i t - \vec{p}_i \cdot \vec{x})} \langle \nu_j | \nu_i \rangle \right|^2 \\ = \left| \sum_{i=1}^3 U_{\alpha i}^* U_{\beta i} e^{-i(E_i t - \vec{p}_i \cdot \vec{x})} \right|^2, \quad (2.30)$$

where we have used the orthogonality relation $\langle \nu_i | \nu_j \rangle = \delta_{ij}$. A usual approximation to

take at this point is to consider ultra-relativistic neutrinos, i.e. $p_i \simeq E$, so we can write

the dispersion relations as:

$$E_i = \sqrt{p_i^2 + m_i^2} \approx E + \frac{m_i^2}{2E}. \quad (2.31)$$

In the end, assuming $t \approx L$ where L is the distance between the production and the

detection points, the probability for the $\nu_\alpha \rightarrow \nu_\beta$ transition becomes:

$$P(\nu_\alpha \rightarrow \nu_\beta) = \sum_{i,j} U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j} e^{-i \frac{\Delta m_{ij}^2}{2E} L} \\ = \delta_{\alpha\beta} - 4 \sum_{i < j} \Re e [U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^*] \sin^2 \left(\frac{\Delta m_{ij}^2}{4E} L \right) \\ + 2 \sum_{i < j} \Im m [U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^*] \sin \left(\frac{\Delta m_{ij}^2}{2E} L \right), \quad (2.32)$$

where Δm_{ij}^2 is the difference of the squared masses of the j th and i th neutrino mass

eigenvalues. At this point, it is usual to write the phase responsible for the oscillations

as:

$$\Delta_{ij} \equiv \frac{\Delta m_{ij}^2}{4E} L \simeq 1.27 \frac{\Delta m_{ij}^2}{(\text{eV}^2)} \frac{L}{(\text{km})} \frac{(\text{GeV})}{E}. \quad (2.33)$$

Notice that, in the case of antineutrinos, the only difference would be the sign of the

last term in the oscillation probability. As the process $\bar{\nu}_\alpha \rightarrow \bar{\nu}_\beta$ is the CP-mirror image

of $\nu_\alpha \rightarrow \nu_\beta$, the differences between their oscillation probabilities would be a measure of

2.4. NEUTRINO OSCILLATION FORMALISM

395 CP symmetry violation:

$$\begin{aligned} A_{CP}^{\alpha\beta} &= P(\nu_\alpha \rightarrow \nu_\beta) - P(\bar{\nu}_\alpha \rightarrow \bar{\nu}_\beta) \\ &= 4 \sum_{i<j} \Im \left[U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^* \right] \sin 2\Delta_{ij}. \end{aligned} \quad (2.34)$$

396 Assuming that CPT invariance holds, then the following relation must be true:

$$P(\nu_\alpha \rightarrow \nu_\beta) = P(\bar{\nu}_\beta \rightarrow \bar{\nu}_\alpha), \quad (2.35)$$

397 as these two process are related by the CPT symmetry. From the definition of probability,
398 we also must have:

$$\sum_{\beta} P(\nu_\alpha \rightarrow \nu_\beta) = \sum_{\beta} P(\bar{\nu}_\alpha \rightarrow \bar{\nu}_\beta) = 1, \quad (2.36)$$

399 where the sum includes all flavours, including α . From these two constraints, one can
400 probe that:

$$A_{CP}^{\alpha\beta} = -A_{CP}^{\beta\alpha}, \quad (2.37)$$

401 and in particular:

$$A_{CP}^{\alpha\alpha} = 0. \quad (2.38)$$

402 A direct consequence of this last relation is that there are no observable CP-violating
403 effects in the so-called disappearance experiments. One needs to perform appearance
404 experiments, where the flavour detected is different from the original flavour, in order
405 to measure the CP asymmetry. Neutrino experiments often report the amount of CP-
406 violation through the Jarlskog invariant. In terms of the parametrisation typically used
407 to write the PMNS matrix, it is given by:

$$J = \frac{1}{8} \cos \theta_{13} \sin 2\theta_{12} \sin 2\theta_{13} \sin 2\theta_{23} \sin \delta_{CP}. \quad (2.39)$$

408 The Jarlskog invariant can be used to compare the amount of CP-violation in the lepton
409 and the quark sectors, where $J = 3.12^{+0.13}_{-0.12} \times 10^{-5}$ in the latter [43].

CHAPTER 2. NEUTRINO PHYSICS

410 2.4.2 Oscillations in matter

411 When neutrinos propagate through matter, their oscillation can be affected in mainly
 412 two ways. First, neutrinos can inelastically scatter with nuclei, thus destroying the
 413 coherent propagation of their quantum state. Nevertheless, in most cases this effect is
 414 negligible (even in very dense mediums like the core of the Sun). Second, neutrinos can
 415 also experience coherent or forward scatterings, that can affect their oscillation but not
 416 lose the coherent propagation of the state.

417 The first proposed model to account for neutrino oscillations in matter was proposed
 418 by Mikhaev, Smirnov and Wolfenstein (MSW) [44]. It relies on the fact that, as the
 419 only charged lepton present in ordinary matter is the electron, electron neutrinos can
 420 undergo both charged and neutral-current interactions with matter whereas for muon
 421 and tau neutrinos just neutral currents are possible.

422 An illustrative way to introduce the MSW mechanism is by considering the two
 423 flavours case. It can be shown that the evolution of the two flavour eigenstates in vacuum
 424 is given by the following time-dependent Schrödinger equation:

$$i \frac{d}{dt} \begin{pmatrix} \nu_e \\ \nu_\mu \end{pmatrix} = H_V \begin{pmatrix} \nu_e \\ \nu_\mu \end{pmatrix}, \quad (2.40)$$

425 with a vacuum Hamiltonian given by:

$$H_V = \frac{\Delta m^2}{4E} \begin{pmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix}, \quad (2.41)$$

426 where Δm^2 is the mass splitting between the two neutrino states and θ the only mixing
 427 angle. For simplicity, I omit the terms of the Hamiltonian that are proportional to the
 428 identity, as they do not affect the oscillation phenomenology.

429 The NC contribution to the matter potential is identical for all the flavours, and has
 430 the form:

$$V_{NC} = -\frac{G_F}{\sqrt{2}} N_n(x), \quad (2.42)$$

2.4. NEUTRINO OSCILLATION FORMALISM

431 where G_F is the Fermi constant and $N_n(x)$ the local neutron density. Because it is
 432 common to all flavours, I do not take it into account in the effective Hamiltonian, as it
 433 would appear as a term proportional to the identity. The CC component only affects
 434 the electron neutrino (and antineutrino). It can be written as:

$$V_{\text{CC}} = \pm \sqrt{2} G_F N_e(x), \quad (2.43)$$

435 with $N_e(x)$ being the local electron density in the material. In the end, the effective
 436 Hamiltonian which describes the propagation of the flavour eigenstates in matter only
 437 contains an extra $\nu_e - \nu_e$ element:

$$H_M = H_V + \begin{pmatrix} V_{\text{CC}} & 0 \\ 0 & 0 \end{pmatrix}. \quad (2.44)$$

438 The solution to the Schrödinger equation greatly simplifies if one considers the case
 439 of a constant matter density. In that case, the effective Hamiltonian can be diagonalised,
 440 obtaining the effective neutrino mass eigenstates in matter. It can be re-written in the
 441 same form as the vacuum Hamiltonian:

$$H_M = \frac{\Delta m_m^2}{4E} \begin{pmatrix} -\cos 2\theta_m & \sin 2\theta_m \\ \sin 2\theta_m & \cos 2\theta_m \end{pmatrix}, \quad (2.45)$$

442 where the effective mass splitting and the effective mixing angle are given by:

$$\begin{aligned} \Delta m_m^2 &= \lambda \Delta m_m^2, \\ \sin 2\theta_m &= \frac{\sin 2\theta_m}{\lambda} \end{aligned} \quad (2.46)$$

443 with:

$$\begin{aligned} \lambda &= \sqrt{(\cos 2\theta - A)^2 + \sin^2 2\theta}, \\ A &= \pm \frac{2\sqrt{2} G_F N_e E}{\Delta m^2}. \end{aligned} \quad (2.47)$$

444 In terms of the effective matter oscillation parameters, the transition probability

CHAPTER 2. NEUTRINO PHYSICS

445 $\nu_e \rightarrow \nu_\mu$ (in the two flavour approximation) reads:

$$P(\nu_e \rightarrow \nu_\mu) = \sin^2 2\theta_m \sin^2 \left(\frac{\Delta m_m^2}{2E} L \right) \quad (2.48)$$

446 From this last equation one can see that, when $\cos 2\theta = A > 0$ the oscillations are
447 greatly enhanced. This effect is known as the MSW resonance. For the neutrinos, this
448 resonant condition is only satisfied if $\Delta m^2 > 0$ (the opposite is true for antineutrinos).
449 This is can be exploited by long baseline experiments, which can gain sensitivity to the
450 neutrino mass hierarchy through matter effects.

451 2.4.3 Current status of neutrino oscillations

452 A wide range of neutrino experiments provide experimental input to the neutrino
453 oscillation framework, both using natural or synthetic neutrino sources. The results
454 from one of the neutrino global fit analyses, shown in Tab. 2.3 ¹, summarise well our
455 current understanding of the different oscillation parameters.

456 **Solar neutrino experiments** detect neutrinos produced in thermonuclear reactions
457 inside the Sun, mainly from the so-called *pp* chain and the CNO cycle. These neutrinos
458 have a typical energy in the range from 0.1 to 20 MeV. These experiments (Homestake
459 [45], GALLEX [24], SAGE [23], Borexino [46], Super-Kamiokande [47] and SNO [48])
460 provide the best sensitivities to θ_{12} and Δm_{21}^2 .

461 **Atmospheric neutrino experiments** detect the neutrino flux produced when
462 cosmic rays scatter with particles in Earth's atmosphere. These collisions generate particle
463 showers that eventually produce electron and muon neutrinos (and antineutrinos). Their
464 energies range from few MeV to about 10^9 GeV. Experiments, like Super-Kamiokande
465 [49] and IceCube [50] use atmospheric neutrinos to measure oscillations and are specially
466 sensitive to θ_{23} and Δm_{32}^2 .

467 **Reactor neutrino experiments** look for the $\bar{\nu}_e$ spectrum produced by nuclear
468 reactors, with energies in the MeV scale. Depending on the distance to the source,

1These are the results reported during M. Tórtola's talk at Neutrino 2024 (see this link). I need to keep an eye and see if they publish these or other updated results in the near future.

2.5. OPEN QUESTIONS IN THE NEUTRINO SECTOR

Table 2.3: Summary of neutrino oscillation parameters determined in the Neutrino Global Fit of 2020 [61].

Parameter	Best fit $\pm 1\sigma$	3σ range
Δm_{21}^2 [eV $^2 \times 10^{-5}$]	$7.55^{+0.22}_{-0.20}$	6.98 – 8.19
$ \Delta m_{31}^2 $ [eV $^2 \times 10^{-3}$] (NO)	$2.51^{+0.02}_{-0.03}$	2.43 – 2.58
$ \Delta m_{31}^2 $ [eV $^2 \times 10^{-3}$] (IO)	$2.41^{+0.03}_{-0.02}$	2.34 – 2.49
$\sin^2 \theta_{12}/10^{-1}$	3.04 ± 0.16	2.57 – 3.55
$\sin^2 \theta_{23}/10^{-1}$ (NO)	$5.64^{+0.15}_{-0.21}$	4.23 – 6.04
$\sin^2 \theta_{23}/10^{-1}$ (IO)	$5.64^{+0.15}_{-0.18}$	4.27 – 6.03
$\sin^2 \theta_{13}/10^{-2}$ (NO)	$2.20^{+0.05}_{-0.06}$	2.03 – 2.38
$\sin^2 \theta_{13}/10^{-2}$ (IO)	$2.20^{+0.07}_{-0.04}$	2.04 – 2.38
δ_{CP}/π (NO)	$1.12^{+0.16}_{-0.12}$	0.76 – 2.00
δ_{CP}/π (IO)	$1.50^{+0.13}_{-0.14}$	1.11 – 1.87

469 long-baseline experiments like KamLAND [51] are sensitive to the solar mass splitting
470 Δm_{21}^2 whereas much shorter baseline experiment such as RENO [52] or DayaBay [53]
471 measure θ_{13} and Δm_{31}^2 .

472 **Accelerator experiments** measure neutrino fluxes generated in particle accelerators.
473 Usually mesons are produced in the accelerator to be focused into a beam, then some
474 decay to muon neutrinos and the rest are absorbed by a target. Depending on the
475 configuration one can obtain a beam made of mostly neutrinos or antineutrinos. The
476 typical energies of these neutrinos are in the GeV range. Experiments such as NOvA
477 [54], T2K [55], MINOS [56], OPERA [57] and K2K [58] (and in the future DUNE [59])
478 are primarily sensitive to θ_{13} , θ_{23} and Δm_{32}^2 . Also, in the coming years DUNE [59] and
479 Hyper-Kamiokande [60] will be sensitive to δ_{CP} .

480 2.5 Open questions in the neutrino sector

481 A crucial question that remains open these days, and is of vital importance for oscillation
482 phenomena, is whether the mass eigenvalue ν_3 is the heaviest (what we call normal
483 ordering) or the lightest (referred to as inverted ordering) of the mass eigenstates. In

CHAPTER 2. NEUTRINO PHYSICS

484 other words, this means that we do not know the sign of Δm_{32}^2 , so we can either have
485 $m_1 < m_2 < m_3$ (NO) or $m_3 < m_1 < m_2$ (IO).

486 Another big puzzle is related to the value of δ_{CP} . Nowadays it is poorly constrained,
487 with all values between π and 2π being consistent with data. A prospective measurement
488 different from $\delta_{CP} = 0, \pi$ will predict CP-violation in the leptonic sector, and thus
489 contribute along with the one measured in the quark sector to the total amount of
490 CP-violation. Although it is true that these two contributions by themselves are not
491 enough to explain the matter anti-matter asymmetry in our universe, the amount of
492 CP-violation in the leptonic sector can be key to explain such imbalance.

493 Both of these questions, because of their nature, could be understood thanks to
494 future oscillation experiments.

495 Notwithstanding, there are other mysteries that can not be unveiled just by conducting
496 oscillation experiments, as certain quantities do not influence these phenomena. Among
497 these there is the question of the absolute values of the neutrino masses. Depending
498 on the value of the lightest of the neutrino masses we can have different mass spectra,
499 from hierarchical $m_1 \ll m_2 < m_3$ (NO) or $m_3 \ll m_1 < m_2$ (IO) to quasi-degenerate
500 $m_1 \simeq m_2 \simeq m_3$.

501 Other open question concerns the nature itself of the neutrinos. If neutrinos are Dirac
502 particles then their mass term can be generated through the usual Higgs mechanism
503 by adding right-handed neutrino fields. However, if they are Majorana particles and
504 therefore their own antiparticles, there is no need to add extra fields to have the mass
505 term in the Lagrangian. Experiments like SuperNEMO [62], SNO+ [63] and NEXT
506 [64], which search for neutrino-less double beta decay, will be able to determine whether
507 neutrinos are Dirac or Majorana.

508 2.6 Neutrino interactions

509 The study of neutrino-nucleus interactions is of great importance for long baseline
510 neutrino oscillation experiments. The interaction model provides a mapping between

2.6. NEUTRINO INTERACTIONS

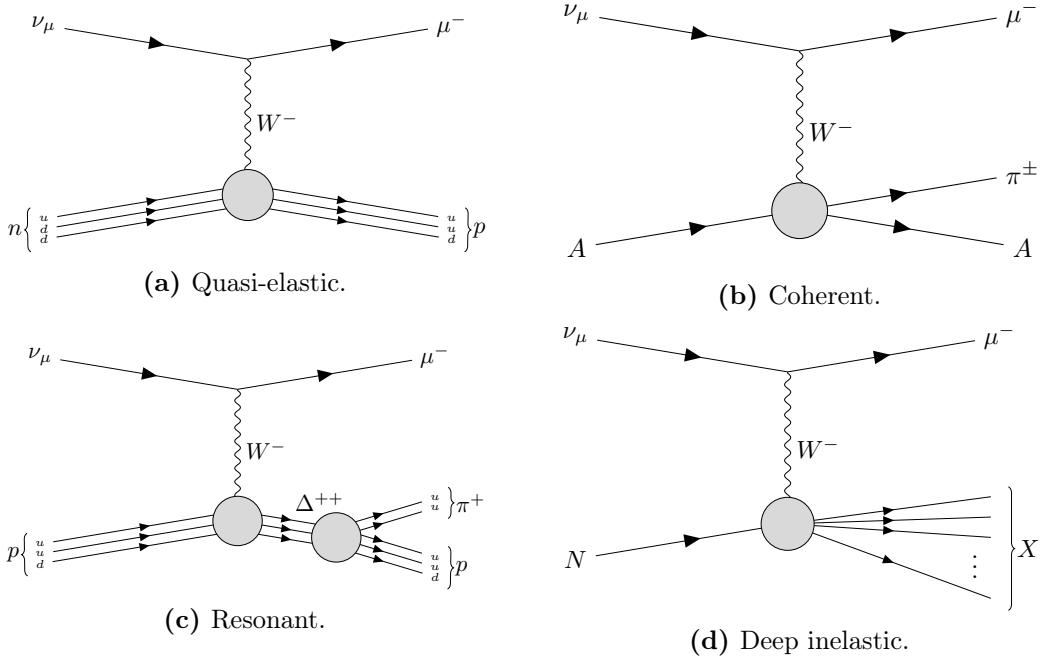


Figure 2.4: Feynman diagrams of the four most relevant CC interactions to long baseline neutrino oscillation experiments.

the energy of the incoming neutrino and the final state particles after the interaction.
 Because in this kind of experiments neutrinos are obtained as secondary decay products of mesons, typically charged pions and kaons, their energies are not known a priori. Not only that, but the kinematics of the interacting nucleon are also unknown. Therefore, we rely on the neutrino interaction models to provide this relation between the observables in the detector and the true kinematics of the neutrino. Interaction modelling is expected to be the one of the leading sources of systematic uncertainties in the next generation of long baseline experiments [65–67].

In the case of neutrino interactions with nuclei, at the energies relevant for long baseline oscillation experiments, around the GeV-scale, the process is dominated by the interaction between the neutrino and a single nucleon within the nuclear medium. Figure 2.4 shows examples of the four most common neutrino CC interactions. In this diagrams A indicated that the interaction happened with the nucleas as a whole, whereas N denotes a single nucleon.

At low energies, below 1 GeV, quasi-elastic (QE) interactions dominate. In a CCQE

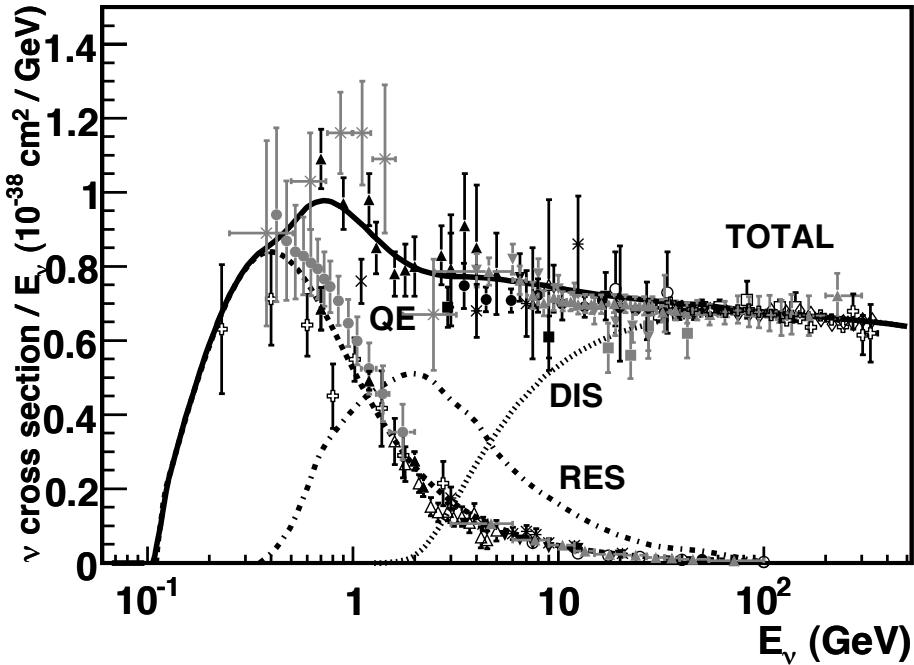


Figure 2.5: Total ν_μ CC cross section per nucleon as a function of the neutrino energy. The contributions from the different channels are shown. Figure taken from Ref. [68].

interaction a neutrino (antineutrino) interacts with a neutron (proton), converting it into a proton (neutron) which is then ejected from the nucleus together with the resulting charged lepton. At energies above 1 GeV the neutrino is able to excite the nucleon into a baryonic resonance, which promptly decays into a nucleon and a pion. These are the so-called resonant (RES) interactions. Neutrinos also interact with entire nucleus coherently, in the process known as coherent (COH) interaction. This kind of reactions also produce a single pion in the final state. At high neutrino energies, above 5 GeV, deep inelastic scattering (DIS) takes place. In these processes, the neutrino interacts with a single quark within the nucleon, breaking the nucleon and producing a hadronic shower.

Figure 2.5 shows a compilation of measurements of the total ν_μ CC cross section (see Ref. [68] for the details of the different experimental results). Also shown are the contributions from the different interaction modes. The contribution of the CCCOH interaction is omitted, as it is negligible compared to the others. This shows how the

2.6. NEUTRINO INTERACTIONS

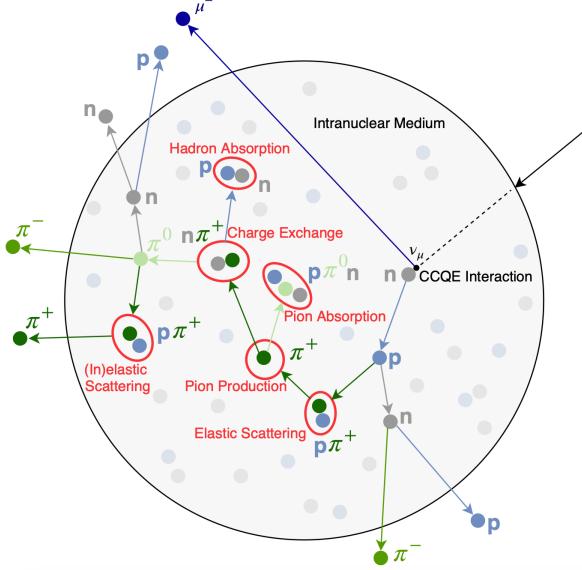


Figure 2.6: Schematic representation of a ν_μ CCQE interaction with a neutron inside a nucleus. The reaction produces a muon and a proton, which travel through the nuclear medium. The outgoing proton undergoes various kinds of hadronic FSIs on its way out. Figure taken from Ref. [69].

540 interaction model needs to accurately predict the neutrino-nucleon cross section for the
 541 different interaction modes across a broad energy range, to obtain the correct relative
 542 contributions.

543 Nuclear effects alter the neutrino cross section, as well as the multiplicities of the
 544 final state particles. Therefore, the interaction models need to account for the effects
 545 introduced by the nuclei. There are several models available to describe the initial state
 546 of the nucleus, like the relativistic Fermi gas model [70], spectral functions [71] or the
 547 random phase approximation [72]. The other main effect that interaction models have to
 548 deal with are the so-called final state interactions (FSI). These are the interactions of the
 549 particles produced in the neutrino-nucleon scattering as they travel through the nuclear
 550 medium. Typically, the lepton exits the nucleus without interacting. However, hadrons
 551 tend to get scattered, absorbed or re-emitted. These effects are usually described by
 552 means of intra-nuclear cascade models [73]. Figure 2.6 illustrates the effects of FSI on
 553 the observable particle content in the detector after a ν_μ CCQE interaction.

554 There exists a rich experimental programme dedicated to the measurement of neutrino

CHAPTER 2. NEUTRINO PHYSICS

555 cross sections. The list of such experiments in the recent years include MiniBooNE
556 [74], MINERvA [75], MicroBooNE [76] and SBND [77]. Additionally, thanks to their
557 near detectors, long baseline experiments can perform cross section measurements.
558 Some recent examples are NOvA [78] or T2K [79]. Future oscillation experiments
559 will greatly benefit from these measurements, as the measurement of the oscillation
560 parameters depends on the cross section modelling. However, there are alternative
561 data-driven approaches to extract the oscillation probabilities without relying on a
562 neutrino interaction model, which are planned to be explored in the next generation of
563 experiments [80, 81].

565

The Deep Underground Neutrino Experiment

567

Deep in the human unconscious is a pervasive need for a logical universe that makes sense. But the real universe is always one step beyond logic.

569

– Frank Herbert, *Dune*

570

The Deep Underground Neutrino Experiment (DUNE) is a next generation long-baseline neutrino experiment [14]. It will aim to address several questions in neutrino physics, study neutrinos from astrophysical sources and search for beyond the standard model physics.

574

This Chapter reviews the main goals of the DUNE experiment, the design of the far detector modules and their data acquisition (DAQ) system, and the role that the near detector plays in the physics program of DUNE.

577

3.1 Overview

578

The main physics goals of DUNE are:

579

- measure the neutrino mass hierarchy, the amount of CP violation in the leptonic sector and the θ_{23} octant,

581

- detect rare low energy neutrino events, like neutrinos from supernova bursts, and

582

- search for proton decay and other beyond the standard model phenomena.

CHAPTER 3. THE DEEP UNDERGROUND NEUTRINO EXPERIMENT

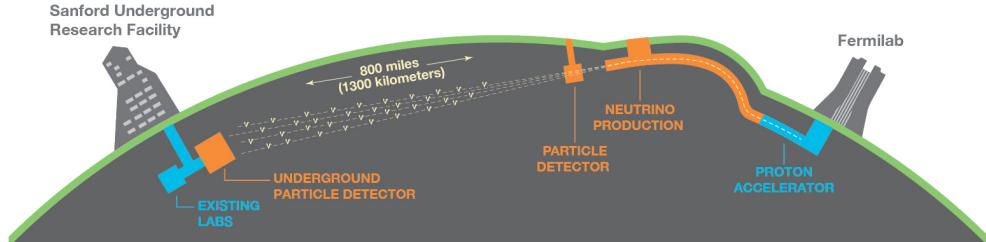


Figure 3.1: Schematic diagram of the DUNE experiment and the LBNF beamline [14].

The design of DUNE has been tailored with these goals in mind. It will consist of two neutrino detectors. A near detector (ND) complex will be placed at Fermilab, 574 m downstream of the neutrino production point, whereas a larger far detector (FD) will be built in the Sandford Underground Research Facility (SURF), South Dakota, approximately 1300 km away. Figure 3.1 shows a simplified view of the various components of DUNE (not to scale).

The beam neutrinos will be provided by the Long-Baseline Neutrino Facility (LBNF) beamline, the multi-megawatt wide-band neutrino beam planned for Fermilab. It will produce neutrinos travelling in the direction of SURF, with the capability to switch between neutrino and antineutrino mode.

Before arriving to the FD, the neutrino beam meets the ND complex, which serves as the experiment's control. The design of the DUNE ND is mainly driven by the needs of the oscillation physics program, as its main role is to measure the unoscillated neutrino energy spectra. From these we can predict the unoscillated spectra at the FD, which can be compared to the spectra measured at the FD to extract the oscillation parameters. Additionally, the ND has a physics programme of its own, including cross section measurements and BSM physics searches.

The technology chosen for the FD modules of DUNE is the liquid Argon time projection chamber (LArTPC). Its four modules will record neutrino interactions from the accelerator-produced beam arriving at predictable times. As it also aims at recording rare and low energy events, like supernovae and solar neutrinos, the FD requires trigger

3.2. PHYSICS GOALS OF DUNE

Table 3.1: Summary of the two-phased plan for DUNE. Adapted from Ref. [82].

Parameter	Phase I	Phase II	Benefit
FD mass	20 kt fiducial	40 kt fiducial	FD statistics
Beam power	up to 1.2 MW	2.4 MW	FD statistics
ND config.	ND-LAr, TMS, SAND	ND-LAr, ND-GAr, SAND	Systematic constraints

604 schemes which can deal with both kinds of physics, and also maximum uptime.

605 DUNE is planned to be built using a staged approach consisting on two phases,
 606 which are summarised in Tab. 3.1. Phase I consists of a FD with 50% of the total
 607 fiducial mass, a reduced version of the ND complex and a 1.2 MW proton beam. It will
 608 be sufficient to achieve some early physics goals, like the determination of the neutrino
 609 mass ordering. For its Phase II, DUNE will feature the full four FD modules, a more
 610 capable ND and a 2.4 MW proton beam. The physics milestones for the two phases are
 611 given in Tab. 3.2, in a staging scenario which assumes that Phase II is completed after
 612 6 years of operation.

613 A summary of the DUNE science program can be found in the DUNE FD Technical
 614 Design Report (TDR) Volume I [14]. For a detailed discussion on the two-phased
 615 approach the reader is referred to the DUNE Snowmass 2021 report [82].

616 3.2 Physics goals of DUNE

617 As noted in the literature (see for instance Ref. [61] for a review), the parameter space of
 618 the neutrino oscillation phenomena within the three-flavour picture is quite constrained
 619 by current experimental data. However, there are still crucial open questions, like the
 620 mass ordering, the value of δ_{CP} or the θ_{23} octant. One of the main goals of DUNE is to
 621 determine precisely the values of these parameters [83].

622 To address these questions DUNE can look to the subdominant oscillation channel
 623 $\nu_\mu \rightarrow \nu_e$ ($\bar{\nu}_\mu \rightarrow \bar{\nu}_e$) and study the energy dependence of the ν_e ($\bar{\nu}_e$) appearance probability.
 624 When we focus on the antineutrino channel $\bar{\nu}_\mu \rightarrow \bar{\nu}_e$ there is a change in the sign of δ_{CP} ,
 625 thus introducing CP-violation. Moreover, due to the fact that there are no positrons in

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Table 3.2: Exposure and time required to achieve the different physics milestones of the two phases. The predictions assume a Phase II staging scenario where FD modules 3 and 4 are deployed in years 4 and 6 and both the beam and ND are upgraded after 6 years. Adapted from Ref. [82].

Stage	Physics milestone	Exposure (kt-MW-years)	Years (staged)
Phase I	5σ MO ($\delta_{CP} = -\pi/2$)	16	1-2
	5σ MO (100% of the δ_{CP} values)	66	3-5
	3σ CPV ($\delta_{CP} = -\pi/2$)	100	4-6
Phase II	5σ CPV ($\delta_{CP} = -\pi/2$)	334	7-8
	δ_{CP} resolution of 10 degrees ($\delta_{CP} = 0$)	400	8-9
	5σ CPV (50% of the δ_{CP} values)	646	11
	3σ CPV (75% of the δ_{CP} values)	936	14
	$\sin^2(2\theta_{13})$ resolution of 0.004	1079	16

the composition of Earth, there is a sign difference for the matter effect contribution when looking to the antineutrino channel. This asymmetry is proportional to the baseline length L and is sensitive to the sign of Δm_{31}^2 , and thus to the neutrino mass ordering.

Another of the main physics goals of DUNE is the search for baryon-number violating processes. Specifically, it will try to answer the question of whether protons are stable or not. There is no symmetry argument that forbids protons from decaying, but its apparent stability seems to suggest that baryon number is conserved [84]. However, proton decay is a usual feature of grand-unified theories, where electromagnetic, weak and strong interactions are unified above a certain energy scale [85].

As the energy deposition scale for this kind of searches is nearly the same as the one for long-baseline neutrino oscillations, DUNE will be able to look for them. It has several advantages over other experiments, such as excellent imaging and particle identification, which can be translated to lower backgrounds.

The last of the main objectives of DUNE is the detection of neutrinos originated in supernovae explosions, what is called a supernova neutrino burst (SNB). These neutrinos carry with them information about the core-collapse process, from the progenitor to the explosion and the remnant; but also may have information about new exotic physics. So far, the only neutrino events ever recorded from such a process were a few dozens of $\bar{\nu}_e$

3.3. LBNF BEAMLINE

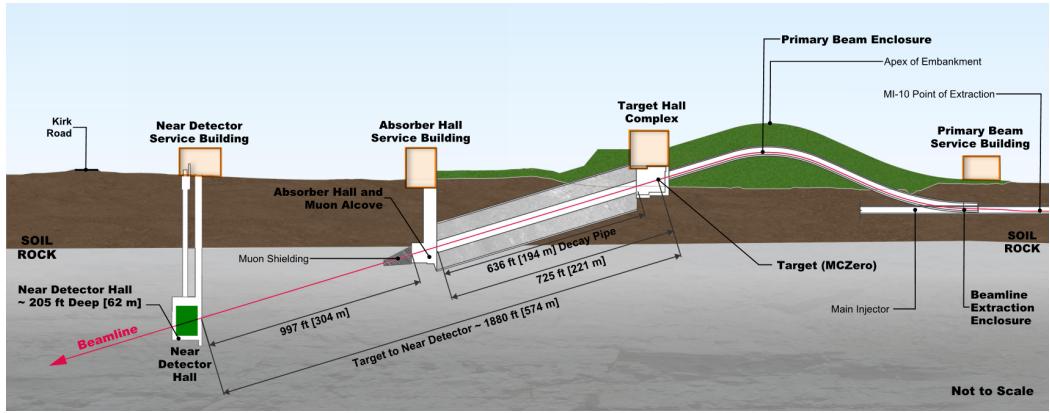


Figure 3.2: Schematic longitudinal section of the LBNF beamline at Fermilab (not to scale). Figure taken from Ref. [88].

644 events from the 1987A supernova located in the Magellanic Cloud, 50 kpc away from
 645 Earth [86,87].

646 DUNE aims to collect SNB events. Although these are quite rare, as the expected
 647 supernovae explosion events are about one every few decades for our galaxy and
 648 Andromeda, the long lifetime of the experiment (around a few decades as well) makes it
 649 reasonable to expect some. Nowadays the main sensitivity to SNB of most experiments
 650 is to the $\bar{\nu}_e$ through inverse beta decay. One of the advantages of DUNE is its expected
 651 sensitivity to ν_e , since the dominant channel will be ν_e CC scattering.

652 Moreover, due to the stringent requirements that the main physics goals set for
 653 DUNE, it will allow also to perform searches for all kind of BSM physics. Among
 654 others, DUNE will be able to look for: active-sterile neutrino mixing, non-unitarity of
 655 the PMNS matrix, non-standard interactions, Lorentz and CPT violations, neutrino
 656 trident production, light-mass DM, boosted DM and heavy neutral leptons. The reader
 657 is referred to the DUNE FD TDR Volume II [83] for a full discussion of the physics
 658 scope of DUNE.

659 3.3 LBNF beamline

660 The LBNF project is responsible for producing the neutrino beam for the DUNE detectors.
 661 A detailed discussion of the LBNF program can be found in the DUNE/LBNF CDR

CHAPTER 3. THE DEEP UNDERGROUND NEUTRINO EXPERIMENT

662 Volume III [88].

663 A schematic diagram of the longitudinal section of the LBNF beamline is shown in
 664 Fig. 3.2. First, a beam of 60 – 120 GeV protons is extracted from the Fermilab Main
 665 Injector. This beam is aimed towards the target area, where it collides with a cylindrical
 666 graphite target to produce pions and kaons.

667 The diffuse, secondary beam of particles is focused by a pair of magnetic horns.
 668 These select the positively charged particles when operated in Forward Horn Current
 669 (FHC) mode, or the negatively charged ones when the current is reversed, also known as
 670 Reverse Horn Current (RHC) mode. The focused secondary beam then enters a 194 m
 671 decay pipe where the pions and kaons will predominantly produce $\mu^+\nu_\mu$ pairs when in
 672 FHC mode (or $\mu^-\bar{\nu}_\mu$ in RHC mode).

673 At the end of the decay pipe a hadron absorber removes the undecayed hadrons and
 674 muons from the beam, which reduces the ν_e ($\bar{\nu}_e$) and $\bar{\nu}_\mu$ (ν_μ) contamination coming
 675 from the μ^+ (μ^-) decays. The resulting neutrino flux at the FD is shown in Fig. 3.3,
 676 both for FHC (left) and RHC (right) modes. These predictions show the intrinsic $(\bar{\nu})_e$
 677 contamination and wrong sign component from wrong sign and neutral meson decays,
 678 as well as muons decaying before reaching the absorber.

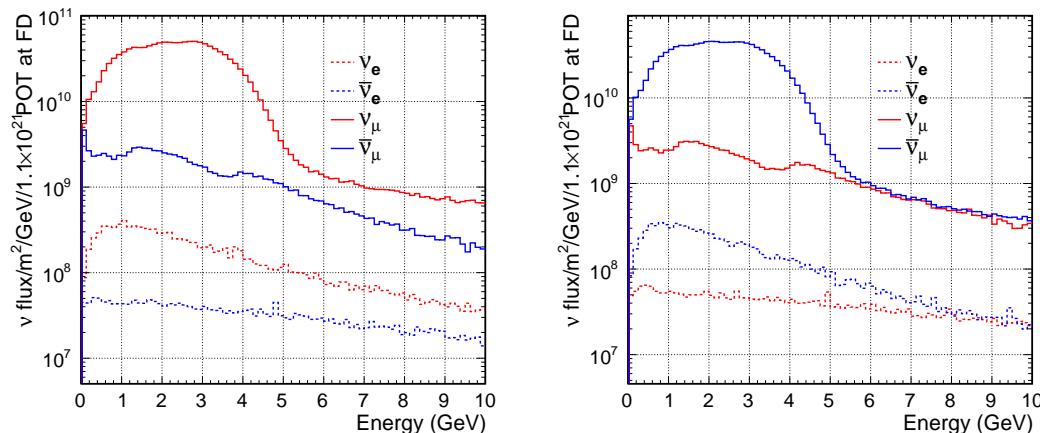


Figure 3.3: Predicted neutrino fluxes at the FD in FHC mode (left panel) and RHC mode (right panel). Figures taken from Ref. [83].

3.4. NEAR DETECTOR

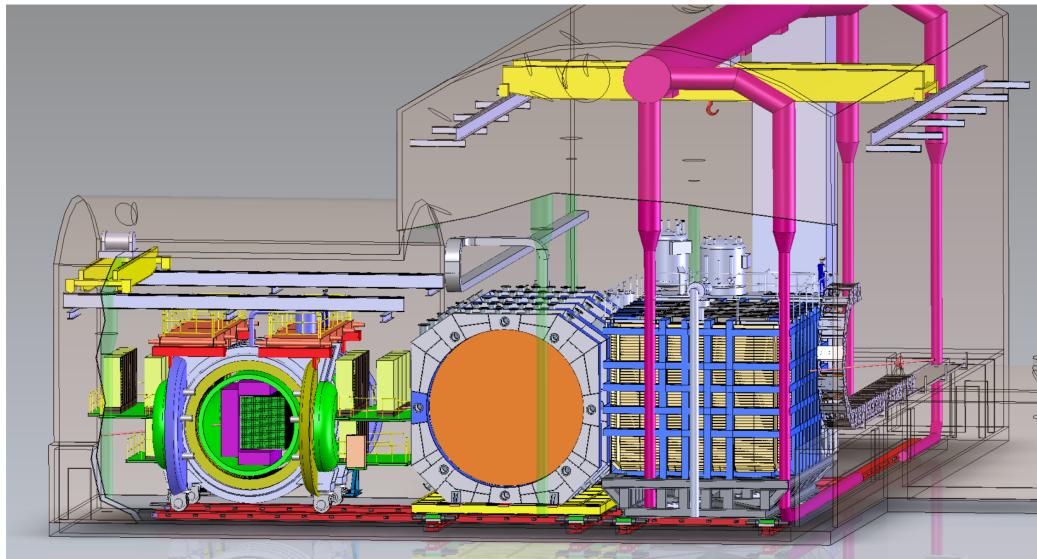


Figure 3.4: Representation of the ND hall in Phase II, showing the different subcomponents. From right to left, in the direction of the beam, we have ND-LAr, ND-GAr and SAND. Figure taken from Ref. [89].

679 3.4 Near Detector

680 To estimate the oscillation parameters we measure the neutrino energy spectra at the FD.
681 This reconstructed energy arises from a convolution of the neutrino flux, cross section,
682 detector response and the oscillation probability. Using theoretical and empirical models
683 to account for the other effects, one can extract the oscillation probability using the
684 measurement. However, these models have associated a number of uncertainties that
685 are then propagated to the oscillation parameters.

686 One of the main roles of the ND is to measure the neutrino interaction rates before
687 the oscillation effects become relevant, i.e. close to the production point. By measuring
688 the ν_μ and ν_e energy spectra, and that of their corresponding antineutrinos, at the ND
689 we can constrain the model uncertainties. A complete cancellation of the uncertainties
690 when taking the ratio between the FD and ND measurements is not possible, as that
691 would require both detectors to have identical designs and the neutrino fluxes to be
692 the same. Because of the distance, the flux probed by the FD will have a different
693 energy and flavour composition than that at the ND, as neutrinos oscillate and the beam

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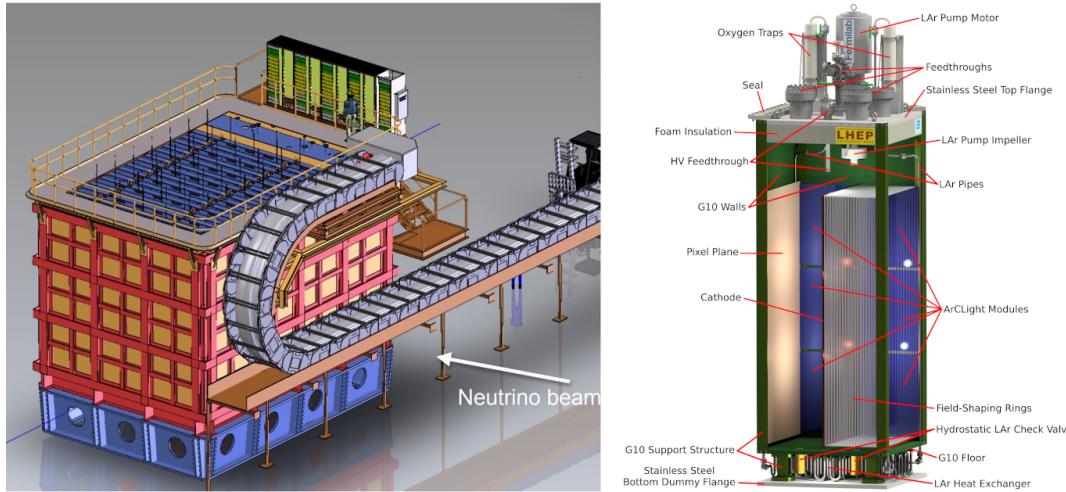


Figure 3.5: Schematic representation of the external components of ND-LAr, including the cryostat and the PRISM movable system (left) and detailed drawing of one ArgonCube module (right). Figure adapted from Ref. [14].

spreads. The differences in the flux also determine the design of the detectors, therefore the ND is limited in its capability to match the FD design.

Nevertheless, having a highly capable ND, DUNE can minimise the systematic uncertainties affecting the observed neutrino energy. The ND data can be used to tune the model parameters by comparison with the prediction. Then, one uses the tuned model to predict the unoscillated FD spectra. Comparing the prediction with the measured spectra it is possible to extract the oscillation parameters.

Additionally, the ND will have a physics program of its own. In particular, it will measure neutrino cross sections that will then be used to constrain the model used in the long-baseline oscillation analysis. It will also be used to search for BSM phenomena such as heavy neutral leptons, dark photons, millicharged particles, etc.

The DUNE ND can be divided in three main components, a LArTPC known as ND-LAr, a magnetised muon spectrometer, which will be the Temporary Muon Spectrometer (TMS) in Phase I and ND-GAr in Phase II, and the System for on-Axis Neutrino Detection (SAND). The layout of the Phase II DUNE ND can be seen in Fig. 3.4. The first two components of the ND will be able to move off-axis, in what is called the Precision Reaction-Independent Spectrum Measurement (PRISM) concept. More details

3.4. NEAR DETECTOR

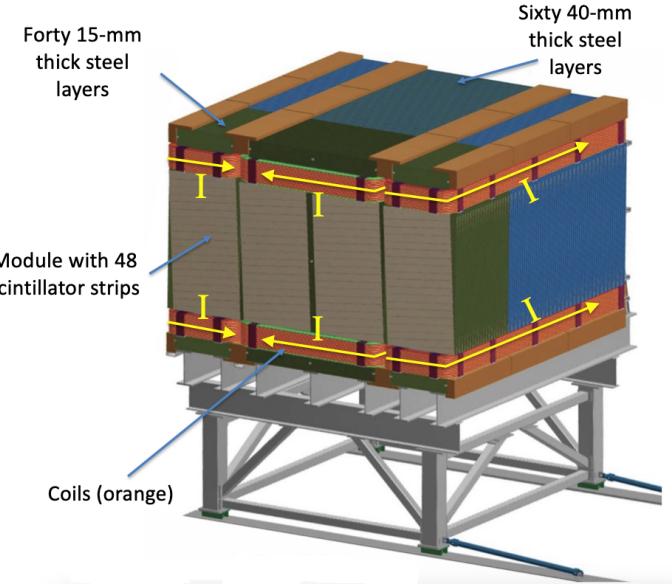


Figure 3.6: Schematic view of the TMS detector, highlighting its main parts. Figure adapted from Ref. [14].

711 on the purpose and design of the ND can be found in the DUNE ND Conceptual Design
 712 Report (CDR) [89].

713 **3.4.1 ND-LAr**

714 ND-LAr is a LArTPC, as the ND needs a LAr component to reduce cross section and
 715 detector systematic uncertainties in the oscillation analysis. However, its design differs
 716 significantly from those proposed for the FD modules. Because of the high event rates
 717 at the ND, approximately 55 neutrino interaction events per $10 \mu\text{s}$ spill, ND-LAr will be
 718 built in a modular way. Each of the modules, based on the ArgonCube technology, is a
 719 fully instrumented, optically isolated TPC with a pixelated readout. The pixelisation
 720 allows for a fully 3D reconstruction and the optical isolation reduces the problems due
 721 to overlapping interactions. Figure 3.5 shows a representation of the external parts of
 722 ND-LAr (left) and a detailed diagram of an ArgonCube module (right).

723 With a fiducial mass of 67 t and dimensions $7 \text{ m (w)} \times 3 \text{ m (h)} \times 5 \text{ m (l)}$, ND-LAr
 724 will be able to provide high statistics and contain the hadronic systems from the beam
 725 neutrino interactions, but muons with a momentum higher than 0.7 GeV will exit the

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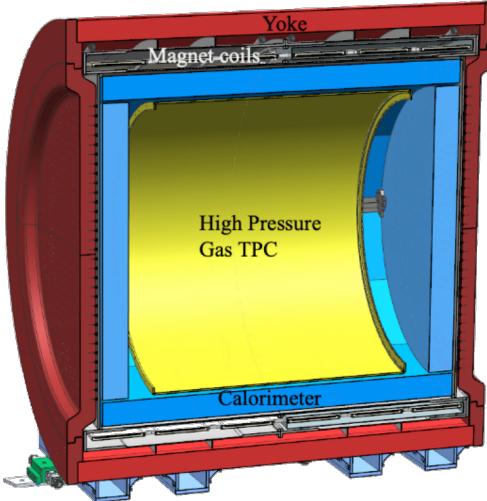


Figure 3.7: Cross section of the ND-GAr geometry, showing the HPgTPC, ECal and magnet. Figure adapted from Ref. [90].

726 detector.

727 **3.4.2 TMS/ND-GAr**

728 To accurately estimate the neutrino energy, the momentum of the outgoing muons needs
 729 to be determined. That is the reason why a muon spectrometer is needed downstream
 730 of ND-LAr.

731 In Phase I that role will be fulfilled by TMS. It is a magnetised sampling calorimeter,
 732 with alternating steel and plastic scintillator layers. Figure 3.6 shows a schematic view
 733 of the TMS detector. The magnetic field allows a precise measurement of the sign of the
 734 muon, so one can distinguish between neutrino and antineutrino interactions.

735 After the Phase II upgrade, TMS will be replaced with a more capable near detector.
 736 The current technology considered is ND-GAr. This detector is a magnetised, high-
 737 pressure GAr TPC (often denoted as HPgTPC) surrounded by an electromagnetic
 738 calorimeter (ECal) and a muon tagger. A cross section of its geometry can be seen
 739 in Fig. 3.7. ND-GAr will be able to measure the momenta of the outgoing muons
 740 while also detect neutrino interactions inside the GAr volume. This allows ND-GAr
 741 to constrain the systematic uncertainties even further, as it will be able to accurately

3.4. NEAR DETECTOR

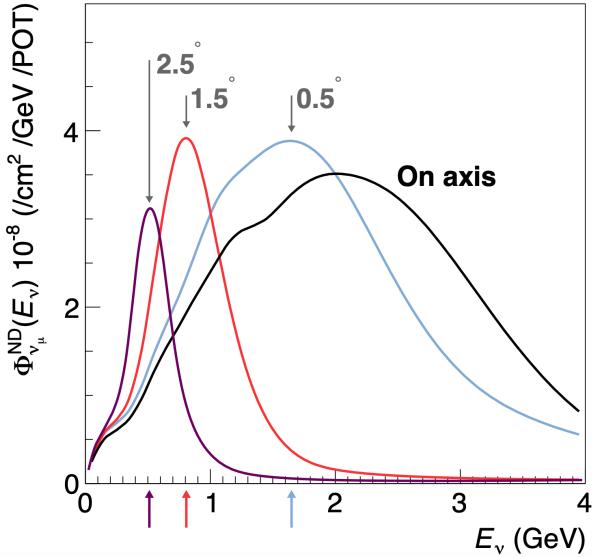


Figure 3.8: Predicted beam muon neutrino flux at the ND location for different off-axis positions. Figure taken from Ref. [89].

742 measure neutrino interactions at low energies thanks to the lower tracking thresholds of
743 GAr.

744 3.4.3 PRISM

745 In general, the observed peak neutrino energy of a neutrino beam decreases as the
746 observation angle with respect to the beam direction increases. This feature has been
747 used in other long-baseline neutrino experiments, like T2K (2.5° off-axis) and NOvA
748 (0.8° off-axis), to achieve narrower energy distributions. The DUNE PRISM concept
749 exploits this effect using a movable ND. Within PRISM both ND-LAr and the muon
750 spectrometer (TMS in Phase I and ND-GAr in Phase II) can be moved up to 3.2°
751 off-axis, equivalent to move the detectors 30.5 m laterally through the ND hall.

752 This allows to record additional data samples with different energy compositions.
753 Figure 3.8 compares the on-axis muon neutrino flux at the ND with the fluxes at different
754 off-axis positions. As the off-axis position increases the neutrino flux becomes closer to
755 a monoenergetic beam with a lower peak energy. These samples can be used to perform
756 a data-driven determination of the relation between true and reconstructed neutrino

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757 energy, to reduce the dependence on the interaction model. The off-axis samples are
758 linearly combined to produce a narrow Gaussian energy distribution centered on a target
759 true energy. From the combination coefficients one can build a sample of reconstructed
760 neutrino events that will determine the energy mapping.

761 The PRISM samples will be used to form a flux at the ND location similar in shape
762 to the oscillated flux measured by the FD. This method can be used to extract the
763 oscillation parameters with minimal input from the neutrino interaction model.

764 3.4.4 SAND

765 The role of SAND is to monitor the beam stability by measuring the on-axis neutrino
766 energy spectra. As the PRISM program requires that ND-LAr and its downstream
767 muon spectrometer spend about half of the time in off-axis positions, it is not possible
768 to monitor the stability with the movable detectors. Moreover, for the success of PRISM
769 it is essential to have a stable beam configuration, or, at least, a quick assessment and
770 modeling of the distortions.

771 The SAND detector is magnetised, and features an inner low density tracker, a LAr
772 target with optical readout and surrounding sampling calorimeter.

773 3.5 A More Capable Near Detector

774 In DUNE Phase II, a more capable near detector is needed to achieve the ultimate physics
775 goals of the experiments. The current leading proposal for this detector is ND-GAr.
776 As mentioned previously, it will fulfill the role of TMS, measuring the momentum and
777 sign of the charged particles exiting ND-LAr. Additionally, it will be able to measure
778 neutrino interactions inside the HPgTPC, achieving lower energy thresholds than those
779 of the ND and FD LArTPCs. By doing so ND-GAr will allow to constrain the relevant
780 systematic uncertainties for the LBL analysis even further. A detailed discussion on the
781 requirements, design, performance and physics of ND-GAr can be found in the DUNE
782 ND CDR [89] and the ND-GAr white paper [91].

3.5. A MORE CAPABLE NEAR DETECTOR

783 3.5.1 Requirements

784 The primary requirement for ND-GAr is to measure the momentum and charge of
785 muons from ν_μ and $\bar{\nu}_\mu$ CC interactions in ND-LAr, in order to measure their energy
786 spectrum. To achieve the sensitivity to the neutrino oscillation parameters described
787 in the DUNE FD TDR Volume II [83], ND-GAr should be able to constrain the muon
788 energy within a 1% uncertainty or better.

789 Another requirement for ND-GAr is the precise measurement of neutrino interactions
790 on argon for the energies relevant to the neutrino oscillation program. The goal is to
791 constrain the cross section systematic uncertainties in the regions of phase space that
792 are not accessible to ND-LAr. This requires the kinematic acceptance for muons in
793 ND-GAr to exceed that of ND-LAr, being comparable to the one observed in the FD.

794 ND-GAr should also be able to help establishing the relationship between true and
795 reconstructed energy from neutrino interactions on argon with low thresholds, being
796 sensitive to particles that are not observed or may be misidentified in ND-LAr. In
797 particular, ND-GAr needs to have low tracking thresholds in order to measure the
798 spectrum of pions and protons produced in final-state interactions (FSI). It also must
799 be able to accurately measure the pion multiplicity in 1, 2 and 3 pions final states, to
800 inform the pion mass correction in the LArTPCs.

801 3.5.2 Reference design

802 The final design of ND-GAr is still under preparation. However, a preliminary baseline
803 design was in place at the time of the ND CDR. This section summarises the main
804 features of that design, as it is also the one used for the default geometry in our simulation.
805 A DUNE Phase II white paper, discussing the different options under consideration for
806 the ND-GAr design, is in progress.

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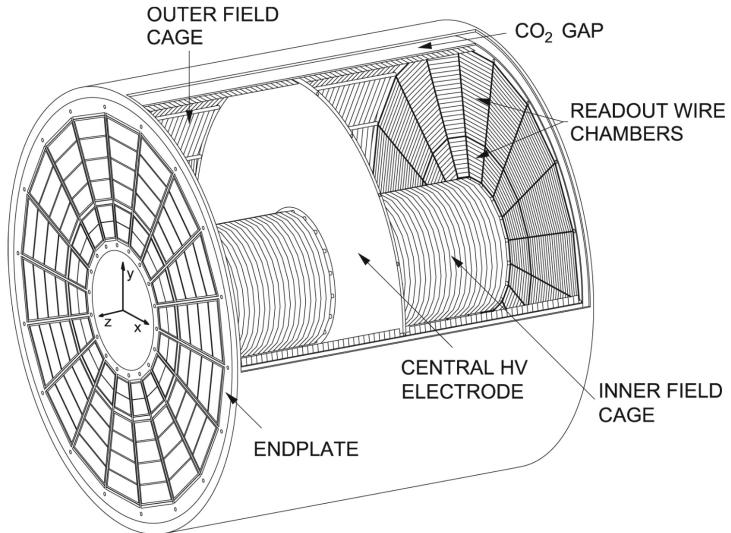


Figure 3.9: Diagram of the ALICE TPC, showing the two drift chambers, inner and outer field cages and readout chambers. Figure taken from Ref. [89].

807 HPgTPC

808 The reference design for the ND-GAr HPgTPC follow closely that of the ALICE TPC.
 809 It is a cylinder with a central high-voltage cathode, generating the electric field for
 810 the two drift volumes, with a maximum drift distance of 2.5 m each. The anodes will
 811 be instrumented with charge readout chambers. The original design repurposed the
 812 multi-wire proportional readout chambers (MWPCs) of ALICE, however some of the
 813 current R&D efforts focus on a gas electron multiplier (GEM) [92] option instead. Figure
 814 3.9 shows a schematic diagram of the ALICE TPC design. The basic ND-GAr geometry
 815 will resemble this, except for the inner field cage.

816 It will use a 90:10 molar fraction Ar:CH₄ mixture at 10 bar. With this baseline gas
 817 mixture light collection is not possible, as the quenching gas absorbs most of the VUV
 818 photons. Additional R&D efforts are underway, to understand if different mixtures allow
 819 for the light signal to be used to provide a t_0 while maintaining stable charge gain.

3.5. A MORE CAPABLE NEAR DETECTOR

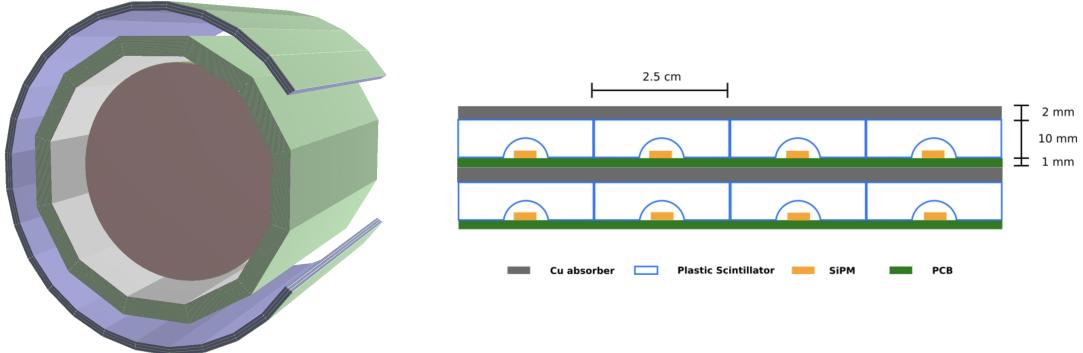


Figure 3.10: View of the 12-sided ECal barrel and outer muon tagger geometries (left) and layout of the ECal tile layers for the 2 mm Cu, 10 mm scintillator option (right). Figure adapted from Ref. [89].

820 ECal

821 The main role of the ND-GAr ECal is the calorimetric measurement of the electron
 822 energies and the reconstruction of photons, in particular those from neutral pion decays.
 823 Also, the ECal is able to provide a t_0 timestamp for neutrino interactions, by associating
 824 its activity to the tracks in the HPgTPC. The ECal will also be able to perform
 825 neutron reconstruction using time of flight and reject external backgrounds, thanks to
 826 its sub-nanosecond time resolution.

827 The ECal design features three independent subdetectors, two end caps at each side
 828 and a barrel surrounding the HPgTPC. Each of the detectors is divided in modules,
 829 which combine alternating layers of plastic scintillator and absorber material readout
 830 by SiPMs. The inner scintillator layers consist of $2.5 \times 2.5 \text{ cm}^2$ high-granularity tiles,
 831 whereas the outer ones are made out of 4 cm wide cross-strips spanning the whole
 832 module length. The current barrel geometry consists of 8 tile layers and 34 strip layers,
 833 while the end caps feature 6 and 36 respectively. The thickness of the scintillator layers
 834 is 7 mm and 5 mm for the Pb absorber layers. The 12-sided geometry of the ECal barrel
 835 (left) and the layout of the tile layers (left)¹ can be seen in Fig. 3.10.

¹The figure shows the layout of the tile layers for a previous design with 2 mm Cu absorber and 10 mm plastic scintillator, as mentioned in the text the current choice is 5 mm Pb absorber and 7 mm scintillator.

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836 Magnet

837 The ND-GAr magnet design, know as the Solenoid with Partial Yoke (SPY), consists of
838 two coupled solenoids with an iron return yoke. The idea behind the design is to have a
839 solenoid as thin as possible, as well as a return yoke mass distribution that minimises
840 the material budget between ND-LAr and ND-GAr. The magnet needs to provide a
841 0.5 T field in the direction perpendicular to the beam, parallel to the drift electric field.
842 It needs to host the pressure vessel and the surrounding ECal, which points to a inner
843 diameter of ~ 6.4 m.

844 The solenoid is a single layer coil, based on niobium titanium superconducting
845 Rutherford cable. The total length of the coil is 7.5 m. The bobbin will be split in four
846 segments grouped in pairs with two identical cryostats, connected in series. The iron
847 yoke features an aperture in the upstream side to allow the muons coming from ND-LAr.
848 Still, its material will be enough to reduce the magnetic field reaching SAND, and also
849 stop the charged pions produced inside the HPgTPC.

850 Muon system

851 The design of the ND-GAr muon system is still in a preliminary stage. Its role is to
852 distinguish between muons and pions punching through the ECal. This is especially
853 important for wrong-sign determination, to separate these from neutral current events.

854 In its current form, the muon system consists of three layers of longitudinal sampling
855 structures. It alternates 10 cm Fe absorber slabs with 2 cm plastic scintillator strips.
856 The transverse granularity required is still under study.

857 3.5.3 R&D efforts

858 There are several ND-GAr-related prototypes, mostly focused on the TPC charge
859 readout and electronics. The priority is to test the full readout chain, in a high-pressure
860 environment, using a gas mixture with high argon fraction. A detailed summary of these
861 can be found in the DUNE Phase II white paper [90].

3.5. A MORE CAPABLE NEAR DETECTOR

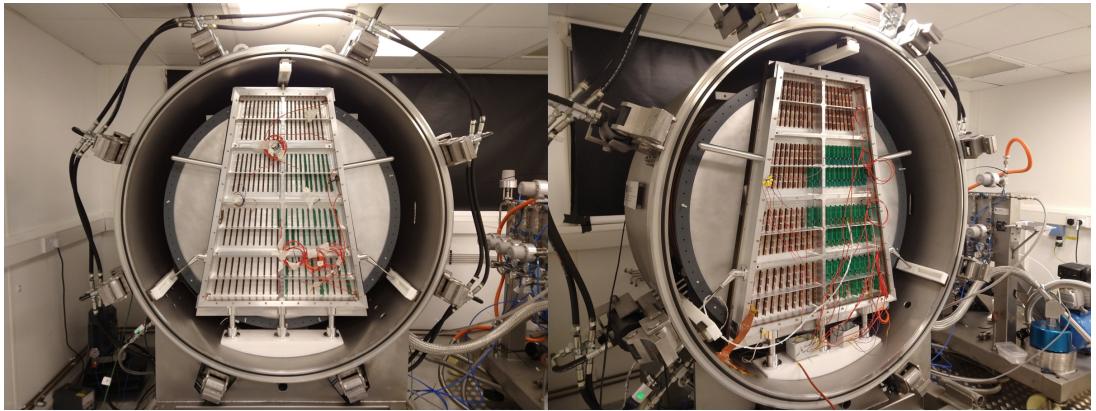


Figure 3.11: Photographs of the TOAD pressure vessel at RHUL. The TPC is mounted inside the vessel, and the OROC is supported by an aluminium frame. Figure taken from Ref. [93].

862 Multi-Wire Proportional Chambers

863 As mentioned before, the original ND-GAr design repurposes the MWPCs of the ALICE
864 TPC, which became available after the recent upgrade [94]. These were operated using
865 a 90:10:5 Ne:CO₂:N₂ gas mixture at 1 atm. Therefore, their performance needed to be
866 studied in an argon gas environment at high pressure.

867 The Gas-argon Operation of ALICE TPC (GOAT) test stand tested the ALICE
868 readout chambers at high pressure. In particular, it used one of the previously operated
869 ALICE inner MWPCs, also known as IROCs, in a pressure vessel rated to 10 atm. It
870 measured the gas gain at various pressure points, voltages and gas mixtures.

871 The Test stand of an Overpressure Argon Detector (TOAD) tested an ALICE outer
872 MWPC, also known as OROC, up to 5 atm. During its time at RHUL, it was used to
873 study the achievable gas gain of the OROC [93]. At the moment, it is being commissioned
874 at Fermilab for a full detector test of the readout electronics and the DAQ.

875 Figure 3.11 shows the interior of the TOAD pressure vessel. The TPC is mounted
876 inside the vessel on three rails. The back of the OROC, supported by an aluminium
877 frame, can be seen at the front.

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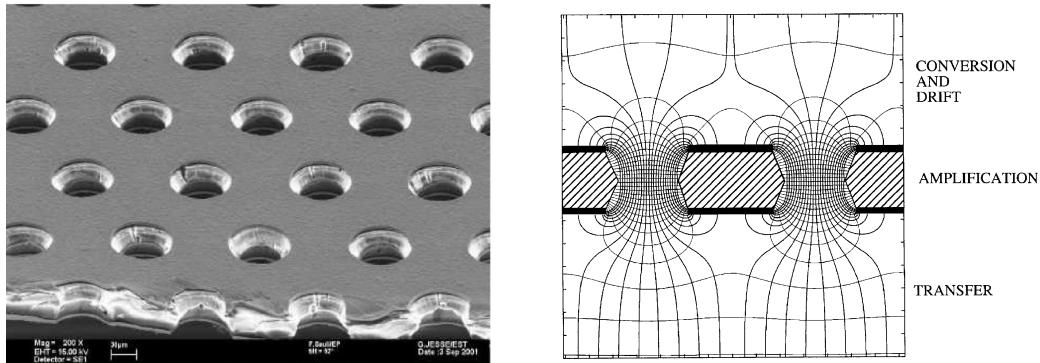


Figure 3.12: Left panel: electron microscope image of a 50 μm thick GEM electrode, with hole pitch and diameter of 140 and 70 μm , respectively. Right panel: Schematics of a GEM electrode cross section, showing the electric field lines around the holes. Figures taken from Ref. [95].

878 Gas Electron Multiplier

879 An alternative to the MWPC option is the use of GEMs. These are a type of micro-patter
 880 detector, where the ionisation electrons passing through the holes in the GEM layers
 881 are accelerated by a high intensity electric field. The acceleration causes the electrons
 882 to ionise the medium, resulting in an avalanche which increase the signal exponentially
 883 [92]. GEMs are used in numerous experiments that need a high spatial resolution, like
 884 ALICE [96] and CMS [97] after their upgrades.

885 Figure 3.12 (left panel) shows an electron microscope picture of a 50 μm thick GEM
 886 electrode, with a pitch between neighbouring holes of 140 μm and a hole diameter of
 887 70 μm . A schematic representation of the cross section of a GEM layer is shown in Fig.
 888 3.12 (left panel).

889 The Gaseous Argon T0 (GAT0²) prototype studies the use of thick GEMs made out
 890 of glass to achieve optical imaging of the primary ionisation. Using a 10 atm pressure
 891 vessel, the goal is to study different argon-based mixtures that allow for a precise t_0
 892 determination.

893 The GEM Over-pressurized with Reference Gases (GORG³) test stand is currently
 894 testing a GEM-based charge readout, using a triple-GEM stack.

²Spanish for cat.

³Persian for wolf.

3.6. FAR DETECTOR

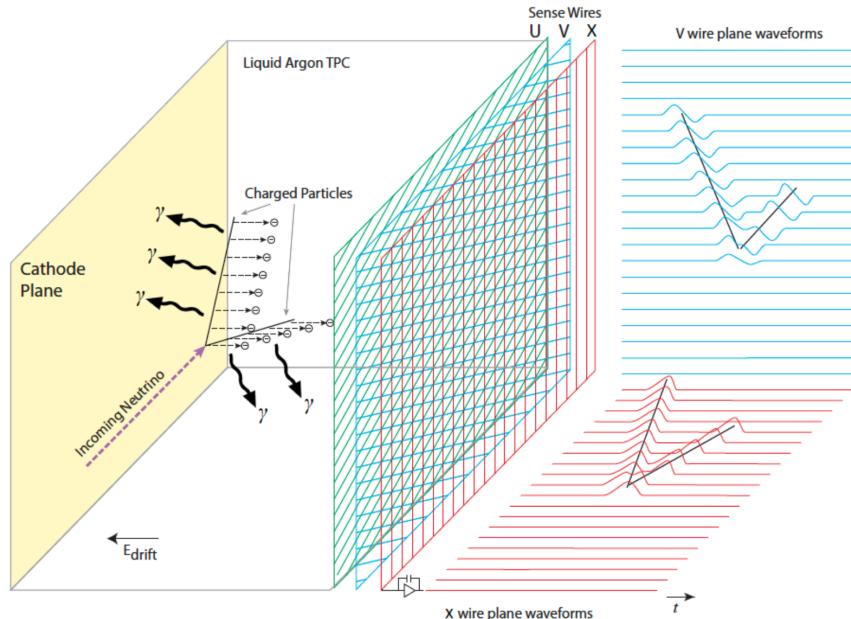


Figure 3.13: Schematic diagram showing the operating principle of a LArTPC with wire readout. Figure taken from Ref. [14].

3.6 Far Detector

The DUNE FD complex will sit 1300 km away from the beam target and 1.5 km underground at SURF, South Dakota. Two caverns will host the four FD modules, two of them per cavern, each embedded in cryostats of dimensions 18.9 m (w) \times 17.8 m (h) \times 65.8 m (l). A central, smaller cavern will host the cryogenic system.

Three out of the four modules will be liquid argon (LAr) time projection chamber detectors, often refer to as LArTPCs, with a LAr fiducial mass of at least 10 kt each. The first and second FD modules, FD-1 and FD-2, will use a Horizontal Drift (HD) technology, whereas the third module, FD-3, will have a Vertical Drift (VD) direction. The technology for the fourth module is still to be decided,

For each event, with energies ranging from a few MeV to several GeV, these detectors collect both the scintillation light and the ionisation electrons created when the charged particles produced in neutrino-nucleus interactions ionise the argon nuclei. In both HD and VD designs the characteristic 128 nm scintillation light of argon is collected by a photon detection system (PDS). This light will indicate the time at which electrons

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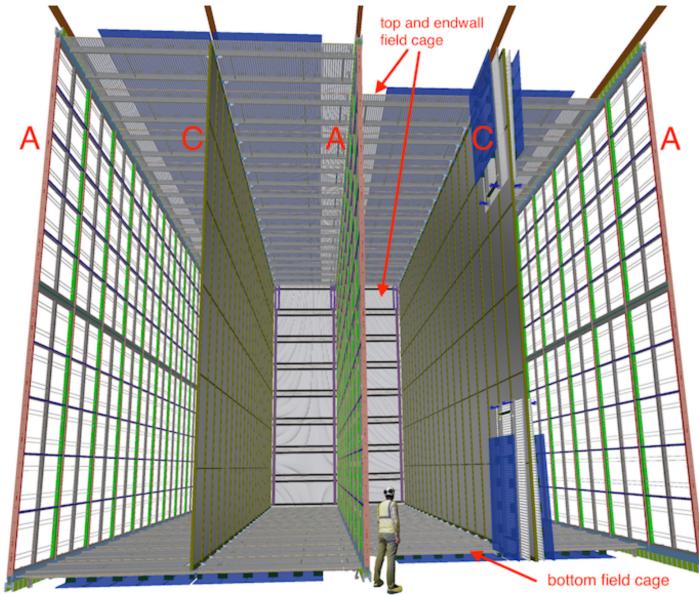


Figure 3.14: Proposed design for the FD-1 and FD-2 modules following the HD principle. Figure taken from Ref. [14].

910 start to drift, thus enabling reconstruction over the drift coordinate when compared
 911 to the time when the first ionisation electron arrives to the anode. Reconstruction of
 912 the topology in the transverse direction is achieved using the charge readout. Fig. 3.13
 913 illustrates the detection principle described, for the case of a HD detector with a wire
 914 readout.

915 3.6.1 Horizontal Drift

916 The HD design the ionisation electrons produced as charged particles traverse the LAr
 917 drift horizontally towards the anode planes, due to the effect of an electric field. These
 918 anode planes are made out of three layers of wire readout. This design, previously
 919 known as single-phase (SP), was tested by the ProtoDUNE-SP detector at CERN. The
 920 prototype collected data from a hadron beam and cosmic rays, providing high-quality
 921 data sets for calibration and performance studies.

922 Each FD HD detector module is divided in four drift regions, with a maximum drift
 923 length of 3.5 m, by alternating anode and cathode walls. The surrounding field cage
 924 ensures the uniformity of the 500 V/cm horizontal electric field across the drift volumes.

3.6. FAR DETECTOR

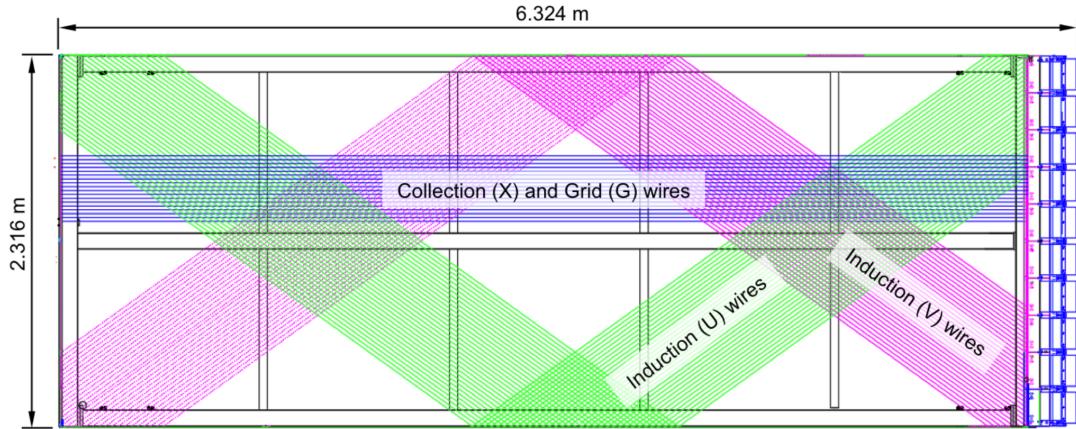


Figure 3.15: Schematic representation of an APA. The black lines represent the APA steel frame. The green and magenta lines correspond to the direction of the U and V induction wires respectively. The blue lines indicate the direction of the X collection wires and the wire shielding G. Figure taken from Ref. [14].

925 The three anode walls, which constitute the charge readout of the detector, are built by
 926 stacking anode plane assemblies (APAs), 2 high times 25 wide. The design of the HD
 927 modules is shown in Fig. 3.14.

928 Each APA is made of 2560 active wires arranged in three layers, plus an extra grid
 929 layer, wrapped around a metal frame. The two induction wire planes, U and V, sit at
 930 $\pm 35.7^\circ$ to the vertical on each side of the APA. The collection and shielding plane wires,
 931 X and G, run parallel to the vertical direction. The ionisation electrons drift past the
 932 induction planes, generating bipolar signals on those wires, and are collected by the
 933 collection plane, producing a monopolar positive signal. The spacing between the wires
 934 is ~ 5 mm, and it defines the spatial resolution of the APA.

935 The front-end readout electronics, or cold electronics as they are immerse in the LAr,
 936 are attached to the top of the up APAs and the bottom of the down APAs. Mounted on
 937 the front-end mother boards we have a series of ASICs that digitize the signals from the
 938 collection and induction planes. Each wire signal goes to a charge-sensitive amplifier,
 939 then there is a pulse-shaping circuit and this is followed by the analogue-to-digital
 940 converter. This part of the process happens inside the LAr to minimise the number of
 941 cables penetrating the cryostat. The digitised signals come out finally via a series of

CHAPTER 3. THE DEEP UNDERGROUND NEUTRINO EXPERIMENT

942 high-speed serial links to the warm interface boards (WIBs), from where the data is sent
943 to the back-end DAQ through optical fibers.

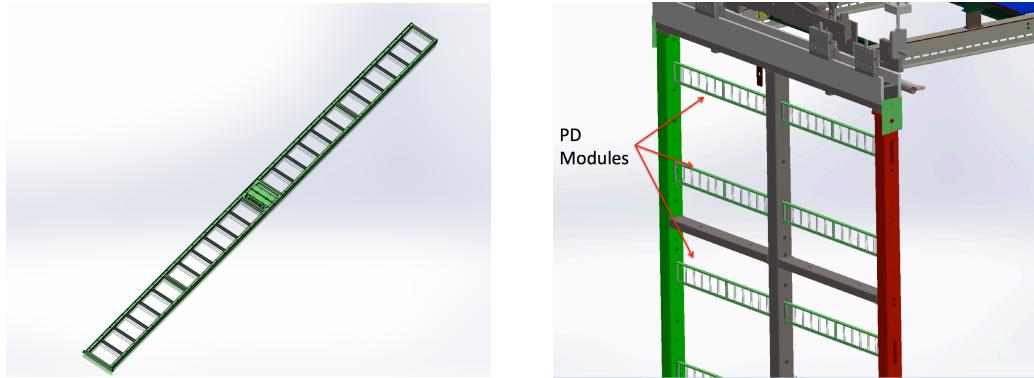


Figure 3.16: A PDS module containing 24 X-ARAPUCAs (left) and the location of the modules on the APAs (right). Figure taken from Ref. [14].

944 The PDS uses modules of X-ARAPUCA devices, mounted on the APA frames
945 between the wire planes. Each X-ARAPUCA consists of layers of dichroic filter and
946 wavelength-shifter. They shift the VUV scintillation light into the visible spectrum,
947 sending then the visible photons to silicon photomultiplier (SiPM) devices. The PDS
948 modules are 209 cm × 12 cm × 2 cm bars, containing 24 X-ARAPUCAs. There are 10
949 of these PDS modules per APA. Fig. 3.16 shows a PDS module (left) and the placement
950 of the modules on the APAs (right).

951 3.6.2 Vertical Drift

952 In the VD case the ionisation electrons will drift vertically until they meet a printed
953 circuit board-based (PCB) readout plane. It is based on the original dual-phase (DP)
954 design deployed at CERN, known as ProtoDUNE-DP, used a vertical drift design with
955 an additional amplification of the ionization electrons using a gaseous argon (GAr) layer
956 above the liquid phase. The VD module incorporates the positive features of the DP
957 design without the complications of having the LAr-GAr interface.

958 The current design of the FD VD module counts with two drift chambers with a
959 maximum drift distance of 6.5 cm. A cathode plane splits the detector volume along the
960 drift direction while the two anode planes are connected to the bottom and top walls

3.6. FAR DETECTOR

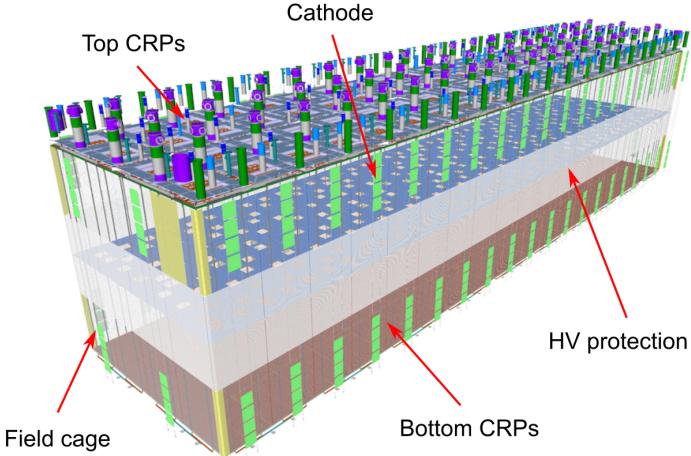


Figure 3.17: Proposed design for the FD-3 module following the VD principle. Figure adapted from Ref. [98].

of the detector. The layout of the VD module is shown in Fig. 3.17. Compared with the HD design, the VD option offers a slightly larger instrumented volume and a more cost-effective solution for the charge readout.

As in the HD design, each drift volume features a 500 V/cm electric field and a field cage that ensures its uniformity. The anode planes are arrays of $3.4\text{ m} \times 3\text{ m}$ charge-readout planes (CRPs). These are formed by a pair of charge-readout units (CRUs), which are built from two double-sided perforated PCBs, with their perforations aligned. The perforations allow the drift electrons to pass between the layers.

The PCB face opposite to the cathode has a copper guard plane which acts as shielding, while its reverse face is etched with electrode strips forming the first induction plane. The outer PCB has electrode strips on both faces, the ones facing the inner PCB form the second induction plane while the outermost ones form the collection plane. Fig. 3.18 shows the layout of the electrode strips for the top (left) and bottom (right) CRUs. The magenta and blue lines represent the first and second induction planes respectively, and the green lines correspond to the collection plane.

The PDS in the VD module will use the same X-ARAPUCA technology developed for the HD design. The plan is to place the PDS modules on the cryostat walls and on

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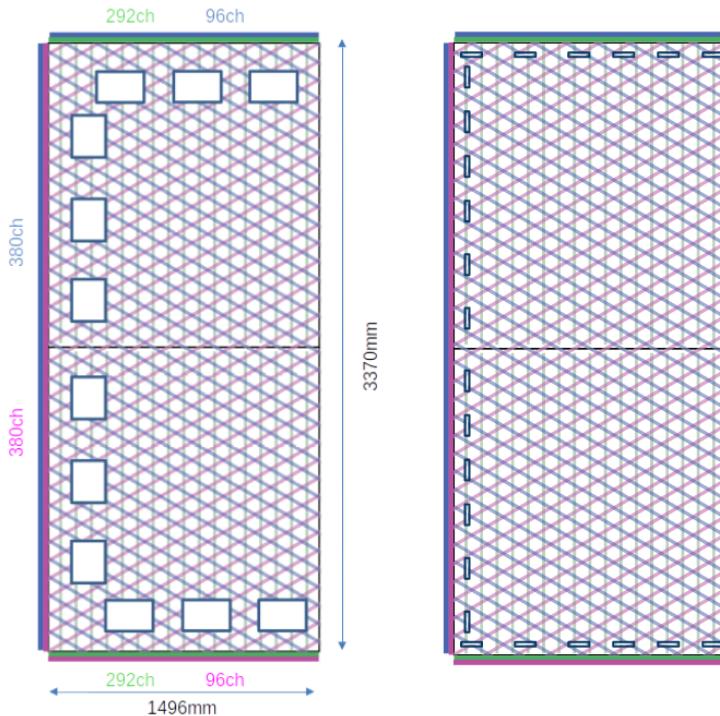


Figure 3.18: Schematic representation of the electrode strip configuration for a top (left) and bottom (right) CRU. Figure taken from Ref. [98].

978 the cathode, in order to maximise the photon yield.

979 **3.6.3 FD Data Acquisition System**

980 The data acquisition (DAQ) system receives, processes and stores data from the detector
981 modules. In the case of DUNE the DAQ architecture is designed to work for all FD
982 modules interchangeably, except some aspects of the upstream part which may depend
983 on the specific module technology.

984 The enormous sample rate and the number of channels in TPC and PD readouts
985 will produce a very large volume of data. These pose really strong requirements and
986 challenges to the DUNE FD DAQ architecture. It will be required to read out data of
987 the order of ten thousand or more channels at rates of a few MHz. To cope with the
988 huge data volume, segmented readouts and compression algorithms are used to reduce
989 the data rate to manageable levels.

990 The DAQ system of the DUNE FD is composed of five different subsystems. The

3.6. FAR DETECTOR

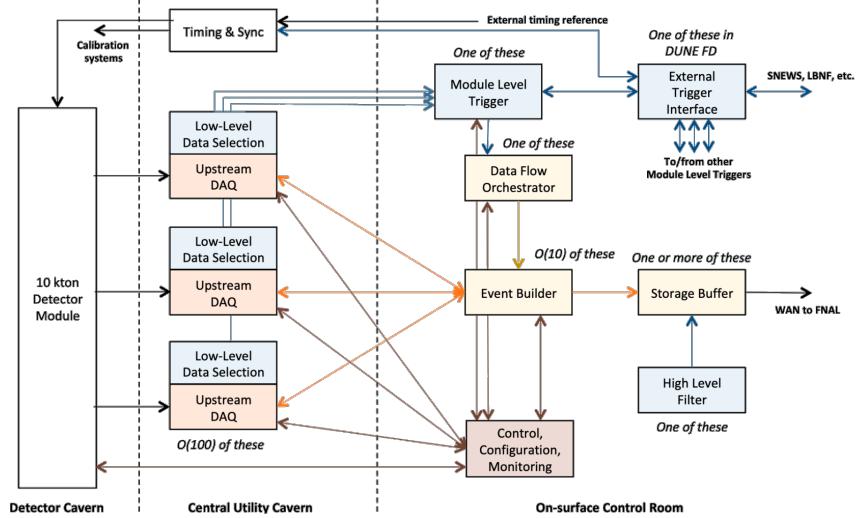


Figure 3.19: Detailed diagram of the DUNE FD DAQ system. Figure taken from Ref. [99].

first one is the upstream DAQ, which receives the raw data from the detector, buffers it and perform some low-level pre-processing. The minimally processed data is then fed into a hierarchical data selection system, which then performs a module level trigger decision. In case of a positive decision a trigger command is produced and executed by the data flow orchestrator, located in the back-end (BE) DAQ subsystem. Subsequently the DAQ BE retrieves the relevant data from the buffers located in the upstream DAQ, adds all the data into a cohesive record and saves it to permanent storage. Watching over all the other subsystems we also have the control, configuration and monitoring subsystem and the time and synchronization subsystem. Figure 3.19 shows a schematic diagram of the DAQ system, showing the different subsystems and their relations.

A notorious challenge for the DUNE DAQ system comes from its broad physics goals. We must be prepared to process events spanning a wide range of time windows (from 5 ms in the case of beam and cosmic neutrinos and nucleon decay to 100 s in the case of SNBs) and therefore this requires a continuous readout of the detector modules. Moreover, because of the off-beam measurements we need to ensure the capabilities of online data processing and self-triggering. Having this into account, together with the technical constraints, the DUNE FD DAQ faces a series of challenges: it needs to

CHAPTER 3. THE DEEP UNDERGROUND NEUTRINO EXPERIMENT

1008 be fault tolerant and redundant to reduce downtime, accommodate new components
1009 while it keeps serving the operational modules, have large upstream buffers to handle
1010 SNB physics, be able to support a wide range of readout windows and last reduce the
1011 throughput of data to permanent storage to be at most 30 PB/year.

4

1012

1013

Matched Filter approach to Trigger

1014

Primitives

1015

It is a capital mistake to theorize before one has data. Insensibly one begins to twist facts to suit theories, instead of theories to suit facts.

1017

– Arthur Conan Doyle, *A scandal in Bohemia*

1018

The DAQ system is responsible of what data will be collected in the DUNE FD.

1019

Therefore, it has the capability of either expanding or limiting our physics reach, depending of its specifications. This is important for the low energy physics program, as more it requires more sensitive and reliable methods to pick the relevant signals.

1022

In this Chapter, I present of a possible method to improve the sensitivity of the DUNE FD by enhancing the production of hits in the online processing. This is possible thanks to a more efficient filter strategy, the matched filter, which benefits the induction channels of the detector.

1026

4.1 Motivation

1027

The lowest-level objects that are formed within the DUNE FD DAQ system are the so-called trigger primitives (TPs). This represent the hits on a channel, and are used as input to the rest of the DAQ trigger chain. The TPs are formed in the hit finder chain.

1030

A schematic representation of it is shown in Fig. 4.1. This chain takes the raw ADC data from the detector, removes the constant pedestal of the signal using a dynamical

1031

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

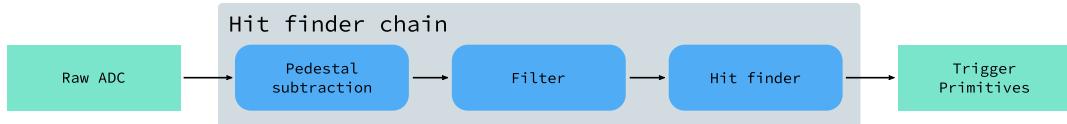


Figure 4.1: Schematic representation of the Trigger Primitive Generation chain in the DUNE FD.

1032 median estimation method, applies a filter to the signal, and tries to find peaks over
 1033 a certain threshold. These peaks form the TPs, which contain information such as the
 1034 start and end time over the threshold, the maximum ADC value and the corresponding
 1035 ADC integral. Currently, there are two implementations of the hit finder chain, one
 1036 firmware-based and other software-based.

1037 The filter implemented in the firmware of the upstream DUNE FD DAQ is a 32nd-
 1038 order low-pass finite impulse-response (FIR) filter. The output of such filter for a discrete
 1039 system can be written as:

$$y[i] = \sum_{j=0}^N h[j]x[i-j], \quad (4.1)$$

1040 where N is the order of the filter, y is the output sequence, x is the input sequence and h
 1041 is the set of coefficients of the filter. The current implementation within `dtp-firmware`
 1042 [100] uses a set of 16 non-zero integer coefficients. For the software case, only a 5th-order
 1043 filter is used, as the filtering turns out to be a very CPU expensive task.

1044 Filtering is a vital step in the hit finder chain. It helps to suppress the noise and
 1045 enhance the signal peaks with respect to the noiseless baseline. A good filtering strategy
 1046 allows us to use lower thresholds when forming the trigger primitives (TPs) and thus
 1047 increasing the sensitivity of our detector to low energy physics events. In such events,
 1048 the hits produced by the ionisation electrons tend to have lower amplitudes than those
 1049 of interest to the LBL physics programme of the DUNE experiment.

1050 This is particularly important for the induction planes. In general, signal peaks in
 1051 the induction channels have smaller amplitude than the ones in the collection plane.
 1052 This, together with the fact that the pulse shapes are bipolar, reduces our capacity to

4.2. SIGNAL-TO-NOISE RATIO DEFINITION

1053 detect the hits on these channels. The inefficiency of detecting TPs in the induction
1054 planes (denoted as U and V planes) leads trigger algorithms to focus mainly on the
1055 TPs from the collection plane (so-called X plane). As a result, the possibility of making
1056 trigger decisions based on the coincidence of TPs across the three wire planes remains
1057 nowadays unexploited in DUNE. This will be beneficial for low energy events, as it
1058 adds redundancy to the algorithms, as well as for other physics that requires online
1059 directionality information, like the supernova pointing.

1060 A possible improvement of the current hit finder chain could require optimising
1061 the existing or choosing a new filter implementation. A filter strategy which improves
1062 the induction signals may be able to enhance the detection efficiency of TPs from the
1063 induction planes and ideally make it comparable to that of the collection plane.

1064 The goal is to implement a better finite-impulse response filter design and to evaluate
1065 its performance relative to the current filter. To do so, we need to take into account the
1066 limitations of the firmware: the FIR filter shall have maximum 32 coefficients (so-called
1067 taps) whose values are 12-bit unsigned integers. Although it is technically possible to
1068 include non-integer coefficients, it would be a technical challenge as we have 40 FIR
1069 instances per APA, as there are 4 FIR per optical link and 10 optical links per APA. With
1070 these restrictions, the task is to provide a set of 32 coefficients which yield an optimal
1071 filter performance for the induction wires. A solution compatible with the software hit
1072 finder implementation is not considered, due to its current limitations concerning the
1073 filtering stage.

1074 4.2 Signal-to-noise ratio definition

1075 I introduce the signal to noise ratio (S/N) as a measure of the FIR filter performance
1076 and demonstrate how to extract its value for a set of ProtoDUNE-SP data. The S/N
1077 metrics allow us to compare different filter implementations and serve as a basis for more
1078 detailed studies presented later in this document. Specifically, I use the ADC capture
1079 `felix-2020-07-17-21:31:44` (data capture taken for firmware validation purposes). I

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

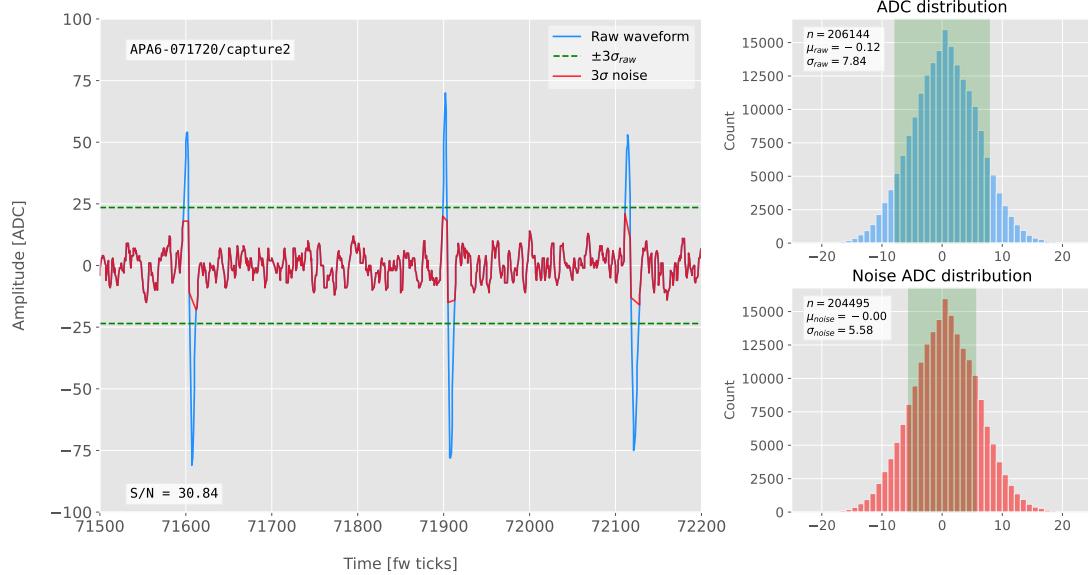


Figure 4.2: Left panel: Zoomed unfiltered waveform corresponding to channel 7840 from the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44` (blue line). The green dashed lines mark the region $\pm 3\sigma_{raw}$. The resulting noise waveform is also shown (red line). Top right panel: ADC distribution for channel 7840, where the green shaded region represents $\pm \sigma_{raw}$. Bottom right panel: noise ADC distribution for channel 7840, where the green shaded region represents $\pm \sigma_{noise}$.

1080 defined S/N as the height of the signal peaks relative to the size of the noise peaks.
 1081 To quantify this quantity channel by channel one first need to estimate the standard
 1082 deviation of the ADC data for each channel, σ_{ADC} . Then, I define the corresponding
 1083 noise waveform to be the ADC values in the range $\pm 3\sigma_{ADC}$. From this new noise data
 1084 one can estimate the mean and standard deviation, μ_{noise} and σ_{noise} , so I can write the
 1085 S/N for any given channel as:

$$S/N = \frac{\max [ADC] - \mu_{noise}}{\sigma_{noise}}, \quad (4.2)$$

1086 where $\max [ADC]$ is simply the maximum ADC value found in the corresponding channel.
 1087 One can apply this definition of the S/N with a waveform from one of the channels
 1088 of the data capture¹. Figure 4.2 shows a zoomed region of the waveform corresponding

¹All the original work was done within the `dtp-simulation` package [101], which offers a variety of tools to read raw data and emulate the TPG block (pedestal subtraction, filtering and hit finder). However, the results shown in this report were re-worked later using the C++ based `dtpemulator` package [102]. Its main purpose is the emulation of the TPG block and, in the same way as its

4.3. LOW-PASS FIR FILTER DESIGN

to channel 7840 (blue line), where one can clearly see three signal peaks and continuous additive noise (we actually see 6 peaks, 3 positive and 3 negative, but, because by design for induction channels the expected signal pulse shapes are bipolar, I treat them as a collection of 3 individual signal peaks). I estimated the standard deviation of this raw waveform to be $\sigma_{raw} = 7.84$ ADC, so I am able to define the noise waveform (red line) as the ADC values in the range ± 23.52 ADC. This way one obtains $\mu_{noise} = 0$ and $\sigma_{noise} = 5.58$ ADC, which gives S/N = 30.84.

We can repeat this calculation now for the corresponding filtered waveform (using the current firmware FIR filter). Figure 4.3 shows the same time window for the filtered waveform from channel 7840 (blue line). In this case, the standard deviation of the waveform is larger than before, giving $\sigma_{raw} = 10.99$ ADC. The noise waveform (red line) is formed by selecting the ADC values in the ± 32.91 ADC range, giving $\mu_{noise} = -0.47$ ADC and $\sigma_{noise} = 7.03$ ADC. Finally, one obtains S/N = 24.68. Notice that the value of S/N decreases after the filtering. Clearly, one can see that the noise baseline has increased by a factor of 1.35 when we applied the FIR filter and at the same time the amplitude of the signal peaks has remained almost unchanged, leading to this poorer S/N value.

4.3 Low-pass FIR filter design

To optimise the frequency response of a digital filter, we can use the Parks-McClellan algorithm, where one finds a set of N real coefficients that give the best response for the specified pass-band and order of the filter [103].

In our case, as the sampling frequency is defined as 1 ticks^{-1} , the Nyquist frequency will simply be $1/2 \text{ ticks}^{-1}$. The current implementation of the filter seems to have as pass-band the range $[0, 0.1] \text{ ticks}^{-1}$. This can be seen in Fig. 4.4, where I show the power spectrum, in decibels, of such filter implementation (blue solid line). For instance, the Park-McClellan algorithm finds the optimal Chebyshev FIR filter [104] taking as

predecessor, it has been cross-checked against the current firmware implementation.

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

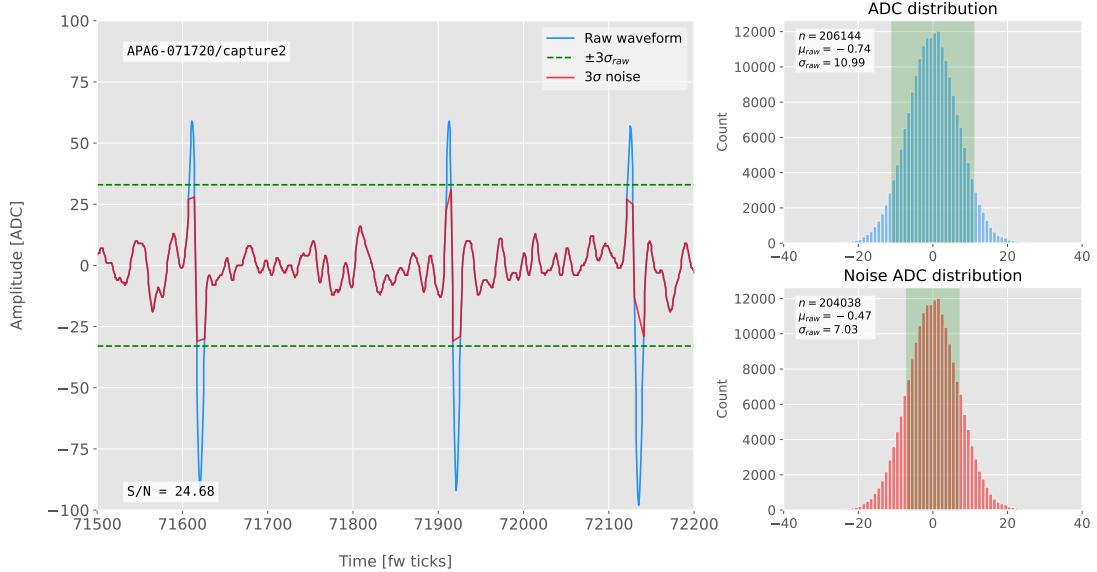


Figure 4.3: Left panel: Zoomed filtered waveform corresponding to channel 7840 from the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44` (blue line). The filter used was the current implementation of the low-pass FIR filter in `dtp-firmware`. The green dashed lines mark the region $\pm 3\sigma_{\text{raw}}$. The resulting noise waveform is also shown (red line). Top right panel: ADC distribution for channel 7840 after filtering, where the green shaded region represents $\pm \sigma_{\text{raw}}$. Bottom right panel: noise ADC distribution for channel 7840 after filtering, where the green shaded region represents $\pm \sigma_{\text{noise}}$.

1115 input the boundaries of the target pass-band and stop-band, which can be written in
 1116 the form:

$$\left\{ \begin{array}{l} [0, f_c] \\ [f_c + \delta f, f_N] \end{array} \right. , \quad (4.3)$$

1117 where f_c is the cut-off frequency, δf is the transition width and f_N is the aforementioned
 1118 Nyquist frequency. A similar behaviour to the one in the current filter can be obtained
 1119 by setting $f_c = 0$ and $\delta f = 0.1 \text{ ticks}^{-1}$. The response of the resulting filter is also shown
 1120 in Fig. 4.4 (blue solid line). Notice that the suppression of the stop-band is enhanced for
 1121 this optimal filter. For comparison I included the power response of the filter obtained
 1122 by taking the integer part of the coefficients resulting from the Parks-McClellan method
 1123 (red dashed line). One can see that it does not suppress that much the stop-band, in a
 1124 similar way to the current implementation of the filter.

1125 At this point, I tried to improve the performance of the FIR filter using the Park-

4.3. LOW-PASS FIR FILTER DESIGN

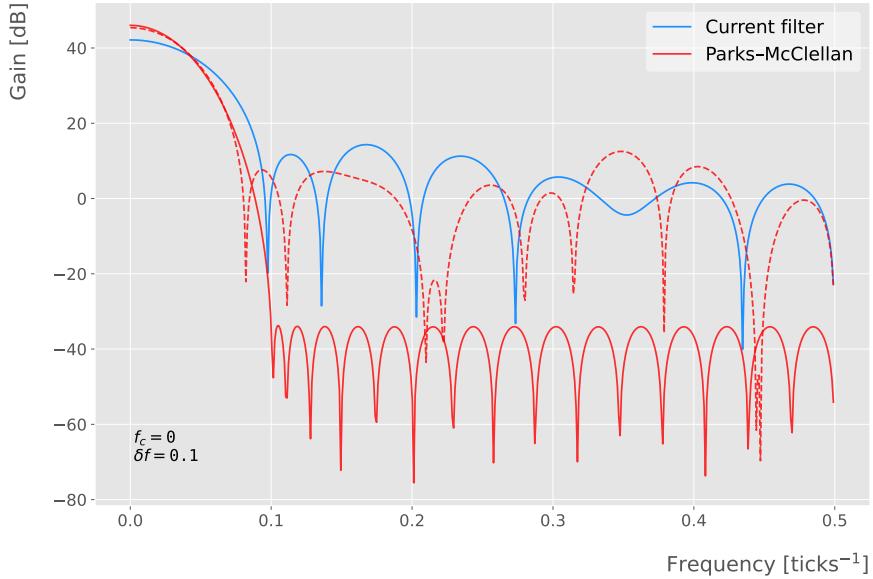


Figure 4.4: Power spectrum in decibels for the current implementation of the low-pass FIR filter in `dtp-firmware` (blue line), compared to the response of an optimal filter obtained using the Parks-McClellan algorithm for the same pass-band (red line). Also for comparison I include the spectrum of the optimal filter when taking only the integer part of the coefficients (red dashed line).

1126 McClellan method, i.e. maximize the overall S/N, using the available data captures. I
 1127 did so by varying the values of the two quantities that parametrize the pass-band and
 1128 stop-band, the cut-off frequency f_c and the transition width δf .

1129 Figure 4.5 shows the average relative change in the S/N (i.e. the ratio between the
 1130 value of the S/N after and before the filtering) for capture `felix-2020-07-17-21:31:44`,
 1131 when using filters designed with the Parks-McClellan algorithm for the specified values
 1132 of the cut-off frequency f_c and the transition width δf , restricted to integer values for
 1133 the filter coefficients. One can clearly distinguish different regions where we get an
 1134 improvement of up to a factor of 1.35 for the U plane. For large values of $f_c + \delta f$ the
 1135 ratio tends to 1, as expected (in that limit the width of the stop-band goes to 0, meaning
 1136 that no frequencies are filtered out and thus the waveform remains the same).

1137 Using the configuration which gives the best mean performance for the three
 1138 planes (see bottom right panel of Fig. 4.5), i.e. $f_c = 0.068$ ticks⁻¹ and $\delta f =$
 1139 0.010 ticks⁻¹, we can see how such filter affects the different channels. Figure 4.6

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

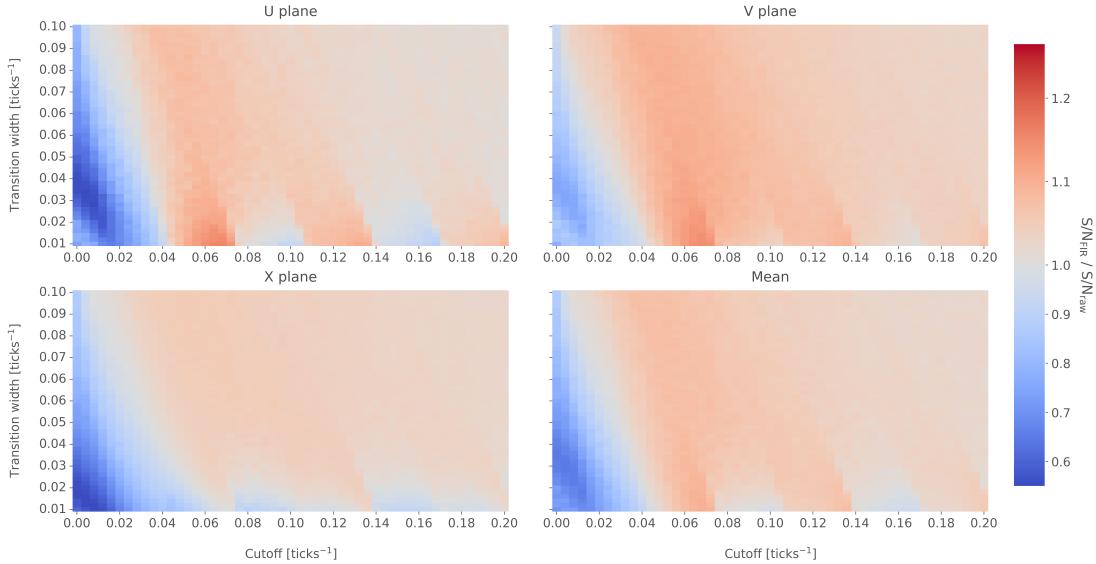


Figure 4.5: Relative change in the S/N for the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44`, using different values of the cutoff frequency f_c and the transition width δf . The optimal Chebyshev filters were applied using just the integer part of the coefficients given by the Parks-McClellan algorithm.

1140 shows the distribution of the S/N improvement values for all the channels in the raw
 1141 ADC capture `felix-2020-07-17-21:31:44`, separated by wire plane, after the optimal
 1142 Chebyshev filter was applied. One can see that there is a clear improvement for both
 1143 U and V induction wire planes, obtaining a mean change of 1.25 and 1.30 for them,
 1144 respectively. However, in the case of the X collection plane the mean of this distribution
 1145 is roughly 1, meaning that a good fraction of channels in that plane get a slightly worse
 1146 S/N after the filter is applied. In any case, this is not a big issue as the S/N for collection
 1147 channels is usually much higher than the one for induction channels.

1148 The results I obtained optimising the low pass filter with the Parks-McClellan method
 1149 are promising. Nonetheless, the improvement found is rather marginal so I wondered
 1150 if there could be an alternative approach to the filtering problem which yields better
 1151 outputs. At this point, I found a possible alternative in matched filters. By construction,
 1152 this kind of filters offer the best improvement on the S/N.

4.4. MATCHED FILTERS

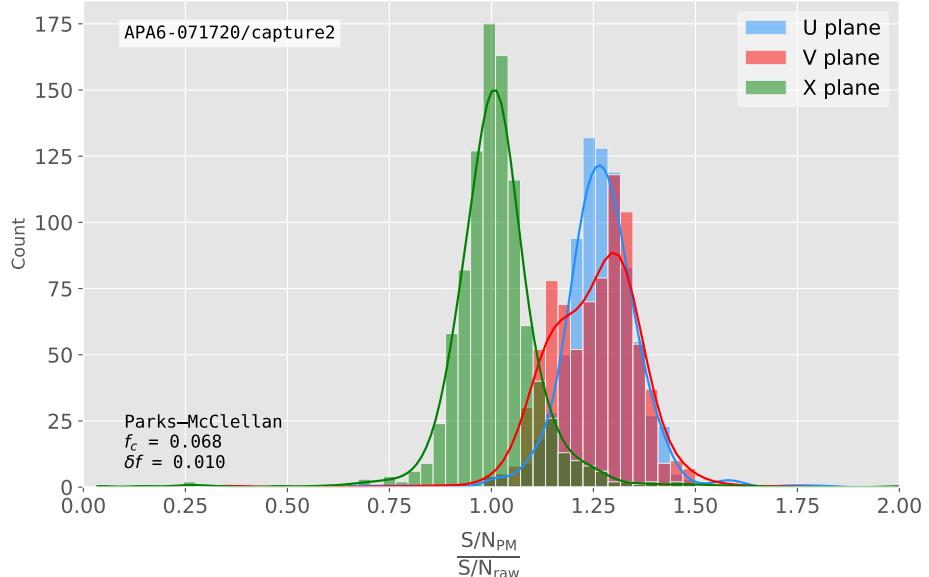


Figure 4.6: Distribution of the relative change of the S/N on the different wire planes from the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44` after the optimal Chebyshev filter was applied. The filter was computed with the Parks-McClellan algorithm using a cutoff of $f_c = 0.068 \text{ ticks}^{-1}$ and a transition width $\delta f = 0.010 \text{ ticks}^{-1}$.

1153 4.4 Matched filters

1154 In the context of signal processing, a matched filter is the optimal linear filter for
 1155 maximising the signal-to-noise ratio (S/N) in the presence of additive noise, obtained
 1156 by convolving a conjugated time-reversed known template with an unknown signal to
 1157 detect the presence of the template in the signal [105].

1158 Given a known signal sequence $s(t)$ and another (a priori unknown) noise sequence
 1159 $n(t)$, the input signal can be written as:

$$x(t) = s(t) + n(t). \quad (4.4)$$

1160 Now, considering a linear time-invariant filter, whose impulse-response function I

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

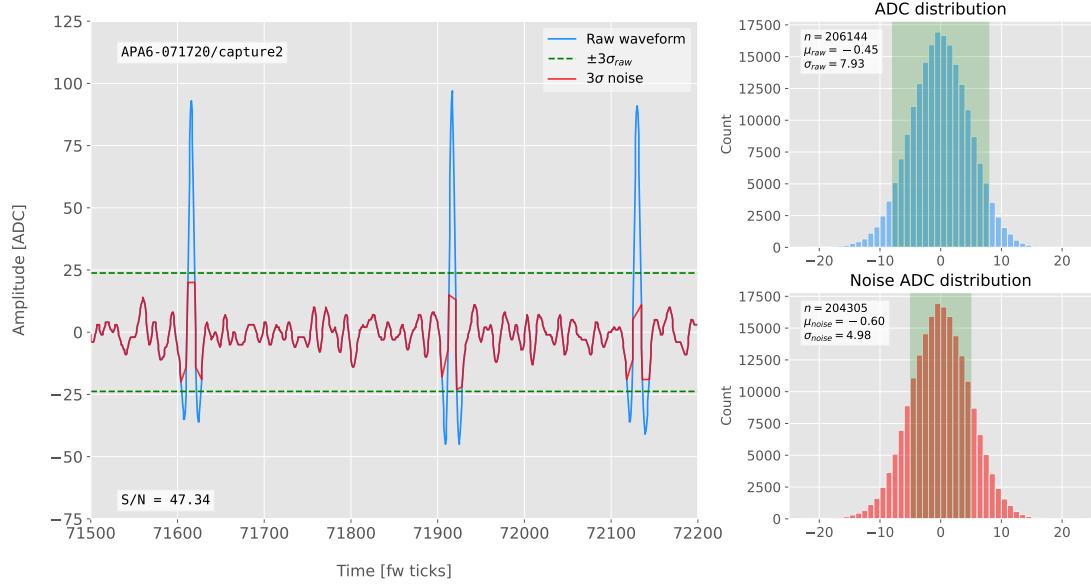


Figure 4.7: Left panel: Zoomed match filtered waveform corresponding to channel 7840 from the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44` (blue line). The filter used was directly extracted from the data, being the 32 values around the first peak in the original waveform. The green dashed lines mark the region $\pm 3\sigma_{\text{raw}}$. The resulting noise waveform is also shown (red line). Top right panel: ADC distribution for channel 7840 after match filtering, where the green shaded region represents $\pm \sigma_{\text{raw}}$. Bottom right panel: noise ADC distribution for channel 7840 after match filtering, where the green shaded region represents $\pm \sigma_{\text{noise}}$

1161 will refer to as $h(t)$, one can write the output signal as:

$$\begin{aligned} y(t) &= x(t) * h(t) \\ &= (s(t) + n(t)) * h(t) \\ &= y_s(t) + y_n(t), \end{aligned} \tag{4.5}$$

1162 where $y_s(t)$ and $y_n(t)$ are simply the outputs of the filter due to the signal and the noise
1163 components respectively.

1164 The goal of the matched filter is to detect the presence of the signal $s(t)$ in the input
1165 sample $x(t)$ at a certain time t_0 , which effectively means we need to maximise the S/N.
1166 This way, what one wants is to have a filter which gives a much bigger output when the
1167 known signal is present than when it is not. Putting it in other words, the instantaneous
1168 power of the signal output $y_s(t)$ should be much larger than the average power of the

4.4. MATCHED FILTERS

1169 noise output $y_n(t)$ at some time t_0 .

1170 For the case of the filtered signal, one can easily re-write it as an inverse Fourier
1171 transform:

$$y_s(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega H(\omega)S(\omega)e^{i\omega t}, \quad (4.6)$$

1172 where $H(\omega)$ and $S(\omega)$ are the Fourier transforms of the impulse-response function (i.e.
1173 the transfer function of the filter) and of the input signal, respectively.

1174 Now focusing on the noise, we can use the Wiener-Khinchin theorem [106] to write
1175 the mean power of the noise after filtering as:

$$E|y_n(t)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega |H(\omega)|^2 S_n(\omega), \quad (4.7)$$

1176 where $S_n(\omega)$ is the power spectral density of the noise.

1177 Having these, one can write the instantaneous S/N at time t_0 as:

$$\begin{aligned} \left(\frac{S}{N} \right)_{t_0} &= \frac{|y_s|^2}{E|y_n(t)|^2} \\ &= \frac{1}{2\pi} \frac{\left| \int_{-\infty}^{\infty} d\omega H(\omega)S(\omega)e^{i\omega t_0} \right|^2}{\int_{-\infty}^{\infty} d\omega |H(\omega)|^2 S_n(\omega)}. \end{aligned} \quad (4.8)$$

1178 Once we have this expression, we need to find the upper limit of it to determine what
1179 would be the optimal choice for the transfer function. One can use the Cauchy-Schwarz
1180 inequality, which in the present case takes the form:

$$\left| \int_{-\infty}^{\infty} dx f(x)g(x) \right|^2 \leq \int_{-\infty}^{\infty} dx |f(x)|^2 + \int_{-\infty}^{\infty} dx |g(x)|^2, \quad (4.9)$$

1181 for any two analytical functions $f(x)$ and $g(x)$. One can prove that making the choice:

$$\begin{aligned} f(x) &= H(\omega) \sqrt{S_n(\omega)} e^{i\omega t_0}, \\ g(x) &= \frac{S(\omega)}{\sqrt{S_n(\omega)}}, \end{aligned} \quad (4.10)$$

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1182 leads to the following upper bound for the S/N:

$$\left(\frac{S}{N}\right)_{t_0} \leq \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{|S(\omega)|^2}{S_n(\omega)}. \quad (4.11)$$

1183 From Eqs. (4.8), (4.9) and (4.10) one can also derive the form of the transfer function
1184 such that the upper bound is exactly reached [107]:

$$H(\omega) \propto \frac{S^*(\omega)e^{-i\omega t_0}}{S_n(\omega)}. \quad (4.12)$$

1185 From this last expression we can clearly see the way the matched filter acts. As the
1186 transfer function is proportional to the Fourier transform of the signal it will try to only
1187 pick the frequencies present in the signal [108].

1188 The matched filter transfer function can be greatly simplified if the input noise is
1189 Gaussian. In that case, the power spectral density of the noise is a constant, so it can be
1190 re-absorbed in the overall normalisation of the transfer function. Moreover, considering
1191 that the input signal is a real function, one can simply set $S^*(\omega) = S(-\omega)$, which gives:

$$H(\omega) \propto S(-\omega)e^{-i\omega t_0}. \quad (4.13)$$

1192 For a discrete signal, one can think of the input and impulse-response sequences as
1193 vectors of \mathbb{R}^N . Then, the matched filter tries to maximise the inner product of the signal
1194 and the filter while minimising the output due to the noise by choosing a filter vector
1195 orthogonal to the later. In the case of additive noise, that leads to the impulse-response
1196 vector:

$$h = \frac{1}{\sqrt{s^\dagger R_n^{-1} s}} R_n^{-1} s, \quad (4.14)$$

1197 where s is a reversed signal template sequence of length N equal to the order of the filter
1198 and R_n is the covariance matrix associated with the noise sequence n . For the Gaussian
1199 noise case, the covariance matrix is simply the unit matrix, so the above expression

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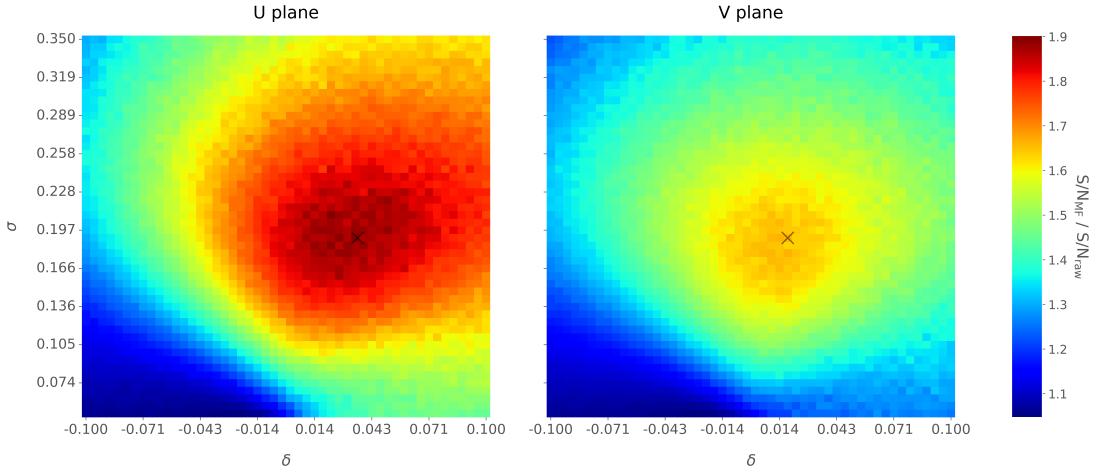


Figure 4.8: Relative change in the S/N for the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44` for different values of δ and σ from the matched filter parametrisation in Eq. (4.16). The black crosses in both panels denote the location of the maximum ratio value.

1200 simplifies again to:

$$h = \frac{s}{|s|}. \quad (4.15)$$

1201 To test whether this choice of filter is appropriate one needs to choose a signal
 1202 template. As an example of how a matched filter would affect our signal, I simply
 1203 took the filter coefficients to be the 32 ADC values around a signal peak present in the
 1204 data. In Fig. 4.7 (left panel) I plotted a zoomed region for channel 7840 in the raw
 1205 data capture `felix-2020-07-17-21:31:44`, after applying the matched filter described
 1206 before (blue line). When compared to the raw and FIR filtered case (see Figs. 4.2 and
 1207 4.3), after applying the match filter the standard deviation of the noise waveform (red
 1208 line) decreases and at the same time the signal peaks are enhanced. This leads to an
 1209 improvement of the S/N by a factor of 1.92 when compared to the raw waveform.

1210 To obtain the matched filter that is more suitable for our data, I explored different
 1211 configurations of signal templates. I parametrised the signal using the bipolar function:

$$f(x) = -A(x + \delta) e^{-x^2/\sigma^2}, \quad (4.16)$$

1212 where the parameter δ controls the asymmetry between the positive and negative peaks

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1213 and σ controls their width. The amplitude parameter A is set such that it keeps the
1214 height of the biggest peak to be less than 200 ADC in absolute value.

1215 As this parametrisation is only adequate for bipolar signals I will focus exclusively
1216 on the induction channels. Also, the optimal configurations I found for the U and V
1217 plane will be kept separate, i.e. I will have two sets of coefficients that will be applied to
1218 either the U and V planes of wires. I do so as I found this was the choice giving the
1219 best performance. Even so, as I will discuss, the differences are not very pronounced. In
1220 case it is not technically possible to separate channels in the firmware according to the
1221 wire plane they come from and use different sets of filter coefficients for them, we can
1222 just find a common unique set of coefficients. In such case, I do not expect our results
1223 to change dramatically.

1224 Figure 4.8 presents the results of the parameter scan, for channels in the induction
1225 planes U (left panel) and V (right panel). For each configuration of σ and δ the resulting
1226 matched filter was applied to all channels in the corresponding plane within the data
1227 capture `felix-2020-07-17-21:31:44`, the S/N improvement was computed with respect
1228 to the raw waveforms and then the S/N mean value was kept as a score for such filter.
1229 One can see that the improvement obtained for the U plane is in general higher than the
1230 one for the V plane. In any case, I got substantially higher ratios than the ones obtained
1231 for the low-pass FIR filters. For the optimal configurations I attained improvements up
1232 to a factor of 1.85 for the U plane and 1.65 for the V plane.

1233 The sets of optimal matched filter coefficients were obtained for the parameters
1234 $\delta = 0.035$, $\sigma = 0.191$ for the U plane and $\delta = 0.018$, $\sigma = 0.191$ for the V plane. I
1235 show these two sets of coefficients in Fig. 4.9 (left panel). In Fig. 4.9 (right panel)
1236 I show the distribution of the S/N improvement after the optimal match filters for
1237 the U and V were applied to the corresponding channels in the raw data capture
1238 `felix-2020-07-17-21:31:44`. As mentioned before, the mean improvement achieved
1239 for the U plane channels is slightly bigger than the one for the V channels. Note, however,
1240 that the spread of the distribution for the V plane is also smaller than the one for the U
1241 plane.

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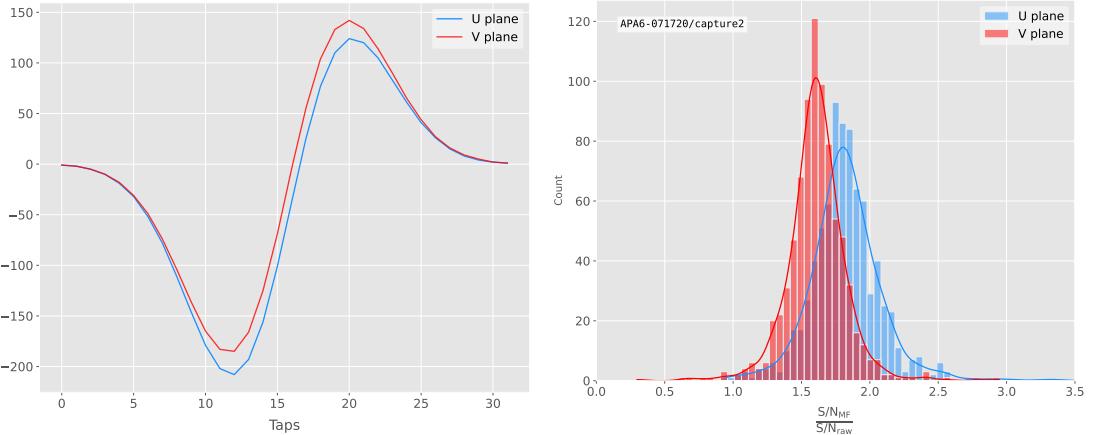


Figure 4.9: Left panel: Optimal matched filter coefficients for the U (blue line) and V (red line) planes. The filters were computed with our parametrisation in Eq. (4.16) for the parameter values $\delta = 0.035$, $\sigma = 0.191$ and $\delta = 0.018$, $\sigma = 0.191$ respectively. Right panel: Distribution of the relative change of the S/N on the two induction wire planes from the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44` after their respective optimal matched filters were applied.

Overall, one can see that the improvements on the S/N are much more significant in the case of the matched filter than it is for the low-pass FIR filters. The analysis of this and other raw data captures from ProtoDUNE-SP suggest that matched filters increase the S/N of induction channels by a factor of 1.5 more than the optimal low-pass FIR filters.

Although these results are by themselves great points in favour of the matched filter, more studies are needed to completely assess the robustness of this approach. I proceeded then to test the matched filter with simulated data samples.

4.5 Monte Carlo studies

To further test the matched filter, the next step was to generate and process data samples using LArSoft [109], the simulation and reconstruction software of the DUNE FD. In this way, one can control the particle content of the samples, the orientation of the tracks and their energy, and therefore see how the matched filter behaves in various situations.

To begin with, I prepared different monoenergetic and isotropic samples containing

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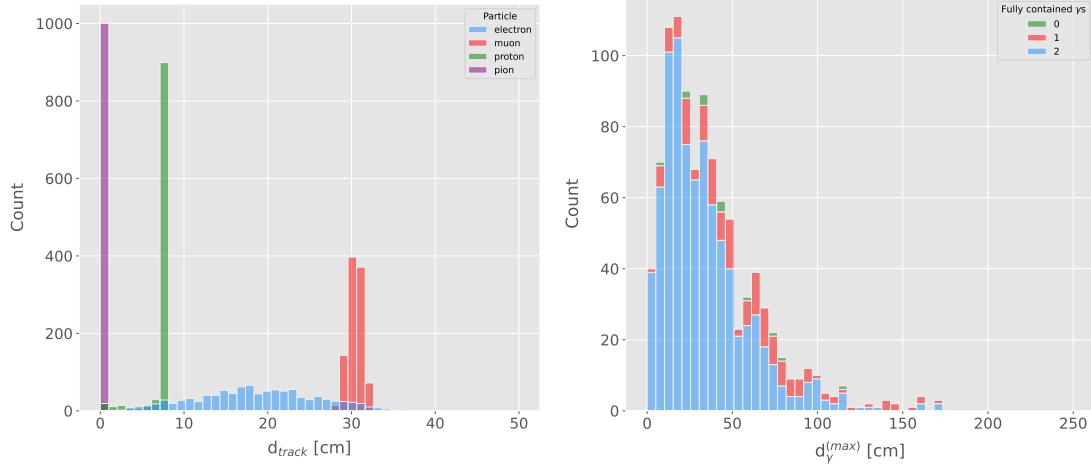


Figure 4.10: Left panel: distributions of the particles track length in the liquid argon for the generated $E_k = 100$ MeV monoenergetic samples, electrons (blue), muons (red), protons (green) and neutral pions (purple). Right panel: distribution of the length of the longest photon in the neutral pion sample after the decay process $\pi^0 \rightarrow \gamma\gamma$.

1256 a single particle per event. Each sample contains a different particle species, namely
 1257 electrons, muons, protons and neutral pions all with a kinetic energy of $E_k = 100$ MeV.
 1258 I chose these because of the fairly different topologies they generate in the liquid argon,
 1259 ranging from shower-like to track-like.

1260 These were generated with the single particle gun and the Geant4 stage of the
 1261 LArSoft simulation [109] was performed with the standard configuration for the DUNE
 1262 FD 10kt module.

1263 For simplicity, I restricted the particles to start drifting in a single TPC volume
 1264 (in this case TPC 0), so I can focus exclusively on the signals coming from one APA.
 1265 The chosen kinetic energy for all the particles in my first trial is $E_k = 100$ MeV, so a
 1266 necessary check is to see if all our tracks will be typically contained in one TPC volume.
 1267 Figure 4.10 (left panel) shows the distributions of the track lengths in the liquid argon
 1268 of all generated particles with $E_k = 100$ MeV. One can see that, in the case of the
 1269 track-like particles (i.e. muons and protons), their length distributions are quite sharp
 1270 and centered at relatively low distances (30 and 8 cm, respectively). For electrons, the
 1271 distribution is quite broad but it does not extend past ~ 30 cm. The case of neutral
 1272 pions can be misleading, as they decay promptly the track length associated with the

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1273 true Monte Carlo particle is always < 1 cm. In Fig. 4.10 (right panel) I show the
1274 effective length distribution of the longest photon after the pion decays as $\pi^0 \rightarrow \gamma\gamma$,
1275 highlighting the number of fully contained photons in the TPC volume per event (either
1276 zero, one or both). One can see that the vast majority of events has both photons
1277 contained and that just a negligible number of them has none of them contained in the
1278 TPC volume. In any case, for the sake of caution, I will only keep the pion events with
1279 both photons contained.

1280 The next step is to process the sample through the detector simulation. To make
1281 adequate estimations of the noise levels, one needs to turn off the default zero-suppression
1282 of the waveforms produced by the simulation. At this first stage I am only concerned
1283 with the waveforms with the noise added, so I keep the noise addition option as true in
1284 the configuration. However, for studies related to the hit finder performance one will
1285 also need to store the noiseless waveforms to retrieve the truth information of the hits. I
1286 will discuss this approach next.

1287 To reduce the amount of data that will go for processing, I used the information from
1288 the Geant4 step of the simulation to select only the active channels, i.e. the channels
1289 where some ionisation electrons arrive. Moreover, as said previously, I only extract the
1290 waveforms from APA 0 and exclusively the ones coming from induction channels. The
1291 resulting ROOT file contains a tree with two branches, one containing the waveforms for
1292 each event and channel and the other with the corresponding offline channel numbers.

1293 Finally, to extract the truth values for the orientation of the tracks and the energies
1294 of the particles I used a modified analysis module. This gives a ROOT file with a single
1295 tree, containing several branches with different information such as the components of
1296 the initial momentum of the particles, initial and final xyz location, track length, etc.

1297 For the analysis of the resulting waveforms and truth values I used a custom set of
1298 Python libraries (available at [??]). Among other functionalities, these enable the user
1299 to read the ROOT files, export the raw data as pandas objects, apply the filters and
1300 compute the S/N of both the raw and filtered signals. So far, the default configuration
1301 for the filtering uses the set of optimal matched filter coefficients that I found using the

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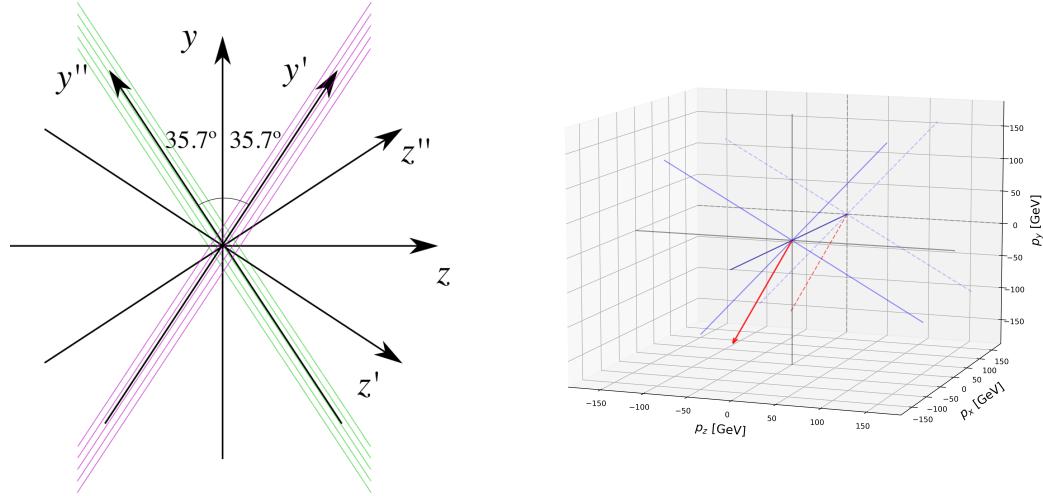


Figure 4.11: Left panel: schematic representation of the two new rotated reference frames used in this analysis (denoted as prime and double prime), viewed from the yz plane. The magenta stack of lines represent the wires in the U plane, whereas the green lines correspond to the wires in the V plane. Right panel: 3D representation of the momentum of one of the generated monoenergetic muons (red arrow) in the original reference frame (black lines), along with the new reference frame used for the U plane waveforms (blue lines). In the yz plane I added the projection of these three.

1302 ProtoDUNE data samples.

1303 Additionally, for the analysis of the samples it was necessary to use two different
 1304 reference frames, to study separately the signals coming from the U and V induction wire
 1305 planes. As I am focussing on a single APA, the U and V wires have a different orientation
 1306 in the yz plane. In the case of U wires, these are tilted 35.7° clockwise from the vertical
 1307 (y direction), whereas the V wires are at the same angle but in the counter clockwise
 1308 direction. Because of this, the best option is to deal with two new coordinate systems
 1309 rotated by $\pm 35.7^\circ$ along the x axis, so the new y' and y'' directions are aligned with the
 1310 U and V induction wires. Figure 4.11 (left panel) shows a schematic representation of
 1311 the original reference frame together with the two rotated ones (denoted by primed and
 1312 double primed). This way, one can easily understand how parallel was a track to the
 1313 wires in the two induction planes. Figure 4.11 (right panel) shows a 3D representation
 1314 of the momentum of a track (red arrow) in the original reference frame (black lines),
 1315 along with the new reference frame for U wires (blue lines). I added the projections in

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1316 the yz plane of these, to show the usefulness of the new reference frame to tell whether
 1317 a track is parallel or normal to the wires in the induction plane.

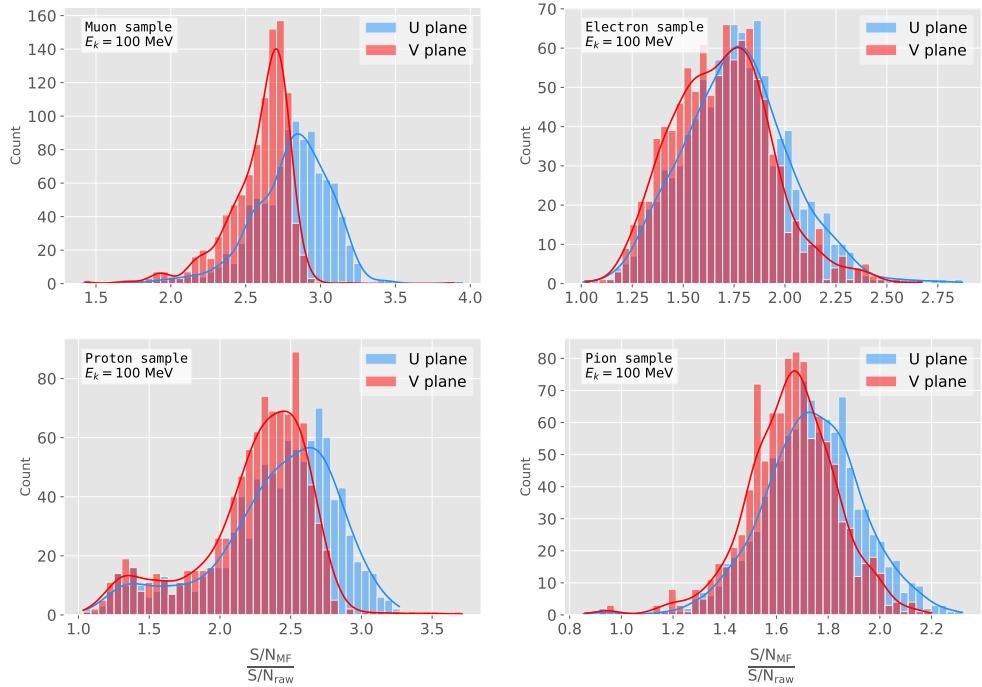


Figure 4.12: Distributions of the mean S/N change per event for the different MC samples after applying the matched filters. Here I separated the change in the U plane (blue) and the V plane (red) channels. From top left to the right: muon, electron, proton and neutral pion. All the events have a fixed kinetic energy of $E_k = 100$ MeV.

1318 Figure 4.12 shows the distribution of the average S/N improvement per event when
 1319 one applies the optimal matched filters. I produced separate distributions for the channels
 1320 in the U (red) and V (blue) induction wire planes. Notice that the S/N distributions
 1321 for the track-like particles, i.e. muons (top left panel) and protons (bottom left panel),
 1322 have significantly larger mean values than the distributions of the shower like particles,
 1323 i.e. electrons (top right panel) and neutral pions (bottom right panel). An important
 1324 difference between these results and the ones seen before for ProtoDUNE data is that,
 1325 overall, the improvements that I get for simulated data are bigger. This could be due
 1326 either to the default noise model used in the *LArSoft* simulation or to the simulated hits
 1327 having higher energy than the ones in the recorded data. Nonetheless, the concluding
 1328 message is that the previously optimised matched filters give an overall significant

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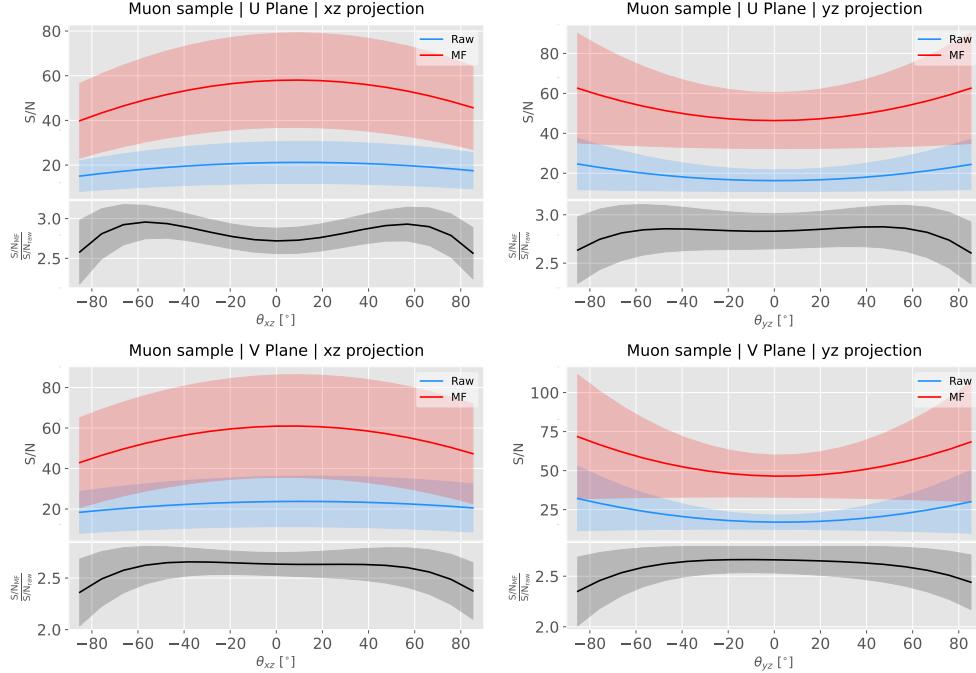


Figure 4.13: Angular dependence of the mean S/N and the S/N improvement for the monoenergetic muon sample. The top and bottom rows correspond to the U and V planes, respectively. The top subplots show the mean S/N for raw (blue) and filtered (red) waveforms whereas the bottom subplots depict the averaged S/N improvement (black).

improvement of the S/N for the different samples.

About the convention I followed for the plots and results, in the case of the raw and filtered S/N of each event in the sample I simply took the average of the quantities over all the active channels in the event. That is, if a certain event has N_{chan} active channels these two quantities are computed as:

$$(S/N_{fir})_{event} = \frac{\sum_{i=0}^{N_{chan}} (S/N_{fir})_i}{N_{chan}},$$

$$(S/N_{raw})_{event} = \frac{\sum_{i=0}^{N_{chan}} (S/N_{raw})_i}{N_{chan}}.$$
(4.17)

However, for the ratio of the raw and filtered S/N (what I called the S/N improvement) per event I am not just taking the ratio of the previous two quantities but computing

4.5. MONTE CARLO STUDIES

1336 the average of the individual ratios per channel in the event:

$$\left(\frac{S/N_{fir}}{S/N_{raw}} \right)_{event} = \frac{\sum_{i=0}^{N_{chan}} \left(\frac{S/N_{fir}}{S/N_{raw}} \right)_i}{N_{chan}}, \quad (4.18)$$

1337 and so:

$$\left(\frac{S/N_{fir}}{S/N_{raw}} \right)_{event} \neq \frac{(S/N_{fir})_{event}}{(S/N_{raw})_{event}}. \quad (4.19)$$

1338 4.5.1 Angular dependence

1339 Having these monoenergetic samples, one can also study the angular dependence of the
1340 performance of the matched filter. This is an important point, as it is a well established
1341 fact that for certain configurations (an extreme case configuration being signals normal
1342 to the wire plane and perpendicular to the induction wires at the same time) the S/N is
1343 much lower than average as the corresponding waveforms are severely distorted. In this
1344 sense, I am interested to see how the matched filter behaves for these cases and how the
1345 S/N improvement on those compare to the average.

1346 Figure 4.13 shows the angular dependence of the S/N for the monoenergetic $E_k =$
1347 100 MeV isotropic muons, for the different induction wire planes and projections. The
1348 angles for each event are given by the components of the initial value of the momentum
1349 of the particles, taking the angles of the projections on the xz and yz planes with respect
1350 to the z axis (more accurately, one needs to compute these angles twice for each event, a
1351 pair for the $xy'z'$ coordinate system and the other for the $xy''z''$). The top row shows the
1352 dependence on the angles corresponding to the U plane, i.e. $\theta_{xz'}$ and $\theta_{y'z'}$, whereas the
1353 bottom row shows the angular dependence viewed from the V plane, $\theta_{xz''}$ and $\theta_{y''z''}$. In
1354 each plot, the top subplot represents the mean values of the S/N for the raw (blue) and
1355 matched filtered (red) signals, and the bottom subplot the averaged S/N improvement
1356 (black). The solid lines represent the mean value obtained for the corresponding angular
1357 value, whereas the semitransparent bands represent one standard deviation around the
1358 mean at each point.

1359 As expected, the S/N is in general higher when tracks are parallel to the APA (i.e.

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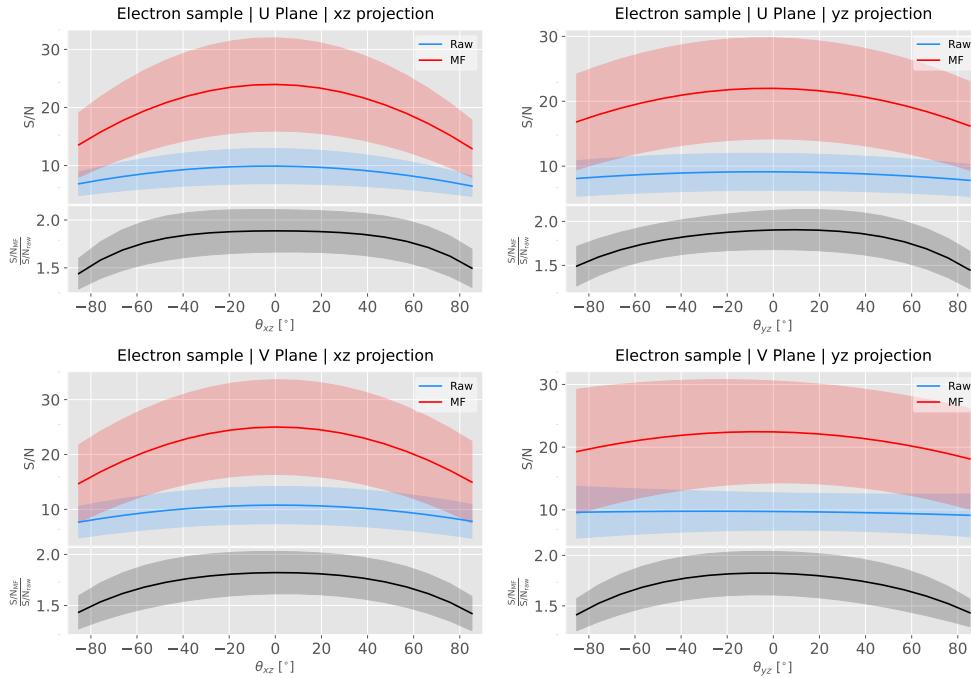


Figure 4.14: Angular dependence of the mean S/N and the S/N improvement for the monoenergetic electron sample. The top and bottom rows correspond to the U and V planes, respectively. The top subplots show the mean S/N for raw (blue) and filtered (red) waveforms whereas the bottom subplots depict the averaged S/N improvement (black).

1360 $\theta_{xz} \sim 0$) and lower when it is normal to the plane ($\theta_{xz} \sim \pm 90^\circ$). In the same way, tracks
 1361 parallel to the wires ($\theta_{yz} \sim \pm 90^\circ$) tend to have higher S/N than those perpendicular to
 1362 these ($\theta_{yz} \sim \pm 0$).

1363 Figure 4.14 shows the corresponding angular dependence information for the $E_k =$
 1364 100 MeV electrons sample. Notice that, in this case, the S/N behaviour discussed above
 1365 does not hold. A possible explanation can be that, because most hits in these events
 1366 are produced by the secondary particles generated in the EM shower, the signal peaks
 1367 whose S/N ratios were computed do not correspond to the directional information of
 1368 the primary electron.

1369 4.5.2 Distortion and peak asymmetry

1370 As a case study, I selected two of the simulated $E_k = 100$ MeV monoenergetic muon
 1371 events. With respect to the U induction plane, one is parallel to the APA (low $\theta_{xz'}$)

4.5. MONTE CARLO STUDIES

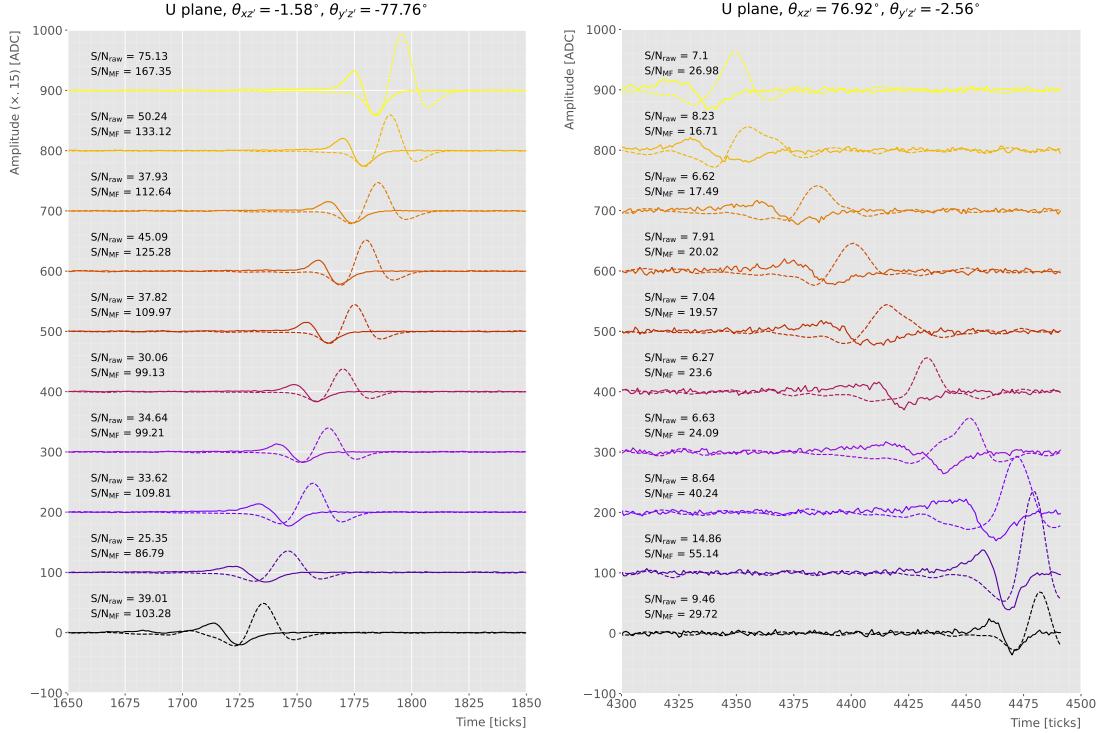


Figure 4.15: Selected consecutive waveforms corresponding to two monoenergetic $E_k = 100$ MeV muon events, one is parallel to the APA and to the wires in the U plane (left panel) and the other is normal to the APA plane and perpendicular to the U plane wires (right panel). The solid lines represent the raw waveforms whereas the dashed lines correspond to the waveforms after the matched filter was applied. The waveforms on the left panel have been scaled by a factor of 0.15 to have similar amplitude to the ones on the right panel.

and to the wires (high $\theta_{y'z'}$) and the other is normal to the APA plane (high $\theta_{xz'}$) and perpendicular to the wires (low $\theta_{y'z'}$). As expected from the results on the angular dependence discussed above, the former has a higher S/N (before and after the filtering) when compared to the latter. An interesting thing to notice about these two samples is that, even though one has a much bigger S/N than the other, it is the one with the smallest S/N the one that got the biggest averaged S/N improvement. In Tab. 4.1 I include all the relevant parameters of these two $E_k = 100$ MeV muon events, namely the angles with respect to the $xy'z'$ reference frame, the values of the S/N, the S/N improvement and also the so-called peak asymmetry Δ_{peak} that I will discuss next.

One can try to understand better what is going on with these two events by looking

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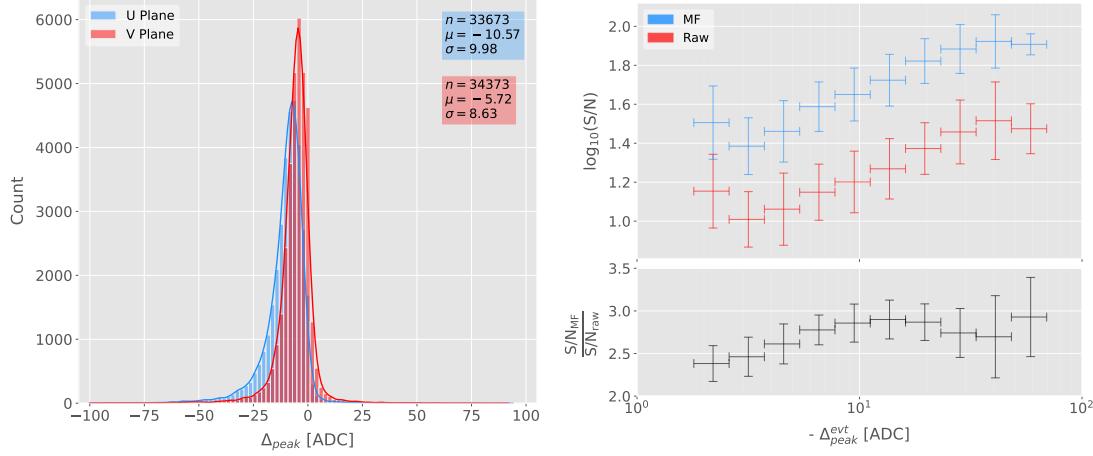


Figure 4.16: Left panel: peak asymmetry distribution for the case of the monoenergetic $E_k = 100$ MeV muon sample. Each value corresponds to a single bipolar signal peak from a channel in any event. The blue distribution represents the peaks on U plane channels, whereas the red corresponds to signal peaks in V wires. Right panel: relation between the mean peak asymmetry per event with the S/N for U channel waveforms from the $E_k = 100$ MeV muon sample. The top subplot shows the decimal logarithm of the mean S/N for the raw (red) and the matched filtered (blue) waveforms. The bottom subplot contains the mean S/N improvement ratio after the matched filter was applied.

Table 4.1: Characteristic parameters of the two monoenergetic muon events selected, relative to the U plane: projected angles in the xz' and $y'z'$ planes, S/N values for the raw and filtered waveforms, mean improvement of the S/N and peak asymmetry.

	$\theta_{xz'}$ ($^\circ$)	$\theta_{y'z'}$ ($^\circ$)	S/N _{raw}	S/N _{MF}	$\frac{S/N_{MF}}{S/N_{raw}}$	Δ_{peak} (ADC)
High ("parallel")	-1.58	-77.76	41.65	112.44	2.83	-35.73
Low ("normal")	76.92	-2.56	8.07	25.46	3.12	-10.38

1382 at the raw and filtered data from some of their active channels. Figure 4.15 shows a
 1383 selection of consecutive raw and filtered U plane waveforms from the event with high S/N
 1384 (left panel) and the one with low S/N (right panel). Notice that to show both collections
 1385 of waveforms at a similar scale I had to apply a factor of 0.15 to the waveforms with
 1386 high S/N. Additionally, next to each waveform I included the values of the raw and
 1387 matched filtered S/N for the corresponding channel. The first thing to notice in this plot
 1388 is that the amplitude of the signal peaks from the normal track have a much smaller
 1389 amplitude, and also appear quite distorted when compared to the others. On the other
 1390 hand, although the matched filtered S/N is still smaller, the relative improvement is
 1391 bigger than in the parallel case.

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1392 A way I found to quantify the difference between the shapes within these two events
 1393 is their different peak asymmetry. One can define the peak asymmetry as the (signed)
 1394 difference between the positive and the negative peaks of the bipolar shape, i.e.:

$$\Delta_{peak} \equiv h_+ - h_-, \quad (4.20)$$

1395 where both heights h_+ and h_- are positive defined. Figure 4.16 (left panel) shows the
 1396 distribution of this peak asymmetry for all the waveforms corresponding to channels
 1397 in the U (blue) and V (red) planes for the monoenergetic muon sample. One can
 1398 see that these distributions are clearly shifted to negative values (with mean values
 1399 $\mu_\Delta^U = -10.57$ ADC and $\mu_\Delta^V = -5.72$ ADC respectively). It is interesting to notice
 1400 that the peak asymmetry value of the sample with high S/N sits at the left tail of the
 1401 distribution whereas the corresponding value of the sample with low S/N lies around
 1402 the mean.

1403 Now, one can try to correlate the peak asymmetry with the S/N and the S/N
 1404 change per event. Figure 4.16 (right panel) shows the result of comparing the mean
 1405 peak asymmetry per event to the averaged raw (red) and matched filtered (blue) S/N
 1406 per event (top subplot). The horizontal lines sit at the mean value obtained in the fit
 1407 and represent the width of the $-\Delta_{peak}$ bins used, while the vertical lines indicate one
 1408 standard deviation around that mean value. Notice that, when taking decimal logarithm
 1409 on both, there is an approximate linear relation between these quantities, except for
 1410 peak asymmetry values bigger than -5 ADC where the S/N remains constant.

1411 Also, in the bottom subplot of Fig. 4.16 (right panel) I show the relation between
 1412 the peak asymmetry and the mean S/N improvement. In this case, one see that there is
 1413 a maximum at $\Delta_{peak} \sim -10$ ADC. As mentioned previously, this is also the value of the
 1414 mean of the peak asymmetry distribution. In fact, it is expected that our filter favours
 1415 the signal peaks with the most common values of the peak asymmetry, as this was one
 1416 of the features I target in our filter coefficient optimisation through the parameter δ .

1417 These results suggest that events with poorer values of the mean S/N, usually

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

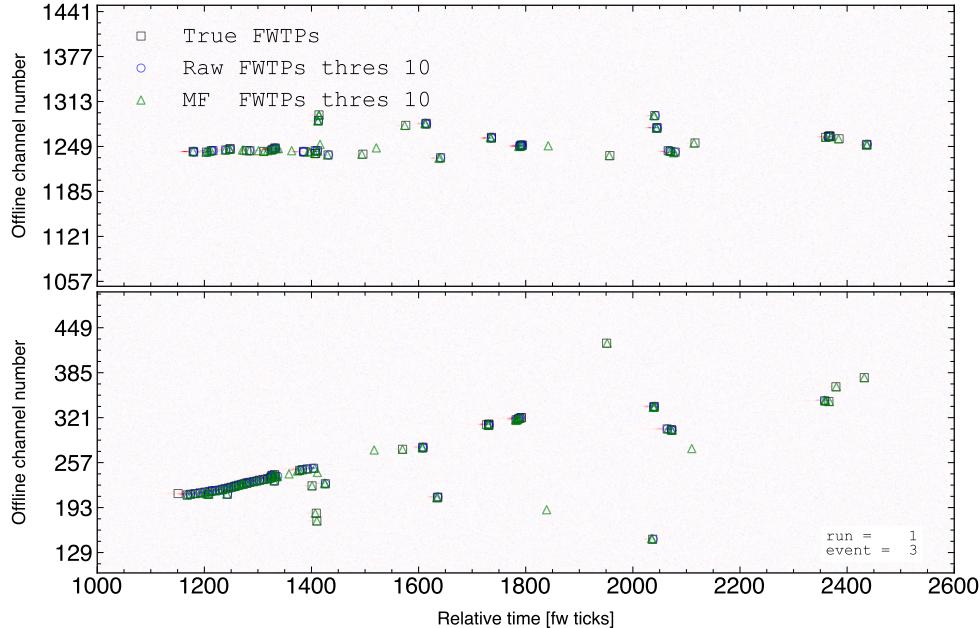


Figure 4.17: Raw event display in the plane time (in firmware ticks) versus offline channel number for a $E_k = 100$ MeV electron event. The produced true hits are superimposed (black boxes) as well as the hits coming from the standard hit finder chain (blue circles) and the hit finder using the matched filter (green triangles).

1418 associated to non-favourable track orientations, tend to have smaller values of the mean
 1419 peak asymmetry (in absolute value). Nonetheless, because our matched filters have
 1420 been optimised to account for these asymmetries, the improvement on the S/N for these
 1421 events is sizeable if not better than the one for events which already had a high S/N.

1422 4.5.3 Hit sensitivity

1423 One of the advantages of the matched filter, directly related to increasing the S/N, is
 1424 the capability of picking hits that before fell below the threshold. For instance, Fig. 4.17
 1425 shows the raw ADC data from an example event (electron, $E_k = 100$ MeV) with the
 1426 produced true hits superimposed (black boxes), together with the hits produced by the
 1427 standard hit finder chain (blue circles), i.e. using the current FIR filter, and the hits
 1428 obtained using the matched filters (green triangles). Both the standard and the matched
 1429 filter hit finders were run with a threshold of 10 ADC. Notice that the standard hits
 1430 match well the true ones at the initial part of the event (where we have a track-like

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object), but they miss most of the hits produced by the EM shower at later times. On the other hand, the hits produced with the matched filter have a better agreement with the true hits even for the more diffuse shower activity.

Even though the matched filter gets more hits as a result of the enhancement of the signal peaks relative to the noise level, it is also true that it picks up some spurious hits not related to any real activity if one lowers the thresholds too much. Therefore, some optimisation of the threshold is needed, as there is a trade-off between precision and sensitivity.

Having this in mind, I tried to compare the produced hits one gets from the standard hit finder and the ones resulting from applying the matched filter with the true hits. By running the hit finders on our samples with different values of the threshold one can understand, for instance, how low one can set the threshold without getting mostly spurious hits and then evaluate the gains obtained from this.

To see how the hit sensitivity changes with the energy, I prepared new isotropic samples with the same types of particles as before (muons, electrons, protons and neutral pions) but with a flat kinetic energy distribution ranging from 5 to 100 MeV.

To estimate the hit sensitivity, given a certain sample, one needs to recover the set of true hits to be able to compare these with the ones produced. To do so, a modification in the procedure I was using to extract the raw waveforms is needed. For this kind of study, I run the detector simulation in two steps, first I produce the waveforms without noise and extract them in the same format I used for the raw data, then the noise is added and the noisy waveforms are then written to a file as well.

To have a better comparison between the true hits and the ones produced from the raw waveforms after applying the two filters, I applied also the FIR filter and the matched filters to the noiseless waveforms and then I run the hit finder with a minimal threshold (in this case I used 1 ADC) on these noiseless filtered waveforms. In this way I generated two sets of true hits, I will refer to them as standard true hits (with the current/default FIR filter) and matched filter true hits respectively. This allows a more precise matching between the different groups of hits produced, as it will account for

CHAPTER 4. MATCHED FILTER APPROACH TO TRIGGER PRIMITIVES

1460 any delays and distortions introduced by the FIR and the matched filters.

1461 In the case of the raw waveforms (with noise), I run the hit finder on them, with
1462 different values of the threshold, after applying either the FIR or the matched filters. I
1463 will name them simply standard hits and matched filter hits respectively. Then, I match
1464 the generated hits to the true hits (the standard hits with the standard true hits and
1465 the matched filter hits with the matched filter true hits). The matching is performed by
1466 comparing the channel number and the timestamp of the hits. To count as a match,
1467 I require that all hits with the same channel number and timestamp have overlapping
1468 hit windows, i.e. the time windows between their hit end and hit start times need to
1469 overlap. If more than one hit in one of the groups have hit overlap with the same hit in
1470 the other group I only count the hit with closer hit peak time value.

1471 To quantify the performance of the two hit finder approaches, I use a classical method
1472 from statistical classification known as confusion matrix [110]. It divides the outputs in
1473 four categories: true positive (TP, both true and predicted values are 1), false negative
1474 (FN, true value is 1 but predicted is 0), false positive (FP, true value is 0 but predicted
1475 is 1) and true negative (TN, both true and predicted values are 0)).

1476 The contents of the confusion matrix allow us to compute other derived scores to
1477 judge the performance of our classifiers. In this study, I will make use of three of these
1478 metrics, namely the precision or positive predictive value:

$$\text{PPV} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \quad (4.21)$$

1479 the sensitivity or true positive rate:

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}, \quad (4.22)$$

1480 and the F_1 score [111]:

$$F_1 = \frac{2\text{TP}}{2\text{TP} + \text{FP} + \text{FN}}, \quad (4.23)$$

1481 which is the harmonic mean of the precision and the sensitivity.

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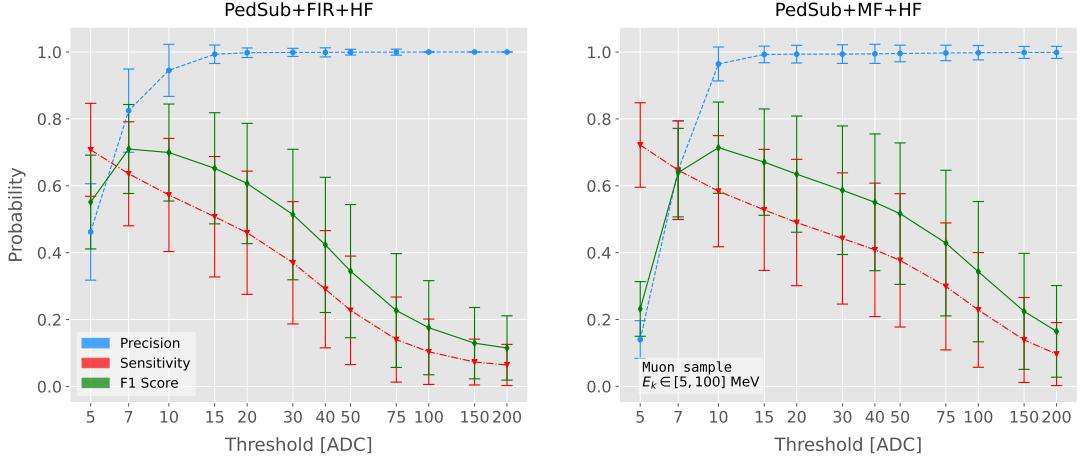


Figure 4.18: Dependence of the precision (blue), sensitivity (red), and F_1 (green) scores on the threshold values used in the hit finder, for the FIR (left panel) and matched filter (right panel) cases. The results were obtained after matching the hits to the true hits in the case of the isotropic muon sample with kinetic energy in the range 5 to 100 MeV, taking only into account the induction plane channels. The points represent the mean value while the error bars indicate one standard deviation around that mean value.

1482 In our specific case I am not going to make use of the true negative value, as its
 1483 definition in this context can be ambiguous because one does not have clear instances in
 1484 the classification process. This way, I will only count the number of true positives as the
 1485 total amount of hits I can match between true and raw populations, the number of false
 1486 negatives will be the number of missing true hits and the false positive the number of
 1487 hits which do not match any true hit.

1488 In Fig. 4.18 I show the precision (blue), sensitivity (red) and F_1 (green) scores I
 1489 obtained for different values of the threshold used in the hit finder for the case of the
 1490 muon sample. Because the matched filters are only applied to induction channels, I only
 1491 consider here hits coming from the U and V planes. The panel on the left corresponds
 1492 to the scores I got when I ran the hit finder on the FIR filtered waveforms, whereas the
 1493 right panel contains the scores for the matched filter case. The points are centered at
 1494 the threshold value used and represent the mean value obtained for each score using all
 1495 the generated events, while the error bars indicate one standard deviation around the
 1496 mean value.

1497 One can see that the precision for the matched filter case is lower when the thresholds

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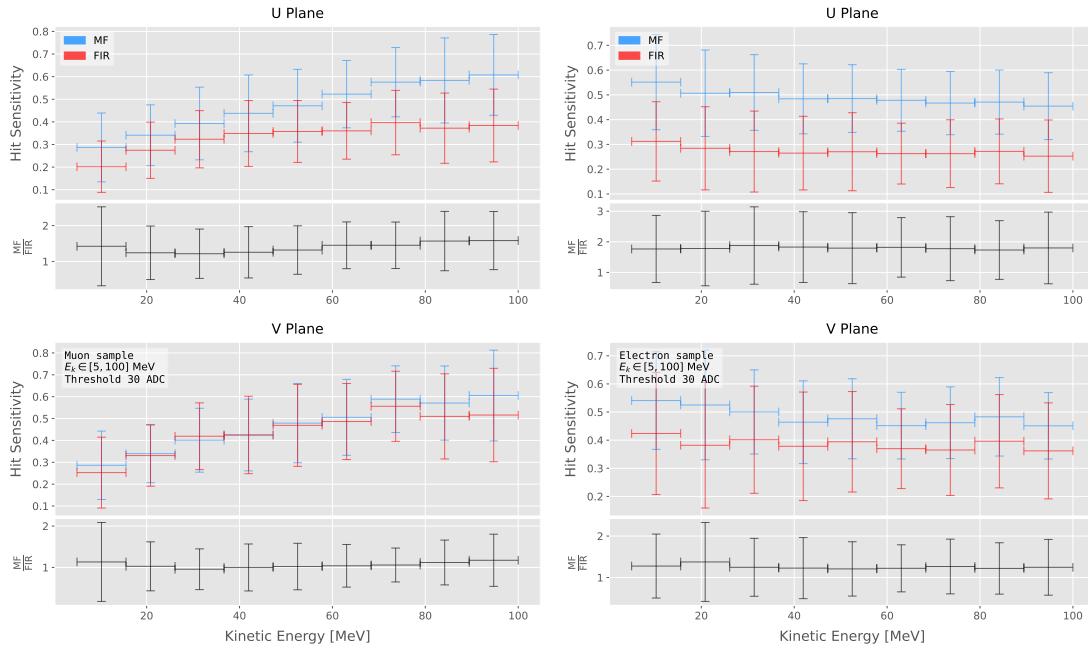


Figure 4.19: Dependence of the averaged hit sensitivity on the kinetic energy of the events for the matched filter (blue) and standard (red) hits, for the case of the muon (left panel) and electron (right panel) samples, separated between U (top plots) and V (bottom plots) induction wire planes. The top subplots contain the hit sensitivities for the two hit finder alternatives, while the bottom subplots show the ratio between the two. The horizontal lines sit at the mean value and represent the size of the energy bins, while the vertical error bars indicate one standard deviation around that mean value.

1498 are very low, as the noise baseline is slightly amplified, but then rises to high values
 1499 quicker than for the FIR case. The other difference one can spot is that the sensitivity
 1500 in the FIR case starts dropping faster at around the same threshold values where the
 1501 precision stabilises around 1, while in contrast for the matched filter this rapid decrease
 1502 starts at higher threshold values. A similar scan for the same thresholds was performed
 1503 for the electron sample in the same energy range, yielding similar results.

1504 In Fig. 4.19 I show the averaged hit sensitivity versus the kinetic energy of the
 1505 events, both for the matched filter hits (blue) and the standard hits (red). The left
 1506 panel corresponds to the muon sample, whereas the one on the right corresponds to the
 1507 electron sample, both with kinetic energies between 5 and 100 MeV. In each panel the
 1508 top plot corresponds to hits in the U plane, while the bottom plot contains the same
 1509 information for the V plane. Each plot contains two subplots, the one on the top shows

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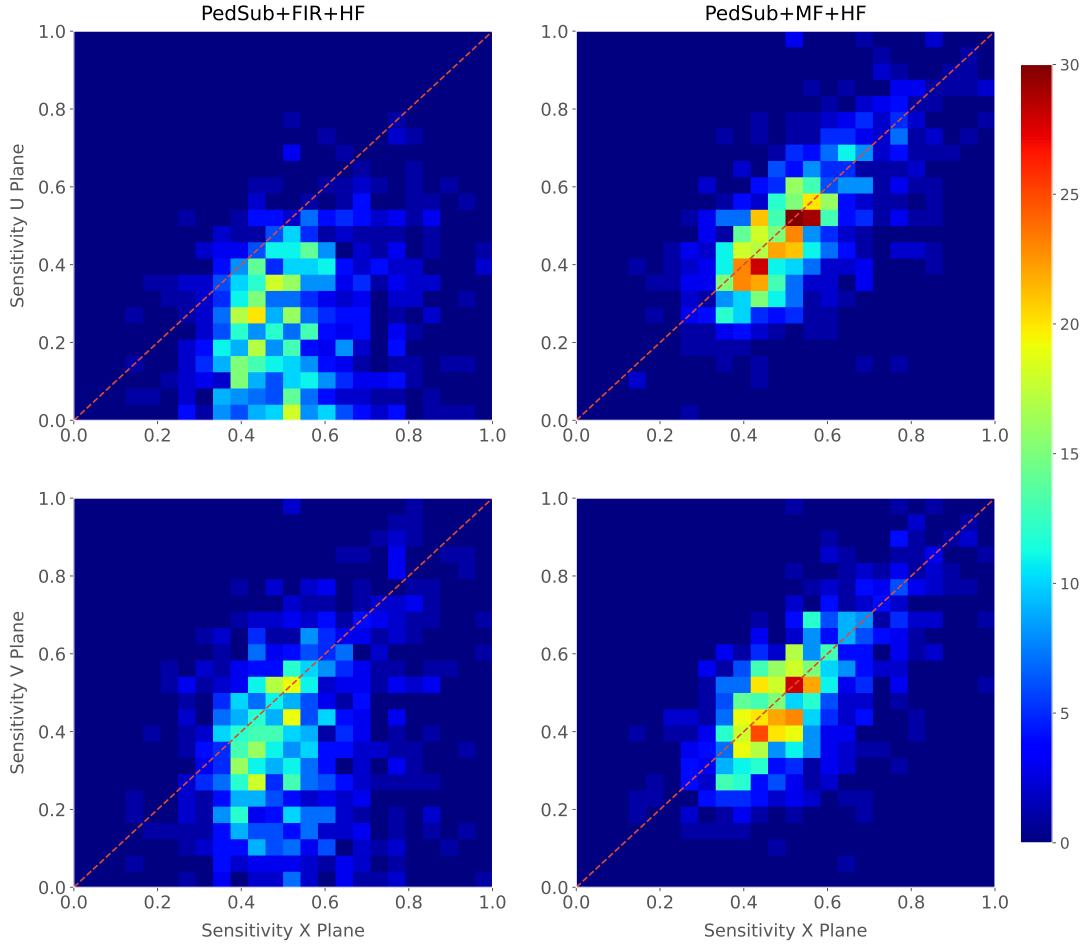


Figure 4.20: Distributions of the hit sensitivity in the U (top panels) and V (bottom panels) planes versus the hit sensitivity in the X plane, both for the standard hits (left panels) and the matched filter hits (right panels), in the case of the electron sample and a threshold of 30 ADC.

the hit sensitivity values for the matched filter and standard hits separate, while the bottom subplot depicts the ratio between the matched filter and standard sensitivities. The horizontal lines are placed at the mean value obtained in the fit and represent the width of the E_k bins used, while the vertical error bars indicate one standard deviation around that mean value. In both cases the threshold used was 30 ADC, as I required the precision to be higher than 0.99 for both matched filter and standard cases.

One can see that, in general, the improvements are better for the U than for the V plane. While for the U channels I achieved a mean improvement of 50% and 80% for muons and electrons respectively, the improvement in the V plane is stalled at 10% and

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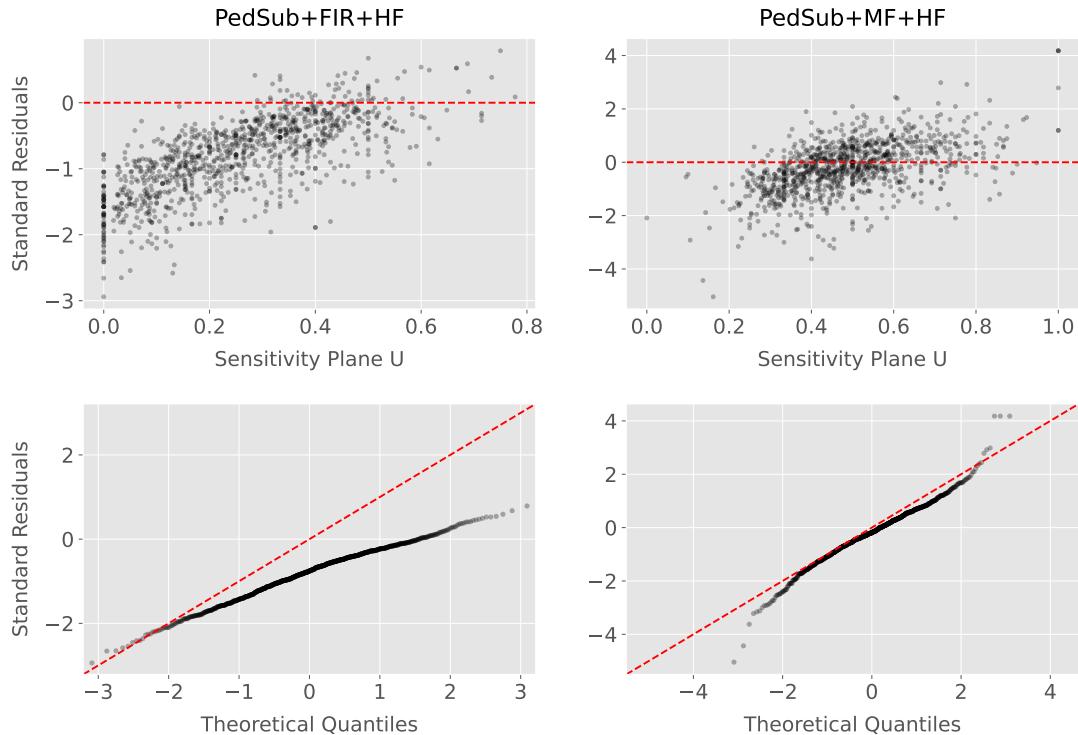


Figure 4.21: Top panels: standard residual plots of the hit sensitivities between the X and U planes. Bottom panels: quantile-quantile plots of the hit sensitivity standard residuals between the X and U planes. In all cases, the left panel corresponds to the standard hits while the right panel represents the matched filter case, all from the electron sample with a 30 ADC threshold.

1519 25%. Nevertheless, if I look at the sensitivities for the matched filter hits in both planes
 1520 one can see these have similar mean values for each energy bin, while on the contrary
 1521 for the standard hits the sensitivity remains relatively high for the V plane. This way, it
 1522 looks there was a less significant gain because the hit sensitivity was already high.

1523 Another interesting observation is the different behaviors for muons and electrons.
 1524 While hit sensitivity for muons grows significantly with energy, in the case of electrons
 1525 this slightly decreases the higher the kinetic energy of the event is. In any case, when it
 1526 comes to the improvement on the sensitivities, this remains almost constant in all cases.

1527 Furthermore, we can look at how the concurrence of hits between the different wire
 1528 planes has changed. For any given event, I expect to have a similar number of hits in the
 1529 three planes. As the ionisation electrons need to cross the U and V planes prior to reach
 1530 the collection plane X they will induce current in those wire planes. A way to check the

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1531 concurrence of hits across planes is looking at the relation between the hit sensitivities
1532 for each individual event. One cannot expect the sensitivities to be exactly equal across
1533 planes, but ideally they should be normally distributed around the diagonal.

1534 Figure 4.20 shows the hit sensitivity in the U (top panels) and V (bottom panels)
1535 planes versus the hit sensitivity in the X plane, for the case of the standard hits (left
1536 panels) and the matched filter hits (right panels). All plots were generated for the
1537 electron sample and a threshold of 30 ADC. From these one can see a clear trend,
1538 when I use the standard hit finder chain the sensitivities in the induction planes are
1539 systematically lower than the hit sensitivity in the X plane, i.e. most of the points sit
1540 below the diagonal (red dashed line). In contrast, when the matched filters are applied,
1541 the majority of the events are distributed around the diagonal. This points out that the
1542 concurrence of hits across planes has improved.

1543 To exemplify the improvement I obtained, one can consider the residuals of the hit
1544 sensitivities for the X and U planes. Assuming the diagonal hypothesis, i.e. given a
1545 dataset of the form (x, y) for any x I take the predicted y value to be equal to the value
1546 of x , I can compute the standard residuals for the hit sensitivities in U given the ones for
1547 X. In Fig. 4.21 (top panels) I show these standard residuals against the corresponding
1548 values of the hit sensitivity in the U plane, for our electron sample with kinetic energy
1549 between 5 and 100 MeV. If I compare the scatter points in the case of the standard
1550 hits (left panel) and the matched filter hits (right panel), I see that the residuals of the
1551 standard hit finder case follow a certain pattern and their mean deviates from 0.

1552 To see clearly if the residuals are normally distributed, in Fig. 4.21 (bottom panels)
1553 I plot the corresponding quantile-quantile plot for both the standard (left panel) and
1554 matched filter (right panel) standard residuals. One can clearly see that the points for
1555 the standard case follow a strongly non-linear pattern, suggesting that the residuals
1556 do not follow a normal distribution. In contrast, for the matched filter hits the points
1557 conform to a roughly linear path, implying that in this case the normality condition is
1558 fulfilled.

1559 All these results hint at the fact that the concurrence of hits across the wire planes

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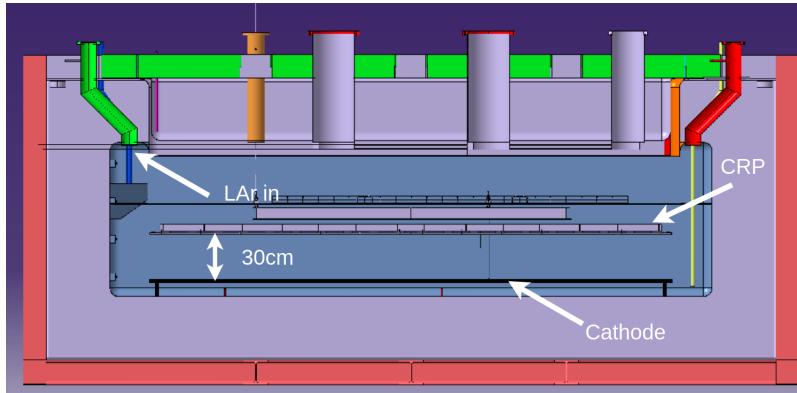


Figure 4.22: Schematic diagram of the vertical drift ColdBox setup at CERN.

1560 can be strengthened by applying the matched filters.

1561 4.6 VD ColdBox data taking

1562 Between February and April 2023 the vertical drift (VD) ColdBox setup at CERN,
 1563 shown in Fig. 4.22, was recommissioned for cold electronics testing with CRP5. That
 1564 provided another opportunity for testing the firmware trigger primitive generation in a
 1565 real LArTPC. However, during the two run periods new software-related complications
 1566 that were not observed in previous running conditions arose.

1567 These prevented us from taking data with the whole system. As a palliative measure,
 1568 new configurations were made that allowed to run with TP generation enabled just in a
 1569 subset of the ADC links. With these workarounds, we managed to run with up to three
 1570 out of twelve ADC links and the horizontal muon trigger algorithm (HMA).

1571 Additionally, an alternative firmware version was prepared featuring the matched
 1572 filter coefficients optimised for the induction plane hit finding. The version of the filter
 1573 we used for the data taking is slightly different from the one of the previous studies, as
 1574 in this case we needed to apply the same filter coefficients to all channels irrespective
 1575 of the readout plane they come from. With this, we also managed to run with three
 1576 ADC links and the HMA trigger. Figure 4.23 shows an example event display from the
 1577 longest run we recorded with the matched filter firmware.

1578 We used the recorded data, together with our standalone TPG simulation tool, to

4.6. VD COLDBOX DATA TAKING

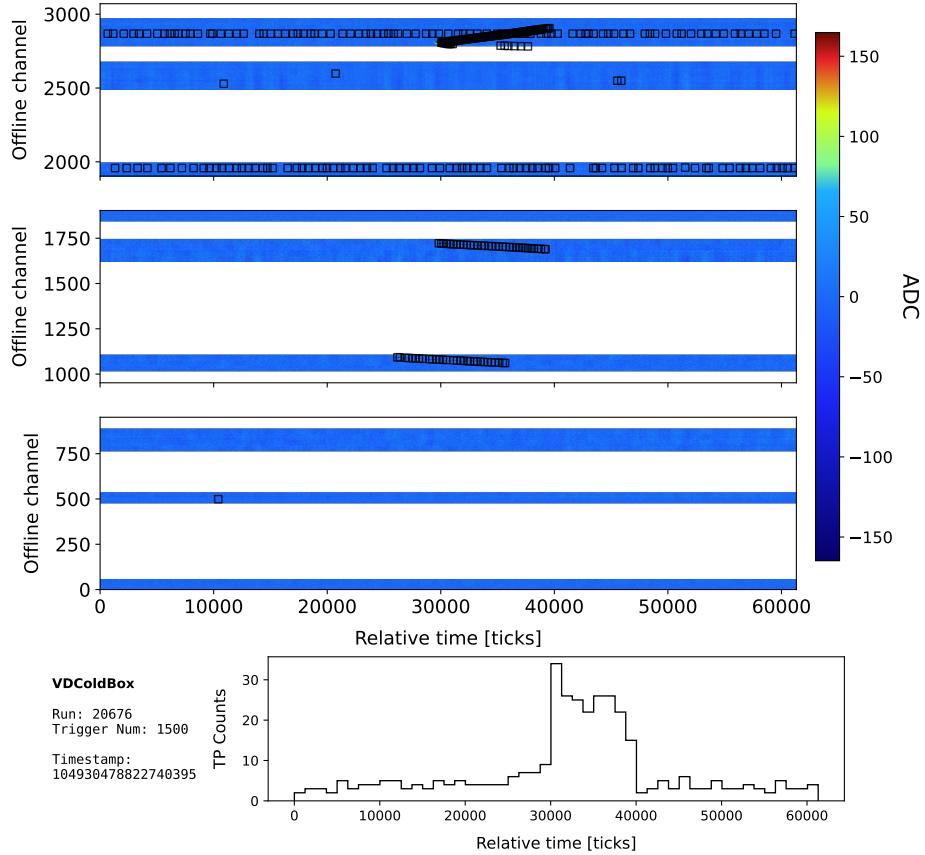


Figure 4.23: Event display of the data taken with the matched filter and HMA trigger at the VD ColdBox. The display shows the data from 3 ADC links for the full trigger window, with the black squares representing the produced TPs. The bottom panel represents the TP counts as a function of time in the trigger window.

1579 perform comparisons between the firmware and simulated TPs. One such comparison
 1580 for a matched filter run can be seen in Fig. 4.24. The agreement achieved is within the
 1581 expectation, from what we have seen in previous samples.

1582 All the studies presented demonstrate the robustness of the matched filter approach
 1583 to form TP. I have used both ProtoDUNE-SP data and MC samples to assess its impact
 1584 on the S/N and TP production of the induction channels. Additionally, I have shown
 1585 that it is possible to run with it in a real detector environment, after the tests at the
 1586 VD ColdBox setup.

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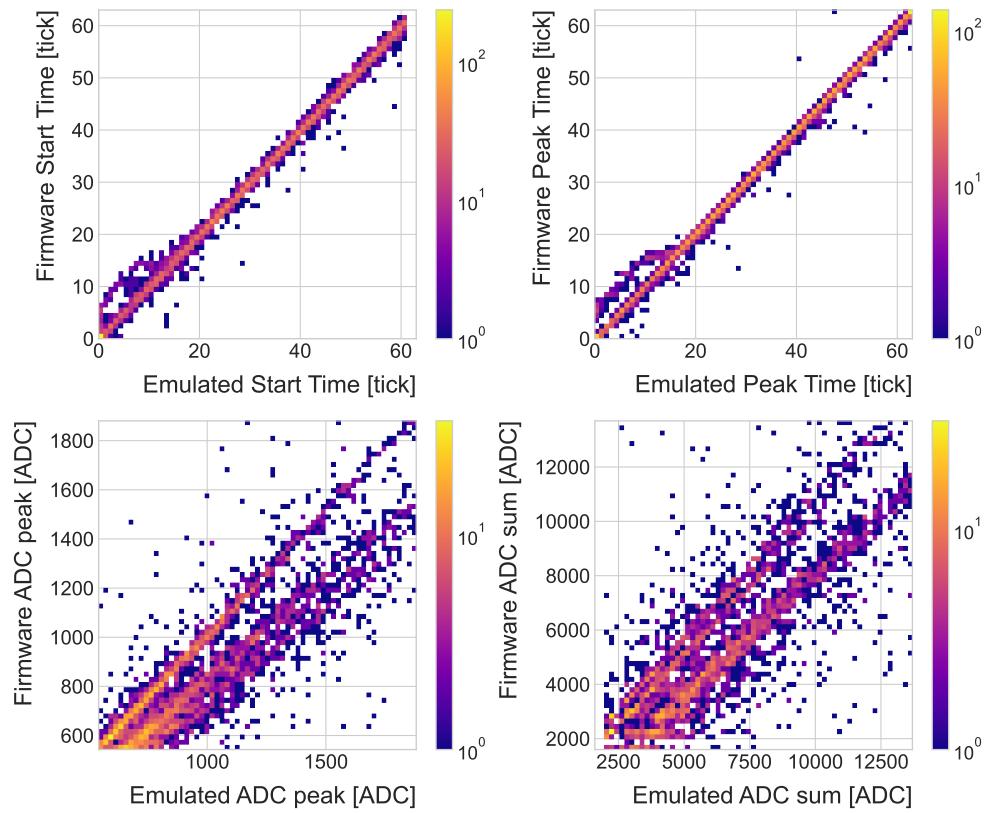


Figure 4.24: Comparison between firmware-produced and simulated TP quantities for a matched filter run at the VD ColdBox.

Dark Matter searches

with neutrinos from the Sun

1590 *He stepped down, trying not to look long at her, as if she were the Sun, yet he
1591 saw her, like the Sun, even without looking.*

1592 – Leo Tolstoy, *Anna Karenina*

1593 The idea of detecting neutrino signals coming from the Sun’s core to probe DM
1594 is not new. The main focus of these searches has usually been high-energy neutrinos
1595 originated from DM annihilations into heavy particles [112–115], although recent studies
1596 have proposed to look at the low-energy neutrino flux arising from the decay of light
1597 mesons at rest in the Sun [116–119] previously thought undetectable.

1598 In this Chapter, I try to demonstrate the capability of DUNE to constrain different
1599 DM scenarios. I used the neutrino fluxes arising from DM annihilations in the core
1600 of the Sun to compute the projected limits that DUNE would be able to set on the
1601 annihilation rates in the Sun and the DM scattering cross sections.

1602 **5.1 Gravitational capture of DM by the Sun**

1603 The Sun and the centre of the Earth are possible sources of DM annihilations, specially
1604 interesting because of their proximity. Their gravitational attraction ensured the capture
1605 of DM from the local halo through repeated scatterings of DM particles crossing them.
1606 Only neutrinos produced from DM annihilations can escape the dense interior of these

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1607 objects. Therefore, neutrino telescopes are the most useful experimental layouts to
 1608 pursue DM searches from their cores.

1609 The neutrino flux from DM annihilations inside the Sun depends on the DM capture
 1610 rate, which is proportional to the DM scattering cross section, and the annihilation rate,
 1611 which is proportional to the velocity-averaged DM annihilation cross section. The total
 1612 number of DM particles inside the Sun follows the Boltzmann equation [116]:

$$\frac{dN_{DM}}{dt} = C_{\odot} - A_{\odot}N_{DM}^2, \quad (5.1)$$

1613 where C_{\odot} and A_{\odot} are the total Sun DM capture and annihilation rates respectively.
 1614 In this expression I neglected the evaporation term, proportional to N_{DM} , which only
 1615 contribute for $m_{DM} \lesssim 4$ GeV [120]. As the current threshold of neutrino telescopes
 1616 is a few GeV, this region falls below the probed range but can be important in future
 1617 low-energy projects.

1618 This equation has an equilibrium solution:

$$N_{DM}^{eq} = \sqrt{\frac{C_{\odot}}{A_{\odot}}}, \quad (5.2)$$

1619 which represents the amount of DM inside the Sun if the capture and annihilation have
 1620 reached equilibrium. As the Sun is approximately 4.6 Gyr old, it is usually assumed that
 1621 equilibrium has been achieved. Therefore, the anomalous neutrino flux from the Sun
 1622 would only depend on the DM scattering cross section, enabling us to set limits on this
 1623 quantity. If one does not assume equilibrium, some assumptions on the DM annihilation
 1624 cross section are necessary to extract predictions from neutrino signals.

1625 Here, I am going to consider three possible scenarios for the DM interactions: DM
 1626 scattering off electrons, spin-dependent (SD) and spin-independent (SI) interactions off
 1627 nuclei. For the case of these last two, the cross sections will be given in terms of the SD
 1628 and SI elastic scattering DM cross section off protons (assuming that DM interactions

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off protons and neutrons are identical), σ_p^{SD} and σ_p^{SI} , as [116, 121]:

$$\sigma_i^{\text{SD}} = \left(\frac{\tilde{\mu}_{A_i}}{\tilde{\mu}_p} \right)^2 \frac{4(J_i + 1)}{3J_i} |\langle S_{p,i} \rangle + \langle S_{n,i} \rangle|^2 \sigma_p^{\text{SD}}, \quad (5.3)$$

$$\sigma_i^{\text{SI}} = \left(\frac{\tilde{\mu}_{A_i}}{\tilde{\mu}_p} \right)^2 A_i^2 \sigma_p^{\text{SI}}, \quad (5.4)$$

where $\tilde{\mu}_{A_i}$ is the reduced mass of the DM-nucleus i system, $\tilde{\mu}_p$ is the reduced mass of the DM-proton system, A_i and J_i the mass number and total angular momentum of nucleus i and $\langle S_{p,i} \rangle$ and $\langle S_{n,i} \rangle$ the expectation value of the spins of protons and neutrons averaged over all nucleons, respectively (see Ref. [122] for a review on spin expectation values).

Since the Sun is mainly composed of Hydrogen, the capture of DM from the halo is expected to occur mainly through spin-dependent scattering. However, since the spin-independent cross section is proportional to the square of the atomic mass, heavy elements can contribute to the capture rate (even though they constitute less than 2% of the mass of the Sun). Heavy elements can also contribute to the spin-dependent cross section if the DM has also momentum-dependent interactions.

DM particles can get captured by the Sun if after repeated scatterings off solar targets their final velocity is lower than the escape velocity of the Sun. In the limit of weak cross sections, this capture rate can be approximately written as [121]:

$$C_{\odot}^{\text{weak}} = \sum_i \int_0^{R_{\odot}} dr 4\pi r^2 \int_0^{\infty} du_{\chi} \frac{\rho_{\chi}}{m_{\chi}} \frac{f_{v_{\odot}}(u_{\chi})}{u_{\chi}} \omega(r) \int_0^{v_e(r)} dv R_i^-(\omega \rightarrow v) |F_i(q)|^2, \quad (5.5)$$

where the summation extends over all possible nuclear targets. In this expression, R_{\odot} is the radius of the Sun, ρ_{χ} is the local DM density, m_{χ} the mass of the DM particle, $f_{v_{\odot}}(u_{\chi})$ the DM velocity distribution seen from the Sun's reference frame, $R_i^-(\omega \rightarrow v)$ is the differential rate at which a DM particle with velocity v scatters a solar target of mass m_i to end up with a velocity ω and $|F_i(q)|$ is the nuclear form factor of target i .

The differential scattering rate takes a rather simple form when considering velocity-

CHAPTER 5. DARK MATTER SEARCHES WITH NEUTRINOS FROM THE SUN

1650 independent and isotropic cross sections. In that case, this quantity is given by [121,123]:

$$R_i^-(\omega \rightarrow v) = \frac{2}{\sqrt{\pi}} \frac{\mu_{i,+}^2}{\mu_i} \frac{v}{\omega} n_i(r) \sigma_i \left[\chi(-\alpha_-, \alpha_+) + \chi(-\beta_-, \beta_+) e^{\mu_i(\omega^2 - v^2)/u_i^2(r)} \right], \quad (5.6)$$

1651 where μ_i is the ratio between the DM mass and the mass of target i , $\mu_{i,\pm}$ is defined as:

$$\mu_{i,\pm} \equiv \frac{\mu_i \pm 1}{2}, \quad (5.7)$$

1652 $n_i(r)$ is the density profile of target i in the solar medium, $u_i(r)$ is the most probable

1653 velocity of target i given by:

$$u_i(r) = \sqrt{\frac{2T_\odot(r)}{m_i}}, \quad (5.8)$$

1654 where $T_\odot(r)$ is the temperature of the Sun, the quantities α_\pm and β_\pm are defined as:

$$\alpha_\pm \equiv \frac{\mu_{i,+}v \pm \mu_{i,-}\omega}{u_i(r)}, \quad (5.9)$$

$$\beta_\pm \equiv \frac{\mu_{i,-}v \pm \mu_{i,+}\omega}{u_i(r)}, \quad (5.10)$$

1655 and the function $\chi(a, b)$ is a Gaussian integral of the form:

$$\chi(a, b) \equiv \int_a^b dx e^{-x^2}. \quad (5.11)$$

1656 Finally, if one assumes the DM halo velocity distribution in the galactic rest frame

1657 to be a Maxwell-Boltzmann distribution, one can write the halo velocity distribution for

1658 an observer moving at the speed of the Sun with respect to the DM rest frame as:

$$f_{v_\odot}(u_\chi) = \sqrt{\frac{3}{2\pi}} \frac{u_\chi}{v_\odot v_d} \left(e^{-\frac{3(u_\chi - v_\odot)^2}{2v_d^2}} - e^{-\frac{3(u_\chi + v_\odot)^2}{2v_d^2}} \right), \quad (5.12)$$

1659 where:

$$\omega^2 = u_\chi + v_e(r)^2, \quad (5.13)$$

1660 is the DM velocity squared, v_\odot the relative velocity of the Sun from the DM rest frame

5.1. GRAVITATIONAL CAPTURE OF DM BY THE SUN

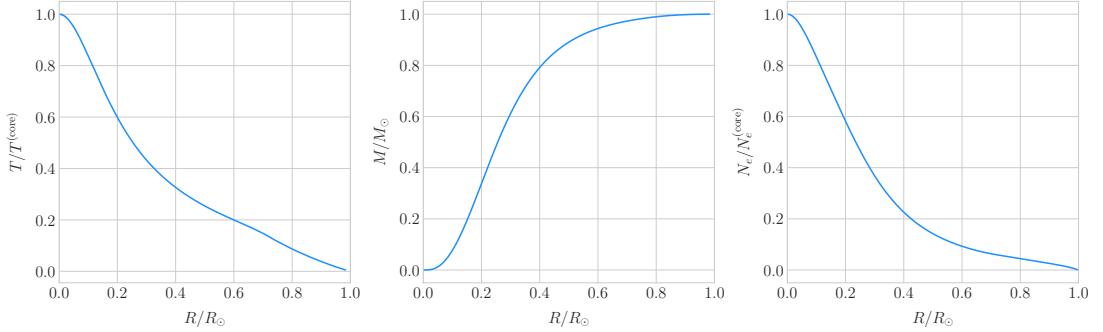


Figure 5.1: Input solar parameters used in the capture rate computation as a function of the solar radius, from left to right: temperature (with respect to the temperature at the core), mass (in solar masses) and electron number density (with respect to the electron density at the core). All quantities shown correspond to the standard solar model BS2005-OP [20].

and $v_d \simeq \sqrt{3/2}v_\odot$ the velocity dispersion.

For the case of strong scattering cross section, Eq. (5.5) ceases to be valid, as it escalates indefinitely with the cross section. In that limit, the capture rate saturates to the case where the probability of interaction is equal to one, which can be written as:

$$C_\odot^{\text{geom}} = \pi R_\odot^2 \left(\frac{\rho_\chi}{m_\chi} \right) \langle v \rangle \left(1 + \frac{3}{2} \frac{v_e^2(R_\odot)}{v_d^2} \right) \xi(v_\odot, v_d), \quad (5.14)$$

where $v_d = \sqrt{8/3\pi}v_\odot$ is the mean velocity in the DM rest frame and the factor $\xi(v_\odot, v_d)$ accounts for the suppression due to the motion of the Sun:

$$\xi(v_\odot, v_d) = \frac{v_d^2 e^{-\frac{3v_\odot^2}{2v_d^2}} + \sqrt{\frac{\pi}{6}} \frac{v_d}{v_\odot} (v_d^2 + 3v_e^2(R_\odot) + 3v_\odot^2) \text{Erf} \left(\sqrt{\frac{3}{2}} \frac{v_\odot}{v_d} \right)}{2v_d^2 + 3v_e^2(R_\odot)}. \quad (5.15)$$

Having these into account, one can write the total capture rate as a combination of both contributions, allowing a smooth transition between the two, as:

$$C_\odot = C_\odot^{\text{weak}} \left(1 - e^{C_\odot^{\text{geom}}/C_\odot^{\text{weak}}} \right). \quad (5.16)$$

I computed the capture rate from Eq. (5.16) in the case of interactions with electrons. To do so, I used the standard solar model BS2005-OP [20]. Fig. 5.1 shows the

CHAPTER 5. DARK MATTER SEARCHES WITH NEUTRINOS FROM THE SUN

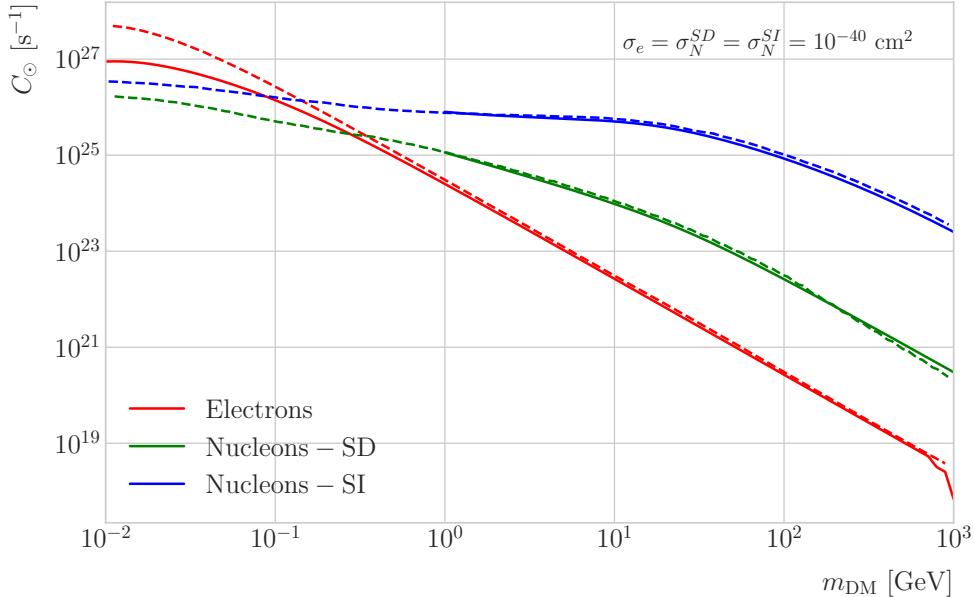


Figure 5.2: Capture rates as a function of the DM mass for the DM-electron interactions (red lines), SD DM-nucleons interactions (green lines), and SI DM-nucleons interactions (blue lines). Solid lines represent the values computed in this work while the dashed lines are the one given in Ref. [121]. All the rates are shown for a choice of scattering cross section of $\sigma_i = 10^{-40} \text{ cm}^2$.

1671 three parameters from the solar model that are needed for the computation, the solar
 1672 temperature (left panel), mass (central panel) and electron density (right panel) profiles.

1673 For the case of the interactions off nuclei, the computations are more convoluted
 1674 as one needs to add up the contributions of the different most abundant nuclei in
 1675 the Sun. Also, in contrast to the electron scenario where the form factor is trivially
 1676 $|F_e(q)|^2 = 1$, for any nucleus i one would need to consider some appropriate nuclear
 1677 density distribution (either a Gaussian approximation, a Woods-Saxon distribution, etc)
 1678 which would complicate the calculations even further.

1679 That is the reason why, at this stage of our study, I decided to take an alternative
 1680 approach to the computation of the DM-nucleus capture rates. I used the **DarkSUSY**
 1681 software, that allows us to compute these quantities performing a full numerical
 1682 integration over the momentum transfer of the form factors. The default standard
 1683 solar model used by **DarkSUSY** is BP2000¹ [124].

¹This is what they say in their manual, but I fear it is somewhat outdated. It appears to me

5.1. GRAVITATIONAL CAPTURE OF DM BY THE SUN

1684 In Fig. 5.2 I show the results I obtained for the capture rates, for the case of
 1685 interactions off electrons (red solid line), SD (green solid line) and SI (blue solid line)
 1686 interactions of nucleons. In all cases I used a value of the scattering cross sections of
 1687 $\sigma_i = 10^{-40} \text{ cm}^2$. Note here one of the limitations of the **DarkSUSY** approach, one can
 1688 not extend the computation below $m_{\text{DM}} = 1 \text{ GeV}$. Nevertheless, this is not something
 1689 to worry about in this case, as I will discuss next. As a comparison, I added also the
 1690 values computed in Ref. [121] (same color scheme, dashed lines). One can see there
 1691 is good agreement between these and the **DarkSUSY** computation of the SD and SI
 1692 interactions for $m_{\text{DM}} \geq 1 \text{ GeV}$. In this regime their computations also matches quite
 1693 well our result for the electron capture rate. However, these start to differ significantly
 1694 below $m_{\text{DM}} = 1 \text{ GeV}$, being their estimate up to a factor of 5 bigger than ours for low
 1695 masses.

1696 Let me comment briefly about the assumption I made before about not including
 1697 an evaporation term in the Boltzmann equation. If I include this term in the equation
 1698 (which will be proportional to the number of DM particles) the equilibrium solution
 1699 takes the form:

$$N_{\text{DM}}^{eq} = \sqrt{\frac{C_{\odot}}{A_{\odot}}} \frac{1}{\kappa + \frac{1}{2} E_{\odot} \tau_{eq}}, \quad (5.17)$$

1700 where E_{\odot} is the total evaporation rate, τ_{eq} is the equilibrium time in the absence of
 1701 evaporation:

$$\tau_{eq} = \frac{1}{\sqrt{C_{\odot} A_{\odot}}}, \quad (5.18)$$

1702 and κ is defined as:

$$\kappa \equiv \sqrt{1 + \left(\frac{E_{\odot} \tau_{eq}}{2} \right)^2}. \quad (5.19)$$

1703 Now, it is easy to proof that in case evaporation dominates $\kappa \gg 1$ and therefore:

$$N_{\text{DM}}^{eq} \simeq \frac{C_{\odot}}{E_{\odot}}. \quad (5.20)$$

this model is relatively old and do not see why they are not using others like [20]. Maybe one can double-check in the code to make sure.

CHAPTER 5. DARK MATTER SEARCHES WITH NEUTRINOS FROM THE SUN

1704 In contrast, if evaporation is irrelevant $\kappa \simeq 1$ and one recovers Eq. (5.2).

1705 In this way, one can define the evaporation mass as the mass for which the number

1706 of DM particles in equilibrium approaches Eq. (5.20) at 10% level:

$$\left| N_{DM}^{eq}(m_{\text{evap}}) - \frac{C_{\odot}(m_{\text{evap}})}{E_{\odot}(m_{\text{evap}})} \right| = 0.1 N_{DM}^{eq}(m_{\text{evap}}). \quad (5.21)$$

1707 This can be regarded as the minimum testable mass one can reach using the annihilation
1708 products of the DM in the Sun.

1709 It was reported in Ref. [121] that, in the case of both SD and SI DM interactions
1710 off nuclei, this value ranges from 2 to 4 GeV depending on the specific scattering
1711 cross section value, compatible with the usual assumptions in the literature. What is
1712 interesting is the case of the electron capture. It was found that, when one applies a
1713 cutoff in the velocity distribution of the DM trapped in the Sun slightly below the escape
1714 velocity, the evaporation mass for the DM-electron interaction decreases remarkably. For
1715 a moderate choice of $v_c(r) = 0.9v_e(r)$ one gets an evaporation mass of around 200 to
1716 600 MeV. This possibility opens a region of the parameter space that could be tested
1717 with neutrino detectors.

1718 5.2 Neutrino flux from DM annihilations

1719 When WIMPs annihilate inside the Sun a flux of high-energy neutrinos is expected from
1720 heavy quarks, gauge bosons and $\tau^+\tau^-$ final states, which decay before losing energy in
1721 the dense solar medium, as they will produce a continuum spectra up to $E_{\nu} \sim m_{\chi}$ (in
1722 the case of direct annihilation to neutrinos one would have a line at $E_{\nu} = m_{\chi}$) [117].
1723 This kind of signal has been extensively studied in the literature, allowing to put strong
1724 limits on the SD WIMP-proton cross section for large m_{χ} . However, the number of
1725 high-energy neutrinos per WIMP annihilation is small and the spectrum depends on the
1726 unknown final state. Moreover, background rejection is easier for large m_{χ} but neutrinos
1727 with $E_{\nu} \gtrsim 100$ GeV are significantly attenuated by interactions in the Sun.

1728 Nevertheless, most WIMP annihilation final states eventually produce a low-energy

5.3. COMPUTING LIMITS FROM SOLAR NEUTRINO FLUXES

neutrino spectrum. In this case one does not just consider the more massive final states but also annihilations into e^+e^- , $\mu^+\mu^-$ and light quarks [116]. In particular, light mesons would be produced and stopped in the dense medium, thus decaying at rest and producing a monoenergetic neutrino signal. The decay-at-rest of kaons will produce a $E_\nu = 236$ MeV ν_μ while in the case of pions one would have a $E_\nu = 29.8$ MeV ν_μ . In practice only K^+ and π^+ contribute to these signals, as K^- and π^- are usually Coulomb-captured in an atomic orbit and get absorbed by the nucleus. There is also a low-energy neutrino signal coming from muon decays, which are produced in kaon or pion decays, leptonic decays of other hadrons and heavy leptons or even directly from WIMP annihilations, which can decay at rest and contribute to the previous low-energy neutrino flux with a well known spectrum below 52.8 MeV.

These monoenergetic MeV neutrinos were previously considered undetectable but, due to the large yield, the known spectra and the modern advances in the detector technology, these low-energy neutrino flux can be a good probe of the SD WIMP-proton cross section in standard solar WIMP capture scenario, as it is sensitive to low WIMP masses and insensitive to the particular final state. A good place to look for these signals are next-generation neutrino experiments such as DUNE.

5.3 Computing limits from solar neutrino fluxes

To use the neutrino fluxes from DM annihilations in the Sun, the first thing I need to do is to determine the expected number of atmospheric background events, for a given exposure, after directionality selection has been applied. I can write this number as:

$$N_B = \eta_B \int d\Omega \int_{E_{min}}^{E_{max}} dE_\nu \frac{d^2\Phi_{atm}^\mu}{dE_\nu d\Omega} \times \left(A_{eff}^{(\mu)}(E_\nu) T \right), \quad (5.22)$$

where η_B is the background efficiency, E_{min} and E_{max} the minimum and maximum energies to integrate over, $d^2\Phi_{atm}^\mu/dE_\nu d\Omega$ the differential flux of atmospheric muon neutrinos, $A_{eff}^{(\mu)}$ is the effective area of DUNE to muon neutrinos and T is the exposure time. The effective area can be expressed as the product of the neutrino-nucleus scattering

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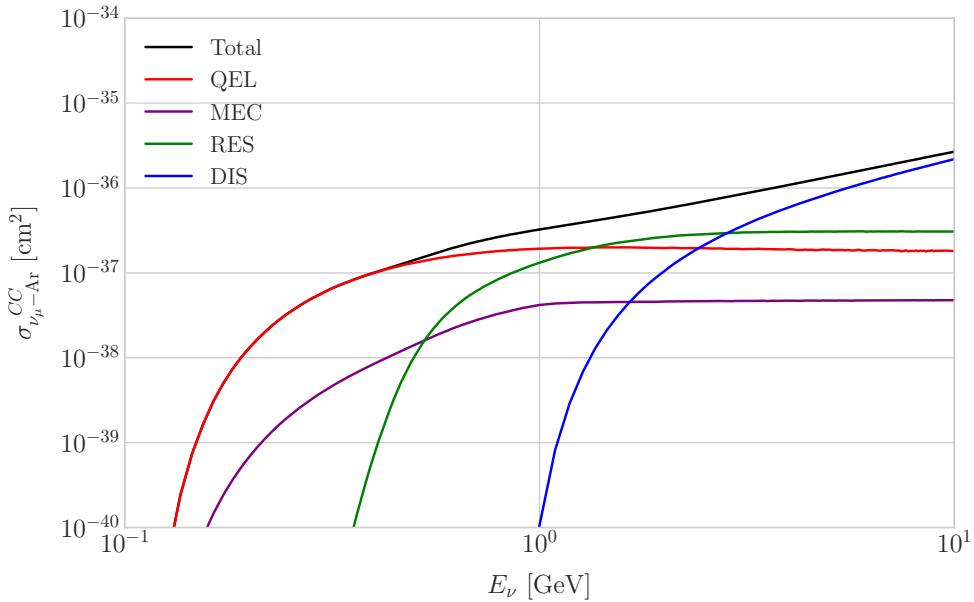


Figure 5.3: NuWro computed $\nu_\mu - {}^{40}\text{Ar}$ charged-current scattering cross section as a function of the neutrino energy. The black line shows to the total cross section, whereas the others correspond to the different contributions (in red quasi-elastic scattering, in green resonant pion exchange, in blue deep inelastic scattering and in purple meson exchange current).

1754 cross section and the number of nuclei in the fiducial volume of the detector. This way
 1755 for DUNE I can write:

$$A_{eff}^{(\mu)}(E_\nu) = (6.0 \times 10^{-10} \text{ m}^2) \left(\frac{\sigma_{\nu-\text{Ar}}^{(\mu)}(E_\nu)}{10^{-38} \text{ cm}^2} \right) \left(\frac{M_{target}}{40 \text{ kT}} \right), \quad (5.23)$$

1756 where $\sigma_{\nu-\text{Ar}}^{(\mu)}$ is the $\nu_\mu - {}^{40}\text{Ar}$ charged-current scattering cross section. In Fig. 5.3 I
 1757 show the computed value of this cross section as a function of the neutrino energy E_ν ,
 1758 in the range of interest both for the atmospheric background and signal events. It was
 1759 computed using the NuWro Monte Carlo neutrino event generator [125], including the
 1760 charged-current contributions of the quasi-elastic scattering (red line), resonant pion
 1761 exchange (green line), deep inelastic scattering (blue line) and meson exchange current
 1762 (purple line).

1763 The background rejection will depend on the resolution of the detector and the
 1764 selection one applies on the events. A geometry argument can be used to estimate

5.3. COMPUTING LIMITS FROM SOLAR NEUTRINO FLUXES

the maximum background rejection one can achieve in this case, considering one can efficiently discriminate all events coming from a direction different from that of the Sun. In that case, the optimal background efficiency will simply be the relative angular coverage of the Sun. Taking the angular diameter of the Sun as seen from the Earth to be 0.5° , I have:

$$\eta_B^{(opt)} \approx \frac{\pi \left(\frac{0.5}{2}\right)^2}{360 \times 180} \simeq 3.03 \times 10^{-6}. \quad (5.24)$$

This value will give a very optimistic estimate of the number of background events. However, it can be regarded as an lower limit, as it represents the best case scenario.

In Fig. 5.4 I show the fluxes of atmospheric neutrinos at the Homestake mine during solar minimum, taken from Ref. [126]. The values are averaged over the two angular directions. In blue I have the flux of muon neutrinos while in red I indicate the flux of electron neutrinos. Additionally, the dashed lines correspond to both antineutrino species.

Using these values for the muon neutrino and the corresponding total CC cross section, one can compute the number of expected background events by integrating over the given energy range (as in this case the angular integral is trivial). As for the energy range to integrate over, I choose the range for DUNE specified in [83], $E_{min} = 10^{-1}$ GeV and $E_{max} = 10$ GeV. Taking all these into account, I found the number of background events to be:

$$N_B \simeq \eta_B \times (3.827 \times 10^4) \times \left(\frac{\text{exposure}}{400 \text{ kT yr}} \right). \quad (5.25)$$

To estimate the sensitivity of DUNE to this kind signal, one can consider a hypothetical data set where the number of observed neutrinos is taken to be the expected number of background events rounded to the nearest integer, $N_{obs} = \text{round}(N_B)$ [127]. Now, if I assume that the number of signal and background events seen by DUNE are given by Poisson distributions with means equal to the expected number of signal and background events, N_S and N_B , one can denote by N_S^{90} to the number of expected signal events such that the probability of having an experimental run with a number of events greater than N_{obs} is 90%. This number can be obtained as the numerical solution

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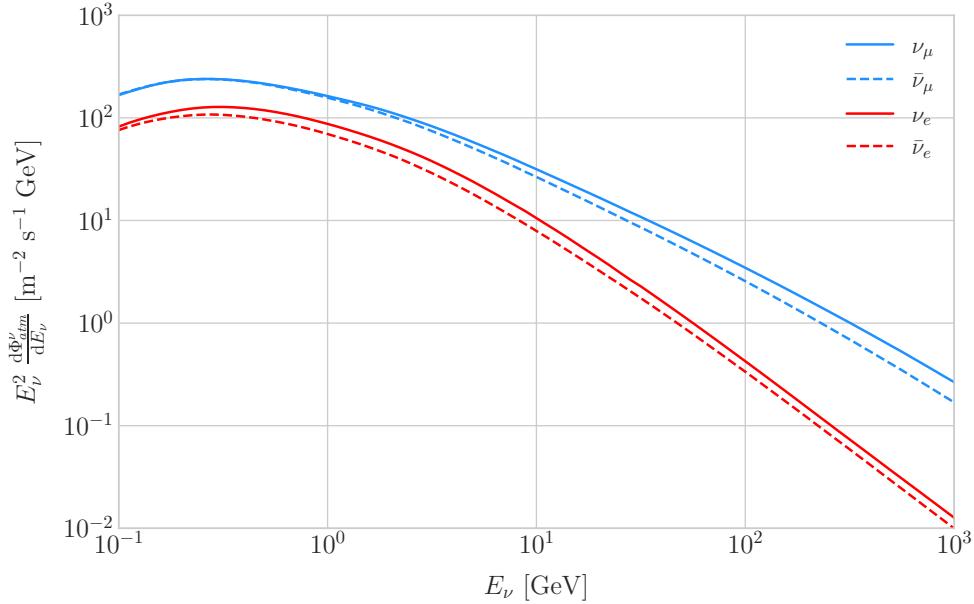


Figure 5.4: Expected atmospheric neutrino flux as a function of the neutrino energy E_ν at Homestake at solar minimum, taken from Ref. [126]. The blue solid (dashed) line correspond to muon neutrinos (antineutrinos) and the red solid (dashed) line correspond to electron neutrinos (antineutrinos).

1791 to the equation:

$$1 - \frac{\Gamma(N_{obs} + 1, N_S^{90} + N_B)}{N_{obs}!} = 0.9, \quad (5.26)$$

1792 where $\Gamma(x, y)$ is the upper incomplete gamma function.

1793 The number of signal events is related to the neutrino flux from DM annihilations in
 1794 a similar way as the background events to the atmospheric neutrino flux. In this case I
 1795 have:

$$N_S = \eta_S \Gamma_A^{eq} \int_{z_{min}}^{z_{max}} dz \frac{dN_\nu}{dAdN_A dz} \times (A_{eff}^\mu(z)T), \quad (5.27)$$

1796 where η_S is the signal efficiency, Γ_A^{eq} is the total annihilation rate of DM particles at
 1797 equilibrium, $\Gamma_A^{eq} = A_\odot (N_{DM}^{eq})^2$, z_{min} and z_{max} the minimum and maximum relative
 1798 energies to integrate over (in such a way that $z_{min,max} \leq E_{min,max}/m_{DM}$ for each m_{DM})
 1799 and $dN_\nu/dAdN_A dz$ the muon neutrino flux per DM annihilation in the Sun.

1800 Knowing N_S^{90} one can use the relation in Eq. (5.27) to obtain $\Gamma_A^{eq,90}$ for different
 1801 values of the DM mass. From there I can directly translate those values into the

5.4. EXAMPLE: KALUZA-KLEIN DARK MATTER

1802 upper limits for DUNE on the DM scattering cross sections, for a given exposure. The
1803 relation between the annihilation rate and the DM-nucleon cross section comes from the
1804 equilibrium condition through the solar DM capture rate, discussed above.

1805 5.4 Example: Kaluza-Klein Dark Matter

1806 Even though there are plenty of BSM theories which provide viable dark matter
1807 candidates, Kaluza-Klein type of models [128, 129] within the universal extra dimensions
1808 (UED) paradigm naturally predict the existence of a massive, stable particle that can
1809 play the role of the dark matter. In the UED scenario all the SM fields can propagate
1810 in one or more compact extra dimensions [130], as opposed to the idea of brane worlds
1811 [131, 132], where just gravity can propagate in the bulk while SM particles live at fixed
1812 points.

1813 Furthermore, in UED there is no violation of the translational invariance along the
1814 extra dimensions, thus leading to degenerate KK modes masses and also the conservation
1815 of the KK number in the effective four dimensional theory. At loop level, radiative
1816 corrections and boundary terms shift the masses of the KK modes and break KK
1817 number conservation into a KK parity. As a result, this theory only contains interactions
1818 between an even number of odd KK modes and therefore the lightest among the first KK
1819 excitations will be stable. This particle is usually denoted as the lightest Kaluza-Klein
1820 particle (LKP) and its mass is proportional to $1/R$, being R the size of the extra
1821 dimension.

1822 A viable DM candidate needs to be electrically neutral and non-baryonic, therefore
1823 good candidates among the first Kaluza-Klein excitations would be the KK neutral
1824 gauge bosons and the KK neutrinos [133]. Another possible candidate is the first KK
1825 excitation of the graviton, which receives negligible radiate contributions and therefore
1826 has a mass almost equal to $1/R$, but it has been shown that the lightest eigenstate from
1827 the mixing of the gauge mass states (B^1, W_3^1) would be lighter, as B^1 and W_3^1 receive
1828 negative radiate corrections [134]. It is also understood that, when these corrections

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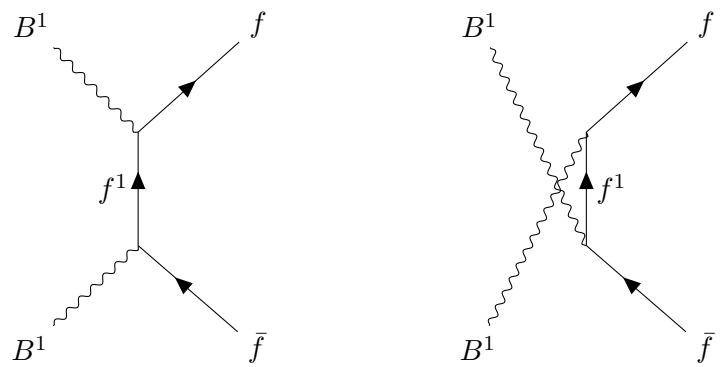


Figure 5.5: Feynman diagrams for B^1B^1 annihilation into SM fermions.

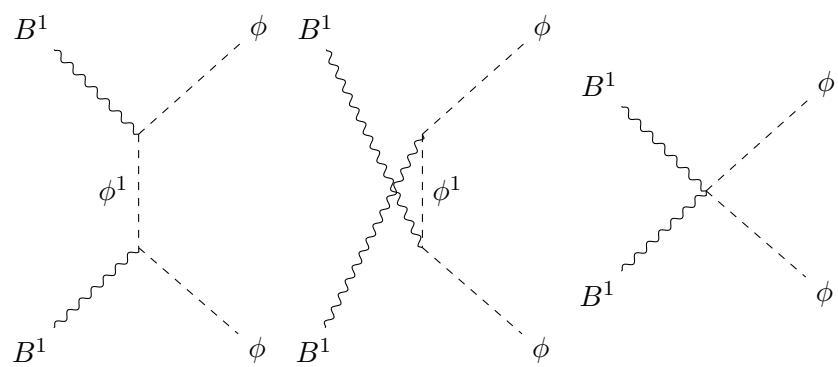


Figure 5.6: Feynman diagrams for B^1B^1 annihilation into a Higgs boson pair.

5.4. EXAMPLE: KALUZA-KLEIN DARK MATTER

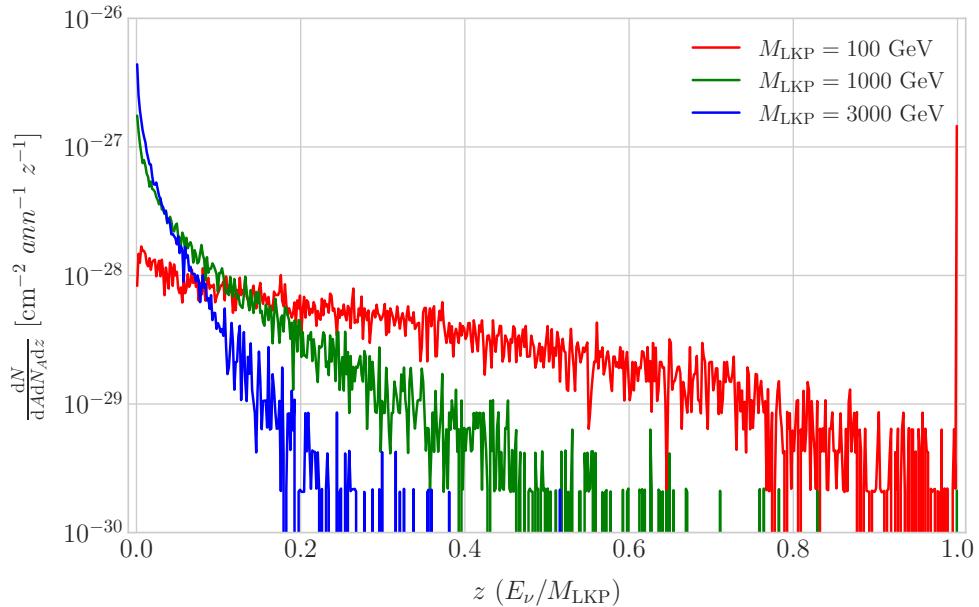


Figure 5.7: Computed spectra of muon neutrinos at the DUNE FD site from B^1 annihilations in the Sun for three different values of M_{LKP} , plotted in relative energy units for legibility.

1829 become sizeable, the eigenstates become approximately pure B^1 and W_3^1 states as the
 1830 Weinberg mixing angle grows small with the KK number [134]. In that case, the LKP
 1831 can be well-approximated as being entirely B^1 .

1832 I need to compute the neutrino flux produced by the annihilations of the LKP in
 1833 the core of the Sun, taking into account their propagation in the solar medium, as
 1834 well as neutrino oscillations. To this end I used `WimpSim` [135, 136] to generate one
 1835 million annihilation events in the Sun over a time span of four years and propagate
 1836 them to the DUNE FD location ($44^\circ 20' \text{ N}, 103^\circ 45' \text{ W}$), for different values of M_{LKP} .
 1837 In Fig. 5.7 I show the obtained muon neutrino spectra arriving to the detector from
 1838 LKP annihilations in the Sun, per unit area and per annihilation, plotted in relative
 1839 energy units for different values of the mass. As one could expect the spectra get
 1840 steeper the higher is the mass, due to the absorption of high-energy neutrinos in the
 1841 solar medium. Also, one can see the peak at $z = 1$ due to the direct annihilation into
 1842 neutrinos $\chi\chi \rightarrow \nu\bar{\nu}$.

1843 Now, one can estimate the sensitivity of DUNE to this particular model by using

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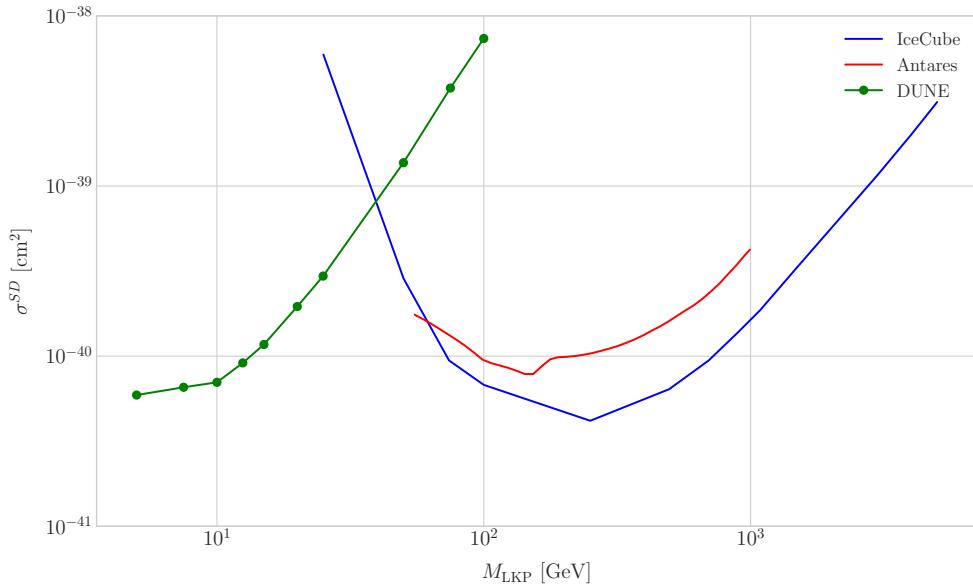


Figure 5.8: Projected 90% confidence level upper limit for DUNE (400 kT yr) on the spin-dependent B^1 -proton scattering cross section as a function of M_{LKP} (green dots). I also show the previous limits from IceCube [137] (blue line) and Antares [138] (red line) on the LKP cross section. The shaded area represents the disfavoured region (at 95% confidence level) on the mass of the LKP from LHC data [139].

1844 the methods I previously discussed. To begin with, I will use the optimistic estimation
 1845 of the background efficiency in Eq. (5.24) to get an upper bound. Using it, one can
 1846 directly compute the number of expected background events to be $N_B = 0.11$ for an
 1847 exposure of 400 kT yr. Then, Eq. (5.26) give us a value of $N_S^{90} = 2.20$ for the 90%
 1848 exclusion number of expected signal events. By using the `NuWro` generated cross sections
 1849 and the computed neutrino fluxes from B^1 annihilations in the Sun I can estimate the
 1850 limits on the SD and SI DM-nucleus cross section using the relation in Eq. (5.2) and
 1851 the capture rates I computed with `DarkSUSY`.

1852 In Fig. 5.8 I show the projected sensitivity for DUNE on the spin-dependent B^1 -
 1853 proton scattering cross section versus the mass of the DM particle, for a exposure of
 1854 400 kT yr (green dots). I also include the previous results from IceCube [137] (blue line)
 1855 and Antares [138] (red line). The shaded area represents the disfavoured region from
 1856 combined searches for UED by ATLAS and CMS [139].

1857 From the experimental point of view, this estimation lacked a detailed simulation of

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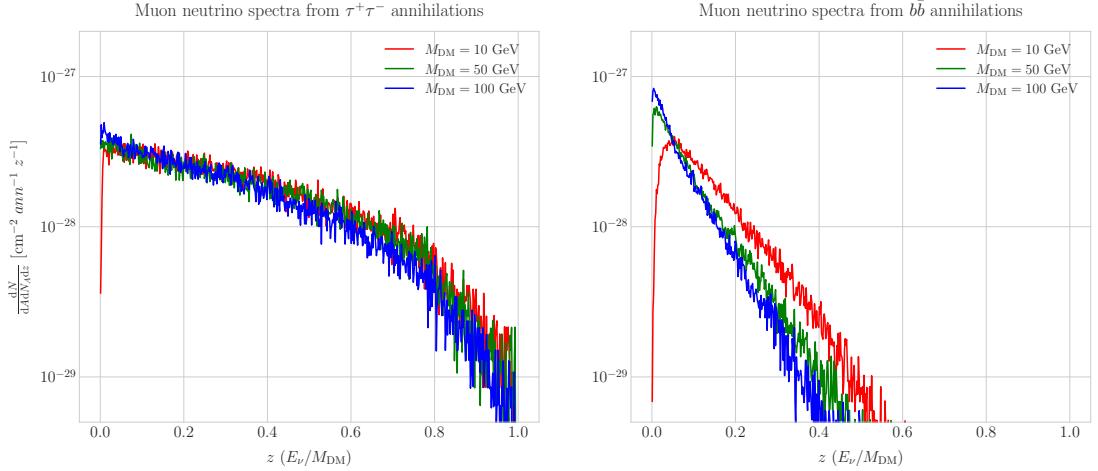


Figure 5.9: Computed spectra of muon neutrinos at the DUNE FD site from $\tau^+\tau^-$ (left panel) and $b\bar{b}$ (right panel) annihilations in the Sun for the DM masses $m_{\text{DM}} = 10 \text{ GeV}$ (red line), 50 GeV (green line) and 100 GeV (blue line), plotted in relative energy units.

the detector response and thus this must be consider as a mere optimistic sensitivity computation. However, it shows the potential of DUNE to constrain this kind of exotic scenarios, showing the region where it will be in a position to compete with other neutrino telescopes. A more detailed analysis is needed if I am to make a realistic estimation. Even though the region of the parameter space where DUNE would be sensitive to this particular model is quite constrained by collider searches [139] and other rare decay measurements [140, 141], it still constitutes an alternative indirect probe.

5.5 High energy DM neutrino signals

To have better estimates on the capability of the DUNE FD to constrain the parameter space of DM using solar neutrino fluxes, I need to start accounting for the detector resolution effects and the topologies of the different signatures. As a starting point, I will focus on specific annihilation channels. For the case of DUNE, the relevant ones are mainly the hard channels $\tau^+\tau^-$ and $\nu\bar{\nu}$ and the soft channel $b\bar{b}$. These are the open annihilation channels for relatively low mass WIMPs that will actually give neutrino fluxes. Other channels, like W^+W^- and ZZ , are open for more massive WIMPs, but those will produce usually a higher energy neutrino flux that will be out of reach for

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1874 DUNE (usually the maximum neutrino energy is taken to be $E_{max} = 10$ GeV).

1875 In Fig. 5.9 I show the `WimpSim` [135, 136] generated muon neutrino spectra at the
1876 DUNE FD location ($44^\circ 20' N$, $103^\circ 45' W$) from $\tau^+\tau^-$ (left panel) and $b\bar{b}$ (right panel)
1877 annihilations in the core of the Sun, for different DM masses. Here, one can clearly see
1878 the meaning of the previous distinction between hard and soft channels. For the same
1879 DM mass value, the muon neutrino spectrum from the $\tau^+\tau^-$ channel is more flat and
1880 reaches higher energies than the one from the $b\bar{b}$ channel, which drops faster.

1881 In this case, I prepared two sets of files, one for $\tau^+\tau^-$ and the other for $b\bar{b}$, for DM
1882 masses in the range from 5 to 100 GeV (for $b\bar{b}$ the first mass point I take is 7.5 GeV, as
1883 this annihilation channel is not kinematically allowed for a WIMP with $m_{DM} = 5$ GeV).
1884 Then, I prepared the `WimpSim` output fluxes in a specific way to use them as inputs to
1885 `NuWro`, which simulates the neutrino interaction with the argon.

1886 Because `WimpSim` outputs an event list together with the fluxes, I can use the former
1887 to generate the events. The direction of these is given in terms of the azimuth and
1888 altitude angles viewed from the specified location, so first I need to convert these into the
1889 DUNE FD coordinates. Once I have done it, each event can be processed with `NuWro`.
1890 To increase the number of samples and optimise the computation time, I generate 100
1891 interactions (i.e. `NuWro` events) for each `WimpSim` event². I restrict the event generation
1892 to charged current interactions, but I allow all the different contributions to the CC
1893 cross section, i.e. quasielastic scattering (QE), meson exchange current process (MEC),
1894 resonant pion production (RES) and deep inelastic scattering (DIS). I just take into
1895 account the CC contribution because I am only interested in final states with charged
1896 leptons, as we have better chances of reconstructing the kinematics of CC events.

1897 For the atmospheric fluxes I follow a similar procedure, only that this time I do not
1898 have a set of events but the fluxes binned in azimuth and altitude angles. This way, I
1899 transform these to DUNE coordinates and process the fluxes for each bin separated with
1900 `NuWro`.

²This also solves a problem related with the generation of the neutrino interactions in `NuWro`, as if you only produce one event each time you launch `NuWro` it will always produce an interaction of the dominant interaction type for that particular energy.

5.5. HIGH ENERGY DM NEUTRINO SIGNALS

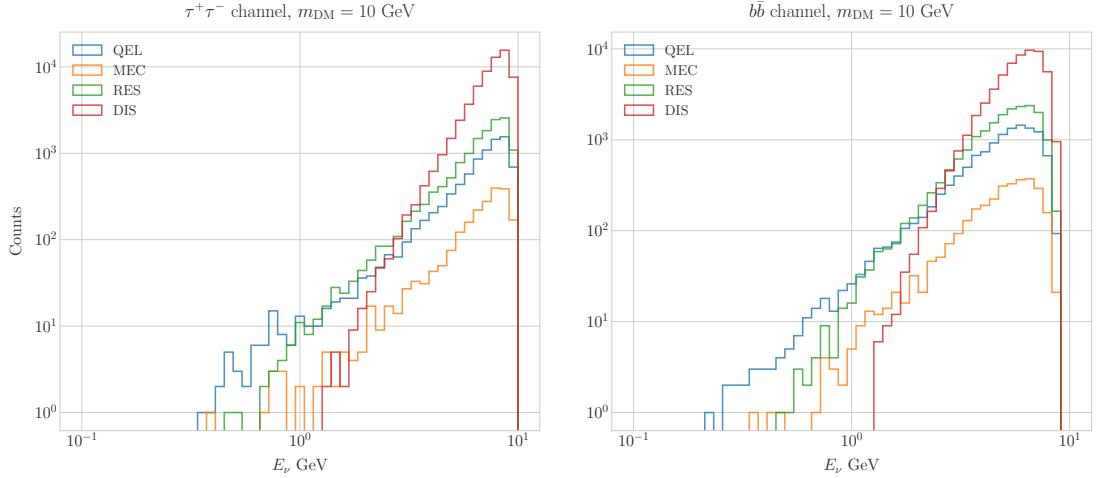


Figure 5.10: Distribution of the muon neutrino energies from the $\tau^+\tau^-$ (left panel) and $b\bar{b}$ (right panel) annihilation channels, for $m_{\text{DM}} = 10 \text{ GeV}$, separated by CC interaction type: QE (blue), MEC (orange), RES (green) and DIS (red).

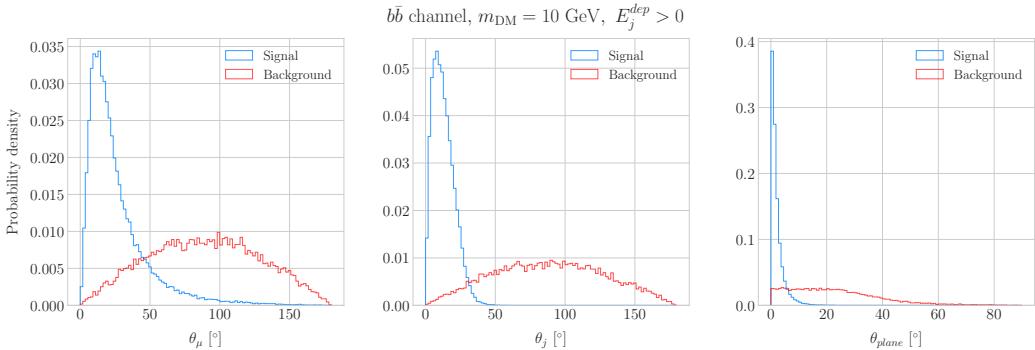


Figure 5.11: Distributions of θ_μ (left panel), θ_j (central panel) and θ_{plane} (right panel) for the $b\bar{b}$ sample with $m_{\text{DM}} = 10 \text{ GeV}$ (blue) and the atmospheric background (red).

1901 At this point, I have two sets of events with different energies and final states.
 1902 In Fig. 5.10 one can see the distribution of the muon neutrino energies for the case
 1903 $m_{\text{DM}} = 10 \text{ GeV}$, both for the $\tau^+\tau^-$ (left panel) and $b\bar{b}$ (right panel) channels, separated
 1904 by interaction. One can clearly see that there are different energy regimes where the
 1905 primary interaction type is different. This leads to a plurality of event topologies,
 1906 therefore making it difficult to implement a general approach to the selection of events
 1907 in detriment of the background. As a way to proceed, I decided to focus on a subset of
 1908 the samples, based on the different interaction modes and contents of the final state.
 1909 Thus, I consider a CC DIS sample and a single proton CC QE sample.

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1910 5.5.1 DIS-like events

1911 To begin with, I consider the high energy part of the spectrum. In this region DIS events
1912 dominate, i.e. interactions of the form $\nu_\mu + q_d(\bar{q}_u) \rightarrow \mu^- + q_u(\bar{q}_d)$. Therefore, our final
1913 estates will contain a muon and a hadronic jet from the fragmentation of the outgoing
1914 quark. As all these events have $E_\nu \gtrsim 1$ GeV the momentum transfer to the remnant
1915 nucleus is negligible, for this reason the neutrino energy can be effectively reconstructed
1916 just taking into account the momenta of the muon and the jet. This technique was
1917 successfully used in Ref. [142] to select monoenergetic DM solar neutrino events from
1918 $\nu\bar{\nu}$ annihilation channels.

1919 Using momentum conservation one sees that the plane generated by the momenta
1920 of the muon and the jet needs to also contain the momentum of the neutrino. As we
1921 are interested in neutrinos coming from the Sun, the momentum of the neutrino can be
1922 regarded as known beforehand. This will allow us to define the angle of the outgoing
1923 muon and jet with respect to the incoming neutrino. Moreover, one can also use that
1924 information to reject poorly reconstructed jets, checking for deviations of these from the
1925 momentum conservation plane.

1926 To account for the limited angular resolution of the detector, I smeared the momenta
1927 of the muons and hadrons. In a liquid argon TPC muons are expected to be tracked with
1928 high precision, therefore I take the associated angular resolution to be 1° . In the case of
1929 jets, it is expected that for the hadrons dominating the cascade a detector like DUNE
1930 has an angular resolution between 1° to 5° [83], so I take the latter, more conservative,
1931 estimate.

1932 As a first selection step, I will just take into account particles with kinetic energies
1933 above the detection threshold of DUNE. For muons and photons the specified threshold
1934 energy is 30 MeV, for charged pions 100 MeV and for other hadrons 50 MeV [83]. This
1935 way, if the outgoing muon in a certain event has an energy lower than the required
1936 threshold I will drop such event. For the case of hadrons and photons, I will only require
1937 to have at least one particle above the energy threshold, so then one can compute the

5.5. HIGH ENERGY DM NEUTRINO SIGNALS

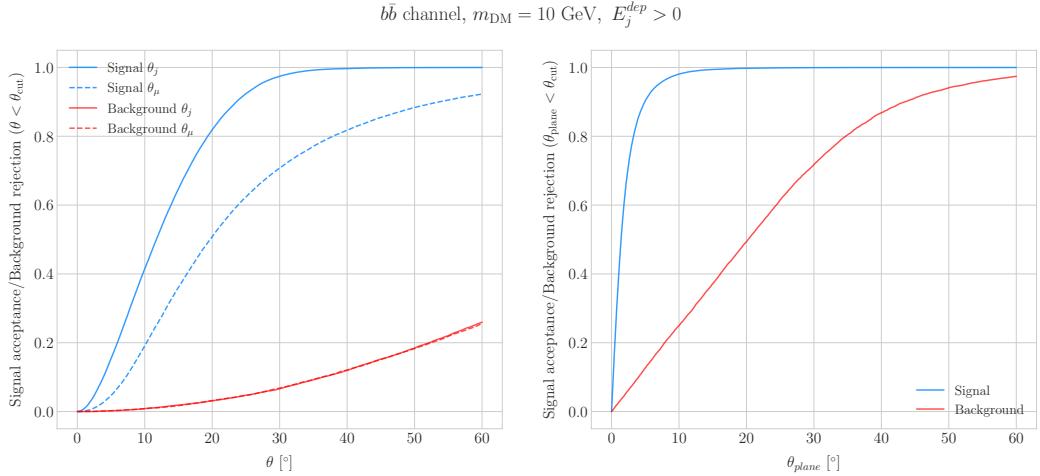


Figure 5.12: Left panel: signal efficiencies (blue lines) and background rejections (red lines) for events passing the cuts $\theta < \theta_{cut}$ for the jet (solid lines) and muon (dashed lines) angles. Right panel: signal efficiency (blue line) and background rejection (red line) for events passing the cut $\theta_{plane} < \theta_{cut}$ for the momentum conservation plane deviation.

1938 jet momentum using the (smeared) momenta of the N particles above threshold as:

$$\vec{p}_j = \sum_{i=1}^N \vec{p}_i. \quad (5.28)$$

1939 Additionally, I will also define an estimation of the deposited hadronic energy as:

$$E_j^{dep} = m_{39\text{Ar}} - m_{40\text{Ar}} + \sum_{i=1}^N \sqrt{|\vec{p}_i|^2 + m_i^2}. \quad (5.29)$$

1940 This quantity is useful to select events with enough hadronic visible energy in the
 1941 detector. For events where most of the hadronic energy is scattered across plenty of
 1942 hadrons with individual energies below the detection threshold, this estimation will
 1943 give $E_j^{dep} \leq 0$. In these cases it could be expected that the jet momentum is poorly
 1944 reconstructed, and therefore I require events to pass the cut $E_j^{dep} > 0$.

1945 For the events I can compute the angles for the muon and jet with respect to the
 1946 incoming neutrino as:

$$\cos \theta_\mu = \hat{p}_\nu \cdot \hat{p}_\mu, \quad (5.30)$$

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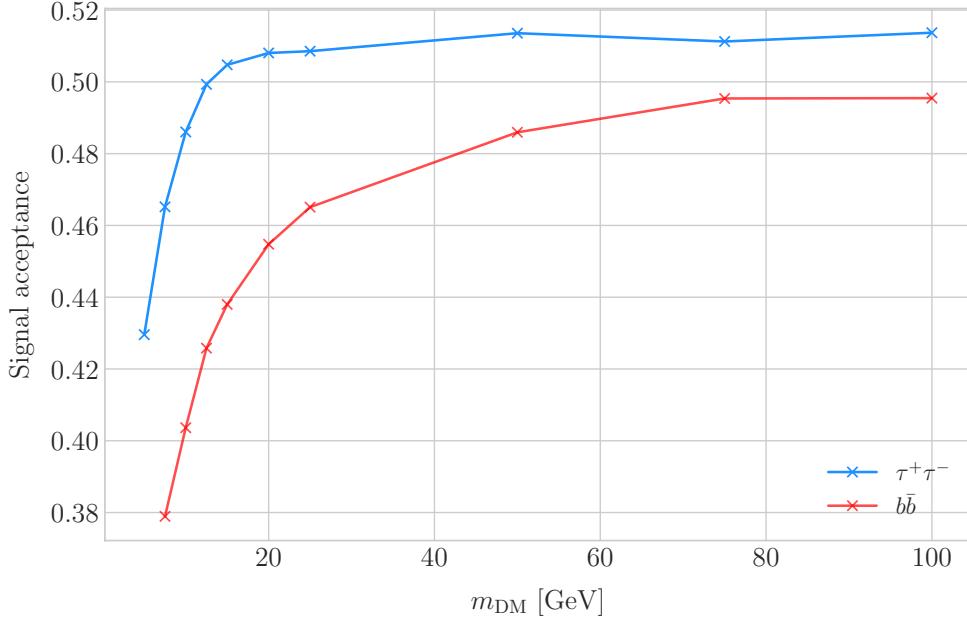


Figure 5.13: Signal efficiencies for the $\tau^+\tau^-$ (blue line) and $b\bar{b}$ (red line) DIS samples as functions of the DM mass, m_{DM} , obtained by applying the optimal angular cuts $\theta_\mu < 27^\circ$, $4^\circ < \theta_j < 26^\circ$ and $\theta_{\text{plane}} < 3.5^\circ$.

$$\cos \theta_j = \hat{p}_\nu \cdot \hat{p}_j, \quad (5.31)$$

and the deviation from the momentum conservation plane as:

$$\sin \theta_{\text{plane}} = \left| \frac{\hat{p}_\mu \times \hat{p}_\nu}{|\hat{p}_\mu \times \hat{p}_\nu|} \cdot \hat{p}_j \right|. \quad (5.32)$$

In Fig. 5.11 I show some distributions of these quantities for the case of the $b\bar{b}$ sample with $m_{\text{DM}} = 10$ GeV (blue histograms) and for the atmospheric backgrounds (red). In order to select the atmospheric events I followed the same criteria as for the signal events. However, because in the signal case I used the true direction of the neutrino as input, as it should be that of the Sun at that time and therefore known, in the atmospheric case I used a set of solar positions as our ansatz for the neutrino direction. From the distributions, one can see that the muon and the jet for the signal events are predominantly forward and also that the deviations from the momentum conservation plane are peaked at zero, as one should expect.

5.5. HIGH ENERGY DM NEUTRINO SIGNALS

Now, I can start applying cuts to maximise our signal selection efficiency while at the same time I try to minimise the amount of atmospheric background events passing the selection. To this end, I will need to find some lower and upper cuts for θ_j and θ_μ and an upper bound for θ_{plane} . In Fig. 5.12 I show how upper bound cuts in the different angular variables affect the signal efficiency (blue lines) and the background rejection (red lines). Notice that the signal efficiency behaves in a quite different way when I apply cuts in the jet and the muon angles. On the contrary, the cuts on both variables have a similar effect on the background rejection.

In order to obtain the optimal set of cuts, I perform a multidimensional scan. I do this separately for the $\tau^+\tau^-$ and the $b\bar{b}$ samples. For each case, I scan the possible cuts for each mass point and then I take the mean value of the signal efficiency for each configuration, to get the mean efficiency for each set of cuts. I do a similar scan for the atmospheric sample independently. Then, I take the sets of cuts such that the background rejection achieved is greater than 99.8% and search for the one which maximises the $\tau^+\tau^-$ and $b\bar{b}$ sample mean efficiencies. I found that with the cuts $\theta_\mu < 27^\circ$, $4^\circ < \theta_j < 26^\circ$ and $\theta_{plane} < 3.5^\circ$ I get a background rejection of 99.80% while achieving a 49.40% and 44.92% mean signal efficiencies for the $\tau^+\tau^-$ and $b\bar{b}$ signals respectively.

In Fig. 5.13 I show the signal efficiencies as a function of the DM mass for the $\tau^+\tau^-$ (blue line) and the $b\bar{b}$ (red line) DIS events, after applying the cuts discussed above, as well as the energy threshold and hadronic visible energy selections. One can see that the efficiency grows with the mass, as annihilations of more massive DM particles will produce a neutrino spectrum centered at higher energies, where DIS events dominate. Notice also that the efficiency is higher for the $\tau^+\tau^-$ case at every mass point, as in general this channel produces neutrinos at higher energies than the corresponding $b\bar{b}$ channel.

5.5.2 Single proton QE-like events

Now, one can try to explore the low energy tail of the neutrino energy distributions. This regime is dominated by the QE interactions, i.e. events of the type $\nu_\mu + n \rightarrow \mu^- + p$.

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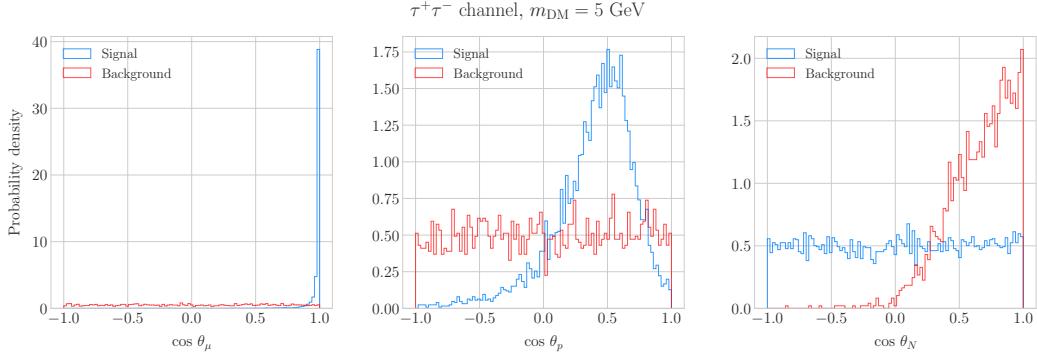


Figure 5.14: Distributions of $\cos \theta_\mu$ (left panel), $\cos \theta_p$ (central panel) and $\cos \theta_N$ (right panel) for the $\tau^+\tau^-$ QE sample with $m_{\text{DM}} = 5$ GeV (blue) and the atmospheric background (red).

1985 In this case, as the typical energies are $E_\nu \lesssim 1$ GeV, the momentum transfer to the
 1986 remnant nucleus is sizeable. Therefore, I can not make the approximation I did before
 1987 and assume that the momentum of the muon and the proton will give an adequate
 1988 estimation of the reconstructed neutrino energy.

1989 In any case, as before, I can take the direction of the incoming neutrino as known.
 1990 That way, one can estimate the energy of the neutrino as:

$$E_\nu^{reco} = E_\mu + E_p + m_{^{39}\text{Ar}} - m_{^{40}\text{Ar}}, \quad (5.33)$$

1991 and using momentum conservation I can write the momentum of the remnant nucleus
 1992 as:

$$\vec{p}_N = \hat{p}_\nu (E_\mu + E_p + m_{^{39}\text{Ar}} - m_{^{40}\text{Ar}}) - \vec{p}_\mu - \vec{p}_p. \quad (5.34)$$

1993 As in the previous case, I need to drop the events where the muon or the proton fall
 1994 below the kinetic energy detection threshold [83]. Also, I again apply a smearing to the
 1995 momenta of the particles, a 1% for muons and 5% for protons.

1996 Having done that, one can compute the following angular variables for our selected
 1997 events:

$$\cos \theta_\mu = \hat{p}_\nu \cdot \hat{p}_\mu, \quad (5.35)$$

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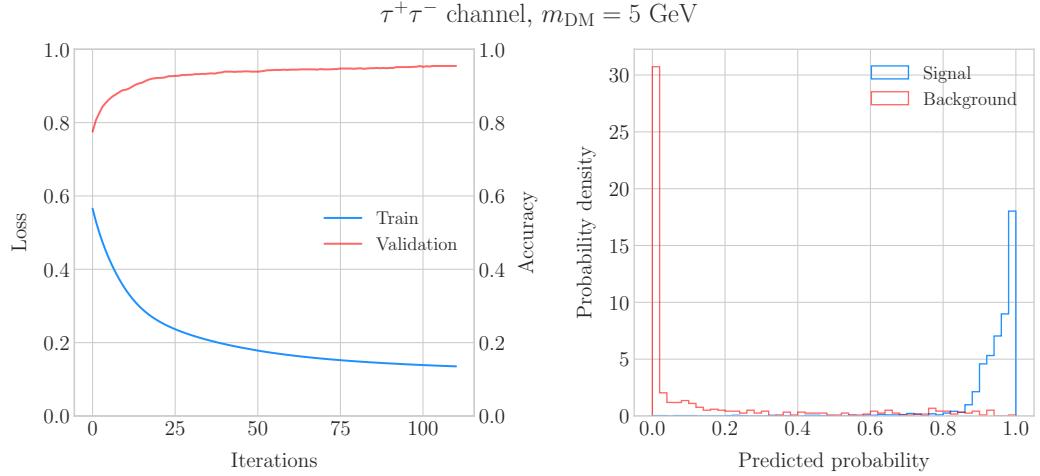


Figure 5.15: Left panel: value of the loss function for the training sample (blue line) and accuracy for the validation sample (red line) versus the number of iterations for the MLP classifier training. Right panel: distributions of the predicted probabilities assigned by the MLP classifier to the test sample for the $\tau^+\tau^-$ QE signal with $m_{\text{DM}} = 5 \text{ GeV}$ (blue) and the atmospheric background (red).

$$\cos \theta_p = \hat{p}_\nu \cdot \hat{p}_p, \quad (5.36)$$

$$\cos \theta_N = \hat{p}_\nu \cdot \hat{p}_N. \quad (5.37)$$

Fig. 5.14 shows the distributions of these angular variables for the $\tau^+\tau^-$ QE sample with $m_{\text{DM}} = 5 \text{ GeV}$ (blue) and the atmospheric background (red). Again, for the atmospheric events I used a random solar position as the ansatz for the incoming neutrino direction. Notice that now, opposed to the DIS case where the signal had very sharp distributions for the variables considered, the shapes of the angular distributions for signal and background are not that much different.

This effectively means that the usual approach of applying simple angular cuts would not work as well as in the previous situation. Therefore, as a possible solution, I tried to use a multilayer perceptron (MLP) classifier to separate between signal and background events. Thus, the power of the hypothesis test will serve as an estimate of the signal efficiency, and in the same way one can take the size of the test to be our background rejection.

For each DM mass value and channel, as well as for the background sample, I divide

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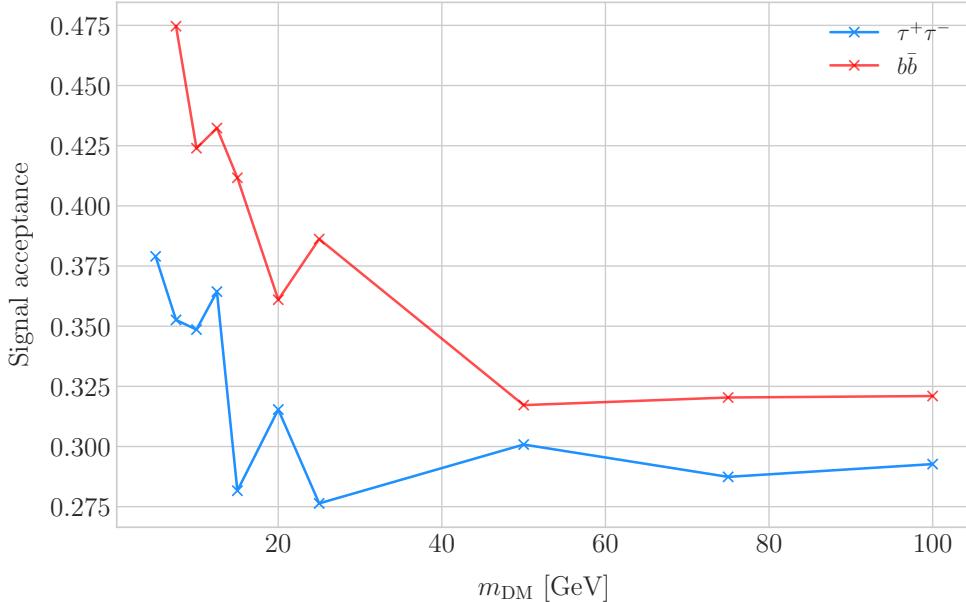


Figure 5.16: Signal efficiencies for the $\tau^+\tau^-$ (blue line) and $b\bar{b}$ (red line) single proton QE samples as functions of the DM mass, m_{DM} , obtained by requiring a minimum predicted probability from the MLP classifier of 0.97 in order to achieve a background rejection greater than 99.8%.

our events into training, validation and test samples. The input variables for the classifier were the reconstructed neutrino energy from Eq. (5.33) and the angular variables defined in Eqs. (5.35 - 5.37). I used the MLP classifier implemented in `scikit-learn` [143], with a total of five hidden layers, the rectified linear unit activation function and adaptive learning rate. In order to account for fluctuations due to artifacts in the training process I repeated the training a thousand times for each sample, redefining each time the training, validation and test subsets, so one can take as our signal efficiency and background rejection the mean values of the powers and sizes of the tests.

The results of one of these training processes for the $\tau^+\tau^-$ QE signal with $m_{\text{DM}} = 5$ GeV is shown in Fig. 5.15. On the left panel I show the loss function values (blue) and accuracy (red) at each iteration for the training and the validation samples respectively. The training stops either when the maximum number of iterations is reached (1000 in this case) or when the accuracy for the validation sample reaches a certain tolerance (I chose 10^{-4} as our tolerance). On the right panel I have the distributions for the

5.5. HIGH ENERGY DM NEUTRINO SIGNALS

predicted probability by the model, separated in true signal (blue) and background (red) events, for the test sample. One can see that both populations are well separated, obtaining a power of 44.97% and a size of 0.17% when I require a predicted probability greater than 0.97.

Applying this criteria for each sample, I obtain the mean signal efficiencies shown in Fig. 5.16. Notice that the efficiencies for the channel $\tau^+\tau^-$ (blue line) are consistently lower than the ones for the $b\bar{b}$ channel (red line). This can be due to the fact that, for each DM mass point, the neutrino spectrum coming from the $b\bar{b}$ annihilation channel is centered at lower energies when compared to the $\tau^+\tau^-$ spectrum. This directly translates into more low energy neutrinos undergoing QE interactions, which give signals that can be easily separated from the atmospheric background. This explanation also help us understand why in both cases the signal acceptance drops when the DM mass increases. In all cases, the background rejection took values between 99.8% to 99.9%. I will assume a 99.8% background rejection value in all cases to keep our estimation conservative.

5.5.3 Results

In order to estimate the DM-nucleon cross section sensitivities in the present case I need again to compute the expected number of background events. As I am now separating events by interaction type Eq. (5.25) does not hold anymore, as in that case I integrated over the total neutrino-argon cross section. In this instance, the expected background events for DIS events is approximately given by:

$$N_B^{DIS} \simeq \eta_B^{DIS} \times (4.655 \times 10^3) \times \left(\frac{\text{exposure}}{400 \text{ kT yr}} \right), \quad (5.38)$$

whereas for QE events we have:

$$N_B^{QE} \simeq \eta_B^{QE} \times (2.248 \times 10^4) \times \left(\frac{\text{exposure}}{400 \text{ kT yr}} \right). \quad (5.39)$$

Now, using these together with Eqs. (5.26) and (5.27) one can obtain the 90% C.L.

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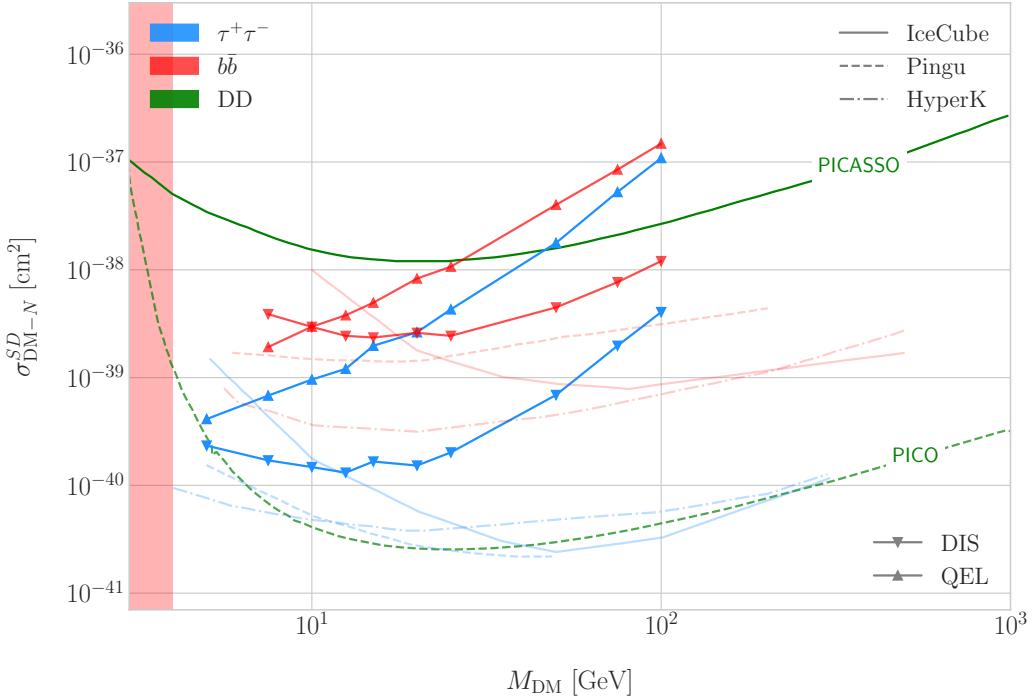


Figure 5.17: Projected 90% confidence level upper limit for DUNE (400 kT yr) on the spin-dependent DM-nucleon scattering cross section as a function of m_{DM} , for the annihilation channels $\tau^+\tau^-$ (blue) and $b\bar{b}$ (red) separated by interaction mode (up triangles denote DIS interactions whereas down triangles represent QE interactions). I also show the previous limits from IceCube [144] (solid lines) and the projected sensitivities for Pingu [145] (dashed lines) and Hyper-Kamiokande [146] (dash-dotted lines), as well as the direct detection limits from PICASSO [147] (solid green line) and PICO-60 C₃F₈ [148] (dashed green line).

2047 upper limit on the total annihilation rate at equilibrium for both kind of events. Then,
 2048 applying the computed DM-nucleons capture rates I can translate these into limits on
 2049 the DM-nucleon cross section by means of Eqs. (5.2), (5.5) and (5.6).

2050 Fig. 5.17 shows the obtained limits on the SD DM-nucleon cross section for DUNE,
 2051 using the DIS (up triangles) and QE (down triangles) events both for the $\tau^+\tau^-$ (blue)
 2052 and the $b\bar{b}$ (red) samples, for an exposure of 400 kT yr. I also include the corresponding
 2053 current limits from IceCube [144] (solid lines), as well as the projected sensitivities
 2054 of Pingu [145] (dashed lines) and Hyper-Kamiokande [146] (dash-dotted lines). For
 2055 comparison, I also show the reported direct detection limits from PICASSO [147] (solid
 2056 green line) and PICO-60 C₃F₈ [148] (dashed green line).

5.6. EXAMPLE: LEPTOPHILIC DARK MATTER

2057 Notice that, for most of the mass range, the limits one can set by using the DIS
 2058 events are stronger than those of the QE interactions, except for the low mass part
 2059 of both the $\tau^+\tau^-$ and the $b\bar{b}$ curves where the QE events dominate. In general, the
 2060 expected sensitivity of DUNE for DM masses $\lesssim 25$ GeV surpasses the stronger current
 2061 indirect limits. However, experiments like Hyper-Kamiokande are foreseen to have an
 2062 overall better sensitivity in this kind of searches, as they have a bigger active volume
 2063 and accept a broader energy range.

2064 A pending question is what happens when we add the RES and MEC charged-current
 2065 interaction contributions. In that case it would probably be more convenient to split
 2066 the samples by final state interaction topologies. Also, another necessary improvement
 2067 would be adding a full detector simulation and reconstructions. This will also require
 2068 considering the effect of poorly reconstructed events or final states containing neutral
 2069 particles such that they mimic the desired topology at the reconstruction level.

2070 5.6 Example: Leptophilic Dark Matter

2071 In general, the capture rate of DM particles by the Sun via interactions with electrons is
 2072 several orders of magnitude smaller than the capture via DM-nucleus scattering. Thus,
 2073 it would be sub-leading even when nucleon capture is loop suppressed. As I showed in
 2074 Fig. 5.2, the capture rate via scattering off electrons only surpasses the capture rates
 2075 via DM-nucleons interactions for DM masses $\lesssim 100 - 500$ MeV.

2076 However, if one considers a model where DM-nucleon interactions are forbidden even
 2077 at loop level, then electron interactions will be the sole contributor to DM capture in
 2078 the Sun. One can describe such scenario where the DM particles couple to leptons but
 2079 not to the quark sector using effective operators.

2080 In general, assuming that the DM particle is a Dirac fermion, the dimension six
 2081 operators describing the interaction between two DM particles and two leptons can be
 2082 written as:

$$\mathcal{L}_{eff} = G \sum_i (\bar{\chi} \Gamma_x^i \chi) (\bar{\ell} \Gamma_\ell^i \ell), \quad (5.40)$$

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where $G = 1/\Lambda^2$ is the effective coupling strength, Λ the cut-off of the effective field theory and ℓ denotes any lepton. In principle, one should consider all the possible Lorentz structures Γ_f^i in order to have a complete set of effective operators.

However, some combinations will induce interactions with nucleons at loop level. As we are specifically interested in interactions which forbid any communication with the quark sector, I will not consider those [149]. In addition, some of the effective operators give rise to velocity-suppressed scattering cross sections between DM particles and leptons. I will also neglect those, as the suppression goes with the square of the DM halo velocity which in units of the speed of light is $\sim 10^{-6}$.

This way, the only Lorentz tensor structure that do not induce interactions with quarks at loop level and gives a contribution to the scattering cross section that is not velocity suppress is the axial-axial interaction. The effective Lagrangian is then given by:

$$\mathcal{L}_{eff} = \frac{c_A^\chi c_A^\ell}{\Lambda^2} (\bar{\chi} \gamma^\mu \gamma^5 \chi) (\bar{\ell} \gamma_\mu \gamma^5 \ell), \quad (5.41)$$

where c_A^χ and c_A^ℓ are the couplings for the different species. As the DM coupling appears as a common factor for any lepton choice, I will redefine the corresponding coupling c_A^ℓ to absorb c_A^χ . Also, for simplicity, I will assume that the couplings between the DM particles and the leptons are flavour independent, i.e. I have just two couplings, c_A^e for charged leptons and c_A^ν for neutrinos.

In the case of a scalar DM particle, the lowest order effective interaction with leptons happens through a dimension five operator, generating scalar and pseudoscalar interactions. However, the former induces interactions with quarks at two loop level whereas the latter gives a velocity suppressed scattering cross section.

From the effective Lagrangian in Eq. (5.41) it can be shown that the axial-axial contribution to the scattering cross section for the fermionic DM and a charged lepton is given by:

$$\sigma_{DM-e}^{AA} = 3 (c_A^e)^2 \frac{m_e^2}{\pi \Lambda^4}. \quad (5.42)$$

If the DM interacts exclusively with fermions, then the only annihilation channels

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that will give us a measurable neutrino flux coming out of the Sun are $\tau^+\tau^-$ and $\nu\bar{\nu}$. The former channel, already explored previously in the more mainstream scenario of the DM capture via scattering off nucleons, is open only for $m_{\text{DM}} > m_\tau \simeq 1776.86 \pm 0.12$ MeV [150], a mass region where the solar DM capture by electrons is at least one order of magnitude smaller than the capture via interactions with nucleons. On the contrary, the latter allows us to explore a region where the capture rate via scattering off electrons dominates over the rest.

One downside of focusing in such low mass range is that it falls below the usual limit of $m_{\text{evap}} \sim 4$ GeV usually explored in the literature. The pretext to explore this region is the result discussed previously reported in Ref. [121], where DM evaporation in the Sun for the case of capture via electron scattering could be negligible for masses as low as $m_{\text{evap}} \sim 200$ MeV. This result is quite sensitive to the high velocity tail of the DM velocity distribution in equilibrium inside the Sun, and therefore full numerical simulations would be needed to assess the impact of this effect. However, this falls out of the scope of our work.

In this case, as I have a specific realisation of the interaction between the DM and leptons, one can estimate the relic density of our DM for different values of the couplings and the effective field theory scale Λ . The first step to do so is compute the self-annihilation cross section. Because I consider cold relics, at the freeze-out time our DM particles were non-relativistic and so one can expand the annihilation cross section in terms of the relative velocity v between two annihilating DM particles as [151]:

$$\sigma_{\text{ann}}^{AA}|v| \approx \frac{1}{2\pi\Lambda^4} \sum_\ell \left(c_A^\ell \right)^2 m_\chi^2 \sqrt{1 - \frac{m_\ell^2}{m_\chi^2} \left[\frac{m_\ell^2}{m_\chi^2} + \frac{1}{12} \left(2 - \frac{m_\ell^2}{m_\chi^2} \right) v^2 \right]}, \quad (5.43)$$

where the sum includes all the possible lepton final states with mass m_ℓ .

Solving the Boltzmann equation for the evolution of the DM density gives as a solution a relic density of:

$$\Omega_\chi h^2 \approx \frac{(1.04 \times 10^9) x_F}{M_{Pl} \sqrt{g_*} (a + 3b/x_F)}, \quad (5.44)$$

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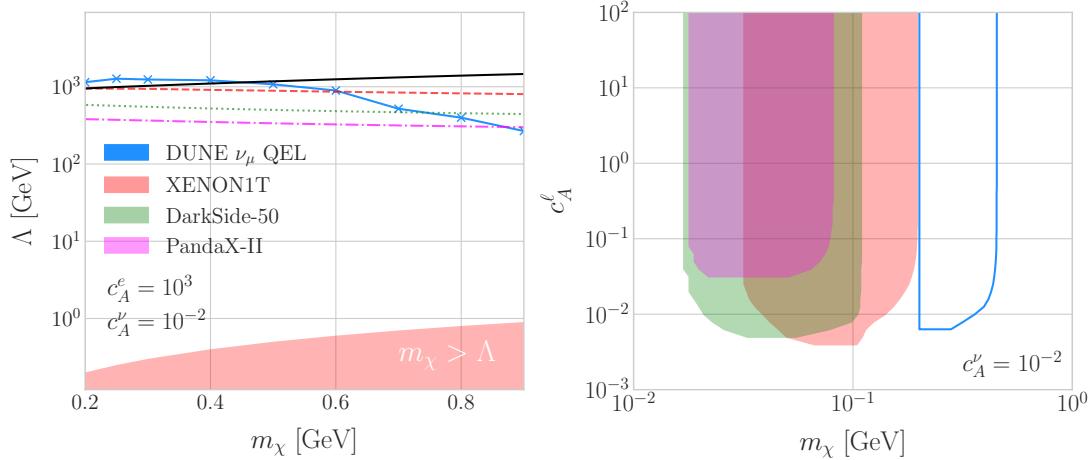


Figure 5.18: Left panel: Projected 90% confidence level sensitivity of DUNE (400 kT yr) to the scale Λ of an EFT containing only leptophilic DM axial-axial interactions (blue line), for the coupling values $c_A^e = 10^3$ and $c_A^\nu = 10^{-2}$. The black line represents the values for which the correct relic density is achieved. Right panel: Excluded values of c_A^ℓ as a function of the DM mass, for a fixed value $c_A^\nu = 10^{-2}$. In both cases the corresponding limits from XENON1T [153] (red), DarkSide-50 [154] (green) and PandaX-II [155] (magenta) are also shown.

2133 where $x_F = m_\chi/T_F$ being T_F the freeze-out temperature, g_* the number of relativistic
 2134 degrees of freedom at freeze-out and a and b the terms in the annihilation cross section
 2135 expansion $\sigma_{ann}|v| \approx a + bv^2 + \mathcal{O}(v^4)$. Using the current best fit for the relic DM density
 2136 $\Omega_\chi h^2 = 0.1198 \pm 0.0012$ [152] one can use these relations to compute the required
 2137 effective theory scale Λ at which the correct density is achieved for any combinations of
 2138 m_χ and c_A^ℓ .

2139 As discussed before, in the low DM mass region QE interactions dominate. Moreover,
 2140 if I focus on direct annihilation to neutrinos, the energy of the muon neutrino flux is
 2141 known as it must be equal to the mass of the DM particle, $E_\nu = m_\chi$. That way, now
 2142 I do not need to use Eq. (5.33) in order to estimate the momentum transfer to the
 2143 remnant nucleus, I can simply take:

$$\vec{p}_N = \hat{p}_\nu m_\chi - \vec{p}_\mu - \vec{p}_p. \quad (5.45)$$

2144 To estimate the signal efficiency and background rejection for this case I used again

5.6. EXAMPLE: LEPTOPHILIC DARK MATTER

the MLP classifier from `scikit-learn`, using the same specifications as before. The only difference now is that I add also the reconstructed neutrino energy as one of the features to train the classifier with, because the characteristic monoenergetic flux for each m_χ value will help to distinguish between signal and background events.

In this case, for masses below ~ 500 MeV I obtain a signal efficiency close to unity while keeping a background rejection of 99.9%. For bigger values of the mass, the signal efficiency drops significantly if I require to keep the background acceptance under 0.01%. However, because this kind of search is dominated by the background, sacrificing the signal acceptance to keep the background rejection to a minimum enhances the reach of the analysis. This way, for DM masses of the order of $m_\chi \sim 1$ GeV I end up with efficiencies as low as 1%.

Now, estimating the number of background events using Eq. (5.39) one can go on and apply Eqs. (5.26) and (5.27) together with Eq. (5.42) to derive the sensitivity of DUNE to this kind of model. Fig. 5.18 (left panel) shows the potential reach of DUNE to constrain the EFT scale Λ this model containing only leptophilic DM axial-axial interactions (blue line), for a choice of couplings $c_A^e = 10^3$ and $c_A^\nu = 10^{-2}$. I also included the current limits on the DM-electron scattering cross section from XENON1T [153] (dashed red line), DarkSide-50 [154] (dotted green line) and PandaX-II [155] (dash-dotted magenta line), reworked with Eq. (5.42) to show their implications for the EFT scale. The values of Λ for which the correct DM relic density value is achieved for each mass are also shown (black line). This tells us that, for that specific choice of couplings, DUNE would be sensitive to DM configurations allowed by the relic density constraint up to a mass of $m_\chi \sim 400$ MeV.

In Fig. 5.18 (right panel) I show similar limits for the excluded values of c_A^ℓ as a function of the DM mass, for a fixed $c_A^\nu = 10^{-2}$. I do not show the limits for other values of c_A^ν , as this parameter has little effect on the phenomenology at hand. From this view one can see that DUNE would be able to offer complementary information to the low energy DM-electron interaction searches performed by direct detection experiments, in a slightly higher mass range.

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Table 5.1: Systematic uncertainties for the solar WIMP signal events. Table adapted from Ref. [156].

Systematic	Value
Form factor	Does not apply to SD [157]
Solar model	3% [157]
Local DM density	Not relevant for relative interpretations [157, 158]
Dynamics of solar system	Negligible [159]
Velocity distributions	20% at 20 GeV [157, 158]
Oscillation parameters	8% for $\tau^+\tau^-$, 5% for $b\bar{b}$ [160]
Neutrino interactions in the Sun	10%
Matter effects in the Earth	10%

2174 With the present example, although it focuses on a very specific realisation of the DM
2175 interactions, I show the potential of DUNE to constrain exotic DM scenarios. Thanks
2176 to its low backgrounds and superb angular resolution DUNE will be able to help with
2177 the systematic searches for dark sectors physics.

2178 5.7 Systematic uncertainties

2179 The estimation of the DM cross sections using neutrinos from WIMP annihilations
2180 inside the Sun is affected by systematic uncertainties from different sources. Surely, the
2181 atmospheric background estimation is also affected by systematic uncertainties. There
2182 are uncertainties common to both types of events, as well as others specific to each. In
2183 this section, I try to provide a comprehensive summary of the main sources of uncertainty
2184 for this analysis, which should be taken into account in any future extensions of the
2185 same.

2186 5.7.1 Systematic uncertainties in the solar WIMP signal

2187 The systematic uncertainties affecting the solar WIMP neutrino signal can be divided in
2188 two categories. On the one hand, we have those affecting the solar WIMP annihilation
2189 rate. On the other hand, there are the ones which modify the neutrino flux resulting

5.7. SYSTEMATIC UNCERTAINTIES

Table 5.2: Systematic uncertainties for the solar WIMP atmospheric background events. Table adapted from Ref. [49].

Systematic	Value
Flux normalisation	25 – 7% for $0.1 < E_\nu \leq 1$ GeV (linear in $\log E_\nu$) 7% up to 10 GeV
$(\nu_\mu + \bar{\nu}_\mu)/(\nu_e + \bar{\nu}_e)$	2% for $E_\nu \leq 1$ GeV 3% for $1 < E_\nu \leq 10$ GeV
$\bar{\nu}_\mu/\nu_\mu$	2% for $E_\nu \leq 1$ GeV 6% for $1 < E_\nu \leq 10$ GeV
K/ π ratio	5% $E_\nu \leq 100$ GeV

2190 from the annihilations reaching our detector.

2191 • **Uncertainties on the annihilation rate.** These include the astrophysical effects
 2192 that affect the normalisation of the solar DM neutrino flux. The main contributions
 2193 are the solar model choice, the form factor uncertainties (only for SI searches), the
 2194 gravitational effect of other planets, the local DM density (not relevant for relative
 2195 comparisons, as it affects direct detection experiments in the same way), and the
 2196 DM halo and dispersion velocities.

2197 • **Uncertainties on the neutrino flux.** These are related to the oscillation effects,
 2198 as well as the absorption and regeneration of neutrinos in the Sun. Matter effects
 2199 inside the Earth also affect the neutrino flux the measured at the detectors.

2200 Table 5.1 summarises the contributions of the different sources of uncertainty for the
 2201 signal events. These are the signal systematic uncertainties that have been taken into
 2202 account in previous solar DM searches with neutrinos [156, 158, 160].

2203 5.7.2 Systematic uncertainties in the atmospheric background

2204 For the atmospheric background events, one needs to take into account the systematic
 2205 uncertainties affecting the atmospheric ν_μ flux. These have been extensively studied
 2206 in the context of atmospheric neutrino oscillation measurements. Among these, the
 2207 energy-dependent flux normalisation uncertainty is the in the low energy regime. Other

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2208 important contributions to the uncertainty come from the ratios between the muon to
2209 electron neutrino and the muon to anti-muon neutrino components of the flux. Additional
2210 uncertainty is introduced by the errors in the pion and kaon production rates calculated
2211 for the hadronic interactions of cosmic rays in the atmosphere [161].

2212 Table 5.2 shows a summary of the leading contributions to the uncertainty on the
2213 atmospheric muon neutrino flux, in the energy range relevant for this analysis.

2214 5.7.3 Common systematic uncertainties

2215 Finally, there are sources of uncertainty common to both signal and backgrounds. These
2216 have two different origins:

2217 • **Uncertainties on the neutrino cross section.** These are introduced by the
2218 modelling of the neutrino-nucleus interactions. In the context of the solar WIMP
2219 analysis, these have been estimated to be 10% for DM masses around 10 GeV
2220 [160].

2221 • **Uncertainties related to the detector.** They affect the measurement of the
2222 neutrino interaction and the final state particles produced. The main detector
2223 uncertainties relevant to this analysis are those of the energy and angular resolutions
2224 of the DUNE FD. Other effects, like the timing and triggering efficiencies, will
2225 also contribute to the uncertainties. The particular values these will take for this
2226 analysis need to be worked out in the context of DUNE.

6

2227

2228

Particle identification in ND-GAr

2229 *I am no bird; and no net ensnares me; I am a free human being with an
2230 independent will.*

2231 – Charlotte Brontë, *Jane Eyre*

2232 In DUNE Phase II, ND-GAr will fulfill the role of TMS measuring the momentum
2233 and sign of the charged particles exiting ND-LAr. Additionally, it will measure neutrino
2234 interactions inside the HPgTPC. This way, ND-GAr will allow to constrain certain cross
2235 section systematic uncertainties and study the effect of FSI in CC interactions. To
2236 do so, it needs to measure the spectrum of protons and charged pions at low energies,
2237 as well as measure the pion multiplicity. This puts strong requirements to the the
2238 particle identification (PID) capabilities of the detector, as well as stimulates the relevant
2239 developments in the reconstruction.

2240 The goal of the present Chapter is to review the status and design of the GArSoft
2241 package, the simulation and reconstruction software of ND-GAr, and present the different
2242 additions and upgrades that I have added to the reconstruction with the PID in mind.

2243 6.1 GArSoft

2244 GArSoft is a software package developed for the simulation and reconstruction of events
2245 in ND-GAr. It is inspired by the LArSoft toolkit used for the simulation of LArTPC
2246 experiments, like the DUNE FD modules. It is based on `art`, the framework for event
2247 processing in particle physics experiments [162]. Other of its main dependencies are

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAr

2248 ROOT, NuTools, GENIE and Geant4. It allows the user to run all the steps of a generation-
2249 simulation-reconstruction workflow using FHiCL configuration files.

2250 **6.1.1 Event generation**

2251 The standard generator FHiCLs in GArSoft run the event generation and particle
2252 propagation simulation (i.e. Geant4) in the same job by default. However, it is possible
2253 to split them up if needed. The current version of GArSoft provides five different event
2254 generators, each of them producing `simb::MCTruth` products defined in NuTools. The
2255 available modules are:

2256 • **SingleGen**: particle gun generator. It produces the specified particles with a given
2257 distribution of momenta, initial positions and angles.

2258 • **TextGen**: text file generator. The input file must follow the `hepevt` format¹, the
2259 module simply copies this to `simb::MCTruth` data products.

2260 • **GENIEGen**: GENIE neutrino event generator. The module runs the neutrino-nucleus
2261 interaction generator using the options specified in the driver FHiCL file (flux file,
2262 flavour composition, number of interactions per event, t_0 distribution, ...). Current
2263 default version is v3_04_00.

2264 • **RadioGen**: radiological generator. It produces a set list of particles to model
2265 radiological decays. Not tested.

2266 • **CRYGen**: cosmic ray generator. The module runs the CRY event generator with a
2267 configuration specified in the FHiCL file (latitude and altitude of detector, energy
2268 threshold, ...). Not tested.

¹In brief, each event contains at least two lines. The first line contains two entries, the event number and the number of particles in the event. Each following line contains 15 entries to describe each particle. The entries are: status code, pdg code for the particle, entry of the first mother for this particle, entry of the second mother for this particle, entry of the first daughter for this particle, entry of the second daughter for this particle, x component of the particle momentum, y component of the particle momentum, z component of the particle momentum, energy of the particle, mass of the particle, x component of the particle initial position, y component of the particle initial position, z component of the particle initial position and time of the particle production.

6.1. GArSOFT

2269 The module **GArG4** searches for all the generated **simb::MCTruth** data products, using
2270 them as inputs to the Geant4 simulation with the specified detector geometry. A constant
2271 0.5 T magnetic field along the drift coordinate is assumed. The main outputs of this step
2272 are **simb::MCParticle** objects for the generated Geant4 particles, **gar::EnergyDeposit**
2273 data products for the energy deposits in the HPgTPC and **gar::CaloDeposit** data
2274 products for the energy deposits in the ECal and muon system.

2275 6.1.2 Detector simulation

2276 The standard detector simulation step in GArSoft is all run with a single FHiCL, but
2277 the different modules can be run independently as well. First the **IonizationReadout**
2278 module simulates the charge readout of the HPgTPC, and later the **SiPMReadout** module
2279 runs twice, once for the ECal and then for the muon system, with different configurations.

2280 The **IonizationAndScintillation** module collects all the **gar::EnergyDeposit**
2281 data products, to compute the equivalent number of ionization electrons for each energy
2282 deposit. The **ElectronDriftAlg** module simulates the electron diffusion numerically
2283 both in the longitudinal and transverse directions and applies an electron lifetime
2284 correction factor. The induced charge on the nearest and neighbouring readout pads
2285 is modeled using the provided pad response functions. The digitisation of the data is
2286 then simulated with the **TPCReadoutSimAlg** module. By default, the ADC sampling
2287 rate used is 50.505 MHz. The resulting raw waveforms for each channel are stored with
2288 zero-suppression, in order to save memory and CPU time. The algorithms keep blocks
2289 of ADC values above a certain threshold, plus some adjustable additional early and late
2290 tick counts. The results of these three steps are **gar::raw::RawDigit** data products.

2291 For the ECal and the muon system the **SiPMReadout** module calls either the
2292 **ECALReadoutSimStandardAlg** or **MuIDReadoutSimStandardAlg** modules. These take
2293 all the **gar::CaloDeposit** data products in the corresponding detector and do the
2294 digitisation depending on whether the hit was in a tile or strip layer. They include single
2295 photon statistics, electronic noise, SiPM saturation and time smearing. The resulting
2296 objects are **gar::raw::CaloRawDigit** data products.

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2297 6.1.3 Reconstruction

2298 The reconstruction in GArSoft is also run as a single job by default. It first runs the hit
2299 finding, clustering, track fitting and vertex identification in the HPgTPC, followed by
2300 the hit finding and clustering in the ECal and muon system. After those it produces the
2301 associations between the associations between the tracks and the ECal clusters.

2302 Focusing first on the HPgTPC reconstruction, the `CompressedHitFinder` module
2303 takes the zero-suppressed ADCs from the `gar::raw::RawDigit` data products. The
2304 reconstructed hits largely correspond to the above threshold blocks, however the hit
2305 finder identifies waveforms with more than one maximum, diving them in multiple hits
2306 if they dip below a certain threshold. The data products produced are of the form
2307 `gar::rec::Hit`. These are the inputs to the clustering of hits in the `TPCHitCluster`
2308 module. Hits close in space and time are merged, and the resulting centroids are found.
2309 This module outputs `gar::rec::TPCClusters` objects and associations to the input
2310 hits.

2311 The following step prior to the track fitting is pattern recognition. The module
2312 called `tpcvechitfinder2` uses the `gar::rec::TPCClusters` data products to find track
2313 segments, typically called vector hits. They are identified by performing linear 2D fits
2314 to the positions of the clusters in a 10 cm radius, one fit for each coordinate pair. A
2315 3D fit defines the line segment of the vector hit, using as independent variable the one
2316 whose sum of (absolute value) slopes in the 2D fits is the smallest. The clusters are
2317 merged to a given vector hit if they are less than 2 cm away from the line segment. The
2318 outputs are `gar::rec::VecHit` data products, as well as associations to the clusters. The
2319 `tpcpatrec2` module takes the `gar::rec::VecHit` objects to form the track candidates.
2320 The vector hits are merged together if their direction matches, their centers are within
2321 60 cm and their direction vectors point roughly to their respective centers. Once
2322 the clusters of vector hits are formed they are used to make a first estimation of the
2323 track parameters, simply taking three clusters along the track. The module produces
2324 `gar::rec::Track` data products and associations between these tracks and the clusters

6.1. GArSOFT

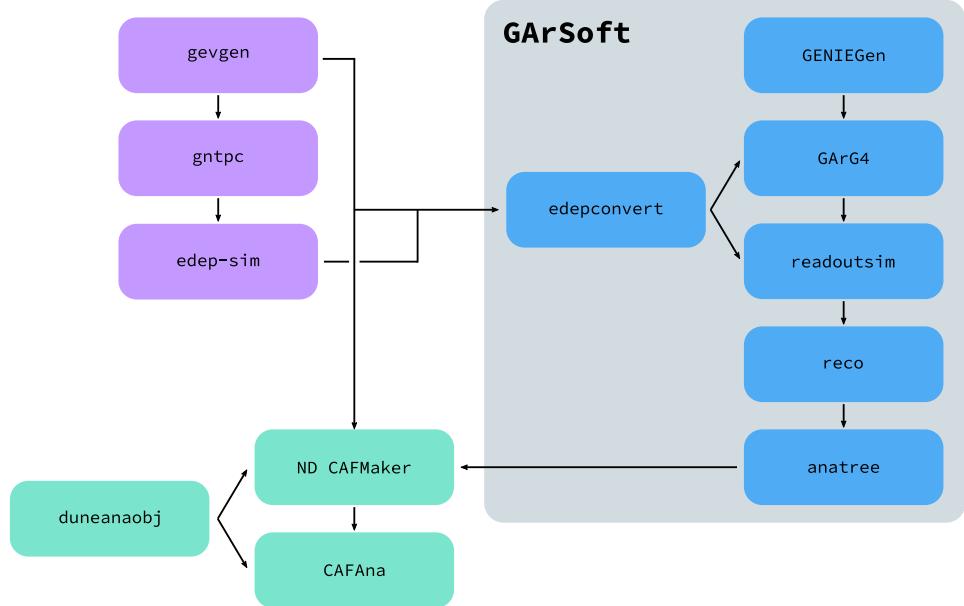


Figure 6.1: Schematic diagram showing the different modules involved in the ND-GAr production.

and vector hits.

The track is fitted by means of a Kalman filter in the `tpctrackfit2` module, using the position along the drift direction as the independent variable. Two different fits are performed per track, a forward and a backwards fit, each starting from one of the track ends. The Kalman filter state vector ($y, z, R, \phi, \tan\lambda$) is estimated at each point along the track using a Bayesian update. The track parameters reported in the forward and backwards fits are the ones computed at the opposite end where the fit started. The main outputs of the track fit are the `gar::rec::Track` objects. Additionally, the module stores the fitted 3D positions along the track in the `gar::rec::TrackTrajectory` data products and the total charge and step sizes for each point also get stored in the form of `gar::rec::TrackIonization` objects.

After the tracking step, the `vertexfinder1` module looks at the reconstructed `gar::rec::Track` products, creating vertex candidates with the track ends that are within 12 cm of each other. The vertices are then fitted using linear extrapolations from the different track ends associated. The results are `gar::rec::Vertex` data products,

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAr

2340 and associations to the tracks and corresponding track ends.

2341 For the ECal and muon tagger, the `SiPMHitFinder` module runs twice with different
2342 configurations, adapted to the particular capabilities of both. The module simply takes
2343 the `gar::raw::CaloRawDigit` products, applies a calibration factor to convert the ADC
2344 counts to MeV and for the strip layer hits it calculates the position along the strip using
2345 the times recorded of both SiPMs. This module produces `gar::rec::CaloHit` data
2346 products. Next, these objects are used as inputs to the `CaloClustering` module. It
2347 merges the hits based on a simple nearest neighbours (NN) algorithm. For the resulting
2348 clusters it also computes the total energy and position of the centroid. The results are
2349 stored as `gar::rec::Cluster` data products, with associations to the hits.

2350 The last step in the reconstruction is associating the reconstructed tracks in the
2351 HPgTPC to the clusters formed in the ECal and muon system. The `TPCECALAssociation`
2352 module checks first the position of the track end points, considering only the points
2353 that are at least 215 cm away from the cathode or have a radial distance to the center
2354 greater than 230 cm. The candidates are propagated up to the radial position, in the
2355 case of clusters in the barrel, or the drift coordinate position, for the end cap cluster, of
2356 the different clusters in the collection using the track parameters computed at the end
2357 point. The end point is associated to the cluster if certain proximity criteria are met.
2358 This module creates associations between the tracks, the end points and the clusters.
2359 The criteria for the associations are slightly different for the ECal and the muon tagger.

2360 6.2 dE/dx measurement in the TPC

2361 Among the parameters extracted from the track fitting, ionisation is particularly useful
2362 for particle identification, as it is a function of the particle velocity. Although for the
2363 case of relativistic particles this dependence is not very strong, measuring the track on
2364 a large number of points may allow us to estimate the amount of ionisation accuratel.
2365 This, paired with a measurement of the momentum, may allow us to identify the particle
2366 type.

6.2. dE/dx MEASUREMENT IN THE TPC

2367 The first calculation of the energy loss per unit length of relativistic particles using a
 2368 quantum-mechanical treatment is due to Bethe [163]. Using this approach, the mean
 2369 ionisation rate of a charged particle traveling through a material medium is (using
 2370 natural units $G = \hbar = c = 1$):

$$\left\langle \frac{dE}{dx} \right\rangle = \frac{4\pi Ne^4}{m_e \beta^2} z^2 \left(\log \frac{2m_e \beta^2 \gamma^2}{I} - \beta^2 \right), \quad (6.1)$$

2371 where N is the number density of electrons in the medium, e the elementary charge, m_e
 2372 is the electron mass, z the charge of the particle in units of e , β is the velocity of the
 2373 particle, $\gamma = (1 - \beta^2)^{-1}$ and I denotes the effective ionisation potential averaged over
 2374 all electrons. This relation is known as the Bethe-Bloch formula.

2375 From Eq. (6.1) one can see that the ionisation loss does not depend explicitly on
 2376 the mass of the charged particle, that for non-relativistic velocities it falls as β^{-2} , then
 2377 goes through a minimum and increases as the logarithm of γ . This behaviour at high
 2378 velocities is commonly known as the relativistic rise. The physical origin of this effect
 2379 is partly due to the fact that the transverse electromagnetic field of the particle is
 2380 proportional to γ , therefore as it increases so does the cross section.

2381 It was later understood that the relativistic rise could not grow indefinitely with γ .
 2382 A way to add this feature in the Bethe-Bloch formula is by introducing the so-called
 2383 density effect term. It accounts for the polarisation effect of the atoms in the medium,
 2384 which effectively shield the electromagnetic field of the charged particle halting any
 2385 further increase of the energy loss [164]. Denoting the correction as $\delta(\beta)$, one can rewrite
 2386 Eq. (6.1) as:

$$\left\langle \frac{dE}{dx} \right\rangle = \frac{4\pi Ne^4}{m_e \beta^2} z^2 \left(\log \frac{2m_e \beta^2 \gamma^2}{I} - \beta^2 - \frac{\delta(\beta)}{2} \right). \quad (6.2)$$

2387 In general, the form of $\delta(\beta)$ depends on the medium and its state of aggregation,
 2388 involving the usage of tabulated parameters and implicit relations [165].

2389 Another standard method to compute the amount of ionisation a charged particle
 2390 produces is the so-called photo-absorption ionisation (PAI) model proposed by Allison
 2391 and Cobb [166]. Within their approach, the mean ionisation is evaluated using a

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAR

2392 semiclassical calculation in which one characterises the continuum material medium by
2393 means of a complex dielectric constant $\varepsilon(k, \omega)$. However, in order to model the dielectric
2394 constant they rely on the quantum-mechanical picture of photon absorption and collision.
2395 Therefore, in the PAI model the computation of the ionisation loss involves a numerical
2396 integration of the measured photo-absorption cross-section for the relevant material.

2397 In a particle physics experiment, the typical way of determining the energy loss
2398 per unit length as a function of the particle velocity is studying identified particles
2399 over a range of momenta. Once we have established this relation we can use it for
2400 other, unknown particles. In this sense, it makes sense to have a regular mathematical
2401 expression for this relation that one can use.

2402 It happens that neither the Bethe-Bloch theory nor the PAI model from Allison and
2403 Cobb offer a close mathematical form for the ionisation curve. This is the reason why a
2404 full parametrisation of the ionisation curves can be useful. A parametrisation originally
2405 proposed for the ALEPH TPC [167] and later used by the ALICE TPC [168] group that
2406 manages to capture the features of the ionisation energy loss is:

$$f(\beta\gamma) = \frac{P_1}{\beta^{P_4}} \left(P_2 - \beta^{P_4} - \log \left[P_3 + \frac{1}{(\beta\gamma)^{P_5}} \right] \right), \quad (6.3)$$

2407 where P_i are five free parameters. Hereafter, we will refer to Eq. (6.3) as the ALEPH
2408 dE/dx parametrisation.

2409 6.2.1 Energy calibration

2410 In order to obtain the amount of energy loss by a charged particle due to ionisation
2411 in our TPC we need to determine the conversion between the charge deposited in our
2412 readout planes and the actual energy depositions. This procedure is known as energy
2413 calibration.

2414 In a general, the first step of the calibration involves a non-uniformity correction,
2415 to make sure that the detector response is uniform throughout the TPC. These are
2416 typically divided into three categories, non-uniformities in the transverse YZ plane,

6.2. dE/dx MEASUREMENT IN THE TPC

2417 non-uniformities along the drift direction X and variations of the detector response
2418 over time (would not apply to us as the detector is not built yet). These would correct
2419 for effects such as electron diffusion and attenuation, space charge effects or channel
2420 misconfiguration. However, because at the moment I am only interested in making sure
2421 we recover a sensible result from our simulation, I will not apply uniformity corrections
2422 to our charge deposits.

2423 Other effects, like electron-ion recombination or ADC saturation, lead to a non-linear
2424 relation between the observed charge and the deposited energy in the detector, with the
2425 observed readout charge saturating at high ionisation energies. In this case, because we
2426 are dealing with gaseous argon and therefore recombination is not as important as in
2427 liquid, we do not simulate recombination effects in the TPC. Even so, the simulation of
2428 the electronic response will still introduce charge saturation, and one needs to correct
2429 for it in order to obtain the exact amount of energy loss due to ionisation.

2430 By default, the track fitting algorithm in GArSoft provides a `TrackIonization`
2431 object associated to each reconstructed track. It contains two collections of charge
2432 deposits, one for each fitting direction, consisting on pairs of charge values (dQ , in ADC)
2433 and step sizes (dx , in cm).

2434 In order to estimate the ionisation loss in the ND-GAr TPC, I have used an MC
2435 sample consisting of single, isotropic protons propagating in the TPC. The starting points
2436 of the protons were sampled inside a $50 \times 50 \times 25$ cm box centered at $(100, -150, 1250)$,
2437 and their momenta are uniformly distributed in the range $0.25 - 1.75$ GeV. I ran the
2438 simulated sample through GArSoft's default detector simulation and reconstruction, and
2439 then a custom analyser module that extracts the ionisation data together with other
2440 reconstructed track information from the Kalman fit.

2441 For studying the energy loss of the protons I select the reconstructed tracks that
2442 range out (i.e. slow down to rest) inside the TPC. A characteristic feature of the energy
2443 loss profile of any stopping ionising particle is the so-called Bragg peak, a pronounced
2444 peak that occurs immediately before the particle comes to rest. From Eq. (6.1) we can
2445 see that this behaviour is expected, as the energy loss for non-relativistic particles is

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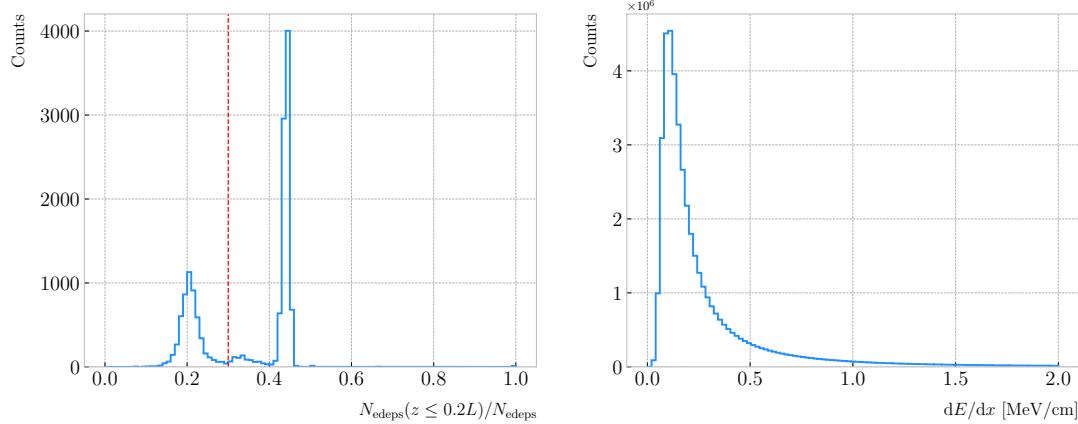


Figure 6.2: Left panel: distribution of the fraction of Geant4-level energy deposits per track with residual range less than 20% of the total track length, for the isotropic proton sample. Right panel: distribution of the ionisation per unit length of the energy deposits in the proton sample after removing the tracks with less than 30% of their energy deposits in the last 20% of the track.

2446 inversely proportional to β^2 . In data, a way of identifying the Bragg peak, and thus
 2447 select the stopping particles, is checking the number of energy deposits towards the
 2448 end of the track. In this case, I count the fraction of the Geant4 simulated energy
 2449 deposits with a residual range value (the distance from a given energy deposit to the
 2450 last deposit in the track trajectory) less than a 20% of the corresponding track length².
 2451 The distribution of this fraction of energy deposits for our proton sample is shown in
 2452 Fig. 6.2 (left panel). We can clearly see two well separated peaks in this distribution,
 2453 one centered at 0.2 and another, narrower, one centered at a higher value. The first
 2454 one corresponds to non-stopping protons, as in that case the number of energy deposits
 2455 towards the end of the track is uniformly distributed due to the absence of the Bragg
 2456 peak. In that way, I apply a cut in this distribution, requiring that at least 30% of the
 2457 simulated energy deposits sit in the last 20% of the tracks, to ensure that the Bragg
 2458 peak is present.

2459 Figure 6.2 (right panel) shows the distribution of the energy loss per unit length for
 2460 the Geant4 simulated energy deposits of the selected stopping protons. We can see that

²As we are applying this selection at the Geant4 level we could have simply selected the stopping protons using the `EndProcess` labels from the simulation. However, the Bragg peak identification method displayed here could serve as a starting point for a selection of stopping protons in real data.

6.2. dE/dx MEASUREMENT IN THE TPC

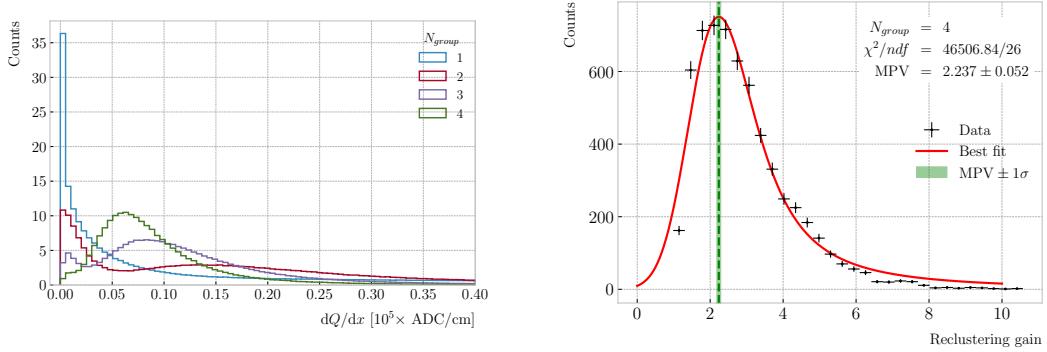


Figure 6.3: Left panel: distribution of the reconstructed ionisation charge per unit length for our MC stopping proton sample. The different colors indicate how many consecutive dQ/dx pairs were grouped together. Right panel: distribution of the median change in dQ/dx per track after $N_{group} = 4$ clusters were reclustered together.

it follows the expected shape of a Landau distribution, which describes the fluctuations of the ionisation energy losses [169]. This distribution has a characteristic asymmetric PDF, with a long right tail that translates into a high probability for high-energy ionisation losses. The origin of these fluctuations is mainly the possibility of transferring a high enough energy to an electron, so it becomes a ionising particle itself.

Now, from the point of view of the reconstruction, the objects that we have available to extract the ionisation information for the different reconstructed tracks are the collections of dQ and dx pairs, as stated before. The dQ values come from adding up the amplitude of all the reconstructed hits in a cluster, which is the input object to the Kalman fit.

Figure 6.3 (left panel) shows the distribution of the ionisation charge deposits per unit length for the track in the stopping proton sample (blue line). As one can notice, this distribution does not resemble the expected shape of the Landau PDF. This distribution peaks sharply at 0 and has a heavy tailed behaviour. Notice, however, how the distribution changes its shape as we group together N_{group} consecutive charge deposit pairs (red, purple and green lines). The distribution in the $N_{group} = 4$ case already has a shape which resembles that of the Geant4-level ionisation per unit length, so I will proceed using this amount of reclustering for the reconstruction-level depositions.

An extra factor I need to account for, when reclustering is applied, is how the overall

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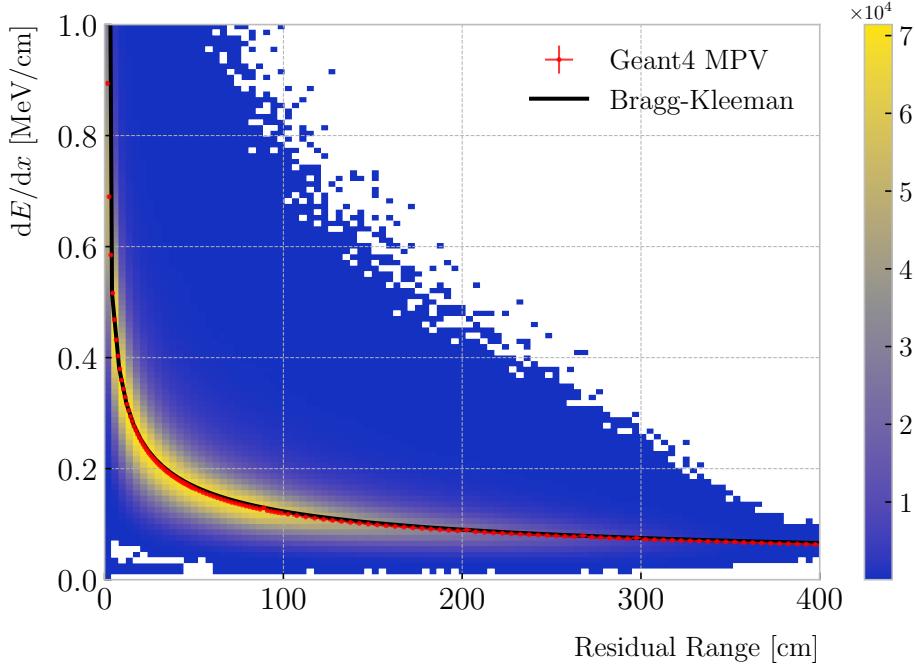


Figure 6.4: Distribution of the Geant4-simulated energy losses per unit length versus residual range for the stopping proton sample. The overlaid points represent the fitted most probable value of the dE/dx distribution in each residual range bin, whereas the curve is their best fit to the Bragg-Kleeman formula from Eq. (6.4).

2480 dQ/dx per track changes. To do so, we can look at the ratio between the median dQ/dx
 2481 after and before the reclustering. Figure 6.3 (right panel) shows the median enhancement
 2482 in dQ/dx per track for the stopping proton sample in the case $N_{group} = 4$. Fitting a
 2483 Landau distribution convolved with a Gaussian³, I estimate the most probable value of
 2484 this ratio to be $G_{group} = 2.24 \pm 0.05$.

2485 At this point, I am left with determining the conversion between the charge deposits
 2486 per unit length dQ/dx and the energy deposits per unit length dE/dx . To this end, we
 2487 need a way of comparing the two. I can use the residual range z to get a prediction of
 2488 the most probable dE/dx by using the following empirical parametrisation [170]:

$$\frac{dE}{dx}(z) = \frac{z^{\frac{1}{p}-1}}{p\Lambda^{\frac{1}{p}}}, \quad (6.4)$$

³In the literature, this distribution is often referred to as Landau+Gaussian or langau. In the following, I will use LanGauss to refer to such PDF.

6.2. dE/dx MEASUREMENT IN THE TPC

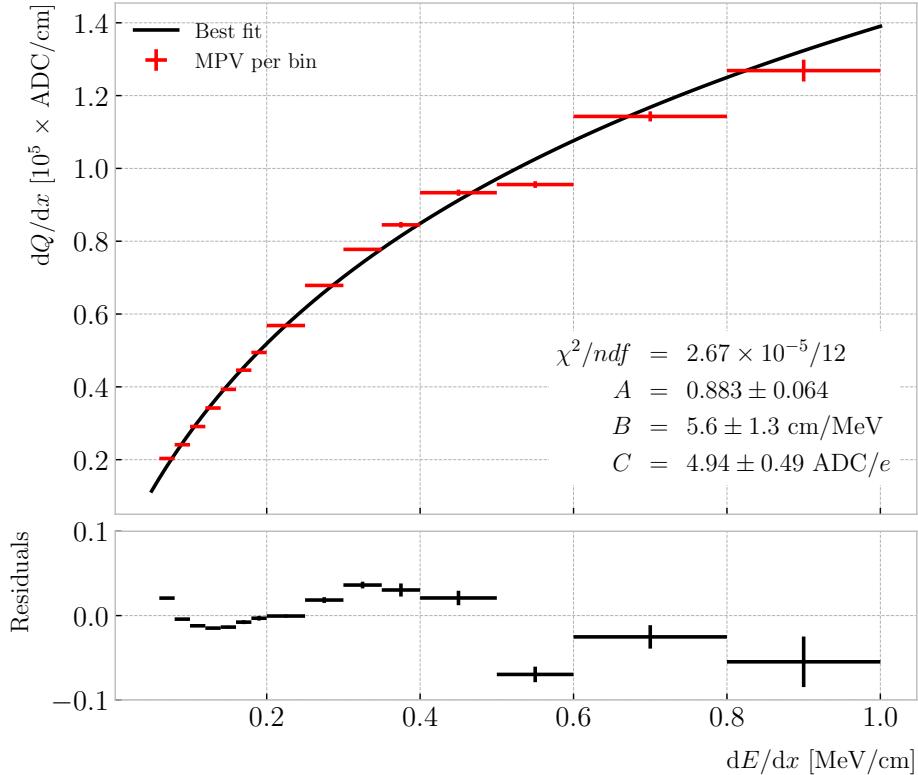


Figure 6.5: Fitted most probable dQ/dx values for each dE/dx bin (red points), obtained from the stopping proton sample. The overlaid curve (black line) represents the best fit to the logarithmic calibration function from Eq. (6.5).

which is quoted in the literature as the Bragg-Kleeman formula. In order to obtain the p and Λ parameters I perform a fit using the energy losses and the residual ranges given by the Geant4 stage of our proton sample.

Within our simulation, the residual range is sampled with a maximum size of 5 mm. Therefore, to perform the fit to the Bragg-Kleeman formula, we can use a fine-grained residual range binning. For each of the residual range bins I extract the dE/dx distribution and fit it to a LanGauss distribution, to obtain the value of the most probable dE/dx in the bin together with a statistical uncertainty. I then fit Eq. (6.4) to these most probable values and the centres of the residual range bins. This procedure is depicted in Fig. 6.4, where I show the distribution of the energy loss per unit length versus the residual range, together with the most probable dE/dx values and their uncertainty in each bin (red points) and the curve with the best fit of the

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAr

2501 Bragg-Kleeman relation to those values (black line). The best fit is obtained for the
 2502 parameter values $p = 1.8192 \pm 0.0005$ and $\Lambda = 0.3497 \pm 0.0008 \text{ cm}/\text{MeV}^p$ ⁴.

2503 Having an analytical expression that relates the residual range to dE/dx , I can take
 2504 our reconstruction-level residual ranges from the stopping proton sample and compute
 2505 the most probable energy loss associated.

2506 In order to parametrise the charge saturation, we can use the following logarithmic
 2507 function inspired by the modified box model for recombination:

$$\frac{dE}{dx} = \frac{e^{\frac{dQ}{dx}B\frac{W_{ion}}{G_{group}C}} - A}{B}, \quad (6.5)$$

2508 where A and B are the calibration parameters we need to determine, W_{ion} is the average
 2509 energy to produce an electron-ion pair, G_{group} is the gain from the reclustering discussed
 2510 above and C is the calibration constant to convert number of electrons to ADC counts,
 2511 commonly refer to as gain (also to be obtained in the fit). In this case, I use a value
 2512 for the electron-ion production energy of $W_{ion} = 26.4 \text{ eV}$ [171]. This value, used in our
 2513 simulation as well, was measured for gaseous argon in normal conditions, and therefore
 2514 should be checked in the future to describe correctly the high-pressure argon-CH₄ mixture
 2515 of ND-GAr.

2516 For the calibration fit I follow a procedure similar to the previous one for Eq. (6.4).
 2517 Binning the dE/dx range, I fit a LanGauss distribution to the corresponding dQ/dx
 2518 distribution to obtain the most probable value. The resulting data points (red bars) are
 2519 shown in Fig. 6.5 (top panel), the horizontal error bars depict the width of the dE/dx
 2520 bin whereas the vertical bars represent the error associated to the most probable value
 2521 estimation. A fit to the logarithmic function in Eq. (6.5) is also shown (black line).
 2522 For this I weighted the data points using the inverse of their relative error, obtaining
 2523 a reduced chi-square value of $\chi^2/ndf = 2.22 \times 10^{-6}$. The best fit parameters I found
 2524 from this fit are $A = 0.883 \pm 0.064$, $B = 5.6 \pm 1.3 \text{ cm}/\text{MeV}$ and $C = 4.94 \pm 0.49 \text{ ADC}/e$.
 2525 Figure 6.5 (bottom panel) shows the residuals between the data points and the fit.

⁴These strange units for Λ come from dimensional analysis, just to keep the Bragg-Kleeman formula (6.4) consistent.

6.2. dE/dx MEASUREMENT IN THE TPC

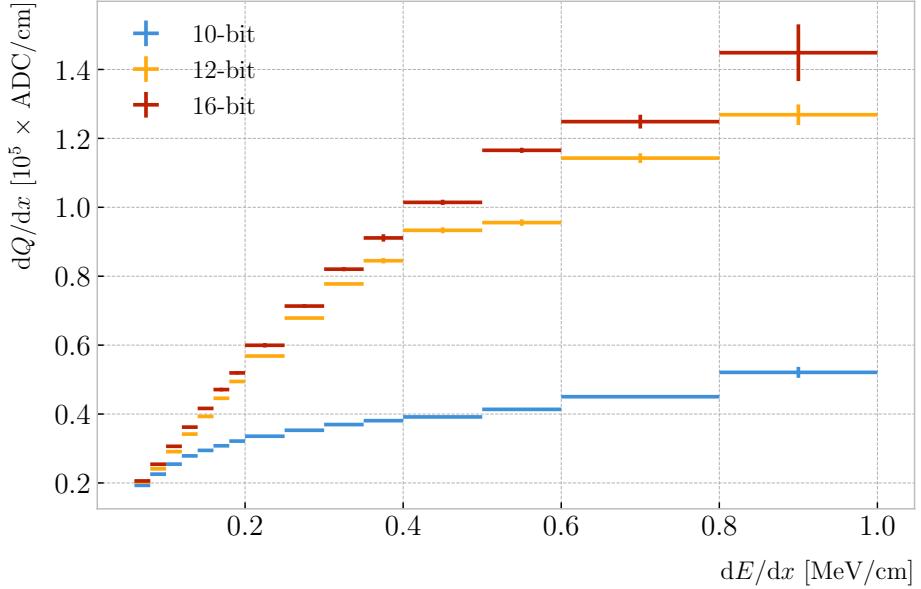


Figure 6.6: Fitted most probable dQ/dx values for each dE/dx bin for three different ADC bit limits, 10 (blue points), 12 (default, yellow points) and 16-bit (red points).

Table 6.1: Calibration parameters obtained from the fit of the ND-GAr simulated stopping proton sample to the calibration function from Eq. (6.5). The fits were performed for the 10, 12, and 16-bit ADC limits.

	χ^2/ndf	Best fit $\pm 1\sigma$		
		A	B (cm/MeV)	C (ADC/e)
10-bit	$1.83 \times 10^{-6}/12$	-9.3 ± 3.9	270 ± 69	27.1 ± 5.4
12-bit	$2.67 \times 10^{-5}/12$	0.883 ± 0.064	5.6 ± 1.3	4.94 ± 0.49
16-bit	$1.44 \times 10^{-5}/12$	0.949 ± 0.024	3.53 ± 0.58	4.52 ± 0.29

2526 The value for the gain I obtained from the fit is in reasonable agreement with our
 2527 expectation. This value is set in GArSoft to 5 ADC/e by default.

2528 One interesting thing to check is what induces this non-linear relation between charge
 2529 and energy. The only effects that modify the amount of electrons reaching the readout
 2530 planes in the simulation are the transverse diffusion and the finite electron lifetime.
 2531 Once the electrons reach the readout chambers, the pad response functions are applied,
 2532 together with an electrons-to-ADC conversion and the ADC saturation limit.

2533 By default, GArSoft applies a 12-bit ADC limit, which can be changed in the
 2534 simulation configuration. However, it can only be increased up to 16-bit, as we represent

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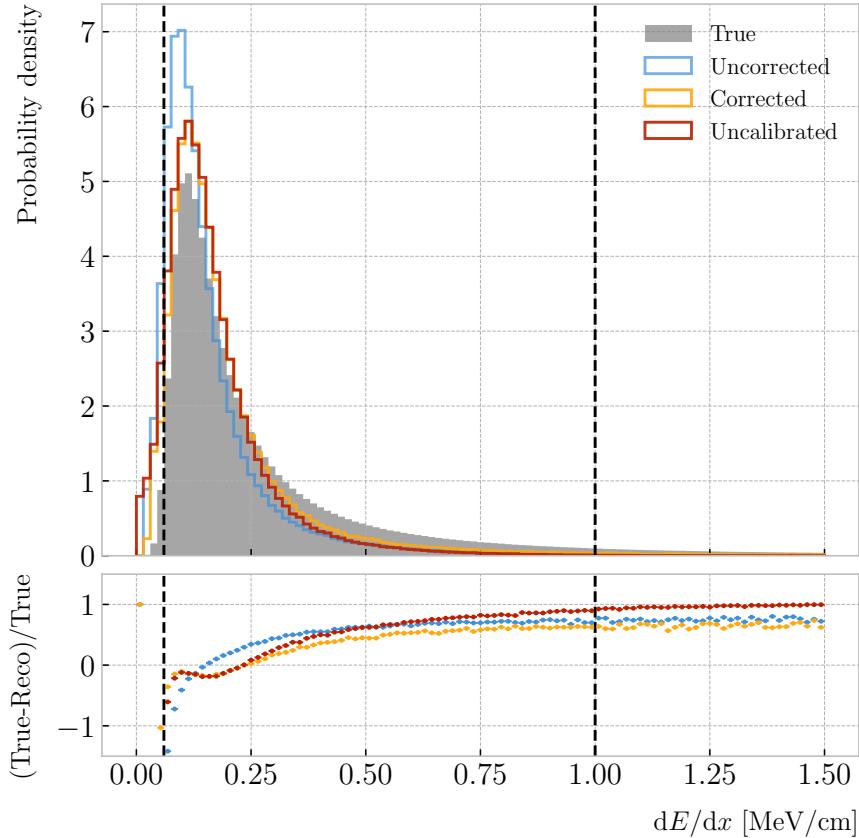


Figure 6.7: Top panel: area normalised dE/dx distributions for the true (solid grey) and the reconstructed energy deposits in the stopping proton sample, both after applying the calibration (blue) and the calibration and the normalisation correction (yellow). Also shown is the distribution obtained by applying a correction factor to the dQ/dx values but not the calibration (red). Bottom panel: fractional residuals for the uncorrected (blue), corrected (yellow) and uncalibrated (red) samples.

2535 the ADC collection as a `std::vector<short>`. This way, I tried to change the saturation
 2536 parameter to see how it affects the relation between reconstructed charge and energy.
 2537 Figure 6.6 shows a comparison between the most probable dQ/dx for 10, 12 and 16-
 2538 bit ADC limits. As expected, the lower the limit is the sooner the charge saturates.
 2539 For higher ADC limits the relation between energy and charge remains linear up to
 2540 higher dE/dx values, but even for the 16-bit limit the saturation is noticeable for values
 2541 $\gtrsim 0.5$ MeV/cm.

2542 Table 6.1 shows the results of fitting the samples with 10 and 16-bits ADC limits to
 2543 the calibration function from Eq. (6.5), using the weights based on their relative error

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as described previously. One interesting feature to notice is how different the best fit points look for the 10-bit ADC saturation when compared to the other two, which are consistent with each other.

At this point we can compare the dE/dx distribution one gets from Geant4, i.e. the true energy loss distribution, and the distribution I found by applying the calibration function to our collection of reconstructed dQ/dx values. Figure 6.7 (top panel) shows the true (solid grey) and reconstructed (blue, labeled as uncorrected) distributions together. The dashed vertical lines indicate the region of validity of the calibration fit, i.e. the left and right edges of the first and last dE/dx bin respectively. Notice that these histograms are area-normalised, as the total number of true energy deposits is much higher than the number of reconstructed charge deposits. This is due to a combination of effects, like the finite spatial resolution of the detector, the hit clustering used in the track fitting and the reclustering we have applied here.

The two distributions are significantly different. That can be seen clearly when looking at the fractional residuals, shown in Fig. 6.7 (bottom panel). In particular, the position of the peak is off, which could bias the mean energy loss predictions. It seems like the difference between these may be due to an overall scaling factor. One possibility is to scale the most probable value of the reconstructed distribution to the most probable value predicted by Geant4. I do this by fitting both distributions using a LanGauss function, obtaining $dE/dx_{MPV, true} = 0.1145 \pm 0.0005$ MeV/cm and $dE/dx_{MPV, reco} = 0.0928 \pm 0.0005$ MeV/cm for the true and reconstructed most probable values respectively. These can be translated into a scaling factor $S = 0.579 \pm 0.006$.

The result of applying the scaling correction can be seen in Fig. 6.7 (top panel). The corrected dE/dx distribution (yellow, labeled as corrected) peaks around the same value the true distribution does, as expected. Moreover, the high energy region is also slightly better described. For low ionisations, below the lower limit of the calibration fit, the differences between true and reconstructed are still significant. This low energy excess may be migration of some events from the peak region. The overall effect of the correction can be seen in the fractional residual plot in Fig. 6.7 (bottom panel).

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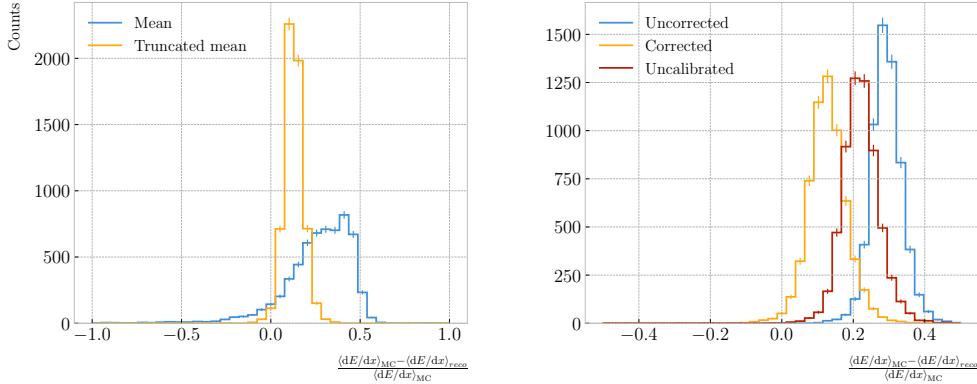


Figure 6.8: Left panel: fractional residuals between the true and the corrected dE/dx means (blue) and the 60% truncated means (yellow), for each event in the stopping proton sample. Right panel: fractional residuals between the true and the uncorrected (blue), corrected (yellow) and uncalibrated (red) dE/dx 60% truncated means, for each event in the stopping proton sample.

One can also check what happens if instead of applying the logarithmic calibration we simply scale the dQ/dx distribution (post reclustering) to have the same most probable value as the true dE/dx distribution. In this case, following an analogous procedure to the one described earlier, I found the scaling factor $S_{uncalibrated} = 0.414 \pm 0.002$ MeV/ADC⁵. The resulting distribution (red, labeled as uncalibrated) is also shown in Fig. 6.7 (top panel). The behaviour of the new distribution is similar to the corrected case at low energy losses, around the peak of the true distribution, but it is worse at describing the high energy tail. This is expected, it is in the high ionisation regime where saturation effects apply and therefore calibration is needed.

6.2.2 Truncated dE/dx mean

Once we have a collection of dE/dx values for each reconstructed track, we can compute the corresponding most probable ionisation loss per unit length of the particle. This is the value predicted by the Bethe-Bloch or the PAI models, and together with a measurement of the momentum it allows for particle identification.

However, estimating the most probable dE/dx value for each reconstructed track is not a trivial task. As mentioned before, the dE/dx distributions follow Landau-like

⁵Notice that now the scaling factor is not dimensionless, as it acts more like a conversion factor here.

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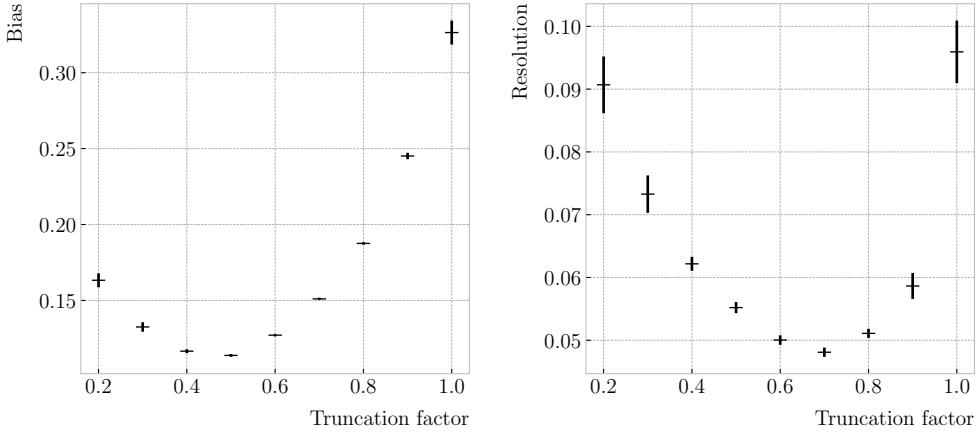


Figure 6.9: Estimated values of the mean dE/dx bias (left panel) and resolution (right panel) obtained using the corrected data from the stopping proton sample, for different values of the truncation factor.

2589 distributions. Therefore, one should perform e.g. a LanGauss fit to correctly estimate
 2590 the most probable values. Automating this kind of fits is often problematic, as they
 2591 usually incur in convergence problems. Moreover, the reconstructed dE/dx distributions
 2592 we obtain tend to have relatively small statistics, which may also produce poor fits. In
 2593 practice, doing these unsupervised fits may degrade our performance, and a more robust
 2594 method is preferred.

2595 A possibility could be taking the mean of the reconstructed dE/dx distribution for
 2596 each particle. The problem with this approach is that the high energy Landau tail,
 2597 combined with our limited statistics, can induce large fluctuations in the computation
 2598 of the mean. Imagine you have two protons with the same kinetic energy, but due to
 2599 reconstruction problems in one case you did not get as many charge deposits reconstructed
 2600 in its high ionisation loss region. If you do not remove the tails the computed dE/dx
 2601 means will be significantly different.

2602 In order to avoid those fluctuations, one can compute the mean of a truncated dE/dx
 2603 distribution instead. By keeping only a given fraction of the lowest energy deposits
 2604 we obtain an estimate of the mean energy loss that is more resilient to reconstruction
 2605 inefficiencies and statistical effects. Figure 6.8 (left panel) shows a comparison between
 2606 the $\langle dE/dx \rangle$ computed by taking the mean of the full distribution (blue line) and the

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2607 60% lowest energy clusters (yellow line), for the stopping proton sample. The fractional
 2608 residuals are computed for each proton, taking the corresponding means using their
 2609 collections of true and reconstructed energy deposits. One can see that using the simple
 2610 mean translates into a high bias and uncertainty in the $\langle dE/dx \rangle$ estimation, whereas
 2611 applying the truncation reduces both significantly.

2612 Additionally, I performed a comparison between the 60% truncated mean dE/dx
 2613 obtained using the different calibration methods discussed earlier, namely the uncorrected
 2614 (blue), corrected (yellow) and uncalibrated (red) distributions. The results are shown
 2615 in Fig. 6.8 (right panel). While the widths of these distributions are similar, the bias
 2616 obtained for the corrected sample, i.e. calibration function and correction factor applied,
 2617 is a factor of ~ 2 lower than in the uncalibrated case and almost three times smaller
 2618 than for the uncorrected sample.

2619 The next step is to optimise the level of truncation we are going to apply to our
 2620 data. To do so, I used different truncation factors, i.e. the percentage of energy-ordered
 2621 reconstructed energy deposits we keep to compute the mean, on the corrected dE/dx
 2622 sample of the stopping protons. Then, following the same procedure of computing the
 2623 fractional residuals as before, I fitted the resulting histograms using a double Gaussian
 2624 function. This is simply the sum of two Gaussian functions of the type:

$$g(x; \mu, \sigma, A) = A e^{-\frac{(x-\mu)^2}{2\sigma^2}}. \quad (6.6)$$

2625 I do not add the classical normalisation factor of the Gaussian, $1/\sqrt{2\pi}\sigma$, therefore
 2626 the amplitude A simply represents the maximum of the function. One of the two
 2627 Gaussian functions describes the core part of the distribution, while the other captures
 2628 the behaviour of the tails.

2629 For each truncation factor, I look at the bias and the resolution I obtain. I define
 2630 these as the weighted means of the corresponding parameters in the fits:

$$\bar{x} = \frac{A_{core} x_{core} + A_{tail} x_{tail}}{A_{core} + A_{tail}}, \quad (6.7)$$

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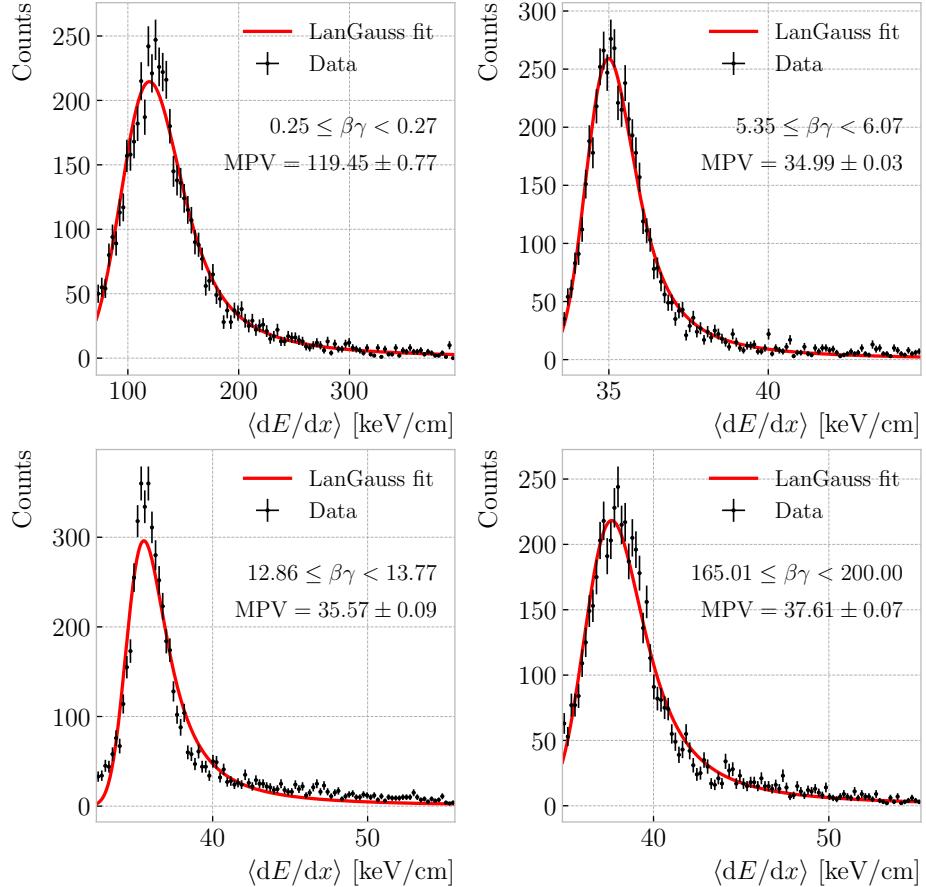


Figure 6.10: Examples of the truncated mean dE/dx LanGauss fits for various $\beta\gamma$ bins, from a simulated FHC neutrino sample.

2631 where A_{core} and A_{tail} are the amplitudes of the core and tail distributions respectively
 2632 and x is either the mean μ or the width σ of said distributions.

2633 Figure 6.9 shows the bias (left panel) and the resolution (right panel) I obtained
 2634 for the stopping proton sample, using different values of the truncation. From these, it
 2635 can be seen that a truncation factor of 50% minimises the bias in the estimation, while
 2636 70% gives the best resolution. That way, I settled on the intermediate value of 60%
 2637 truncation, which yields a $\langle dE/dx \rangle$ resolution of 5.00 ± 0.08 % for stopping protons.

2638 6.2.3 Mean dE/dx parametrisation

2639 Now that we have a way to estimate the mean energy loss of a particle in the HPgTPC,
 2640 we can determine the value of the free parameters in the ALEPH formula, Eq. (6.3).

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2641 For this, I used a sample of 10^5 reconstructed FHC neutrino events inside ND-GAr. In
2642 this case I cannot use the stopping proton sample, as we need to cover the full kinematic
2643 range of interest for the neutrino interactions in our detector.

2644 The original data does not contain an estimation of the velocity of the tracks, instead
2645 the tracks have a value for the reconstructed momentum and the associated PDG code
2646 of the Geant4-level particle that created the track. Therefore, one can select some of the
2647 particles in the data, in this case I selected electrons, muons, pions and protons, and
2648 compute β and γ using the reconstructed momentum and their mass. In terms of $\beta\gamma$
2649 the mean dE/dx does not depend on the particle species, so one can consider all the
2650 dataset as a whole. For this fit, I will express β in terms of the $\beta\gamma$ product as:

$$\beta = \frac{\beta\gamma}{\sqrt{1 + (\beta\gamma)^2}}, \quad (6.8)$$

2651 which can be easily proven from the definition of γ .

2652 Next, I bin the data in $\beta\gamma$. I chose a fine binning so as to capture the different
2653 features of the ionisation curve. Instead of fixing the bin width, I select them so each one
2654 has approximately the same statistics. Then, for each $\beta\gamma$ slice, I compute the median
2655 and the interquartile range (IQR) of the $\langle dE/dx \rangle$ distribution. Using these, I make a
2656 histogram in the range [median - IQR, median + 5 IQR], which I fit to a LanGauss
2657 function in order to extract the MPV. Using this range accounts for the asymmetric
2658 nature of the distributions, while also helps avoiding a second, lower maximum present
2659 at low $\beta\gamma$, probably a result of reconstruction failures.

2660 A few examples of these fits are shown in Fig. 6.10. The chosen values of $\beta\gamma$ sit in
2661 very distinct points along the $\langle dE/dx \rangle$ curve, going from the high ionisation region at
2662 low velocities (top left panel), to the minimum point (top right panel), the beginning of
2663 the relativistic rise (bottom left panel), and the plateau produced by the density effect
2664 (bottom right panel).

2665 I used the resulting most probable $\langle dE/dx \rangle$ values and the centres of the $\beta\gamma$ bins as
2666 the points to fit to the ALEPH formula. For this particular fit I used the least-squares

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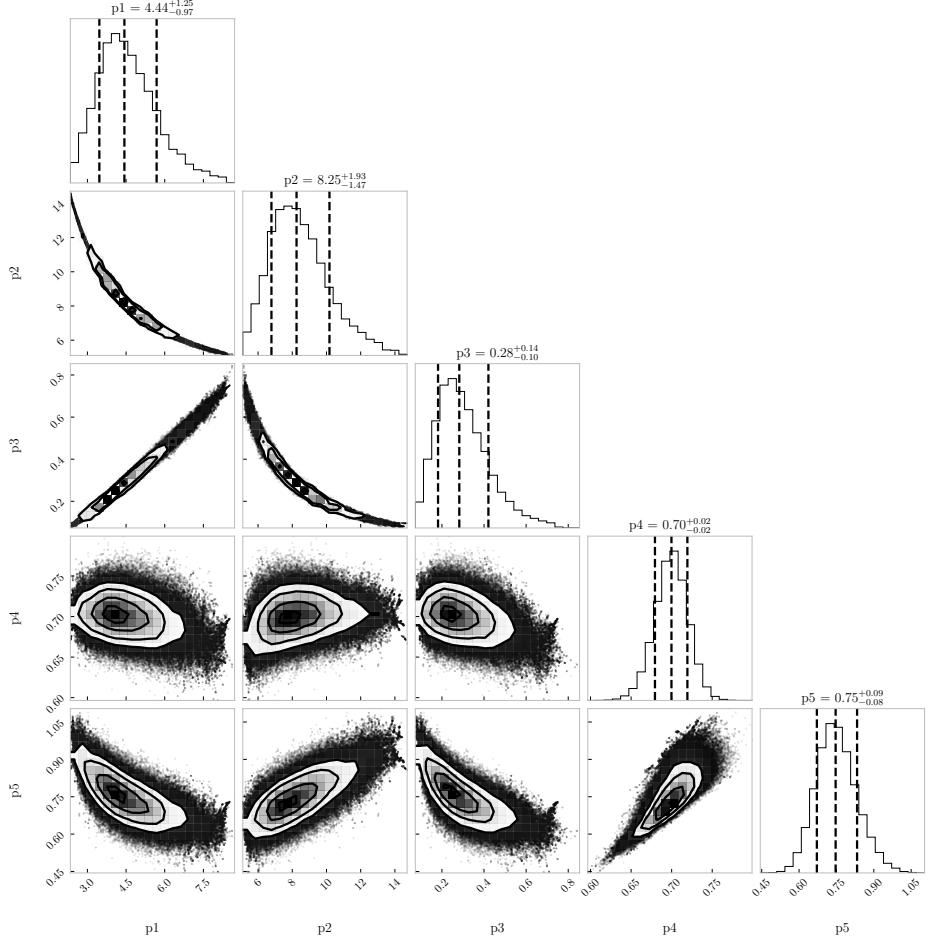


Figure 6.11: Resulting one and two dimensional projections of the posterior probability distributions of the ALEPH $\langle dE/dx \rangle$ parameters obtained by fitting the 60% truncated mean dE/dx values from a FHC neutrino sample in ND-GAr. The vertical dashed lines in the 1D distributions represent the 16th, 50th and 84th percentiles.

method to get a first estimation of the ALEPH parameters. Applying some uniform priors, I then used these values as the starting point of a 100000 steps MCMC. Figure 6.11 shows the posterior probability distributions I obtain for each parameter. The reported best fit points are based on the 16th, 50th, and 84th percentiles in the marginalised distributions.

The resulting fit (black line), compared to the data points (red points) and the underlying distribution is shown in Fig. 6.12 (top panel). The overall fit is good, with a reduced chi-squared of $\chi^2/ndf = 1.02$. However, there are some regions where the fit does not describe the data correctly, like the very low $\beta\gamma$ regime, where the fit severely

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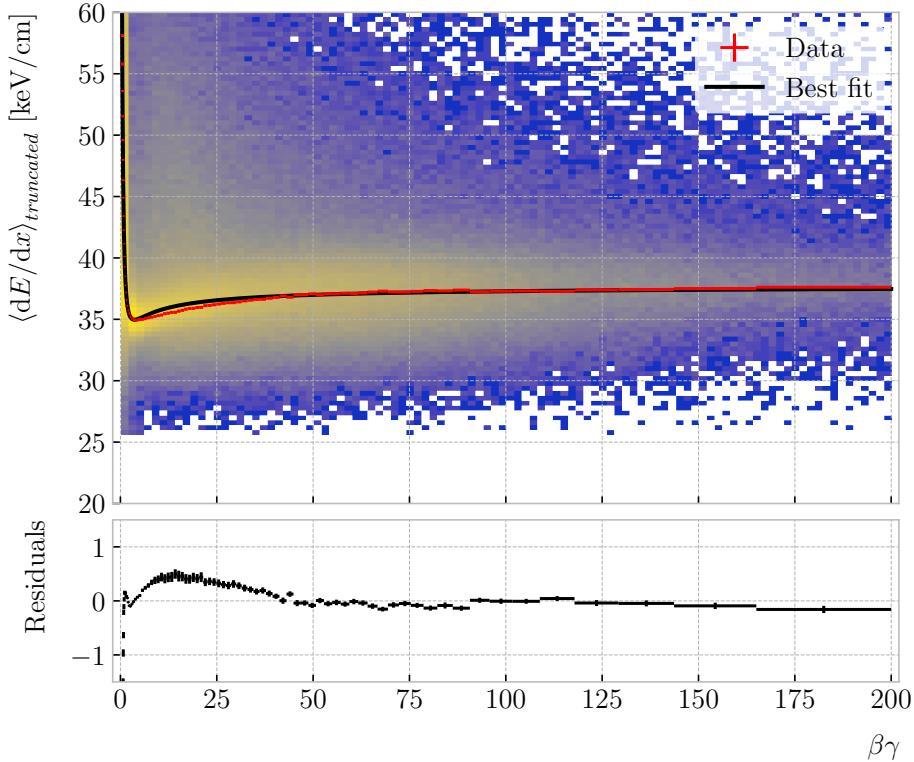


Figure 6.12: Truncated mean dE/dx obtained for the FHC neutrino sample as a function of the $\beta\gamma$ product (upper panel). Also shown are the fitted most probable values for each $\beta\gamma$ bin (red points) and the best fit obtained using the ALEPH parametrisation (black line). The residuals resulting from the fit are shown in the lower panel.

underestimates for energy losses $\gtrsim 50$ keV/cm, and the start of the relativistic raise, where we have a slight overestimation. This is a result of those points having a larger uncertainty when compared to the ones around the dip or the plateau areas. These differences can be better seen in the residual plot, Fig. 6.12 (bottom panel).

It is interesting to look at the results of the fit in momentum space, for the different particle species. Figure 6.13 shows the truncated mean dE/dx values versus the reconstructed momentum for the neutrino sample. Using a logarithmic scale for the momentum helps visualising the curves corresponding to the various particles. The resulting fits for electrons, muons, pions and protons are also shown (solid black lines). Notice that each curve stops at different momentum values, as the fits only extend up to $\beta\gamma = 200$ and translating this limit into momentum depends on the particle.

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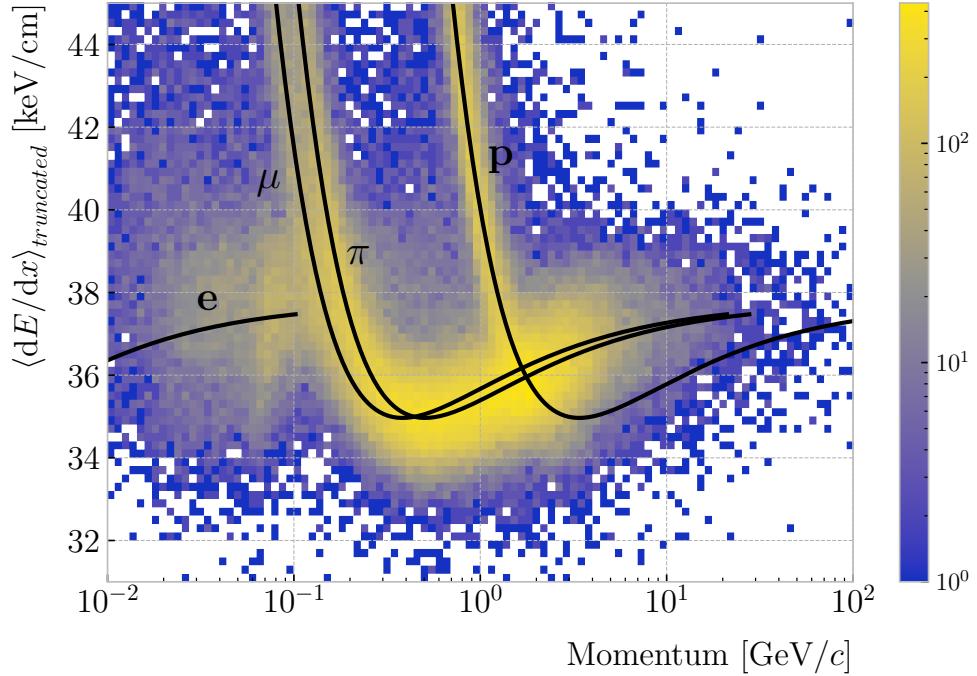


Figure 6.13: Distribution of the 60% truncated mean $\langle dE/dx \rangle$ versus reconstructed momentum for the FHC neutrino sample. The black lines indicate the predictions of the ALEPH parametrisation for electrons, muons, charged pions and protons.

From this plot, the particle separation power of the $\langle dE/dx \rangle$ measurement is evident.

In the low momentum regime separating electrons, muons and pions is possible, while protons can be reliably identified up to $1.5 \text{ GeV}/c$.

Relevant to the separating power is the $\langle dE/dx \rangle$ resolution. This can be obtained from the fit, by taking the ratio of the difference between the expected energy loss for a given particle type and momentum and the measured value over the expectation. Then, performing a double Gaussian fit we can extract the bias and the resolution by means of Eq. (6.7). Figure 6.14 presents the values of the $\langle dE/dx \rangle$ bias (left panel) and resolution (right panel) as a function of the momentum for the true protons in the neutrino sample.

When compared to the values for the resolution obtained for the stopping proton sample (see e.g. Fig. 6.9), it appears that the performance now is much lower. For that low energy sample the resolution obtained was 5%, whereas now we only achieve those numbers for momenta $\geq 0.75 \text{ GeV}/c$. However, there are several differences between these two cases. The former was obtained for a single proton sample, with tracks are fully

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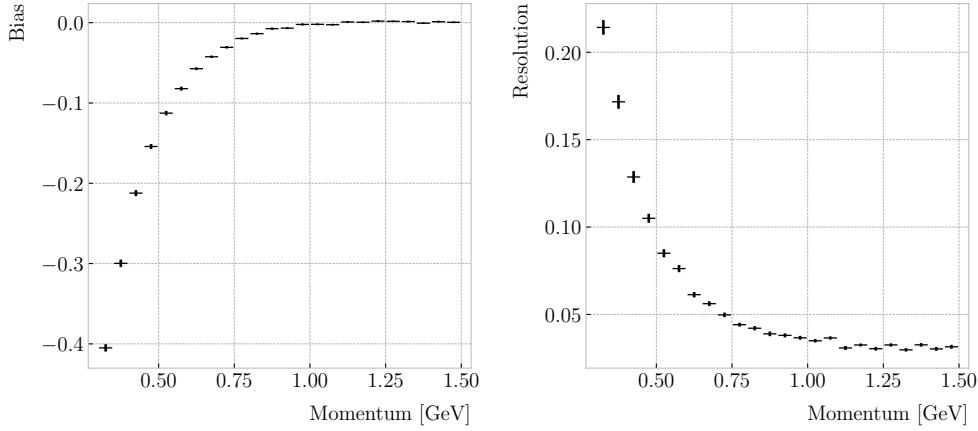


Figure 6.14: Estimated values of the mean dE/dx bias (left panel) and resolution (right panel) obtained for the true protons in the FHC neutrino sample.

2701 contained in the detector volume. On top of that, I refined the selection requiring a single
 2702 reconstructed track per event, which eliminates any misreconstruction effects. In this
 2703 case, we are dealing with tracks that may have fragmented, or even have contributions
 2704 from different true particles. Also, note that at low energies the $\langle dE/dx \rangle$ for protons is
 2705 much higher than it is for other particles. Therefore, having a poor resolution in that
 2706 range does not have an impact on the proton separation.

2707 6.3 Muon and pion separation in the ECal and MuID

2708 As it could be seen from Fig. 6.13, it is not possible to separate muons and charged pions
 2709 in the HPgTPC using dE/dx for momenta $\gtrsim 300$ MeV/ c . In ND-GAr, approximately
 2710 70% of the interactions in FHC mode will be ν_μ CC (compared to the 47% of $\bar{\nu}_\mu$ CC
 2711 interactions when operating in RHC mode), while 24% are neutral currents. Out of
 2712 these, around 53% and 47% of them will produce at least one charged pion in the final
 2713 state, respectively. Figure 6.15 shows a comparison between the spectra of the primary
 2714 muons and the charged pions for ν_μ CC interactions in ND-GAr producing one or more
 2715 charged pions. From this, one can see that (i) the majority of muons and charged pions
 2716 are not going to be distinguishable with a $\langle dE/dx \rangle$ measurement, and that (ii) particle
 2717 identification is necessary both to classify correctly the ν_μ CC events and identify the

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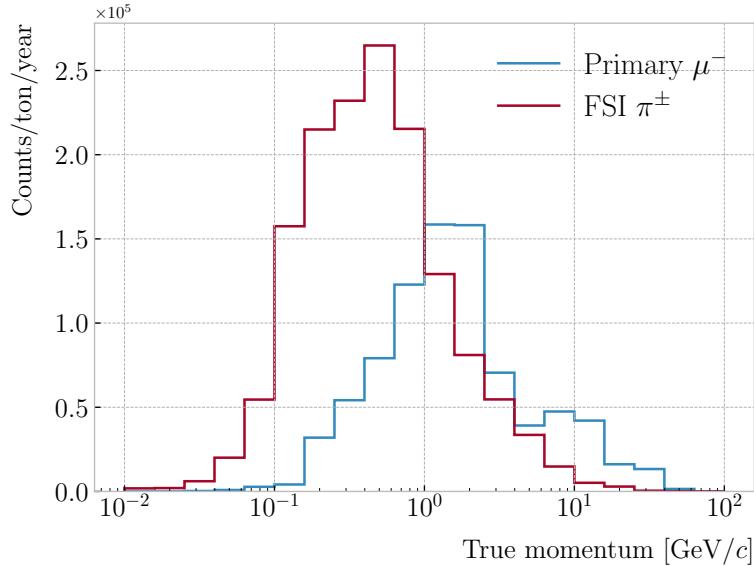


Figure 6.15: True momentum distribution for the primary muon in ν_μ CC $N\pi^\pm$ interactions inside the fiducial volume of ND-GAr (blue line), compared to the post FSI charged pion spectrum (red line).

2718 primary muon within them.

2719 ND-GAr features two other subdetectors which can provide additional information
 2720 for this task, namely the ECal and MuID. The current ECal design, described in (ref
 2721 section), consists of 42 layers, made of 5 mm of Pb, 7 mm of plastic scintillator and a
 2722 1 mm PCB board. The total thickness of this calorimeter is 1.66 nuclear interaction
 2723 lengths or 1.39 pion interaction lengths. The MuID design is in a more conceptual
 2724 stage, however it is envisioned to feature layers with 10 cm of Fe and 2 cm of plastic
 2725 scintillator⁶. With its three layers, it will have a thickness of 1.87 or 1.53 nuclear or pion
 2726 interaction lengths, respectively.

2727 Because pion showers are dominated by inelastic nuclear interactions, the signatures
 2728 of these particles in the calorimeter will look significantly different from those of muons.
 2729 Although our ECal is not thick enough to fully contain the hadronic showers of the
 2730 charged pions at their typical energies in FHC neutrino interactions, they can still be
 2731 used to understand whether the original particle was more hadron-like or MIP-like. In

⁶It is not mentioned anywhere, but I assume that there should also be another layer of PCB board of 1 mm. However, in this case its contribution to the total thickness of the sampling calorimeter would be negligible.

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2732 Fig. 6.16 I show two examples of energy distributions created by a muon (left panel)
2733 and a charged pion (right panel) of similar momenta interacting in the ECal. These
2734 figures represent the transverse development of the interactions. For each of them, I
2735 computed the principal component and centre of mass of the interaction, projecting
2736 the position of the hits onto the plane perpendicular to that direction, and taking the
2737 distances relative to the centre. It can be seen that the muon follows an almost MIP-like
2738 behaviour, being the central bin in the histogram the one with the highest deposited
2739 energy. On the other hand, the pion not only deposits more energy overall, but also this
2740 energy is more spread-out among the different hits. It is this kind of information that
2741 would allow us to tell apart muons from pions.

2742 This way, I identify three main action points that need to be addressed if one wants
2743 to use these detectors to distinguish between muons and charged pions. These are:

- 2744 1. the way we make the associations between tracks in the HPgTPC to the activities
2745 (what in GArSoft we call clusters) in the ECal and the MuID,
- 2746 2. what variables or features one can extract from the calorimeters that encapsulate
2747 the information we are interested about,
- 2748 3. and how to carry out the classification problem.

2749 6.3.1 Track-ECal matching

2750 One of the main players in the muon and pion separation is the way we associate clusters
2751 in the ECal to reconstructed tracks in the TPC. Missing some associations or making
2752 wrong ones can bias the ECal quantities that we can use for classifying particles. The
2753 current algorithm in GArSoft provides precise associations, i.e. most of the associations
2754 that it produces are correct, but it appears to miss an important number of associations
2755 (at least when using the default configuration).

2756 The current TPC track-ECal cluster association algorithm is divided in four parts.
2757 It first checks whether the track end point fulfils certain conditions to be extrapolated.
2758 There are two cut values in this step, one for the drift direction and other radial.

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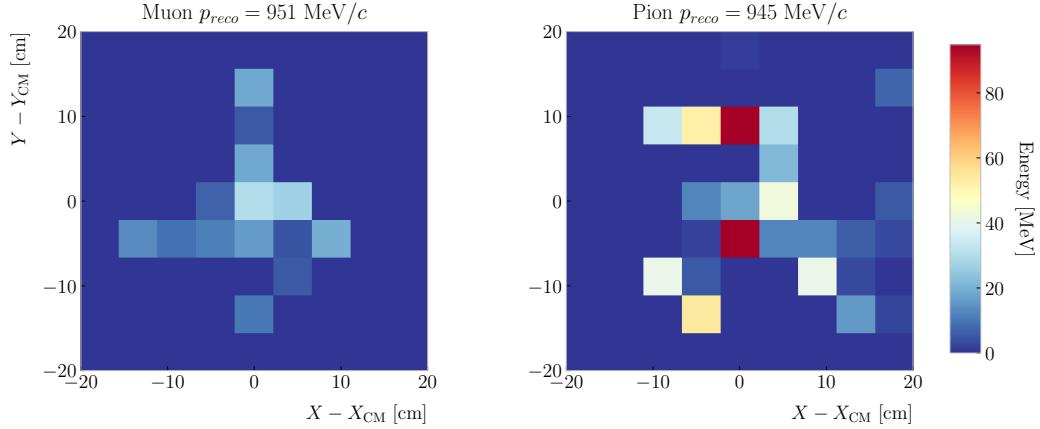


Figure 6.16: Distributions of energy deposits in the ECal for a muon (left panel) and a charged pion (right panel) with similar momenta. The energy is projected onto the plane perpendicular to the principal component of the hits, and the positions are relative to the center of the interaction.

If the point can be extrapolated, the code computes the coordinates of the centre of curvature using the Kalman fit estimates at the track end (y , z , $1/R$, ϕ , $\tan\lambda$). It then compares the distance between this and the cluster in the (z, y) plane with R . This introduces another cut in the perpendicular direction.

The next step is different for clusters in the barrel or in one of the end caps. If it is a barrel cluster the algorithm extrapolates the track up to the radial distance of the cluster. There are three possible outcomes, the extrapolated helix can cut the cylinder of radius r_{clus} two, one or zero times. I get the cut point that is closer to the cluster and check that it is either in the barrel or the end caps. Computing the difference between the x coordinates of the cluster and the extrapolated point, the module checks that this is not greater than a certain cut. If the cluster is in an end cap, I propagate the track up to the x position of the cluster. Then, the algorithm computes the angle in the (z, y) plane between the centre of curvature and the cluster, α , and the centre of curvature and the propagated point, α' . A cut is applied to the quantity $(\alpha - \alpha')R$.

If the cluster contains more than a certain number N of hits, I apply an extra cut to the dot product of the direction of the track at the propagated x value and the cluster direction.

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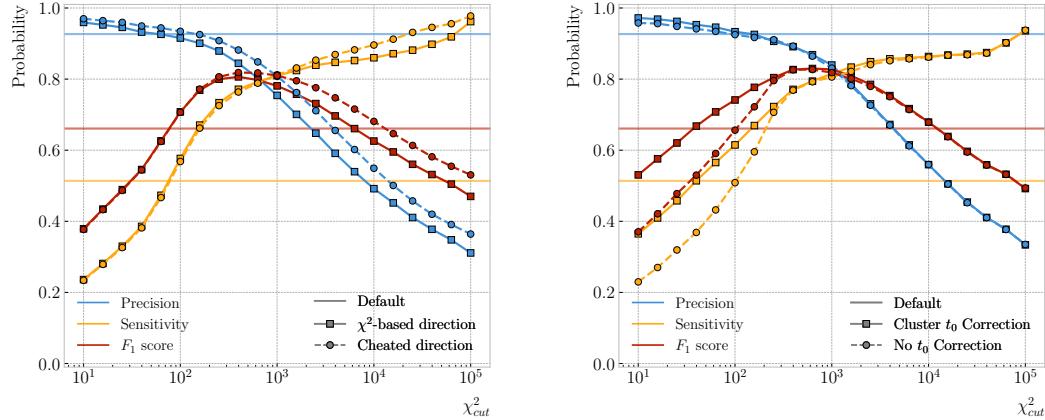


Figure 6.17: Left panel: comparison between the precision (blue), sensitivity (yellow) and F_1 score (red) obtained for the default (horizontal lines) and new algorithms, both with the χ^2 -based direction estimator (squares) and cheating the directions (circles), for different values of the χ^2 cut. Right panel: comparison of the performance of the new algorithm when applying the cluster t_0 correction (squares) and when (circles).

2776 The code makes sure to only associate one end of the track (if any) to a cluster.
2777 However, it can associate more than one track to the same cluster. This makes sense,
2778 as different particles can contribute to the same cluster in the ECal, but it makes it
2779 difficult to quantify the relative contributions of the tracks to a certain cluster.

2780 As a way of comparing the performance of this algorithm, a new, simpler association
2781 module was written. The goal was to have a simple and robust algorithm, which depends
2782 on as few parameters as possible and that can produce a one-to-one matching between
2783 tracks and ECal clusters.

2784 For each reconstructed track, the new algorithms applies the same procedure to the
2785 forward and the backward fits irrespective of their end point positions. It first gets the
2786 Kalman fit parameters at the corresponding end point together with the X position, x_0 ,
2787 $(y_0, z_0, 1/R, \phi_0, \tan\lambda)$.

2788 For each ECal cluster, I compute the radial distance to the centre of the TPC and
2789 find the ϕ value in the range $[\phi_0, \phi_0 + \text{sign}(R)\phi_{max}]$ that makes the propagated helix
2790 intersect with the circle defined with such radius. The (x, y, z) position of the helix for
2791 the ϕ value found (if any) is then computed. In case there are two intersections, I keep
2792 the one that minimises the distance between (y, z) and (y_c, z_c) .

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2793 I then calculate χ^2 value based on the Euclidean distance between the propagated
2794 point and the cluster:

$$\chi^2/ndf = \frac{\sum_{n=0}^2 (x^{(n)} - x_c^{(n)})^2}{3}. \quad (6.9)$$

2795 If there was no intersection I store a -1 instead. In the end, for each reconstructed track
2796 in the event one ends up with two collections of χ^2 values, one for each ECal cluster
2797 and fit directions.

2798 The current code only supports having ECal clusters associated to one end of each
2799 track. We have two options to decide what track end to keep. The first one tries to
2800 cheat the selection, looking at the distance between the two track ends and the true
2801 start position of the associated MC particle. The second one keeps the track end with
2802 more χ^2 entries below the cut.

2803 This feature of only considering one track end limits the algorithm, making it not
2804 suitable for reconstructing events with particles originating outside the TPC. However,
2805 as for the moment the main concern of the group is the study of neutrino interactions
2806 off the gaseous argon, this is an acceptable assumption.

2807 In order to associate a cluster to a track, I take all clusters with a χ^2 value in the
2808 range $[0, \chi_{cut}^2]$. If a cluster has been assigned to more than one track we leave it with
2809 the one with the lowest χ^2 .

2810 This default behaviour of the algorithm can be modified to associate more than one
2811 track to each cluster. Not only that, but the χ^2 values can be used to assign relative
2812 weights to the different contributions.

2813 To evaluate the performance of the association method, I use a binary classification
2814 approach. In this case, I check the leading MC Track IDs associated to the reconstructed
2815 tracks and ECal clusters. I count an association as true positive (TP) if both Track
2816 IDs coincide. An association is considered false positive (FP) when the Track IDs are
2817 different. If a cluster has not been associated to any track but it shares the Track ID
2818 with a reconstructed track it is counted as a false negative (FN).

2819 For the testing, I used a sample of 10000 FHC neutrino events inside the HPgTPC.

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAr

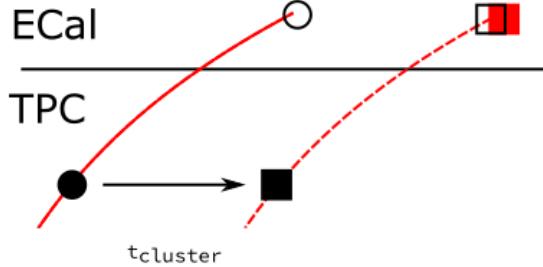


Figure 6.18: Schematics of a possible option to deal with track-ECal associations in non-zero t_0 neutrino interaction events, trying to correct for the drift direction uncertainty in a cluster-by-cluster basis using the cluster time, $t_{cluster}$.

2820 Figure 6.17 (left panel) shows the precision (blue line), sensitivity (yellow line), and F_1
 2821 score (red line) I obtained for different values of χ^2_{cut} . For comparison, the same metrics
 2822 computed for the default algorithm with the current configuration are also shown (dashed
 2823 lines). In the case of the new algorithm, I used both the χ^2 -based method to estimate
 2824 the track direction described earlier (square markers) and the cheated direction from the
 2825 Geant-level information (circle markers). For either of these we achieve similar values of
 2826 the precision compared to the old code, while having a considerably higher sensitivity.
 2827 It can be seen that cheating the direction of the tracks only makes a difference at high
 2828 χ^2_{cut} , past the optimal value of the cut around the F_1 score maximum. Therefore, I set
 2829 the χ^2 method as the default.

2830 One of the possible weak points of this approach is that it relies on the position along
 2831 the drift direction to make the decisions. Within the current ND-GAr design implemented
 2832 in GArSoft, the timing information is provided by the ECal. That effectively means
 2833 that prior to make the track-ECal associations the reconstructed x positions of the track
 2834 trajectories differ from the simulated ones by an amount:

$$x_{reco}^{(n)} - x_{sim}^{(n)} = v_{drift} t_0, \quad (6.10)$$

2835 where v_{drift} is the mean drift velocity in our medium and the initial time is in the range
 2836 $t_0 \in [0, t_{spill}]$ where t_{spill} is the spill length. For a $10 \mu\text{s}$ spill this translates into a
 2837 maximum 30 cm uncertainty on the drift direction position.

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2838 The current default in GArSoft sets $t_0 = 0$, but the functionality to randomly sample
2839 this within the spill time is in place. Therefore, we need to understand what is the impact
2840 of a non-zero t_0 on the associations algorithm and foresee possible ways of minimising a
2841 loss in performance.

2842 Figure 6.18 represents a possible option to tackle the association problem when
2843 having events with a non-zero initial time t_0 . The black and white circles represent the
2844 original points, whereas the squares indicate the corrected positions. The end points of
2845 the track and the propagated points up to the cluster radius are indicated using filled
2846 and unfilled markers respectively. The red square represents the position of the cluster.

2847 Here I try to correct for the drift coordinate position using the time associated to the
2848 cluster. Assuming that the drift time is much larger than the propagation time, $t_{cluster}$
2849 could be used as a good estimation of the t_0 . An alternative can be using the earliest
2850 time associated to a hit in said cluster. Doing this for each cluster before computing
2851 the χ^2 value could be used as an alternative to knowing the specific value of the t_0 , as
2852 when the association is correct this will provide the right correction but its impact is
2853 small enough to not change the position significantly in the case the cluster does not
2854 correspond to a given track.

2855 I tested the effect of this correction again using a sample of 10000 FHC neutrino
2856 events. Figure 6.17 (right panel) shows the precision (blue line), sensitivity (yellow line),
2857 and F_1 score (red line) for the case the cluster t_0 correction is applied (square markers)
2858 and for the no correction case (circle markers), as a function of χ^2_{cut} . In this case, the
2859 differences are particularly notorious at low values of the cut. It makes sense, as the t_0
2860 effect becomes subdominant when the distance we consider grows large. Overall, the
2861 correction increases the sensitivity while keeping the precision almost unchanged. As a
2862 result, I apply the t_0 correction to the generated samples as the default.

2863 6.3.2 Classification strategy

2864 The problem of the muon and charged pion separation has to be viewed in the broader
2865 context of the particle identification in our detector. Focusing on the beam neutrino

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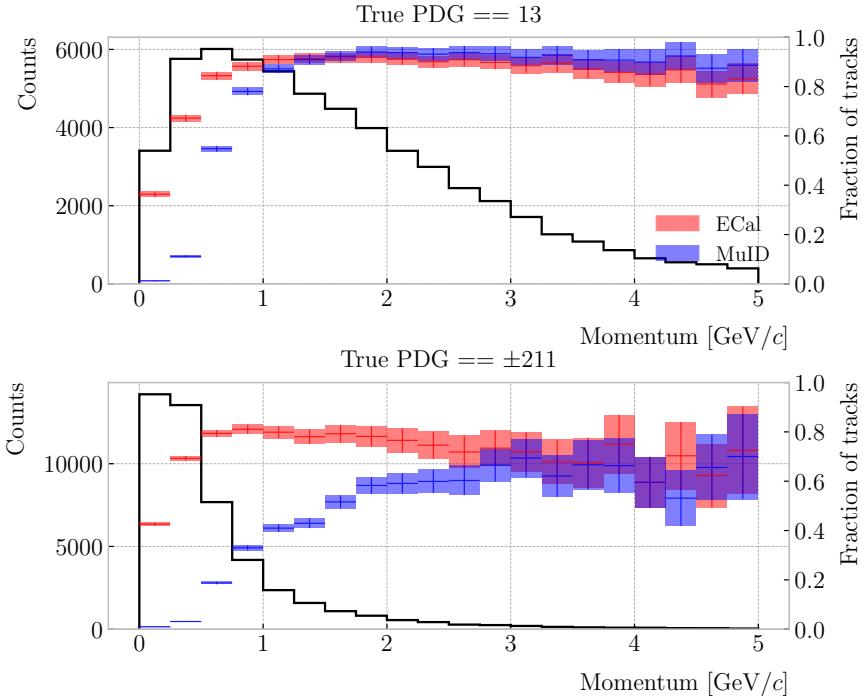


Figure 6.19: Momentum distribution for the reconstructed muons (top panel) and charged pions (bottom panel) in a FHC neutrino sample, together with the fraction of them reaching the ECal (red) and MuID (blue). Each entry corresponds to a reconstructed track, backtracked to a true muon or pion which has not produced any other reconstructed track.

interactions, it is clear that we are going to have muons and pions spanning a broad momentum range. Not only that, but we will also have other particles with similar characteristics that will make the classification even more challenging. Therefore, we are presented with a task that will depend heavily on the kinematic range we are looking at each time, as both the available information and the possible impurities of other particle species vary.

For instance, distinguishing muons from pions could be difficult at low momenta, as a great number of them do not reach the ECal. Therefore, we could think of tailoring a version of the classification for that particular case, which could be complemented with a dE/dx measurement. Likewise, for momenta $\gtrsim 1$ GeV muons and pions reach the calorimeters efficiently, but so do protons. Because of this, one can try to train another classifier for this energy range, and rely on other methods to remove as many of the

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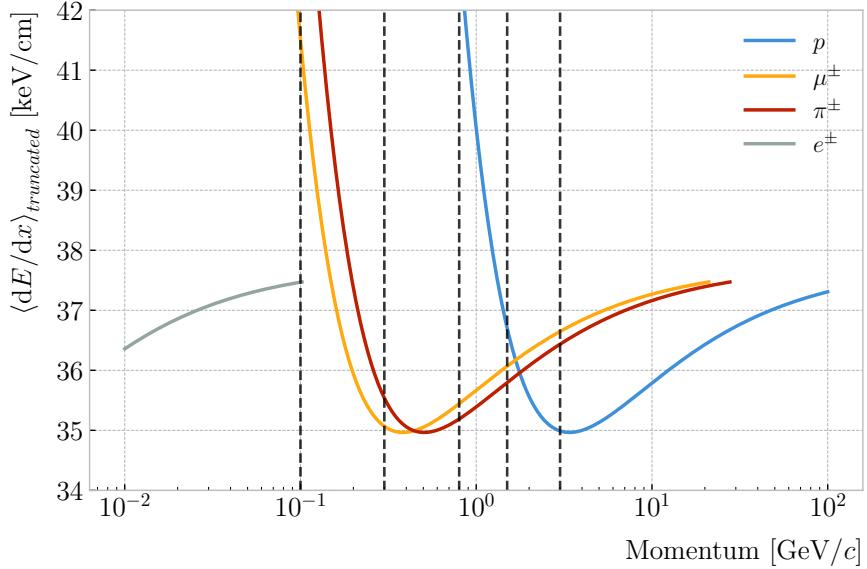


Figure 6.20: Predicted truncated mean dE/dx versus momentum, for electrons, muons, charged pions and protons, obtained using the ALEPH parametrisation. The vertical dashed lines represent the boundaries of the six regions used for the muon and pion classification training.

2878 protons as possible.

2879 Figure 6.19 shows the momentum distribution of the reconstructed muons (top) and
 2880 pions (bottom) in a FHC sample. It also contains the fraction of particles reaching the
 2881 ECal (red) and MuID (blue), for the different momentum bins. In Fig. 6.20 I show the
 2882 mean dE/dx of different particles as a function of the momentum, computed using the
 2883 ALEPH parametrisation with the best fit parameters found in Subsec. 6.2.2.

2884 Using these two figures as references, I decided to approach the classification by
 2885 dividing the problem into six different momentum regions. A summary of these can be
 2886 found in Tab. 6.2. The basic idea is to exploit all the information that is available in
 2887 each region and . For the problem at hand, I prepared separated samples of isotropic
 2888 single muons and pions, with momenta uniformly distributed along the corresponding
 2889 momentum range. Each sample contains 50000 events of the corresponding particle
 2890 species. I did not generate samples for the first region, as it is assumed that the separation
 2891 can be achieved using dE/dx only. For the last region, I generated particles up to a
 2892 momentum of 10 GeV/c , as that is well above the typical energies of muons and pions

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Table 6.2: Momentum ranges and description of the PID approach assumed for the muon and pion classification task.

Momentum range	Description
< 0.1 GeV/c	All tracks can be separated with dE/dx
[0.1, 0.3) GeV/c	Use ECal for reaching muons and pions, dE/dx for the rest
[0.3, 0.8) GeV/c	Use ECal for muons and pions, dE/dx for protons
[0.8, 1.5) GeV/c	Use ECal and MuID for muons and pions, dE/dx for protons
[1.5, 3.0) GeV/c	Use ECal and MuID for muons and pions, ToF for protons
≥ 3.0 GeV/c	Use ECal and MuID for muons and pions, dE/dx and ToF for protons

2893 from FHC neutrino interactions in ND-GAr.

2894 Additionally, I prepared another sample of 100000 FHC neutrino events. For each
 2895 interaction, I select the reconstructed particles which were backtracked to true muons or
 2896 charged pions. I use this dataset to perform validation checks, to see how the models
 2897 trained with the single particle data generalise to a more realistic scenario.

2898 To tackle this classification problem, I make use of Boosted Decision Trees (BDT). A
 2899 decision tree uses a flowchart-like structure to make decisions based on some input data.
 2900 It starts from a root node, which represents the complete dataset, and then it splits
 2901 this based on the variable or feature which gives the best separation between classes,
 2902 creating two new nodes. The process repeats for each node until it reaches a certain
 2903 limit, like a maximum number of splits or some tolerance criteria. The last set of nodes
 2904 are often called leave nodes, and represent the final prediction of the classifier.

2905 Boosting refers to a family of methods to combine the predictions from multiple
 2906 classifiers, following a sequential approach where each new model learns from the errors
 2907 of the previous one. The process starts with a simple decision tree, which is used to
 2908 make predictions on the training data. Then, the data points misclassified by the first
 2909 model are assigned higher weights, and another decision tree is trained on the data with
 2910 adjusted weights. The predictions of the two trees are then combined, and the cycle
 2911 repeats for a predefined number of iterations. Gradient boosting uses the direction of
 2912 the steepest error descent to guide the learning process and improve the accuracy with

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2913 each iteration.

2914 6.3.3 Feature selection and importance

2915 Using the reconstructed tracks as a starting point, I compute a number of ECal and
2916 MuID variables for each of them. As there can be more than one cluster associated to a
2917 track, what I do is collect all associated clusters and compute these variables from the
2918 complete collection of associated hits. For the MuID, because it only features three layers
2919 and typically there will be less hits, I also allow single hits to be associated with tracks⁷.
2920 I can roughly divide the variables in three types: energy-related, geometry-related and
2921 statistical. In the following, I briefly describe the variables related exclusively to the
2922 ECal:

2923 • Energy-related ECal

- 2924 – ECal total energy (ClusterTotalEnergy): sum of the energy of all the ECal
2925 hits.
- 2926 – Mean ECal hit energy (HitMeanEnergy): mean of the hit energy distribution.
- 2927 – Standard deviation ECal hit energy (HitStdEnergy): standard deviation of
2928 the hit energy distribution.
- 2929 – Maximum ECal hit energy (HitMaxEnergy): maximum of the hit energy
2930 distribution.

2931 • Geometry-related ECal

- 2932 – Mean distance hit-to-cluster (DistHitClusterMean): mean of the distance
2933 distribution between the hits and the corresponding cluster's main axis.
- 2934 – RMS distance hit-to-cluster (DistHitClusterRMS): root mean square of the
2935 distance distribution between the hits and the corresponding cluster's main
2936 axis.

⁷At the reconstruction level what happens is that non-clustered hits are put into single hit clusters, instead of being thrown away. This is necessary to keep the consistency of the track-cluster association code.

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- 2937 – Maximum distance hit-to-centre (DistHitCenterMax): maximum of the
2938 distance distribution between the hits and the centre of the TPC.
- 2939 – Time-of-Flight velocity (TOFVelocity): slope obtained when fitting a straight
2940 line to the hit time versus hit distance to the centre (i.e. $d = v \times t$).

2941 • Energy and geometry ECal

- 2942 – Radius 90% energy (Radius90E): distance in the hit-to-cluster distribution
2943 for which 90% of the total energy is contained in the hits that are closer to
2944 the axis (i.e. radius that contains 90% of the energy).

2945 • Statistical ECal

- 2946 – Number of hits (NHits): total number of hits associated to the track.
- 2947 – Number of layers with hits (NLayers): not really a count of all layers with
2948 hits but the difference between the last and the first layer with hits.

2949 Figure 6.21 shows the distributions of three different ECal variables, separating true
2950 muons (blue) and charged pions (red), for the five momentum ranges considered. I chose
2951 to show one feature from each category, namely the mean energy per hit (left column),
2952 the mean distance between the hits and the centre of the cluster (middle column), and
2953 the number of ECal layers with hits (right column). These give an idea of the separating
2954 power of the different features, and how it changes considerably with the energy. In
2955 the number of layers with hits distributions, the peak at 6 is due to the fact that the
2956 first six ECal layers sit inside the pressure vessel⁸. Therefore, some of the particles get
2957 stopped crossing it, never making it to the seventh layer.

2958 In the case of the MuID, because at low momenta a significant fraction of the particles
2959 do not make it past the ECal, I only consider the information coming from this detector
2960 for momenta ≥ 0.8 GeV/ c , i.e. for the last three momentum regions. The variables I
2961 extract from it are the following:

⁸Note to self: check this. I thought the ECal barrel had 8 layers of tiles, and that all of them were inside the pressure vessel.

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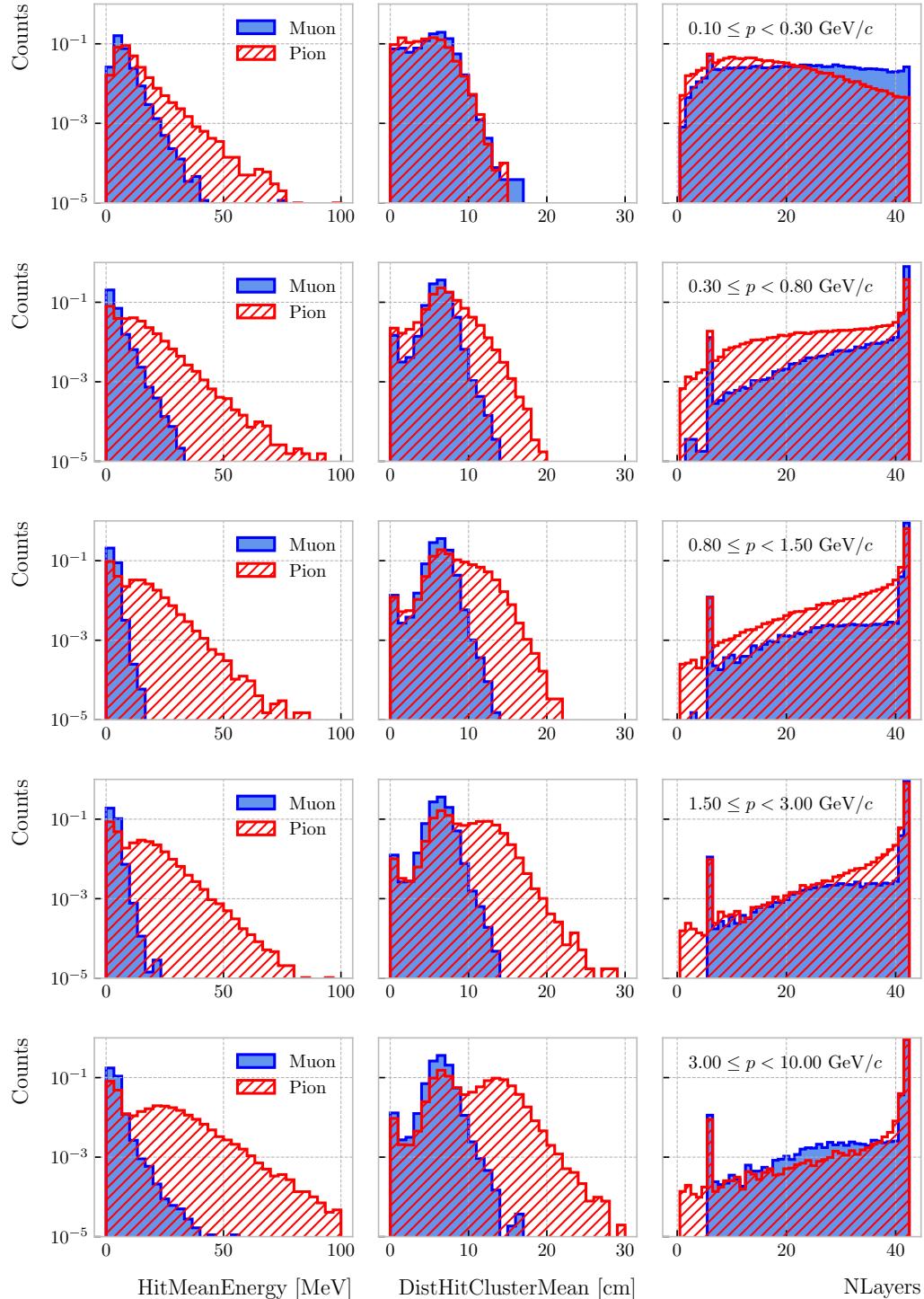


Figure 6.21: Example ECal feature distributions for muons (blue) and charged pions (red) in the five different momentum ranges considered (from top to bottom, in ascending momentum order). From left to right: mean hit energy, mean distance hit-to-cluster, and number of layers with hits.

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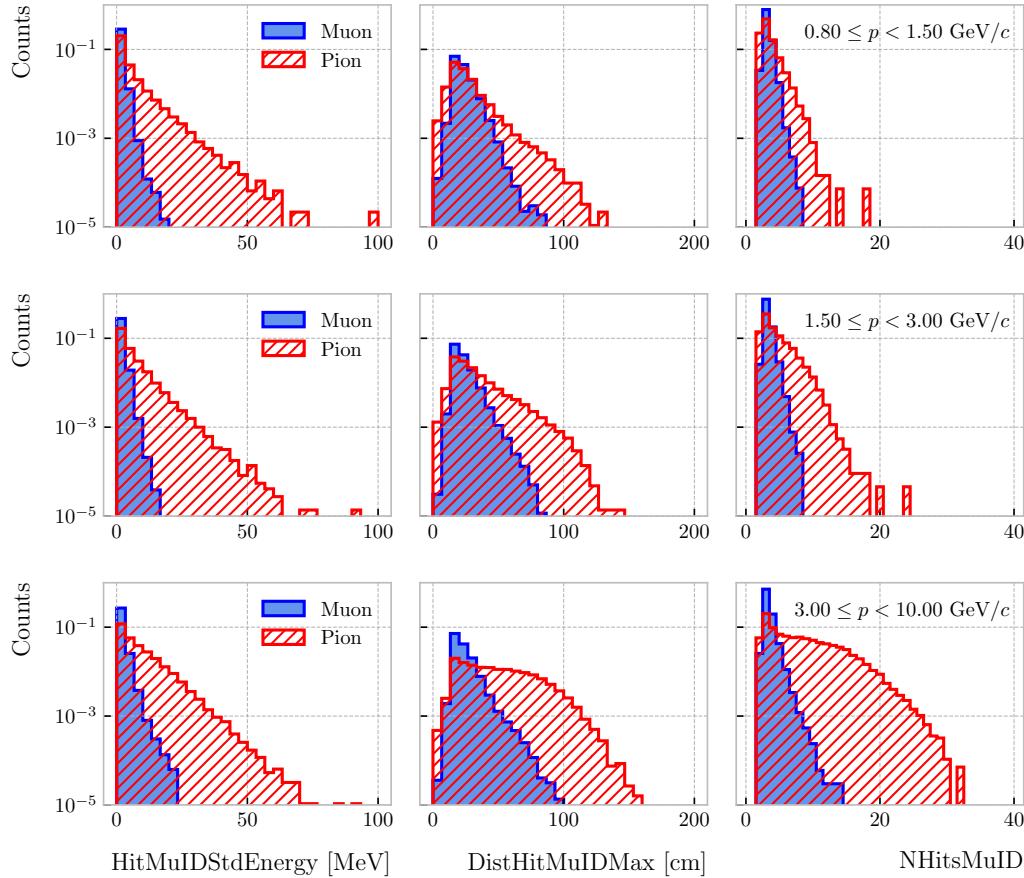


Figure 6.22: Example MuID feature distributions for muons (blue) and charged pions (red) in the three different momentum ranges considered (from top to bottom, in ascending momentum order). From left to right: standard deviation hit energy, maximum distance hit-to-hit, and number of hits.

• Energy-related MuID

- MuID total energy (ClusterMuIDTotalEnergy): sum of the energy of all the MuID hits.
- Mean MuID hit energy (HitMuIDMeanEnergy): mean of the MuID hit energy distribution.
- Standard deviation MuID hit energy (HitMuIDStdEnergy): standard deviation of the MuID hit energy distribution.
- Maximum MuID hit energy (HitMuIDMaxEnergy): maximum of the MuID hit energy distribution.

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• Geometry-related MuID

- 2972 – Maximum distance MuID hit-to-hit (DistHitMuIDMax): maximum distance
- 2973 between pairs of MuID hits (not sure this is a good variable, distribution
- 2974 looks nuts).
- 2975 – Maximum distance MuID hit-to-centre (DistHitCenterMuIDMax): maximum
- 2976 of the distance distribution between the MuID hits and the centre of the
- 2977 TPC.

• Statistical MuID

- 2979 – Number of hits (NHitsMuID): total number of MuID hits associated to the
- 2980 track.
- 2981 – Number of layers with hits (NLayersMuID): not really a count of all layers
- 2982 with MuID hits but the difference between the last and the first layer with
- 2983 MuIDhits.

2984 Figure 6.22 shows the distributions of three different MuID variables, separating true
2985 muons (blue) and charged pions (red), for the three momentum ranges which use the
2986 muon tagger information. In this case I decided to standard deviation of the MuID hit
2987 energy distribution (left column), the maximum distance between the MuID hit pairs
2988 (middle column), and the number of MuID hits (right column). These variables are used
2989 together with the ECal features at high momenta, providing additional disambiguation
2990 power.

2991 Once our features have been defined, one can do some exploratory analysis to
2992 understand how well the variables describe the target class, and avoid the black-box
2993 approach by what features are most relevant for the learning process. This way, I
2994 performed a feature analysis for each of the momentum ranges I divided this classification
2995 problem into. It follows three steps: first a principal component analysis (PCA), followed
2996 by a feature importance study using Gini and Shapley values, and finally a feature
2997 permutation importance analysis.

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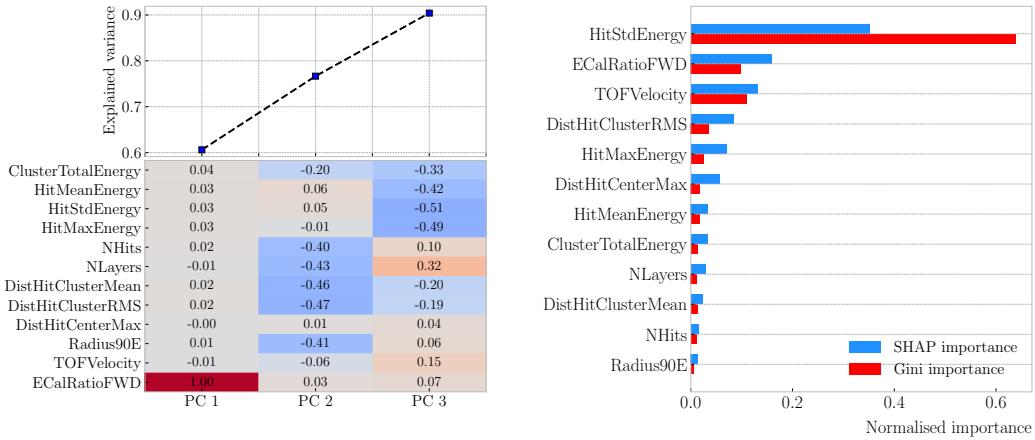


Figure 6.23: Left panel: cumulative explained variance for the first three principal components (top panel) and contribution of the different features to the principal axes in feature space (bottom panel). Right panel: Shapley (blue) and Gini (red) feature importances for the different input features. Both figures correspond to the samples in the momentum range $0.3 \leq p < 0.8 \text{ GeV}/c$.

2998 The PCA is useful to understand the variance of the feature space. It is an
 2999 unsupervised machine learning technique that allows the user to perform a dimensionality
 3000 reduction. It uses a singular value decomposition of the input features to project them
 3001 into a lower dimensional space. The idea is to find the matrix \mathbf{C}_m , whose columns are
 3002 the first m orthonormal eigenvectors of the input covariance matrix. Consider the $n \times p$
 3003 real matrix of input data \mathbf{X} , where n is the number of samples and p the number of
 3004 features. If \mathbf{X} is centred, i.e. the means of its columns are equal to zero, we can write the
 3005 covariance matrix of \mathbf{X} as $\mathbf{C} = \mathbf{X}^\top \mathbf{X} / (n - 1)$. This matrix can be diagonalised, yielding:

$$\mathbf{C} = \mathbf{V} \mathbf{L} \mathbf{V}^\top, \quad (6.11)$$

3006 where \mathbf{V} is a matrix of eigenvectors and \mathbf{L} a diagonal matrix with eigenvalues λ_i . Then,
 3007 performing SVD on \mathbf{X} gives us:

$$\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{W}^\top, \quad (6.12)$$

3008 where \mathbf{U} is a unitary matrix, whose columns are called left singular vectors, \mathbf{S} is a
 3009 diagonal matrix of single values s_i , and \mathbf{W} is another unitary matrix, its columns known

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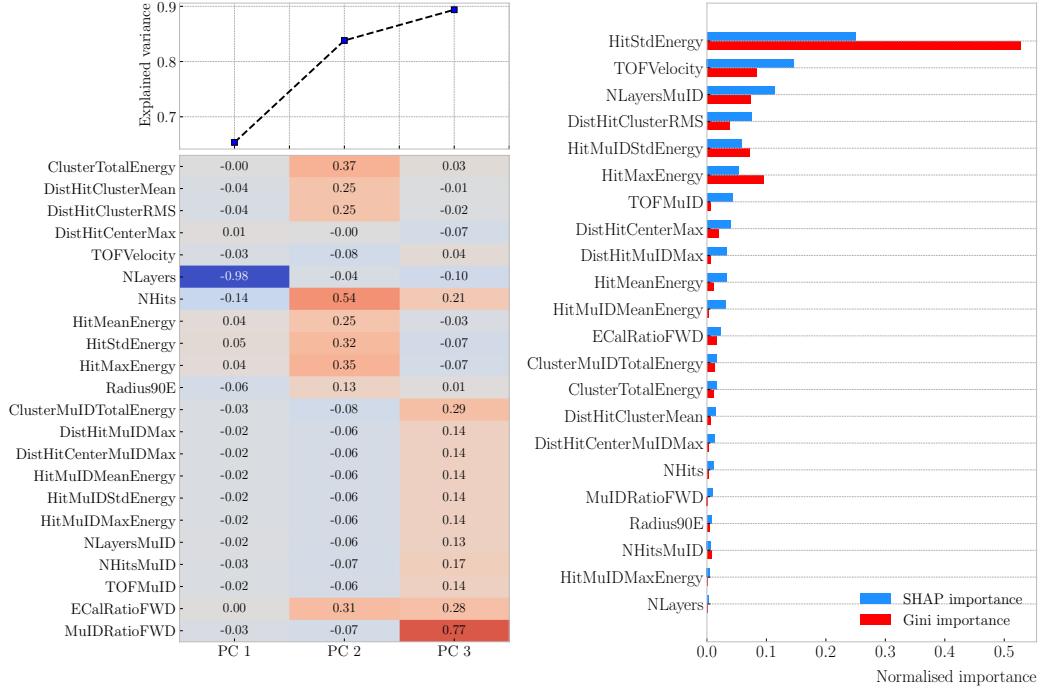


Figure 6.24: Left panel: cumulative explained variance for the first three principal components (top panel) and contribution of the different features to the principal axes in feature space (bottom panel). Right panel: Shapley (blue) and Gini (red) feature importances for the different input features. Both figures correspond to the samples in the momentum range $0.8 \leq p < 1.5$ GeV/c.

as right singular vectors. This way, we can write:

$$\mathbf{C} = \mathbf{W}\mathbf{S}\mathbf{U}^\top\mathbf{U}\mathbf{S}\mathbf{W}^\top/(n-1) = \mathbf{W}\frac{\mathbf{S}^2}{n-1}\mathbf{W}^\top. \quad (6.13)$$

meaning that the right singular vectors are also the eigenvectors of the covariance matrix.

The SVD can be computed numerically following an iterative approach.

This way, taking an input data vector $X \in \mathbb{R}^n$, the resulting feature vector $Y \in \mathbb{R}^m$

is given by:

$$Y = \mathbf{C}_m^\top X. \quad (6.14)$$

The new features capture most of the variance of the original sample, while being lower dimensional, as $m < n$.

Before applying the PCA reduction one needs to centre and scale the input data.

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3018 Centring is necessary when using SVD to obtain the eigenvectors of the covariance
3019 matrix, as only in that case we can do the identification with the right singular vectors
3020 from the input data. Scaling is needed when variables are on different scales, as some
3021 can then dominate the PCA procedure.

3022 I used the PCA module of `scikit-learn`, together with the `RobustScaler`, which
3023 centres the data and scales it based on the interquartile range. In Fig. 6.23 (left panel)
3024 and Fig. 6.24 (left panel) I show the results I obtained from the PCA for the momentum
3025 ranges $0.3 \leq p < 0.8 \text{ GeV}/c$ and $0.8 \leq p < 1.5 \text{ GeV}/c$, respectively. Notice that in
3026 the second case the number of features increases considerably, as this is the first region
3027 which uses the MuID variables. I found that, in all the cases, adding a fourth PC does
3028 not add additional information. As it can be seen in the top panels of the figures, the
3029 cumulative explained variance is already over 80% with three PCs.

3030 The bottom panels show the contribution of the variables to the principal axes. For
3031 the two first momentum regions, I observe a tendency of the energy-related and the
3032 geometry-related ECal variables to be clustered together. For the other ranges, when
3033 I include the MuID variables, there seems to be a division between ECal and MuID
3034 variables. For these, it seems like the number of ECal layers with hits also plays an
3035 important role.

3036 The next step in the analysis is to quantify the importance of the features based on
3037 two additional metrics, namely the Gini and the Shapley values. The Gini importance,
3038 often called mean decrease impurity, is based on how much a feature contributes to the
3039 purity improvement at the splits in each decision tree. The purity is measured in terms
3040 of the Gini impurity index, defined as:

$$I_G = 1 - \sum_i f_i, \quad (6.15)$$

3041 where f_i is the fractional abundance of the i -th class. Then, for each split one can

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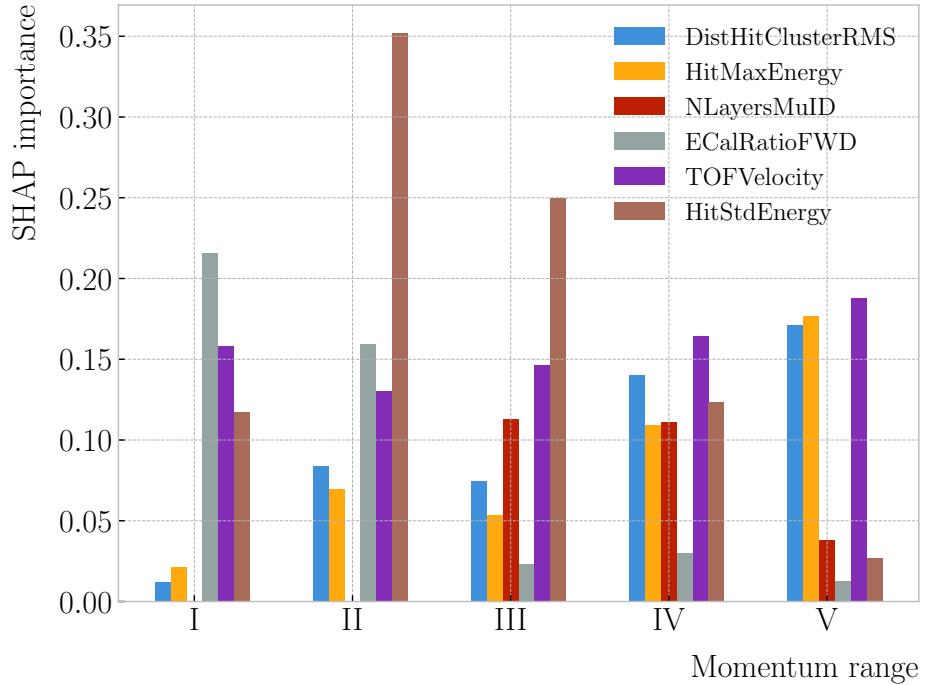


Figure 6.25: Evolution of the SHAP importance for the top six most important features across all five momentum ranges.

3042 compute the weighted decrease in impurity as:

$$\Delta_G = \frac{N_t}{N} \left(I_G - \frac{N_t^R}{N_t} I_G^R - \frac{N_t^L}{N_t} I_G^L \right), \quad (6.16)$$

3043 where N represents the total number of samples, N_t the number of samples at the current
 3044 node, N_t^R and N_t^L the number of samples in the right and left children respectively,
 3045 I_G is the Gini impurity at the current node, and I_G^R and I_G^L the Gini impurities of the
 3046 resulting right and left children.

3047 For each decision tree, one will have a normalised vector with the accumulated
 3048 decrease in Gini impurity for each feature. In the case of a BDT, the feature importances
 3049 are simply the mean for all the estimators in the ensemble⁹.

3050 The concept of Shapley values originated in the context of game theory, and it
 3051 measures the marginal contribution of a feature in enhancing the accuracy of a classifier.

⁹Note to self: this appears not to be the case. If you get the `feature_importance` for each tree in the BDT and take the average, the result is not the same to be one reported in the `feature_importance` attribute of the BDT.

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3052 Take F to be the set of all features in a problem, and $S \subseteq F$ the subset of features. To
 3053 compute the Shapley value of the i -th feature, one has to train a model with that feature
 3054 present, $f_{S \cup \{i\}}$, and another model trained without it, f_S . This has to be repeated for
 3055 all possible combinations of subsets $S \subset F \setminus \{i\}$, and evaluating the models predictions
 3056 on the appropriate sets of data x_S . This way, the Shapley value results:

$$\varphi_i = \sum_{S \subset F \setminus \{i\}} \frac{|S|! (|F| - |S| - 1)!}{|F|!} [f_{S \cup \{i\}}(x_{S \cup \{i\}}) - f_S(x_S)]. \quad (6.17)$$

3057 I trained the `GradientBoostingClassifier` from `scikit-learn` with the default
 3058 configuration in order to evaluate both the Gini and Shapley importances. The Gini
 3059 scores are automatically computed by `scikit-learn`, using the training data. For the
 3060 Shapley importance, I used the implementation from the `SHAP` package, computing
 3061 it using the test sample. The results can be seen in Fig. 6.23 (right panel) and
 3062 Fig. 6.24 (right panel), again for the momentum ranges $0.3 \leq p < 0.8 \text{ GeV}/c$ and
 3063 $0.8 \leq p < 1.5 \text{ GeV}/c$. The length of the bars denote either the SHAP (blue) or the Gini
 3064 (red) importance of the feature. One interesting thing to notice is that, when looking at
 3065 the Gini importance, there is always one feature that dominates over the rest. This is
 3066 not the case for the SHAP importance, where importances tend to be more balanced.

3067 Across all momentum ranges, I observe that the most important features are. For
 3068 the five momentum ranges considered, only six variables sit in the top five at least once.
 3069 Figure 6.25 shows the evolution of the SHAP importance of these six features. It is
 3070 interesting to see that the time-of-flight variable keeps its importance almost unchanged
 3071 for all momenta. Also, it looks like the ECal energy ratio gets less relevant the higher the
 3072 momentum is, but the RMS of the hit-to-cluster distance distribution and the maximum
 3073 ECal hit energy become more important in the last momentum ranges.

3074 The last step in the feature selection analysis is the feature permutation. This
 3075 technique measures the contribution of each feature to the performance of a model by
 3076 randomly shuffling its values and checking how some scores degrade. For the present
 3077 case, I am interested in the precision or purity, and the sensitivity or efficiency, as these

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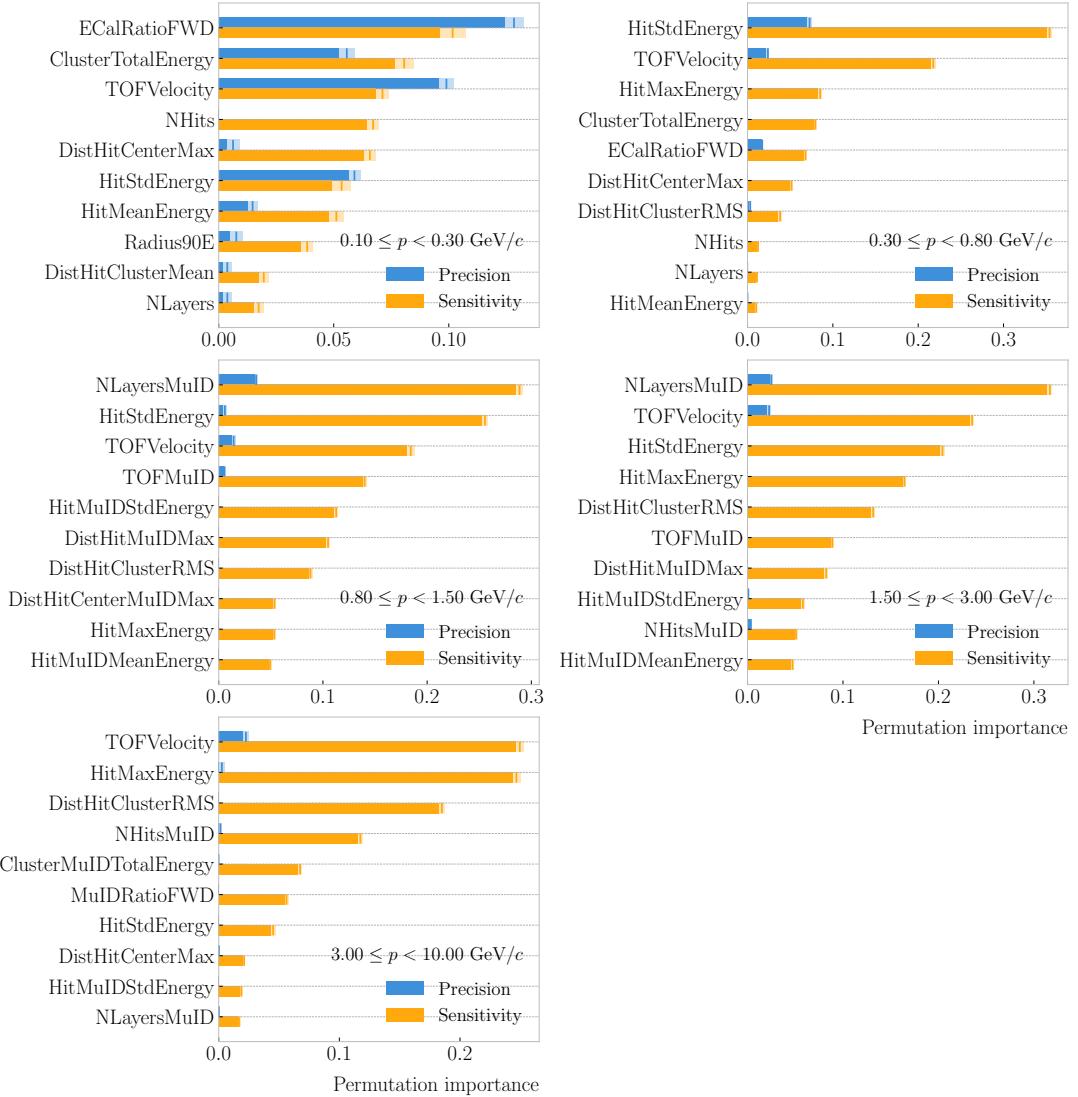


Figure 6.26: Permutation importances for the ten most important features in the different momentum ranges (from left to right, top to bottom, in increasing momentum order). The bars indicate the effect that permutations of each feature have on the purity (blue) and the sensitivity (yellow), the translucent regions representing one standard deviation around the central value.

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3078 two are the most relevant metrics from a physics point of view. The `scikit-learn`
3079 module provides the user with a method to perform the permutation scans.

3080 The results of these are shown in Fig. 6.26. For the different momentum ranges
3081 I show the permutation importances for the ten most important features. For each
3082 of the variables I report the effect the permutations have on the precision (blue) and
3083 sensitivity (yellow) of the models. The bars indicate the importance value, with the
3084 lighter part representing one standard deviation around the mean (hinted as an additional
3085 vertical line). Something to notice is that, in the first momentum region, the feature
3086 permutations have an effect on both the precision and the sensitivity. However, for the
3087 rest the precision is almost unaffected, while the sensitivity changes are considerably
3088 larger.

3089 It is also interesting to see that most of the variables identified as important here
3090 are the same I found when looking at the Shapley values. The behaviour of these across
3091 the momentum ranges is also similar, with the same patterns of some features being
3092 important at low momenta and then dropping in importance for the high momentum
3093 ranges.

3094 Wit this, I conclude the study of the features. I have prepared the training and
3095 testing datasets and understood what features are likely to have the largest impact on
3096 the performance of the classifiers.

3097 6.3.4 Hyperparameter optimisation

3098 Any BDT requires the user to specify a number of parameters that will dictate its
3099 behaviour. They can be divided into two categories: (i) tree-specific parameters, which
3100 affect each individual tree in the model, and (ii) boosting parameters, which control the
3101 boosting operation in the model. The value of these so-called hyperparameters affect the
3102 performance and predictive power of the models. Therefore, one needs to carefully select
3103 their optimal values in order to extract as much information as possible from the data.

3104 From all the parameters used to define a tree in the `scikit-learn` implementation
3105 of the BDT classifier, I only consider a subset of them. This is due to the fact that some

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3106 are mutually exclusive, but also because I noticed that others have little effect on the
3107 problem at hand. Therefore, the parameters I investigate are the following:

- 3108 • `min_samples_split`: defines the minimum number of samples required in a node
3109 to be considered for splitting. Higher values prevent a model from learning relations
3110 which might be highly specific to the particular sample, but may lead to under-fitting
3111 if the value is too low.
- 3112 • `min_samples_leaf`: defines the minimum samples required in a leaf node. For
3113 imbalanced problems it should take a low value, as there will not be many cases
3114 where the minority class dominates.
- 3115 • `max_depth`: maximum depth of a tree. Useful to prevent over-fitting, as higher
3116 depth will allow a model to learn relations specific to the training sample.

3117 In the case of the boosting parameters, the ones I look at are:

- 3118 • `learning_rate`: determines the impact of each tree on the final outcome. Low
3119 values make the model robust to the specific characteristics of a tree, and thus
3120 allow it to generalise well. However, that usually requires a large number of trees
3121 to model the data properly.
- 3122 • `n_estimators`: number of sequential trees to be trained. In general, BDTs are
3123 fairly robust at higher number of trees but it can still overfit at a point.
- 3124 • `subsample`: fraction of observations to be selected for each tree. Values slightly
3125 less than 1 make the model robust by reducing the variance.

3126 In general, hyperparameters depend on each other. Thus, it is not possible to
3127 optimise them independently. In the literature, we find two main strategies to explore
3128 the hyperparameter space. We could use a grid search, in which one discretises a
3129 portion of the space of hyperparameters and evaluates the model at each point. Another
3130 approach is the randomised search, where a certain number of random configurations of
3131 hyperparameters are explored.

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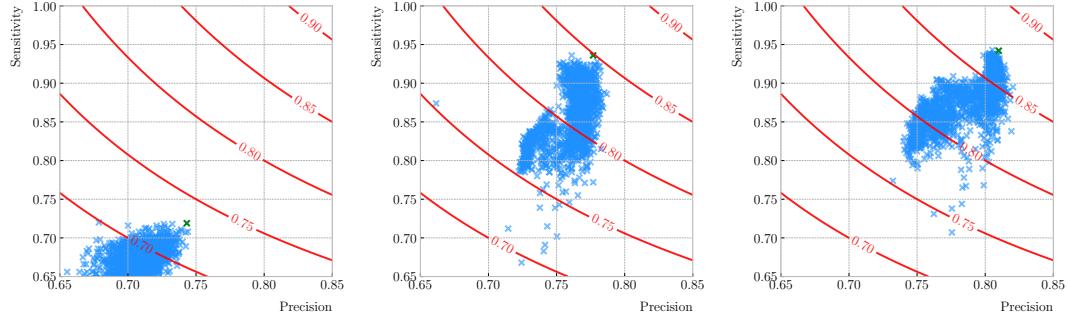


Figure 6.27: Values of the precision and sensitivity obtained for 10000 BDT hyperparameter configurations, for the momentum regions I, III and V. The red contours indicate the curves of equal F_1 -score, while the green crosses are the selected configurations.

3132 In this case, I used the random search to scan the hyperparameter space. Also,
 3133 because it is not guaranteed that a set of hyperparameters can be efficiently applied
 3134 across different datasets, I perform the optimisation for each of the momentum ranges
 3135 considered. Table 6.3 shows the list of hyperparameters considered, and the range within
 3136 which I let them vary. I decided to fix the number of estimators to 400 in all cases, as
 3137 its value is correlated with that of the learning rate.

3138 I evaluate 10000 different hyperparameter configurations for each momentum range.
 3139 For the hyperparameter tuning, I used subsamples containing 10% of the full datasets,
 3140 keeping the original proportions between classes, in order to reduce the computational
 3141 load. The performance of the models was assessed using a stratified 3-fold cross-validation
 3142 with replacement. Cross-validation involves dividing the data in a number of subsets,
 3143 training the model using some of them, and testing it with the rest. In our case, I
 3144 divide the data in 3 equal-sized subsets, maintaining the class proportions of the original
 3145 dataset. Then, for 3 consecutive iterations, I train the models using 2 of the subsets
 3146 while I compute the precision and sensitivity scores with the other. This approach
 3147 provides a more robust estimate of the performance on unseen data.

3148 Figure 6.27 shows the results in the precision versus sensitivity plane, for the
 3149 momentum regions I, III and V (from left to right). The contours represent the curves
 3150 of equal F_1 -score, i.e. the harmonic mean of the precision and the sensitivity. In order

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Table 6.3: Optimal values of the hyperparameters used by the BDT, for each momentum range.

Hyperparameter	Range	Best value				
		I	II	III	IV	V
<code>min_samples_split</code>	[0.001, 1]	0.10	0.06	0.05	0.27	0.06
<code>min_samples_leaf</code>	[0.001, 1]	0.02	0.03	0.01	0.02	0.07
<code>max_depth</code>	{2, 3, ..., 8}	8	2	4	2	7
<code>learning_rate</code>	[0.05, 1]	0.10	0.23	0.07	0.13	0.09
<code>subsample</code>	[0.01, 1]	0.75	0.65	0.79	0.86	0.95

Table 6.4: Performance metrics of the BDTs with optimal hyperparameters, for the different momentum ranges.

Metric	Value $\pm 1\sigma$				
	I	II	III	IV	V
Accuracy	0.779 ± 0.003	0.812 ± 0.003	0.846 ± 0.002	0.861 ± 0.003	0.874 ± 0.002
Precision	0.769 ± 0.003	0.752 ± 0.005	0.788 ± 0.002	0.805 ± 0.003	0.815 ± 0.003
Sensitivity	0.745 ± 0.009	0.921 ± 0.006	0.965 ± 0.002	0.967 ± 0.002	0.976 ± 0.001
F_1 -score	0.757 ± 0.004	0.828 ± 0.003	0.867 ± 0.002	0.879 ± 0.002	0.889 ± 0.002
ROC AUC	0.868 ± 0.003	0.865 ± 0.003	0.899 ± 0.002	0.902 ± 0.002	0.911 ± 0.001

3151 to select the optimal configurations (indicated in the plots with a green cross), I chose
 3152 the point with the highest F_1 -score.

3153 The results for the different momentum ranges are summarised in Tab. 6.3. One
 3154 can see some consistency in hyperparameter choices, with models generally preferring
 3155 small values for the tree-specific parameters, small learning rate, and relatively large
 3156 subsample sizes.

3157 Now that I have obtained the optimal values of the hyperparameters, I can train
 3158 the different BDTs. In this case I use the complete datasets, keeping 20% of the data
 3159 for testing. Table 6.4 shows the values of the different performance metrics obtained
 3160 using the selected hyperparameters and 5-fold cross-validation. The last row indicates
 3161 the value of the area under the receiver operating characteristic (ROC) curve. This
 3162 represents the sensitivity of a model as a function of the false positive rate. I have

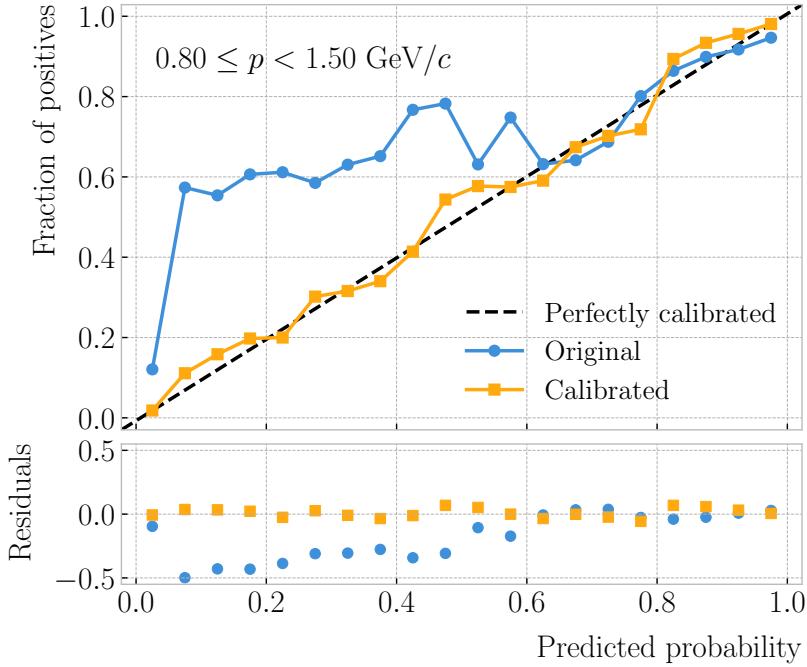


Figure 6.28: Reliability diagrams for the BDT classifier used in the momentum range $0.3 \leq p < 0.8 \text{ GeV}/c$, both for the original (blue circles) and calibrated (yellow squares) responses. For reference, the response of a perfectly calibrated classifier is also shown (black dashed line).

3163 included it here as it is a classic model metric used in the machine learning community.

3164 Overall, there is a clear trend of models performing better at higher momentum.

3165 6.3.5 Probability calibration

3166 So far, the trained BDTs are able to provide predictions of the class labels. Ideally,
3167 one would like the output of a classifier to give a confidence level about the prediction.
3168 However, it is not straightforward to interpret the outputs of our BDTs in terms of
3169 probabilities.

3170 A way to visualise how well the predictions of a classifier are calibrated is using
3171 reliability diagrams [172]. They represent the probability of the positive label versus the
3172 probability predicted by the classifier. These can be obtained by binning the predicted
3173 probabilities, and then compute the conditional probability $P(y_{true} = 1 | y_i \leq y_{pred} <$
3174 $y_{i+1})$ by checking the fraction of true positive instances in each bin. The reliability

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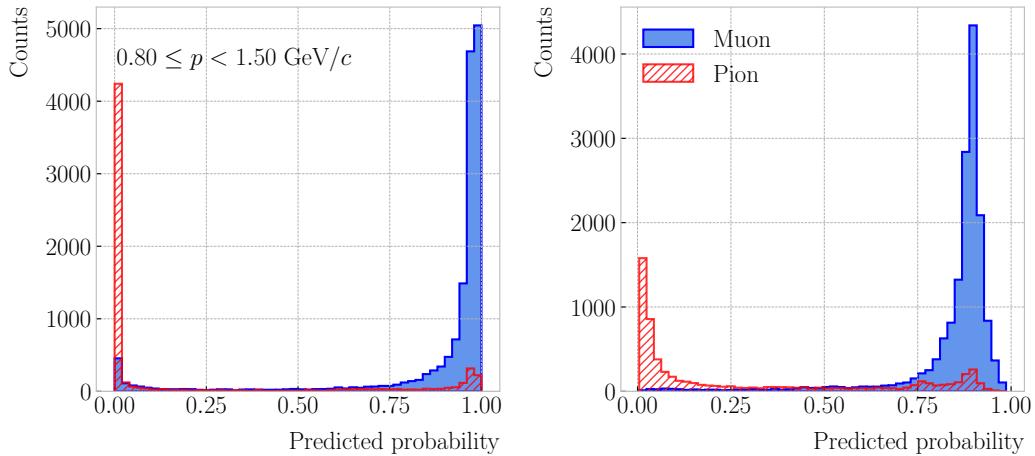


Figure 6.29: Uncalibrated (left panel) and calibrated (right panel) predicted probabilities assigned by the BDT classifiers for true muons (blue) and charged pions (red) in the momentum range $0.3 \leq p < 0.8 \text{ GeV}/c$.

3175 diagram of a perfectly calibrated classifier would be a diagonal line.

3176 In this case, I try to correct the raw response of the classifiers by applying a sigmoid
3177 function:

$$\sigma(x; A, B) = \frac{1}{1 + e^{Ax+B}}, \quad (6.18)$$

3178 where the parameters A and B are real numbers determined using the method of least
3179 squares.

3180 For each classifier, I perform a grid search to obtain the optimal values of A and B .
3181 For any pair, I compute the predicted probabilities as $y_{pred} = \sigma(y_{raw}; A, B)$, where y_{raw}
3182 are the raw predictions of the classifier¹⁰. Then, I calculate the corresponding reliability
3183 curve, and take the sum of the squared residuals between it and the response of the
3184 perfectly calibrated classifier.

3185 Figure 6.28 shows the reliability diagrams for the original (blue) and calibrated
3186 (yellow) probability predictions of the classifier for the III momentum range, $0.3 \leq p <$
3187 $0.8 \text{ GeV}/c$. The original response of the classifier is given by $y_{pred} = \sigma(y_{raw}; -2, 0)$,
3188 which is the transformation applied by `scikit-learn` to produce the probability estimate.
3189 Notice how the calibrated prediction matches the ideal response much better than the

¹⁰In `scikit-learn` these correspond to the outputs of the `decision_function` method.

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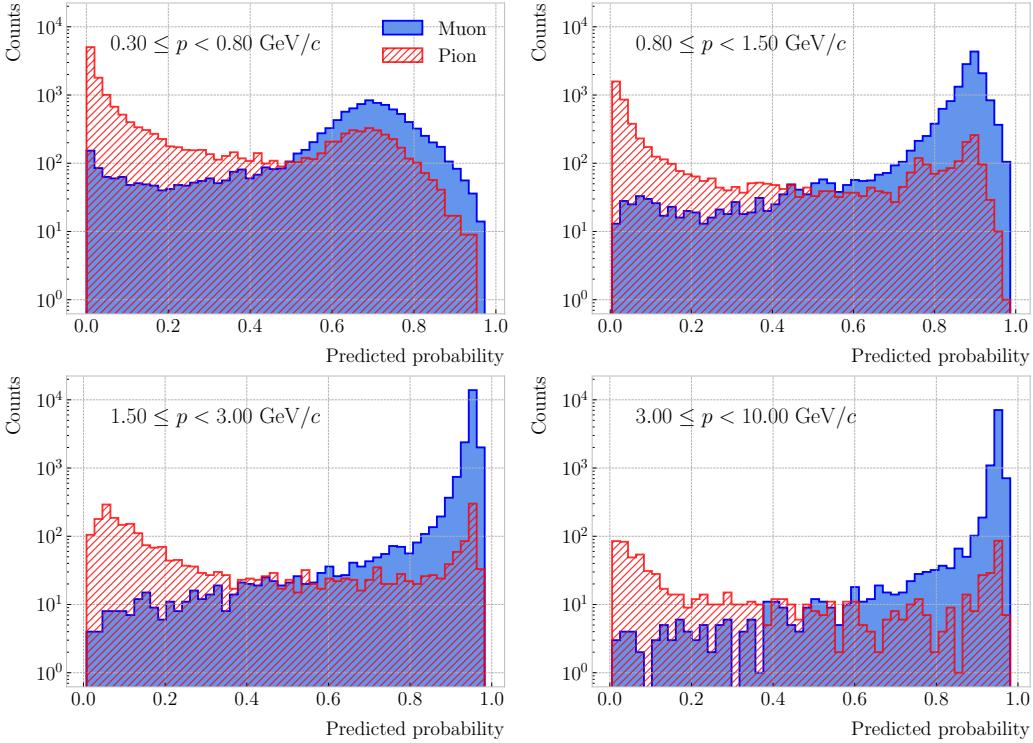


Figure 6.30: Calibrated predicted probabilities assigned by the BDT classifiers for the true muons (blue) and charged pions (red) in a FHC neutrino sample.

3190 original, across all the probability range.

3191 One can also compare the responses of the uncalibrated and calibrated classifiers
 3192 broken down by true particle type, as shown in Fig. 6.29. It can be seen that the
 3193 distributions for both muons (blue) and charged pions (red) smoothen after calibration,
 3194 but still the separating power of the classifier remains unchanged.

3195 6.3.6 Performance

3196 At this point, having the trained classifiers and the probability calibration parameters, I
 3197 am able to assess the performance of the classification strategy in a physics-relevant case.
 3198 For this, I prepared a sample of 10^5 FHC neutrino interaction events in the HPgTPC.
 3199 Using the truth matching information, I select all true muons and pions, and apply the
 3200 corresponding BDT classifier based on their momentum.

3201 Figure 6.31 shows the resulting calibrated output of the classifiers for the different

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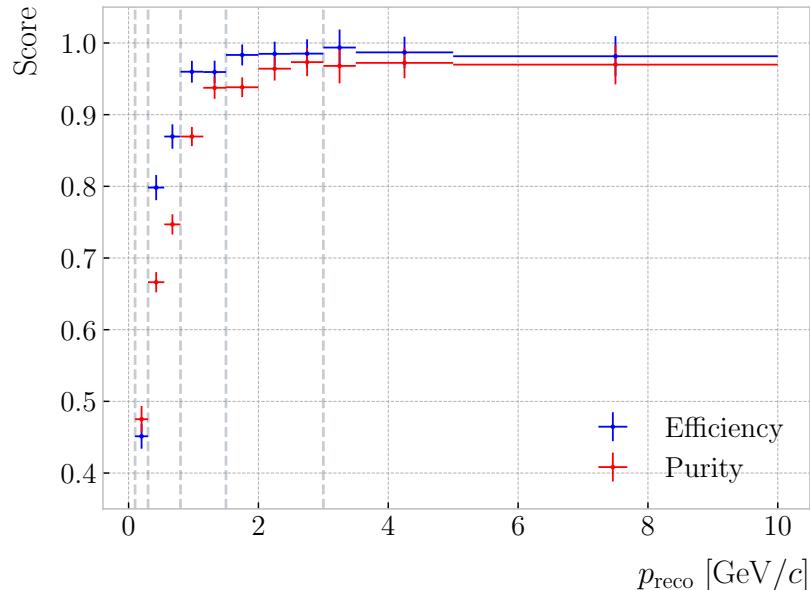


Figure 6.31: Efficiency (blue) and purity (red) of the muon selection as a function of the reconstructed momentum for the FHC neutrino sample.

3202 momentum regions. I do not include the first region, $0.10 \leq p < 0.30$ GeV/ c , as it only
 3203 contains a small fraction of signal events. The distributions obtained for this validation
 3204 sample

3205 I also studied the performance of the muon identification in a track-by-track selection.
 3206 To do so, I apply a simple cut on the output of the BDT classifiers. Every particle
 3207 with a predicted probability higher than the cut is considered a muon, while the ones
 3208 not passing the cut are taken to be pions. The results obtained for a cut of 0.50 are
 3209 shown in Fig. 6.31. Both the efficiency (blue) and the purity (red) of the selection are
 3210 displayed as a function of the momentum. The binning was chosen so that there were no
 3211 bins in between different momentum ranges and each had roughly the same number of
 3212 events. Even without optimising the value of the cut, the performance of the selection
 3213 is excellent. The only issues the first momentum range, where efficiency and purity sit
 3214 slightly below 0.50. However, a dE/dx measurement could help enhance the selection
 3215 there.

3216 This shows that the method behaves as expected when using unseen data, generalising
 3217 without problems from single particle to full neutrino events. In the coming Chapter, I

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3218 will study how to use the outputs of the BDT, hereafter referred to as muon scores, to
3219 perform realistic event selections in ND-GAr.

3220 6.4 ECal time-of-flight

3221 Looking at Fig. 6.20, it is clear that for momentum values in the range $1.0 - 3.0 \text{ GeV}/c$
3222 it is not possible to separate pions and protons using a $\langle dE/dx \rangle$ measurement in the
3223 HPgTPC. However, in the previous section I assumed that protons at those energies
3224 could be identified by other means, and therefore were not an issue for the muon and
3225 pion discrimination.

3226 Some detectors, like ALICE [173] or the ILD concept [174], complement the PID
3227 capabilities of their gaseous trackers with time-of-flight measurements. The use of
3228 fast timing silicon sensors, with hit time resolutions under 100 ps, would allow for the
3229 identification of charged hadrons via a ToF measurement up to $5.0 \text{ GeV}/c$. In the case
3230 of ND-GAr, one could think of using the inner layers of the ECal, the ones consisting of
3231 high-granularity tiles, to obtain a ToF-based PID, with some inputs from the TPC.

3232 Measuring the momentum and the velocity of a charged particle allows for a
3233 determination of the mass through the relativistic momentum formula:

$$m = \frac{p}{\beta} \sqrt{1 - \beta^2}. \quad (6.19)$$

3234 In our case, the momentum is measured in the TPC, using the curvature and the dip
3235 angle of the helix inside the magnetic field. The velocity of the particle can be written
3236 as:

$$\beta = \frac{\ell_{track}}{c\tau}, \quad (6.20)$$

3237 where ℓ_{track} is the length of the track, and τ the arrival time to the ECal.

3238 In GArSoft, the track length is computed at the Kalman filter stage. It is simply the
3239 sum of the line segments along the track, either in the forward or backward fit. In this
3240 case, because we are only interested in the particles that make it to the ECal, I choose

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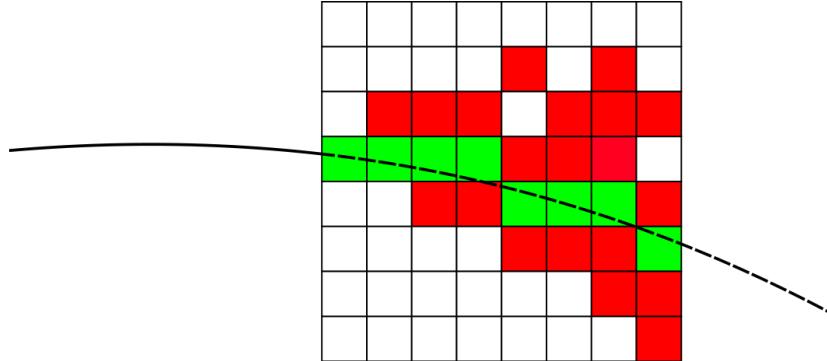


Figure 6.32: Schematic of the hit selection used for the ToF measurement. The grid represents the layers of the inner ECal, with coloured squares indicating the tiles with hits. Green squares indicate the selected hits.

3241 the fit direction based on the results of the track-cluster associations.

3242 Additionally, because the last 30 cm of the TPC radius are uninstrumented¹¹, I need
 3243 to correct for the length of the tracks. Using the track fit parameters to propagate the
 3244 helix to its entry point in the ECal, one can write the total track length as:

$$\ell_{track} = \ell + \left| \frac{\phi_{EP} - \phi}{R^{-1}} \right| \sqrt{1 + \tan^2 \lambda}, \quad (6.21)$$

3245 where ϕ_{EP} is the angle of rotation at the entry point to the calorimeter, and ℓ , ϕ , R and
 3246 λ are the track length, angle of rotation, radius of curvature and dip angle at the last
 3247 point in the fit, respectively.

3248 To test the idea of performing a ToF measurement with the inner ECal, I generated
 3249 two data samples. Each consists of 10000 single particle events, either charged pions or
 3250 protons. Their momenta are uniformly distributed in the range $0.5 - 5.0$ GeV/ c , and
 3251 their directions are isotropic. I process each sample using different values of the time
 3252 resolution, from $\Delta\tau = 0$, the perfect time resolution case for comparison, to the current
 3253 nominal value of $\Delta\tau = 0.7$ ns, and the worse scenario of $\Delta\tau = 1.0$ ns.

¹¹Note to self: check this number.

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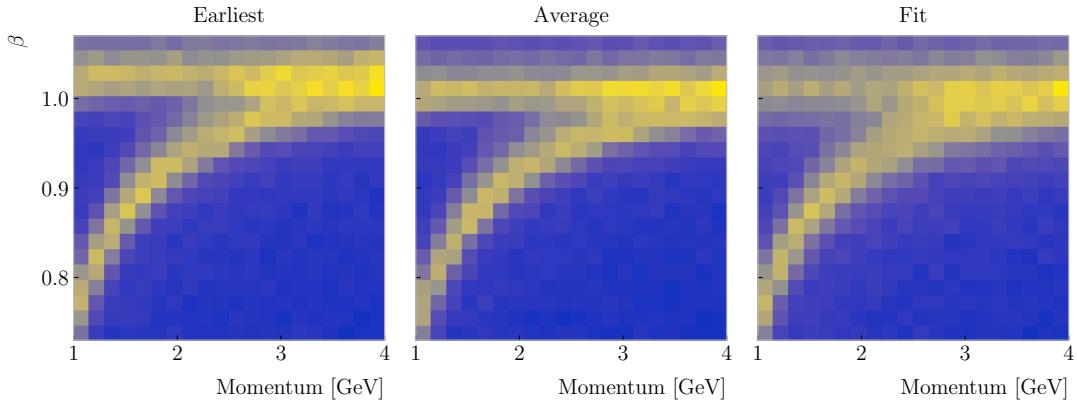


Figure 6.33: Particle velocity versus momentum measured with different ECal arrival time estimations. From left to right: earliest hit time, average hit time, and fitted hit time. In all cases the time resolution is $\Delta\tau = 0.1$ ns.

3254 6.4.1 Arrival time estimations

3255 In the simulation, the limited time resolution of the ECal is taken into account by
 3256 applying a Gaussian smearing to the true hit times. Other effects, like the digitisation
 3257 of the signals, are not taken into account and fall beyond the scope of this study. After
 3258 the track-cluster, one ends up with a collection of ECal hits associated to each particle.
 3259 From these, the arrival time of the particle to the ECal can be extracted.

3260 The simplest possibilities are to either take the time of the earliest hit or the hit
 3261 closest to the entry point. Because these two coincide, in general, I focused only in
 3262 the earliest hit time. However, this needs to be corrected, to account for the distance
 3263 travelled from the entry point to the position of the hit:

$$\tau_{earliest} = \tau_{hit} - \frac{d_{EP-hit}}{c}, \quad (6.22)$$

3264 where τ_{hit} is the time of the earliest hit, and d_{EP-hit} is the distance between that hit
 3265 and the entry point of the particle to the ECal. This is computed as the arc length
 3266 between the entry point and the point of the extrapolated helix up to the layer of the
 3267 hit. This way of correcting the time assumes c for the propagation of the particle, which
 3268 may lead to biased estimates.

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3269 I also tried to estimate the arrival times using information from the rest of the hits.
3270 In order to do this, as a simplifying assumption, I approximate the hadronic shower
3271 considering only its MIP component. For each layer, I keep only the hit in the tile closest
3272 to the point of the extrapolated track up to that layer. Figure 6.32 shows an example of
3273 how this hit selection works. The dashed line represents the extrapolated track, while
3274 the coloured squares are the tiles containing hits. Green indicates the tiles closer to the
3275 track in each layer (in the sketch they correspond to the grid columns).

3276 Now, I can use these collections of hits to estimate the arrival times. A possibility
3277 is to take the average of the times of the selected hits, denoted $\tau_{average}$. For that to
3278 work, one needs to correct these times, in a similar way as in Eq. (6.22), before taking
3279 the average. However, as before, this correction assumes that the particle travels at the
3280 speed of light inside the ECal. Another option is to perform a linear fit to the hit times
3281 and the distances to the entry point. In that case, the arrival time would be the fitted
3282 value of the intercept, τ_{fit} . This method would not assume a speed of light propagation.

3283 Figure 6.33 shows the velocity estimations as a function of the particle momentum,
3284 for the earliest hit time (left panel), average hit time (middle panel), and fitted hit time
3285 (right panel). The two bands correspond to the π^\pm and the p particles. $\Delta\tau = 0.1$ ns.
3286 Notice how, for the earliest hit time method, the velocities are significantly biased
3287 towards larger values. For the multi-hit methods, the τ_{fit} estimate appears to produce a
3288 larger variance than when using the $\tau_{average}$ method.

3289 6.4.2 Proton and pion separation

3290 Once we have the velocities of the particles, one can estimate their masses through
3291 Eq. (6.19). The resulting mass spectra are shown in Fig. 6.34. I computed the masses
3292 for the three arrival time estimates discussed above, and three different values of the
3293 time resolution: $\Delta\tau = 0.00$ (perfect time resolution), $\Delta\tau = 0.10$ ns, and $\Delta\tau = 0.70$ ns.
3294 Although in all cases we have the same number of events, it appears as if the entries
3295 in the histograms decrease as the time resolution increases. Sometimes, the particles
3296 get unphysical values of $\beta > 1$, and in turn they do not contribute to the mass spectra.

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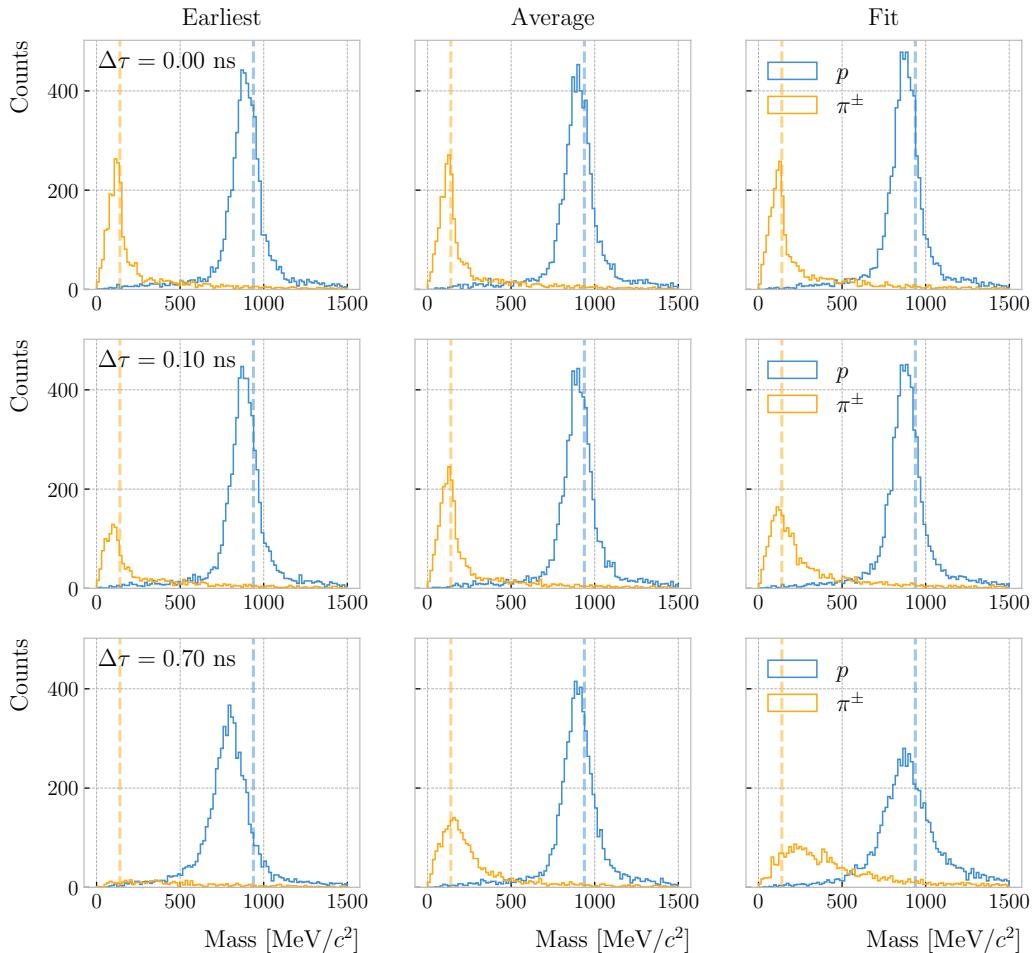


Figure 6.34: Mass spectra for p (blue) and π^\pm (yellow) particles, using different ECal time resolution values (from top to bottom, in ascending order), and arrival time estimates. From left to right: earliest hit time, average hit time, and fitted hit time. The dashed lines indicate the true masses of the particles.

3297 This is more likely to happen for higher values of $\Delta\tau$.

3298 As noted before, the average hit time method produces the most robust estimates
 3299 when increasing $\Delta\tau$. Intuitively this makes sense, as by taking the mean one averages
 3300 out the effect of the Gaussian smearing. Going forward, I will use this arrival time
 3301 estimator, as it appears to be the best performing one.

3302 It is possible to use the velocity estimations to select a sample of protons. In this
 3303 case, I do so by dividing the relevant momentum range in bins of $0.1 \text{ GeV}/c$. For each
 3304 momentum bin, I compute the expected velocity for the protons via the inverse of Eq.

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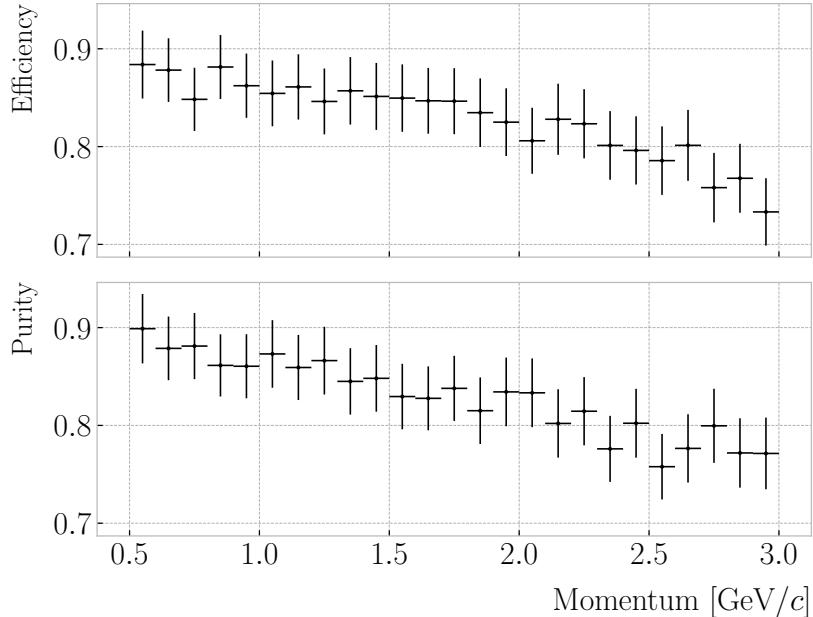


Figure 6.35: Efficiency (top panel) and purity (bottom panel) for the proton selection as a function of the momentum, for $\Delta\tau = 0.10$ ns.

3305 (6.19), and then take the fractional residuals of the measured velocities. Using that
 3306 distribution, I choose the cut that maximises the F_1 -score of the proton selection.

3307 The results can be seen in Fig. 6.35, for the case $\Delta\tau = 0.10$ ns. As expected from
 3308 Fig. 6.33, the performance of the selection degrades rapidly with increasing momentum.
 3309 However, the purity is still around 75% at 3.0 GeV/ c . This is likely to be sufficient, as
 3310 we do not expect protons or charged pions with higher energies from the beam neutrino
 3311 interactions.

3312 Figure 6.36 shows a few examples of the ToF velocity estimation in a FHC neutrino
 3313 sample. Here, for the different momentum bins, I have taken the fractional residual of
 3314 the expected value of β for a proton and the measured values (black data points). The
 3315 coloured lines represent Gaussian fits to the distributions of the different true particle,
 3316 with the gray line being the sum of these. It can be seen that, even for momenta close
 3317 to 2.0 GeV/ c , a good proton separation can be achieved. This idea will be explored
 3318 further later, in the context of the event selection.

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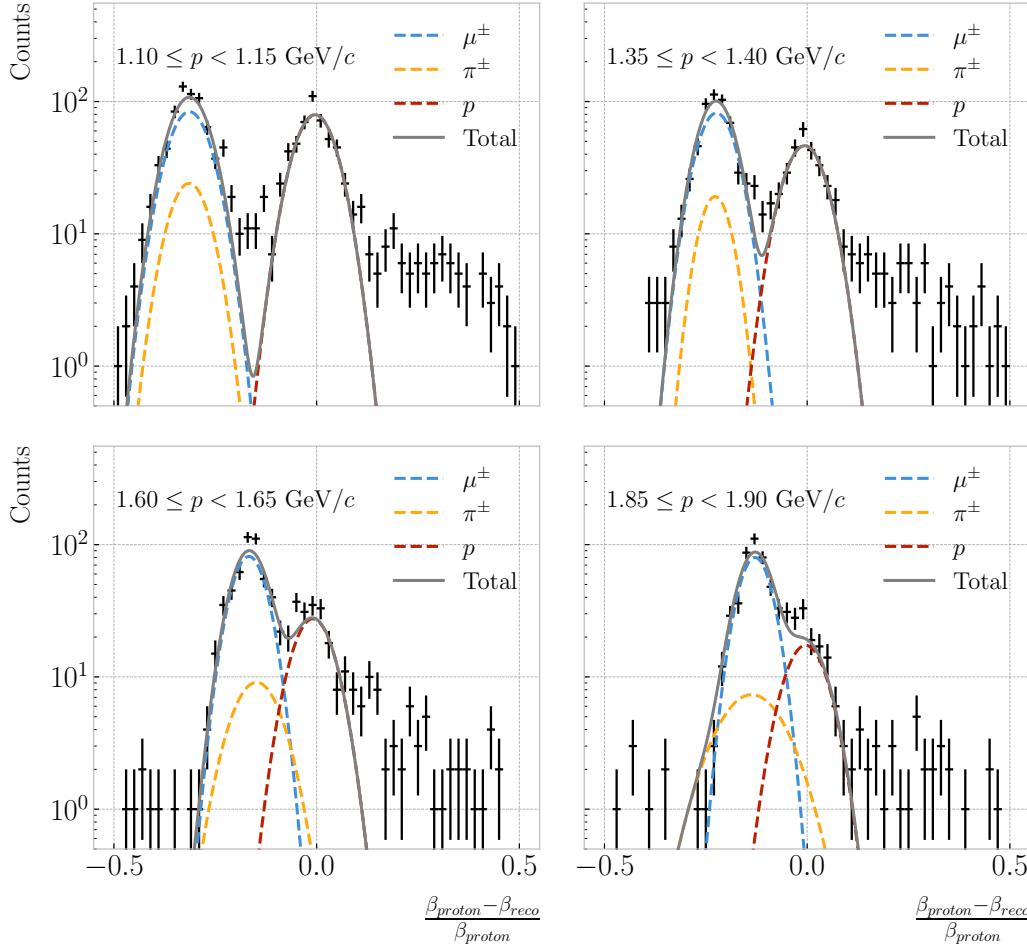


Figure 6.36: Distributions of the velocities measured by ToF with the inner ECal, for different momentum bins, in a FHC neutrino interaction sample. The Gaussian fits are performed around the maxima for each particle species.

3319 6.5 Charged pion decay in flight

3320 As discussed previously, in GArSoft the TPC tracks are formed after a pattern recognition
 3321 algorithm and a Kalman filter are applied to the TPC clusters. These two steps can
 3322 find discontinuities in the track candidates (e.g. due to a particle decay) when these
 3323 so-called breakpoints are large enough. However, for some, more subtle, cases they may
 3324 miss them and form a single reconstructed track. It has been noted in the literature
 3325 that Kalman filters offer, as a by-product, additional information to form test statistics
 3326 to identify these breakpoints [175, 176].

6.5. CHARGED PION DECAY IN FLIGHT

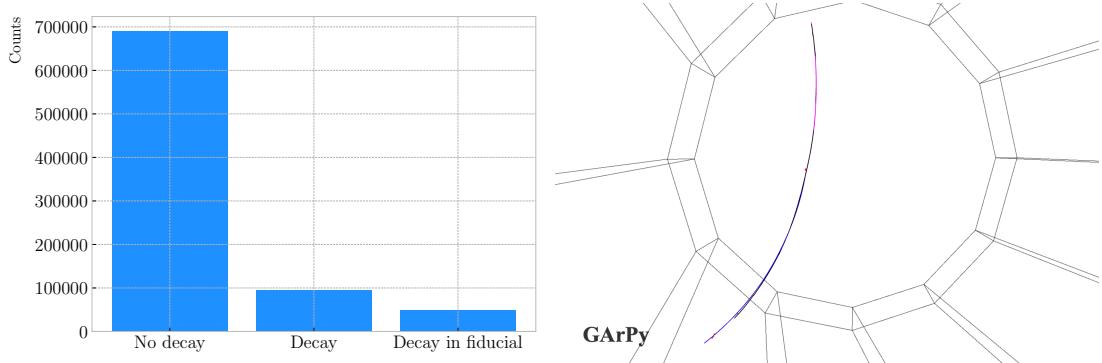


Figure 6.37: Left panel: number of non-decaying, decaying and decaying in the fiducial volume pions for a MC sample of 100000, $p = 500 \text{ MeV}/c$ isotropic positively charged pions inside the TPC. Right panel: event display for a positive pion decaying inside the fiducial volume, with a single reconstructed track for the pion and muon system.

3327 Considering the mean life of the charged pion, $\tau = (2.6033 \pm 0.0005) \times 10^{-8} \text{ s}$, one
 3328 can estimate that about 12% of the pions with momentum $p \sim \mathcal{O}(500 \text{ MeV}/c)$ (roughly
 3329 the peak of the pion momentum distribution in ν_μ CC interactions off argon) decay
 3330 inside the TPC. Figure 6.37 (left panel) shows the amount of charged pions decaying in
 3331 the full TPC and fiducial volumes from an isotropic, monoenergetic sample of 100000
 3332 negatively charged pions with $p = 500 \text{ MeV}/c$. We see that about 10% of those decayed,
 3333 with more than half of them decaying inside the TPC fiducial volume.

3334 Figure 6.37 (right panel) shows an example event display of a charged pion (magenta
 3335 line) decays in flight inside the TPC, but because the angle of the muon (blue line) is
 3336 small both were reconstructed as one single track (black line). In this case, the composite
 3337 track reaches the ECal, where it undergoes a muon-like interaction, thus being classified
 3338 as a muon.

3339 A way to understand what decaying pion tracks were totally or partially reconstructed
 3340 together with the daughter muon is looking at the relative energy contributions to the
 3341 reconstructed track. In order to select a sample of such events, I require that a minimum
 3342 50% of the total energy comes from the pion and at least 20% from the muon.

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3343 6.5.1 Track breakpoints

3344 To identify potential decays we can use the information we obtain from the Kalman
3345 filter at each step of the fitted track. The simplest test we can think about is computing
3346 the χ^2 of the mismatch between all the parameters in the forward and the backward fits:

$$\chi_k^{2(FB)} = (\hat{x}_k^B - \hat{x}_k^F)^T [V^{(\hat{x}_k, B)} + V^{(\hat{x}_k, F)}]^{-1} (\hat{x}_k^B - \hat{x}_k^F), \quad (6.23)$$

3347 where \hat{x}_k^F , \hat{x}_k^B are the Kalman filter state vector estimates at step k in the forward and
3348 backward fits and $V^{(\hat{x}_k, F)}$, $V^{(\hat{x}_k, B)}$ the covariance matrices of \hat{x}_k^F and \hat{x}_k^B respectively.
3349 Using the values of the χ^2 at measurement k for the forward and backward fits we can
3350 compute another χ^2 value that characterises the overall track fit:

$$\chi_{track}^2 = \chi_k^{2(F)} + \chi_k^{2(B)} + \chi_k^{2(FB)}, \quad (6.24)$$

3351 which remains approximately constant for all k .

3352 An alternative approach proposed in the context of the NOMAD experiment was
3353 using a fit with a more elaborate breakpoint hypothesis, so we can perform a comparison
3354 of the χ^2 with and without breakpoints. This can be achieved by using some alternative
3355 parametrisation with extra parameters, which allows some of the track parameters to
3356 be discontinuous at certain points. A decay changes the momentum magnitude and
3357 direction, so we can use the new state vector:

$$\alpha = (y, z, 1/R_F, 1/R_B, \phi_F, \phi_B, \tan\lambda_F, \tan\lambda_B)^T. \quad (6.25)$$

3358 As we already have the estimates from the standard Kalman filter and their
3359 covariance matrices at each point, we do not need to repeat the Kalman fit for the new
3360 parametrisation. Instead, I can compute the values of α at each point k that minimise

6.5. CHARGED PION DECAY IN FLIGHT

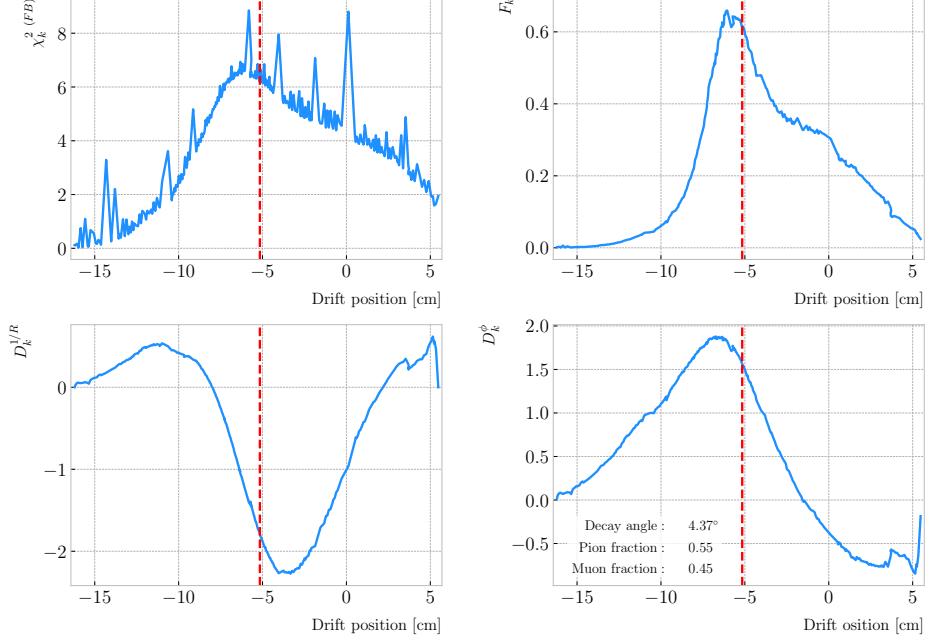


Figure 6.38: Values of $\chi_k^2(FB)$ (top left panel), F_k (top right panel), $D_k^{1/R}$ (bottom left panel) and D_k^ϕ (bottom right panel) versus position along the drift direction for a reconstructed track in a positive pion decay event. The vertical red dashed line indicates the true location of the decay point.

3361 the χ^2 resulting from comparing them to $\{\hat{x}_k^B, \hat{x}_k^F\}$. Introducing the two 5×8 matrices:

$$H^F = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad H^B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (6.26)$$

3362 we can write this as:

$$\begin{aligned} \chi_k^2(FB)(\alpha) &= (\hat{x}_k^F - H^F \alpha)^T \left[V^{(\hat{x}_k, F)} \right]^{-1} (\hat{x}_k^F - H^F \alpha) \\ &\quad + (\hat{x}_k^B - H^B \alpha)^T \left[V^{(\hat{x}_k, B)} \right]^{-1} (\hat{x}_k^B - H^B \alpha). \end{aligned} \quad (6.27)$$

3363 The minimum of $\chi_k^2(FB)(\alpha)$ is found when the measured new state vector takes the
3364 value:

$$\hat{\alpha}_k = V^{(\hat{\alpha}_k)} H^T (V^{(\hat{x}_k)})^{-1} \hat{X}, \quad (6.28)$$

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAR

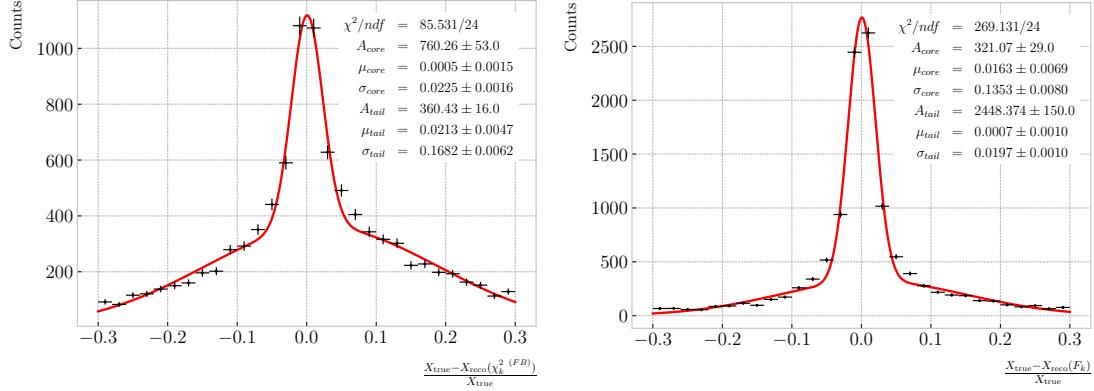


Figure 6.39: Fractional residual distributions of the true and reconstructed decay position along the drift coordinate, using the position of the maximum of $\chi_k^2(FB)$ (left panel) and F_k (right panel) as estimates of the decay position. Also shown are double Gaussian fits to these points (red lines).

3365 where $\hat{\mathbf{X}} = \{\hat{\mathbf{x}}_k^B, \hat{\mathbf{x}}_k^F\}$, $V^{(\hat{\mathbf{x}}_k)}$ is the block diagonal matrix formed by $V^{(\hat{\mathbf{x}}_k, F)}$ and $V^{(\hat{\mathbf{x}}_k, B)}$
 3366 and $V^{(\hat{\alpha}_k)}$ is the covariance matrix of $\hat{\alpha}_k$, given by:

$$V^{(\hat{\alpha}_k)} = \left(H^T (V^{(\hat{\mathbf{x}}_k)})^{-1} H \right)^{-1}. \quad (6.29)$$

3367 From these new fit estimates we can compute the F statistic, which tells us whether
 3368 the model with breakpoint provides a statistically significant better fit:

$$F_k = \left(\frac{\chi_{\text{track},k}^2 - \chi_{\text{full},k}^2}{8 - 5} \right) / \left(\frac{\chi_{\text{full},k}^2}{N - 8} \right). \quad (6.30)$$

3369 One can also compute the signed difference of the duplicated variables divided by
 3370 their standard deviation at each point. These represent how significant the discontinuity
 3371 in each variable is. For any variable η we can write it as:

$$D_k^\eta = \frac{\hat{\eta}_k^B - \hat{\eta}_k^F}{\sqrt{\text{Var}[\hat{\eta}_k^F] + \text{Var}[\hat{\eta}_k^B] - 2\text{Cov}[\hat{\eta}_k^F, \hat{\eta}_k^B]}}, \quad (6.31)$$

3372 In our case, the relevant ones to look at are $D_k^{1/R}$ and D_k^ϕ .

3373 Figure 6.38 shows the values of $\chi_k^2(FB)$, F_k , $D_k^{1/R}$ and D_k^ϕ as functions of the position
 3374 along the drift direction, for an example reconstructed track with 55.5% of the energy

6.5. CHARGED PION DECAY IN FLIGHT

coming from the charged pion and 45.5% from the daughter muon. The true position of the decay is indicated (dashed red lines). Notice how $\chi_k^2(FB)$ and F_k , $D_k^{1/R}$ reach their maxima near the decay point. In the former case this indicates a large forward-backward difference in the track fit. In the later it represents that the extended state vector improves the fit particularly around that point.

I can estimate the decay position finding resolution by computing the difference between the X position of the maxima of $\chi_k^2(FB)$ and F_k and the X position of the true decay. Figure 6.39 represent the the fractional residual distributions for both cases, from the sample of tracks containing pion decays. Fitting a double Gaussian to the distributions (red lines) I find a resolution of $(3.31 \pm 0.15)\%$ and $(6.94 \pm 0.31)\%$ respectively.

In principle, the F -statistic should follow a Fisher distribution with $(8 - 5)$ and $(N - 8)$ degrees of freedom under the null hypothesis. In most of our cases $N \sim \mathcal{O}(100)$, so the probability density functions will look very similar. In this case, it is safe to take the limit $N \rightarrow \infty$ in the Fisher PDF:

$$\begin{aligned} \tilde{f}(x; a - b) &= \lim_{N \rightarrow \infty} f(x; a - b, N - a) \\ &= \frac{2^{-\frac{a-b}{2}}}{\Gamma\left(\frac{a-b}{2}\right)} (a - b)^{\frac{a-b}{2}} x^{\frac{a-b}{2}-1} e^{-\frac{a-b}{2}x}. \end{aligned} \quad (6.32)$$

In our case $a - b = 8 - 5 = 3$, so we would obtain a p-value of 0.05 at $x = 2.60$.

Figure 6.40 contains the distributions of the maxima of $\chi_k^2(FB)$, F_k and D_k^ϕ and the minima of $D_k^{1/R}$ for a sample of non-decaying pion tracks (blue) and another sample of reconstructed tracks containing part of the pion and the daughter muon from a decay inside the fiducial volume (red). Notice that, even though the values of $F_k^{(max)}$ for the decay sample are typically larger than for the non-decaying one, just a small fraction of the events go beyond the aforementioned value of $F = 2.60$. Therefore, from a practical point of view, it is not the most efficient variable to use for selecting the decay events.

However, looking at the $D_k^{1/R \text{ (min)}}$ distribution we can see there is a big difference between non-decaying and decaying events in this variable. One can use a combination

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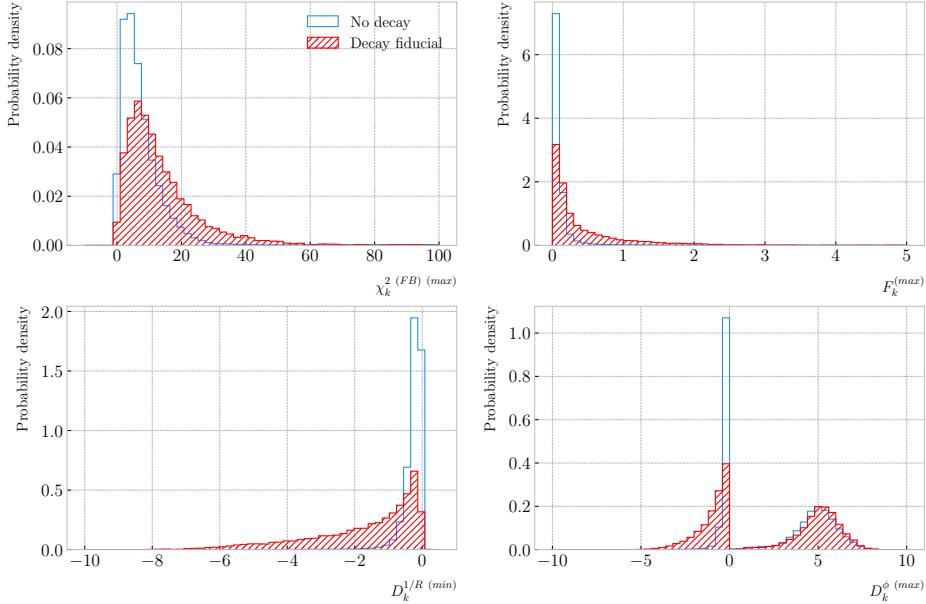


Figure 6.40: Distributions of the extreme values of $\chi_k^2(FB)$ (top left panel), F_k (top right panel), $D_k^{1/R}$ (bottom left panel) and D_k^ϕ (bottom right panel) for non-decaying reconstructed pion tracks (blue) and tracks which include the decay inside the fiducial volume (red).

3400 of these four variables to distinguish between the pion decay events (signal) and the
 3401 non-decaying pions (background).

3402 An approach to this classification could be using a boosted decision tree (BDT). One
 3403 of the advantages of BDTs is that they are easy to interpret and identify the relative
 3404 importance of the different input variables. Training a BDT with 400 estimators and a
 3405 maximum depth of 4 I can obtain an efficient classification without overtraining. Figure
 3406 6.41 (left panel) shows the distribution of probabilities predicted by the BDT for a test
 3407 sample. The signal efficiency as a function of background acceptance, the so-called ROC
 3408 curve, is shown in Fig. 6.41 (right panel). With a relative importance of 0.83, the most
 3409 important variable turned out to be $D_k^{1/R}(\min)$.

3410 One thing we can check is how the resolution to the decay and the signal efficiency in
 3411 the classification changes with the true decay angle. Using an equal-frequency binning
 3412 for the decay angles, we can repeat the previous steps for each bin.

3413 Figure 6.42 (left panel) shows the dependence on the decay angle of the decay finding

6.5. CHARGED PION DECAY IN FLIGHT

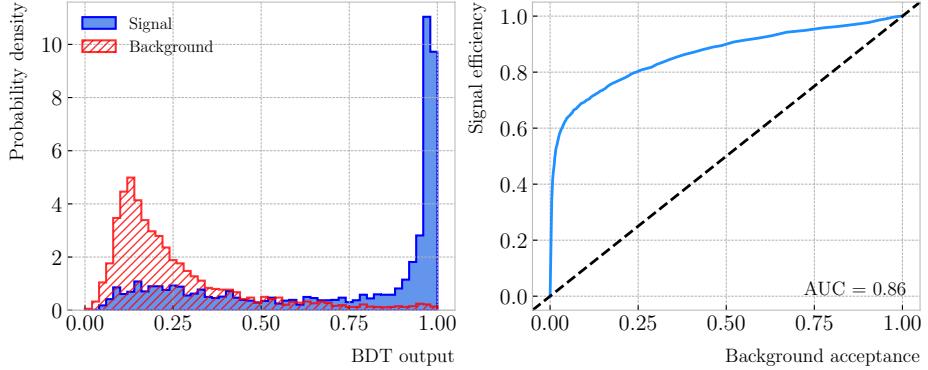


Figure 6.41: Left panel: distributions of the predicted probabilities assigned by the BDT classifier to a test sample of decaying pion+muon tracks (blue) and non-decaying pion tracks (red). Left: signal efficiency versus background acceptance (ROC curve) obtained from the BDT for the test sample.

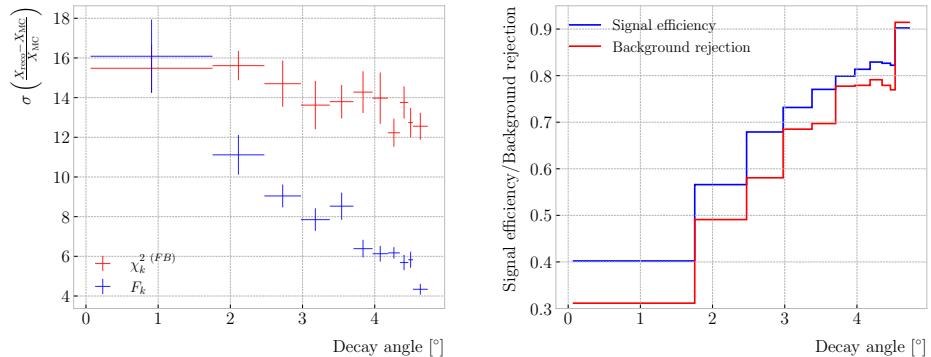


Figure 6.42: Left panel: dependence of the decay position finding resolution on the true value of the decay angle for the $\chi_k^2(FB)$ (red) and F_k (blue) methods. Right panel: signal efficiency (blue line) and background rejection (red line) from the BDT classifier versus true decay angle.

resolution. We can see that for the $\chi_k^2(FB)$ maximum location method the resolution consistently lies between 12 to 16%. However, the $F_k^{(\max)}$ approach gives a significantly better resolution for high angle values, reaching the 4 – 6% range for decay angles $\geq 4^\circ$.

For the classification dependence on the angle, I use the same classifier I trained before but evaluating the test sample for each individual angular bin. I compute the signal efficiency in each bin for a fixed value of the background rejection, in this case 90%. Similarly, for the background rejection estimation I use a fixed signal efficiency value of 90%. Figure 6.42 (right panel) represents the change in signal efficiency (blue)

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3422 and background rejection (red) with the value of the true decay angles.

3423 6.6 Neutral particle identification

3424 6.6.1 ECal clustering

3425 Another important reconstruction item is the clustering algorithm of ECal hits in
3426 GArSoft. The default module features a NN algorithm that treats all hits in the same
3427 way, independently of the layer each hit comes from. However, the current ECal design
3428 of ND-GAr has two very different types of scintillator layers. The inner layers are made
3429 out of tiles, which provide excellent angular and timing resolutions. On the other hand,
3430 the outer layers are cross scintillator strips. That way, an algorithm that treats hits
3431 from both kinds of layers differently may be able to improve the current performance.

3432 Inspired by the reconstruction of T2K’s ND280 downstream ECal [177], the idea
3433 was to put together a clustering module that first builds clusters for the different ECal
3434 views (tiles, strips segmented in the X direction and strips segmented in Y direction),
3435 and then tries to match them together to form the final clusters.

3436 Working on a module-by-module basis, the algorithm first separates the hits depending
3437 on the layer type they come from. Then, it performs a NN clustering for the 3 sets of
3438 hits separately. For the tile hits it clusters together all the hits which are in nearest-
3439 neighbouring tiles and nearest-neighbouring layers, for strip hits it looks at nearest-
3440 neighbouring strips and next-to-nearest-neighbouring layers (as the layers with strips
3441 along the two directions are alternated). For strip clusters an additional cut in the
3442 direction along the strip length is needed.

3443 After this first clustering I then apply a recursive re-clustering for each collection
3444 of strip clusters based on a PCA method. In each case, we loop over the clusters with
3445 $N_{hits} \geq 2$, computing the centre of mass and three principal components. Propagating
3446 these axes up to the layers of the rest of the clusters, we check if the propagated point
3447 and the centre of mass of the second cluster are within next-to-nearest-neighbouring
3448 strips. An additional cut in the direction along the strip length is also needed. Moreover,

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Table 6.5: Summary of parameters and sampled values used in the optimisation of the clustering algorithm.

Name	Units	Sampled values	Description
PrimMinorCut	strips	2, 3, 4	Distance along strip length in NN clustering
RecMinorCut	strips	3, 5, 8	Distance between propagated point and CM along strip length in re-clustering
RecPerpCut	strips	2, 3, 4	Closest hit pair distance in re-clustering
StripDistCut	strips	3, 5, 8	Distance between CMs in strip cluster merging
StripDirCut	cos	0.5, 0.7, 0.9	Main axes direction cut in strip cluster merging
PointDistCut	tiles	3, 5, 8	Distance between propagated point and CM in strip-tile matching
MergePerpCut	cm	10, 20, 30	Closest hit pair distance in module merging
MergeDirCut	cos	0.5, 0.7, 0.9	Main axes direction cut in module merging

3449 I require that the two closest hits across the two clusters are at most in next-to-nearest-
3450 neighbouring strips. I merge the clusters if these three conditions are satisfied. The
3451 re-clustering is repeated until no more cluster pairs pass the cuts.

3452 The clusters in each strip view are combined if their centres of mass are close enough
3453 and they point in the same direction. An alternative approach for the strip cluster
3454 merging could be to compute the overlap between the ellipsoids defined by the principal
3455 axes of the clusters, and then merge the pair if the overlap exceeds some threshold.
3456 Further study is needed to understand if this change would have an impact in the overall
3457 clustering performance.

3458 To merge the tile clusters to the combined strip clusters I propagate the principal
3459 axis of the strip cluster towards the inner layers, up to the centre of mass layer of the
3460 tile cluster. I merge the clusters if the distance between the propagated point and the
3461 centre of mass is below a certain cut.

3462 The last step is to check if clusters in neighbouring modules should be merged
3463 together, both across two barrel modules, across end cap modules and between barrel
3464 end cap modules. I check the distance between the two closest hits in the pair of clusters
3465 and merge them if it passes this and an additional direction cut.

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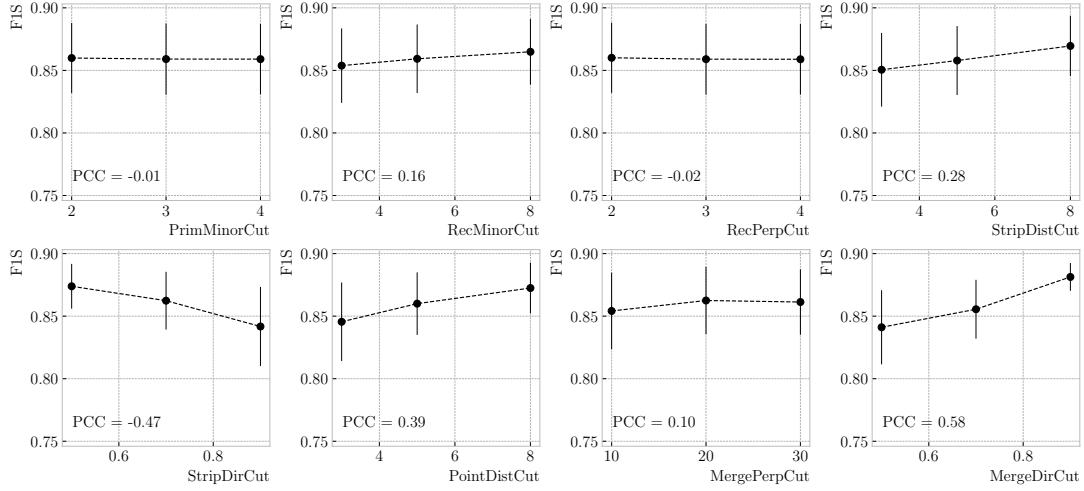


Figure 6.43: Mean values of the F_1 -score marginal distributions for the different free parameters of the new clustering algorithm, with the error bars representing one standard deviation around the mean. The F_1 -score values were computed for the 6561 possible parameter configurations using 1000 ν_μ CC interaction events.

3466 This algorithm has a total number of eight free parameters that need to be optimised.
 3467 I used a sample of 1000 ν_μ CC interactions in order to obtain the optimal configuration of
 3468 clustering parameters. This sample was generated up to the default ECal hit clustering
 3469 level, so then I could run the new clustering algorithm each time with a different
 3470 configuration of parameters. As the number of parameters is relatively large, I only
 3471 performed a coarse-grained scan of the parameter space. Sampling each of the eight
 3472 parameters at three different points each I obtain 6561 different configurations. These
 3473 parameters, together with the used values, are summarised in Tab. 6.5.

3474 In order to measure the performance of the clustering, I use a binary classification
 3475 approach. For each formed cluster, I identify the Geant4 Track ID of the matching MC
 3476 particle and the energy fraction of each hit. Then, I assign to each cluster the Track ID
 3477 with the highest total energy fraction. For each of the different Track IDs associated to
 3478 the clusters, I select the cluster with the highest energy (only from the hits with the
 3479 same Track ID). I identify such a cluster as the main cluster for that Track ID. I count
 3480 as true positives (TPs) the hits with the correct Track ID in each main cluster. False
 3481 positives (FPs) are the hits with the incorrect Track ID for the cluster they are in, not

6.6. NEUTRAL PARTICLE IDENTIFICATION

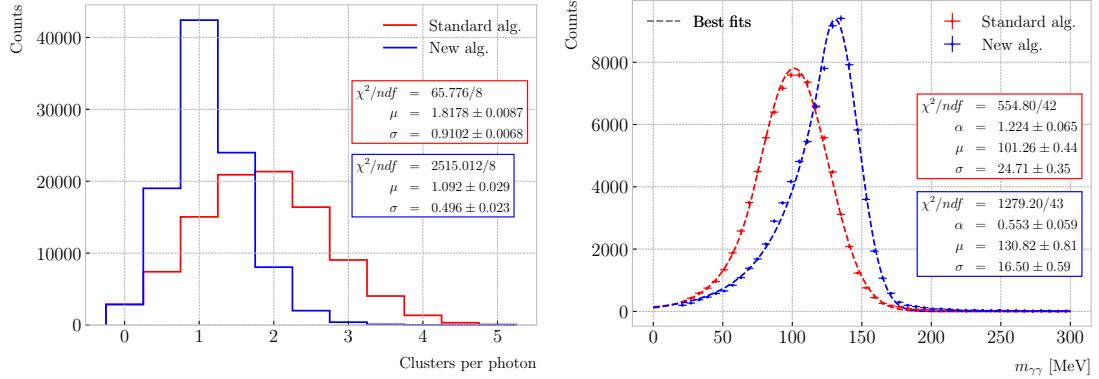


Figure 6.44: Left panel: distributions of the number of ECal clusters per photon from π^0 decays for the standard (red) and new (blue) clustering algorithms. Right panel: reconstructed invariant mass distributions for photon pairs from single π^0 events using the standard (red) and new (blue) ECal clustering algorithms.

only main clusters. The false negatives (FNs) are the hits with the correct Track ID in clusters other than the main.

Figure 6.43 shows the computed F_1 -score values for the different cuts. In each case, the central value represents the mean of the F_1 -score distribution for the specified value of the corresponding variable and the vertical error bar represents one standard deviation around the mean. Also shown are the Pearson correlation coefficients of these central values. We can see that five of the variables have a sizeable effect on the F_1 -score, with an absolute difference between the last and first values as big as 4%.

The working configuration is obtained as follows. I first select all configurations with purity $\geq 90\%$. Among those, I choose the combinations that yield the maximum F_1 -score. If more than one configuration remains I select the one with the highest sensitivity. Doing so, I end up with a parameter configuration with an efficiency of 88% and a 90% purity. Compared with the default algorithm, which gives an efficiency of 76% and a purity of 91% for the same sample, I have managed to improve the efficiency by a factor of 1.16.

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3497 6.6.2 π^0 reconstruction

3498 One of the potential applications of the new ECal hit clustering is the reconstruction of
3499 neutral particles, in particular pions. Neutral pions decay promptly after being produced,
3500 through the $\pi^0 \rightarrow \gamma\gamma$ channel (98.823 ± 0.034)% of the time. The photon pair does
3501 not leave any traces in the HPgTPC (unless one or both of them converts into an
3502 electron-positron pair), but each of them will produce an electromagnetic shower in
3503 the ECal.

3504 To test the potential impact of the new algorithm in π^0 reconstruction, I generated
3505 a MC sample of single, isotropic neutral pions inside the HPgTPC. All pions were
3506 generated with a momentum $p = 500$ MeV and their initial positions were uniformly
3507 sampled inside a $2 \times 2 \times 2$ m box aligned with the centre of the TPC. I ran both the
3508 default and the new clustering algorithms, using for the latter the optimised configuration
3509 discussed above.

3510 The first thing to notice is that the number of clusters produced per photon has
3511 decreased. Figure 6.44 (left panel) shows these distributions for the default (red) and
3512 new (blue) algorithms. Using a simple Gaussian fit, we see that the mean number of
3513 ECal clusters per photon went from 1.82 ± 0.01 to 1.09 ± 0.03 . This effectively means that
3514 with the new algorithm the ECal activity of one true particle is typically reconstructed
3515 as a single object. From the reconstruction point of view this can be an advantage. As
3516 now most of the photon energy ends up in a single ECal cluster, I can simply use cluster
3517 pairs to identify the π^0 decay.

3518 In general, one calculates the invariant mass of the photon pair as:

$$m_{\gamma\gamma} = \sqrt{2E_1E_2(1 - \cos \theta)}, \quad (6.33)$$

3519 where E_i are the energies of the photons and θ the opening angle between them. In this
3520 case I can use the energies deposited in the ECal and their incident directions. This
3521 quantity is computed for all possible pairs of clusters, using their position together with
3522 the true decay point. In a more realistic scenario, e.g. ν_μ CC interaction, one could use

6.7. INTEGRATION IN GArSOFT

3523 the position of the reconstructed primary vertex instead. I also tried to use the principal
3524 direction of the clusters, but that approach gave considerably worse results. For each
3525 event I only keep the pair with an invariant mass closer to the true π^0 mass value.

3526 Figure 6.44 (right panel) shows the invariant mass distributions for the photon pairs
3527 we get using the default (red) and the new (blue) ECal clustering algorithms. For the fit
3528 I used a modified version of the Crystal Ball function [178], obtained by taking the limit
3529 where the parameter controlling the power-law tail goes to infinity:

$$f(x; N, \mu, \sigma, \alpha) = N \cdot \begin{cases} e^{\frac{\alpha(2x-2\mu+\alpha\sigma)}{2\sigma}}; & x \leq \mu - \alpha\sigma, \\ e^{-\frac{(x-\mu)^2}{2\sigma^2}}; & x > \mu - \alpha\sigma. \end{cases} \quad (6.34)$$

3530 Comparing the fitted mean and standard deviation values for the Gaussian cores, we
3531 see that the distribution for the new algorithm is a 67% narrower and also peaks much
3532 closer to the true m_{π^0} value, going from 101.3 ± 0.4 MeV to 130.8 ± 0.6 MeV.

3533 6.7 Integration in GArSoft

3534 All the additions and improvements to the reconstruction discussed in this Chapter
3535 had to be integrated in the GArSoft framework. This is necessary both to allow a
3536 more streamlined path for development, as this makes testing and adding features
3537 straightforward, as well as make the changes usable in future productions of simulated
3538 data. In this section, I outline the current status of the integration in GArSoft of the
3539 reconstruction work presented above.

3540 The new track-cluster association code has been implemented in GArSoft, under
3541 the name of `TPCECALAssociation2`, and has now become the new default in the
3542 reconstruction. The structure of the module is similar to the previous implementation,
3543 and the data products they output are identical in form. Therefore, any existing code
3544 using the association objects does not need to be modified.

3545 The computation of the truncated mean dE/dx of the tracks, the evaluation of
3546 the muon score for muon and pion separation, and the estimation of the velocity from

CHAPTER 6. PARTICLE IDENTIFICATION IN ND-GAr

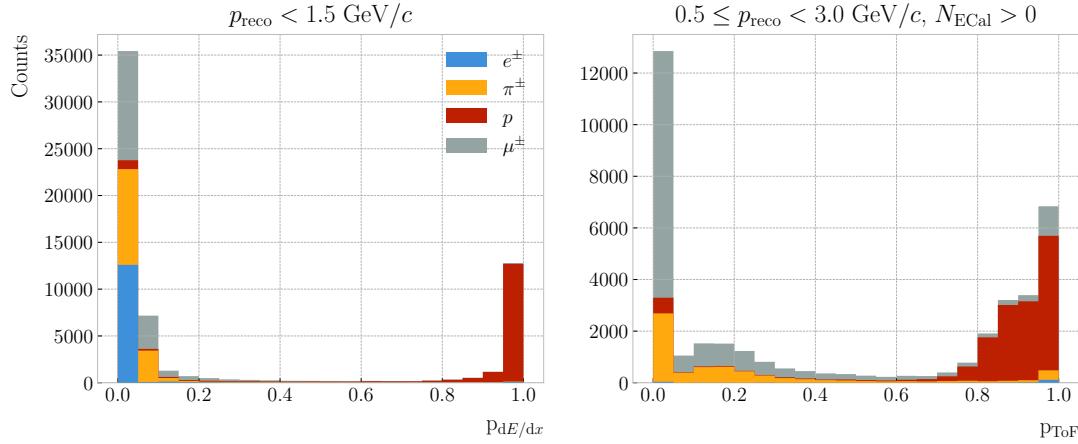


Figure 6.45: Distributions of proton dE/dx (left panel) and ToF (right panel) scores for a sample of 100000 FHC neutrino interactions in the HPgTPC. The distributions are broken down by the true particle type associated to the reconstructed particle.

time-of-flight are all orchestrated by the `CreateRecoParticles` module. Each one of these is implemented as a separate algorithm, which is then called by the parent module. This generates the `gar::rec::RecoParticle` products, a new high-level data object in GArSoft. These combine the information from the HPgTPC, ECal, and μ ID to create an object useful for analysers. At the moment, these data products are only generated for charged particles. However, in the future the module can be extended to incorporate other algorithms used for the identification of neutral particles, like neutral pions and neutrons.

Additionally, analogous to the muon score, the `gar::rec::RecoParticle` objects contain two other scores based on the $\langle dE/dx \rangle$ and ToF estimates which measure the “protoness” of a reconstructed particle. These are obtained in a number of momentum bins, and are a measure of the distance to the point in the corresponding distribution that maximises the F_1 -score for the proton separation. This distance is then transformed applying a sigmoid function, which produces a score in the 0 – 1 range, with coefficients obtained following a procedure similar to the one used to calibrate the response of the muon score. The dE/dx proton score is defined for all particles with momenta $p_{\text{reco}} < 1.5 \text{ GeV}/c$, whereas the ToF proton score is available for the particles with at least one associated hit in the inner ECal and momentum in the range $0.5 \leq p_{\text{reco}} < 3.0 \text{ GeV}/c$.

6.7. INTEGRATION IN GArSOFT

3565 As an example, Fig. 6.45 shows the distributions of the dE/dx (left panel) and ToF
3566 (right panel) proton scores for the reconstructed particles in a 100000 FHC neutrinos
3567 sample.

3568 The calculation of the track breakpoint variables for pion decay identification is
3569 currently implemented as an analysis module in GArSoft. It would be interesting to add
3570 this information to the `gar::rec::RecoParticle` products, possibly calling the code as
3571 an additional algorithm in the `CreateRecoParticles` module. However, the best way
3572 to propagate the information to the high-level objects is still unclear.

3573 About the new ECal clustering algorithm, it is still in a development phase, and
3574 as such it has not replaced the current clustering module. At the moment, its latest
3575 version is integrated in GArSoft as the `CaloClustering2` module. The algorithm used
3576 is implemented separately, and then invoked in the main code. The module can be
3577 run standalone on the outputs of the reconstruction, creating a second instance of the
3578 `gar::rec::Cluster` collection. In the future it may replace the current algorithm as
3579 the default in the reconstruction chain. However, more work is needed in order to
3580 understand its performance in all the different use cases.

3581

3582

Event selection in ND-GAr

3583 *You have power over your mind, not outside events. Realise this, and you will
3584 find strength.*

3585

– Marcus Aurelius, *Meditations*

3586 As discussed previously, it is necessary to evaluate the capabilities of ND-GAr at
3587 identifying different particles. In the context of the LBL analysis, we want ND-GAr to
3588 provide data samples containing events of specific topologies, like ν_μ CC $1\pi^\pm$, ν_μ CC
3589 $1p1\pi^\pm$, etcetera. Thus, developing a strategy for the event selection using the current
3590 reconstruction is required.

3591 In this Chapter, I present the results of a number of preliminary studies focused on
3592 the event selection in ND-GAr, particularly the ν_μ CC selection and the pion tagging
3593 strategies. I also investigate the neutrino energy reconstruction, as well as the systematic
3594 uncertainties relevant for our detector.

3595 7.1 Data sample

3596 For the event selection studies I used a MC sample consisting of 10^5 FHC neutrino
3597 interaction events inside the HPgTPC volume. The version of **GENIE** used was v3_04_00,
3598 with the G18 tune. This is a preliminary version of the re-tune produced from CCQE,
3599 CC1 π , CC2 π , and CC inclusive bubble chamber cross section data [179]. It uses the local
3600 Fermi gas as a description of the nuclear model. The quasielastic-like events are described
3601 by the Nieves quasielastic [180] and Valencia 2p2h [181] models. The Berger-Seghal

CHAPTER 7. EVENT SELECTION IN ND-GAR

3602 model [182, 183] is used for the resonant and coherent pion production. As in all the
3603 GENIE tunes, the Bodek-Yang model [184] describes the DIS interactions. Finally, the
3604 FSI are described using the effective intranuclear transport model in INTRANUKE.

3605 For this sample, I used `GArG4` instead of `edep-sim` for the particle propagation.
3606 Because both `Geant4` wrappers use different configurations for the simulation, the results
3607 obtained are different. The default `edep-sim` configuration used by the DUNE ND
3608 is appropriate for ND-LAr, where thresholds for particle production are higher. In
3609 the case of ND-GAr, these parameters need to be adjusted accordingly. For the time
3610 being, in these first productions of analysis files, we will use our standalone `Geant4`
3611 implementation.

3612 The detector simulation and reconstruction used was GArSoft version v02_21_00. I
3613 made use of the standard routines for the readout simulation and the reconstruction,
3614 which include the additions described in section 6.7. A summary of the GArSoft outputs
3615 is extracted in the form of a plain `ROOT TTree`. These are then used, together with the
3616 GENIE output files, to produce the files known within DUNE as common analysis files
3617 (CAFs). The version of the CAF format used in this analysis is `duneanaobj v3_07_00`.

3618 This sample only includes single interaction events. In the future, we will move
3619 to simulate full neutrino spills. Also, we will need to include neutrino interactions in
3620 the other detector volumes (ECal, magnet, . . .), as well as rock muons making it to
3621 ND-GAr. However, this will require a significant amount of work to go into the so-called
3622 interaction slicer, the part of the reconstruction in charge of splitting the reconstructed
3623 events.

3624 Looking forward, these sort of small samples are useful to prepare for launching a
3625 full production of ND-GAr events. In the original DUNE TDR LBL analysis, the event
3626 rates are calculated with a 1.1×10^{21} POT/year assumption, which assumes a combined
3627 uptime and efficiency of the accelerator complex and the LBNF beamline of 57% [59].
3628 If we have one spill every 1.2 s, that translates into 7.5×10^{13} POT/spill. Therefore,
3629 assuming that the POT/spill scales linearly with beam power, in Phase II we will have
3630 1.3×10^{14} POT/spill for the for the 2.1 MW beam. Or equivalently, 1.9×10^{21} POT/year

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Table 7.1: Estimated event rates in ND-GAr, divided by interaction type and pion multiplicity, for two different values of the POT/year.

Process	Events/ton/year	
	1.1×10^{21} POT/year	1.9×10^{21} POT/year
All ν_μ -CC	1.60×10^6	2.83×10^6
CC 0π	5.28×10^5	9.35×10^5
CC $1\pi^\pm$	3.02×10^5	5.34×10^5
CC $1\pi^0$	1.65×10^5	2.92×10^5
CC 2π	3.18×10^5	5.63×10^5
CC 3π	1.36×10^5	2.41×10^5
CC other	1.52×10^5	2.69×10^5
All $\bar{\nu}_\mu$ -CC	7.54×10^4	1.33×10^5
All NC	5.50×10^5	9.73×10^5
All ν_e -CC	2.70×10^4	4.78×10^4

3631 using the same efficiency. The event rates per year in ND-GAr computed for these two
 3632 possible values of the POT/year are shown in Tab. 7.1.

3633 The latest PRISM plan requires 1.50 POT · years of data on-axis, followed by
 3634 0.25 POT · years at each off-axis position ($2, 4, 8, 12, 16, 20, 24$, and 28 m), both for
 3635 FHC and RHC mode. This implies that a full on-axis ND-GAr production will require
 3636 a total of 2.85×10^{21} POT for both horn currents. The production of these samples
 3637 is necessary to understand the impact of ND-GAr on the LBL sensitivities, and the
 3638 studies presented here should be considered as a first step towards the realisation of
 3639 such analysis.

3640 7.2 ν_μ CC selection

3641 In a ν_μ CC inclusive selection, the signal topology we look for is a neutrino-induced
 3642 muon with or without other final state particles. Here, I also require the neutrino vertex
 3643 to be located inside the fiducial volume (FV) of ND-GAr.

3644 The FV is defined as a smaller cylinder within the cylindrical volume of the HPgTPC.

CHAPTER 7. EVENT SELECTION IN ND-GAR

3645 The FV has a radius R_{FV} and a half-length L_{FV} . For a particle position to lie within
3646 the FV it must satisfy:

$$\vec{x}_i \in \left\{ \vec{x} \in \mathbb{R}^3 \mid |x_0| \leq L_{\text{FV}} \text{ \& } \sqrt{x_1^2 + x_2^2} \leq R_{\text{FV}} \right\}, \quad (7.1)$$

3647 in the reference frame of the HPgTPC. For convenience, I define:

$$\begin{aligned} \Delta R_{\text{FV}} &= R_{\text{HPgTPC}} - R_{\text{FV}}, \\ \Delta L_{\text{FV}} &= L_{\text{HPgTPC}} - L_{\text{FV}}, \end{aligned} \quad (7.2)$$

3648 where R_{HPgTPC} and L_{HPgTPC} refer to the radius and the half-length of the HPgTPC,
3649 respectively. Figure 7.1 shows the HPgTPC volume with the FV inside of it. In that
3650 representation, the FV is defined as $\Delta L_{\text{FV}} = 30.0$ cm and $\Delta R_{\text{FV}} = 30.0$ cm. Also shown
3651 is the HPgTPC reference frame, with x being the drift direction and z aligned along the
3652 beam direction.

3653 In some cases, it is interesting to divide the signal events in different categories
3654 based on their true interaction mode. In this work, I will distinguish between charged-
3655 current quasi-elastic (CCQE), coherent (CCCOH), resonant (CCRES), and deep-inelastic
3656 (CCDIS) interactions. I also use a separate category for the interactions not included in
3657 any of the other categories (CCOther).

3658 Any other events are considered backgrounds. For this selection, I use the following
3659 categorisation of background events:

- 3660 • Out of FV: if the true neutrino vertex lies outside the defined FV.
- 3661 • NC: if the event is a true neutral-current event.
- 3662 • $\bar{\nu}_\mu$ CC: if the true neutrino candidate is of muon antineutrino flavour.
- 3663 • Other: if the event is not signal nor falls in any of the other background categories.

3664 The key to the CC selection is the identification of a primary muon candidate.
3665 Typically, this is the longest track in the event. However, sometimes protons and pions

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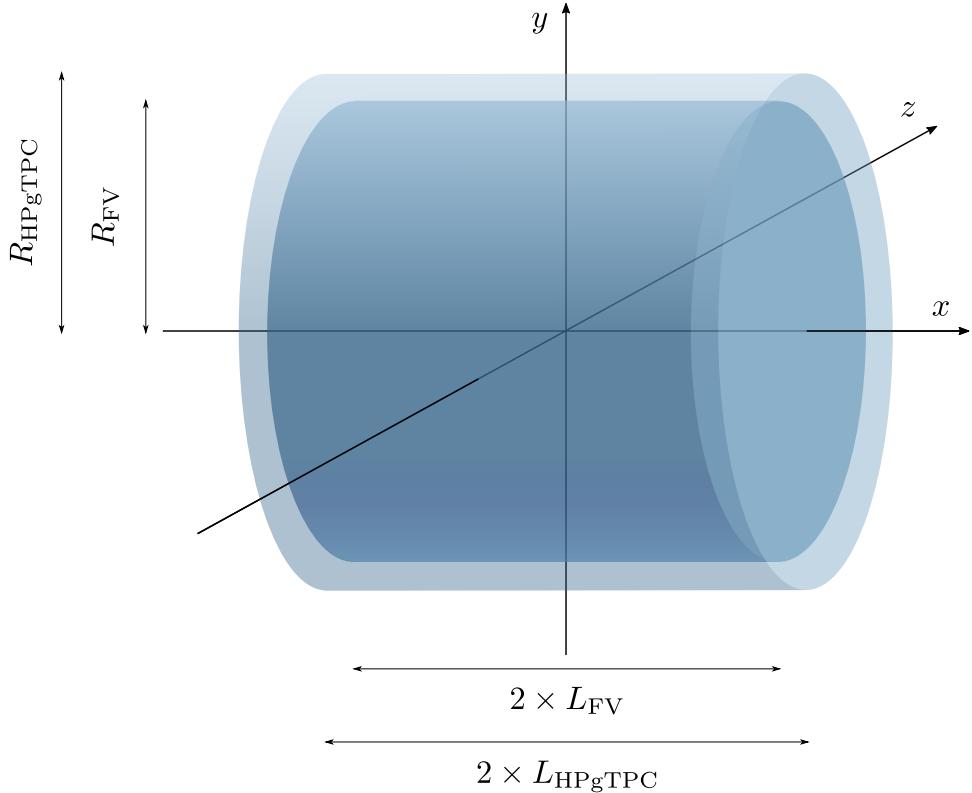


Figure 7.1: Schematic diagram of the HPgTPC including the fiducial volume (FV). In this case the FV is given by $\Delta L_{\text{FV}} = 30.0$ cm and $\Delta R_{\text{FV}} = 30.0$ cm.

3666 leave tracks longer than that of the muon. This is particularly important in the GAr
 3667 medium, considerably less dense than the LAr. For this reason, the muon identification
 3668 in ND-GAr relies heavily on the capabilities of the ECal.

3669 The selection strategy proposed combines the information coming from the three
 3670 main detection systems of ND-GAr: the HPgTPC charge readout, and the ECal and
 3671 μ ID detectors. It consists of five steps:

- 3672 1. Event contains reconstructed particles.
 3673 2. Select particles with reconstructed negative charge, $q_{\text{reco}} = -1$.
 3674 3. Select particles passing the muon score cut, $\mu_{\text{score}} \geq \mu_{\text{score}}^{\text{cut}}$.
 3675 4. Keep reconstructed particle with the highest momentum, $\max [p_{\text{reco}}]$.
 3676 5. Check that the remaining particle starts within the FV.

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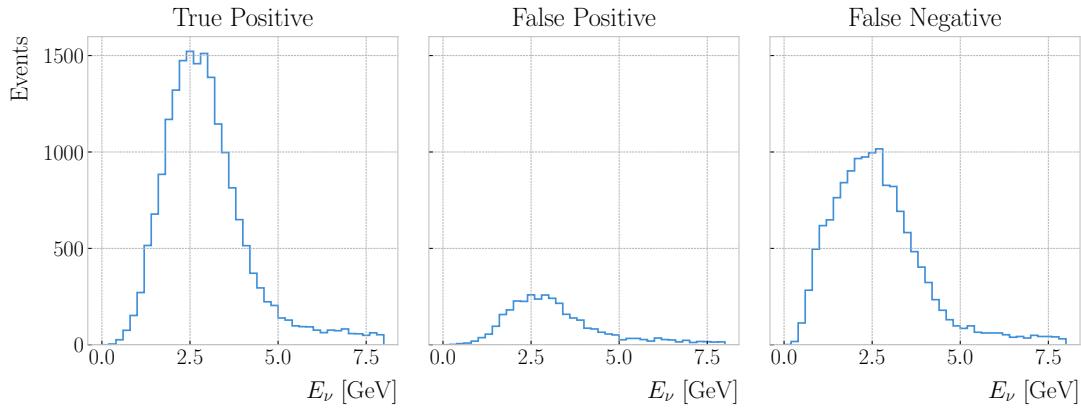


Figure 7.2: True positive (left panel), false positive (middle panel), and false negative (right panel) true neutrino energy distributions for the ν_μ CC selection given by a muon score cut of $\mu_{\text{score}}^{\text{cut}} = 0.75$, and a FV defined as $\Delta L_{\text{FV}} = 30.0$ cm and $\Delta R_{\text{FV}} = 30.0$ cm.

3677 All the events passing these cuts are classified as signal, and the selected particle is
 3678 regarded as the primary muon candidate.

3679 **7.2.1 Selection optimisation**

3680 I performed an optimisation of this selection, comparing the performance of a number of
 3681 configurations. For the muon selection, I varied the value of $\mu_{\text{score}}^{\text{cut}}$ from 0.05 to 0.95,
 3682 using a step size of 0.05. Additionally, to optimise the FV, I systematically explored a
 3683 number of different parameter configurations, moving within the 10.0 – 70.0 cm range for
 3684 ΔL_{FV} and 25.0 – 75.0 cm for ΔR_{FV} , in increments of 10.0 cm and 5.0 cm respectively.

3685 For each parameter configuration, I extract three different true neutrino energy
 3686 distributions. These are built combining the results of the selection described previously,
 3687 which we can refer to as the “reco” selection, and a “true” selection. The later identifies
 3688 the true ν_μ CC events using the GENIE event records, and checks that the true neutrino
 3689 vertices are contained in the FV.

3690 The first distribution consists of the events passing both selections, i.e., these are
 3691 the true ν_μ CC events which pass the “reco” selection. The second distribution contains
 3692 the events passing the “reco” selection but failing the “true” selection. These are
 3693 the background events that the selection misidentifies. Finally, the third distribution

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3694 corresponds to the events picked by the “true” selection but not by the “reco” one. In
 3695 other words, these are the true ν_μ CC events that our selection misses. In analogy to
 3696 the machine learning jargon, I refer to these distributions as the true positive (TP),
 3697 false positive (FP), and false negative (FN) spectra, respectively. Figure 7.2 shows an
 3698 example of these three distributions for the case $\mu_{\text{score}}^{\text{cut}} = 0.75$, $\Delta L_{\text{FV}} = 30.0$ cm, and
 3699 $\Delta R_{\text{FV}} = 30.0$ cm.

3700 By making different combinations of these distributions one can compute a series of
 3701 performance metrics. Using the full information from the spectra allows to obtain the
 3702 scores as a function of the true neutrino energy, whereas the totals can be obtained by
 3703 integrating the histograms. This way, the efficiency of the selection is given by:

$$\begin{aligned} \text{Efficiency} &= \frac{\text{Selected true } \nu_\mu \text{ CC events}}{\text{Total true } \nu_\mu \text{ CC events}} \\ &= \frac{\text{TP}}{\text{TP} + \text{FN}}, \end{aligned} \quad (7.3)$$

3704 while the purity can be written as:

$$\begin{aligned} \text{Purity} &= \frac{\text{Selected true } \nu_\mu \text{ CC events}}{\text{Total selected events}} \\ &= \frac{\text{TP}}{\text{TP} + \text{FP}}. \end{aligned} \quad (7.4)$$

3705 Another scoring metric typically used when quantifying the performance of a selection
 3706 is the significance. It is defined as:

$$\text{Significance} = \frac{S}{\sqrt{S+B}} = \frac{\text{TP}}{\sqrt{\text{TP}+\text{FP}}}. \quad (7.5)$$

3707 The significance measures the relative size of the true signal within the selection, $S = \text{TP}$
 3708 with respect to one standard deviation of the counting experiment. Assuming Poisson
 3709 statistics, the variance is equal to the number of observations, and therefore the standard
 3710 deviation equals to $\sqrt{N} = \sqrt{S+B} = \sqrt{\text{TP}+\text{FP}}$. I use this metric to

3711 Figure 7.3 shows the change in efficiency (blue) and purity (red) of the ν_μ CC
 3712 selection as a function of the different cuts. From left to right, I vary $\mu_{\text{score}}^{\text{cut}}$, ΔL_{FV} ,

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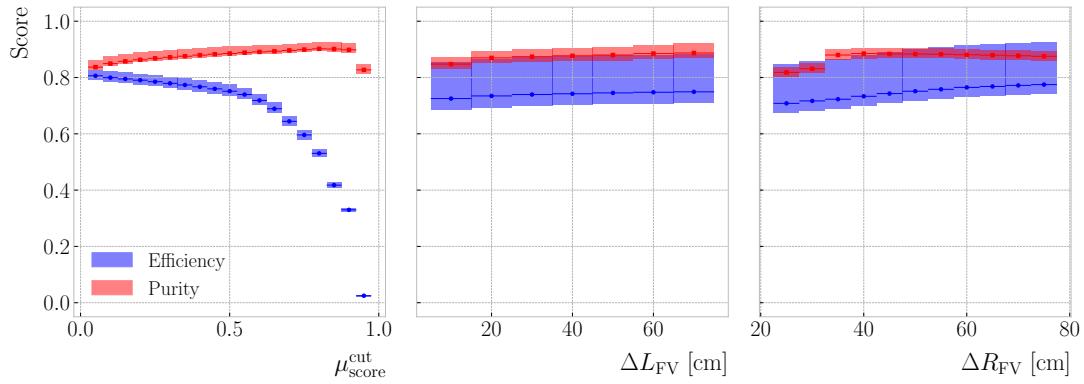


Figure 7.3: Efficiency (blue) and purity (red) for the ν_μ CC selection as a function of the muon score cut (left panel), FV half-length cut (middle panel), and radial cut (right panel). The height of the boxes represents the IQR of the conditional distributions, whereas the horizontal line corresponds to the median.

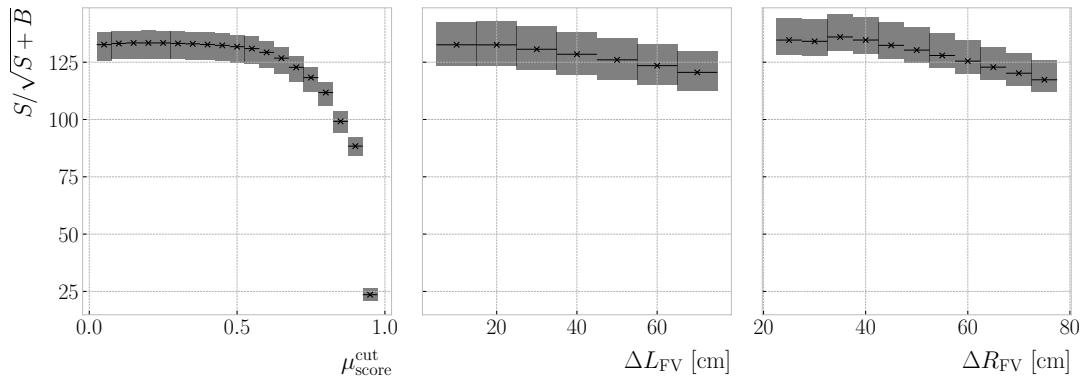


Figure 7.4: Significance for the ν_μ CC selection as a function of the muon score cut (left panel), FV half-length cut (middle panel), and radial cut (right panel). The height of the boxes represents the IQR of the conditional distributions, whereas the horizontal line corresponds to the median.

3713 and ΔR_{FV} . For each value of the cuts, I compute the median and IQR (represented
 3714 by the horizontal lines and the heights of the boxes, respectively) of the corresponding
 3715 conditional distributions of efficiency and purity. This representation is useful to get
 3716 an idea of the general trend the scores follow with the cuts, as well as the spread. It
 3717 is clear that the muon score cut has the biggest impact on the efficiency, which ranges
 3718 between 0.05 to 0.80, whereas the purity remains stable with values around 0.85.

3719 A similar depiction of the significance can be found in Fig. 7.4. In this case, one can
 3720 see that the $S/\sqrt{S+B}$ decreases as the cuts grow tighter. However, there are hints of

7.2. ν_μ CC SELECTION

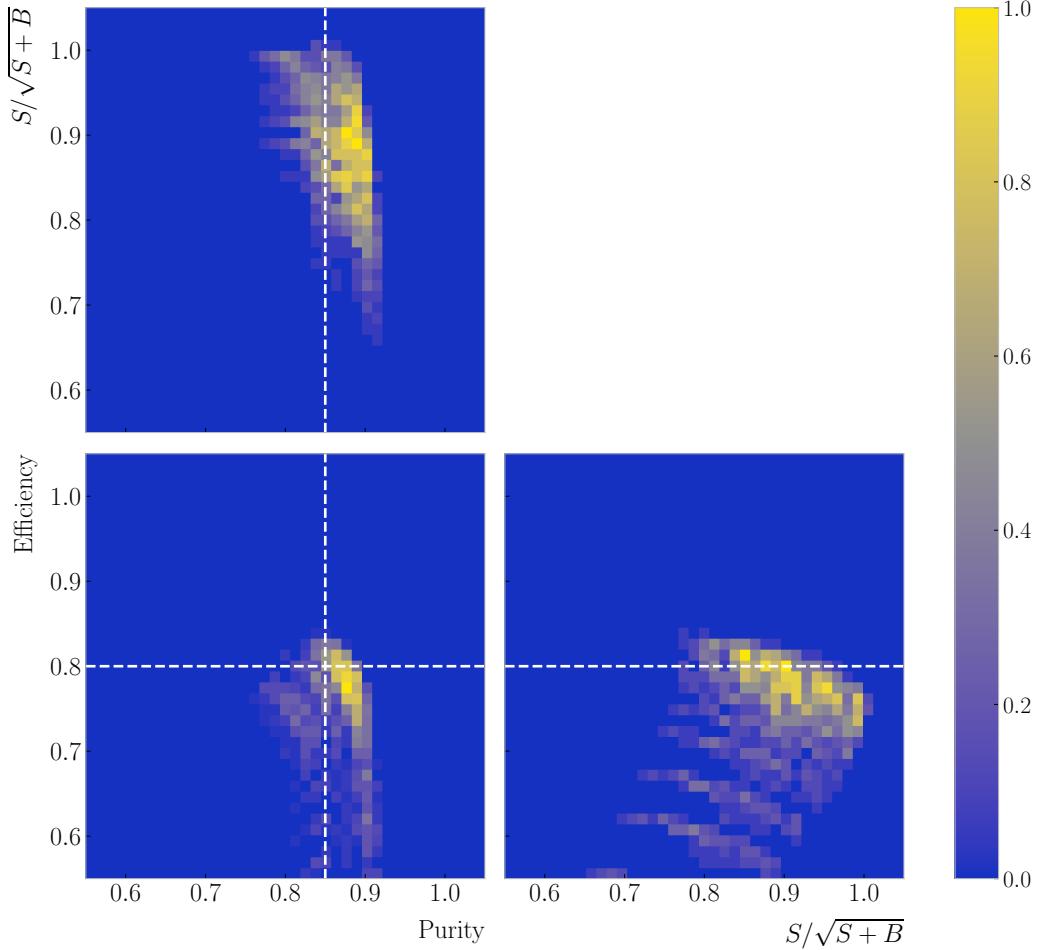


Figure 7.5: Normalised 2D distributions of efficiency, purity and significance for the ν_μ CC selection. The $S/\sqrt{S+B}$ is normalised to the highest value achieved. The vertical dashed line indicates a purity value of 0.85, whereas the horizontal one corresponds to an efficiency of 0.80.

3721 local maxima at intermediate values.

3722 Selecting the cut configuration with the highest significance, 147 ± 11 for the parameter
 3723 values explored here, results in an efficiency and purity of 0.754 ± 0.006 and 0.833 ± 0.007 ,
 3724 respectively. Figure 7.5 shows the 2D distributions resulting when combining pairs of
 3725 efficiency, purity and significance, obtained for the cut configurations explored. The
 3726 significance is normalised to the highest value obtained in the parameter scan. Looking
 3727 at this, it is clear that a selection with highest efficiency and purity can be achieved,
 3728 maintaining a similar significance level.

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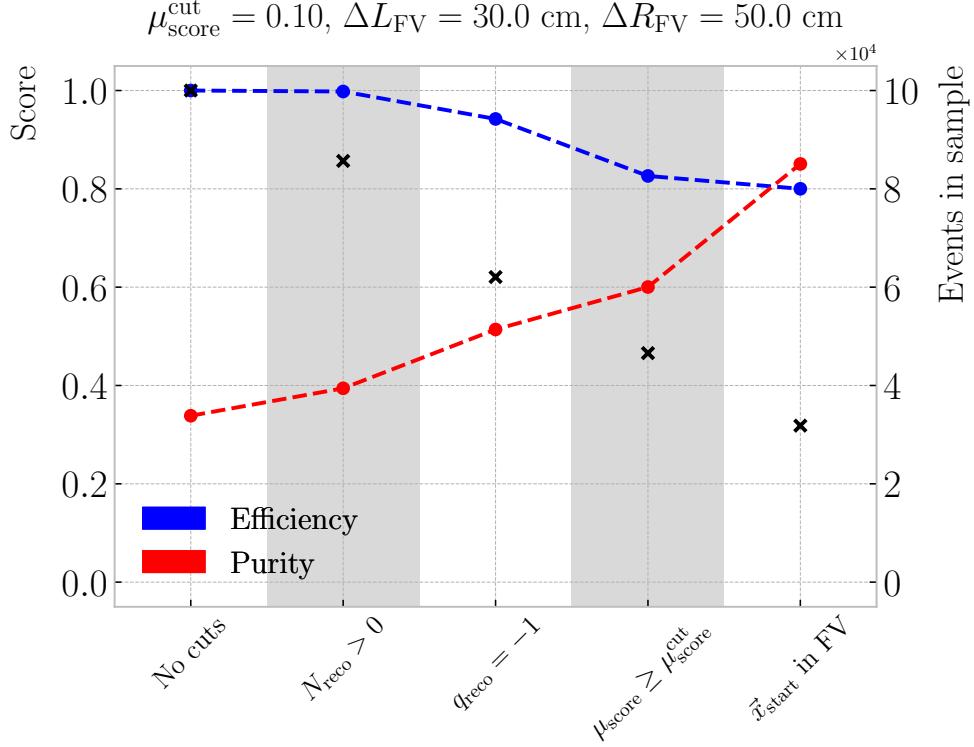


Figure 7.6: Cumulative efficiency (blue) and purity (red) of the ν_μ CC selection. The secondary axis indicates the number of events in the sample after each cut (black crosses).

Table 7.2: Step-by-step ν_μ CC selection cuts and cumulative passing rates. Relative passing rates are indicated in parentheses.

Cut #	Selection cut	Events	Passing rates
0	Total number of events (No cuts)	100000	100.00% (100.00%)
1	At least one reconstructed particle	85680	85.68% (85.68%)
2	Negatively charged particles only	62054	62.05% (72.43%)
3	$\mu_{\text{score}} \geq \mu_{\text{score}}^{\text{cut}}$	46585	46.59% (75.07%)
4	Candidate \vec{x}_{start} in FV	31834	31.83% (68.34%)

3729 Therefore, to get a more refined selection, I first select the configurations with a
 3730 purity and an efficiency higher than 0.85 and 0.80, respectively. After that, I select the
 3731 tuple of cuts yielding the highest significance. The resulting value for the muon score
 3732 cut is $\mu_{\text{score}}^{\text{cut}} = 0.10$, and the FV is given by $\Delta L_{\text{FV}} = 30.0 \text{ cm}$ and $\Delta R_{\text{FV}} = 50.0 \text{ cm}$.
 3733 With these, one obtains a total efficiency of 0.800 ± 0.007 and purity of 0.851 ± 0.008 ,

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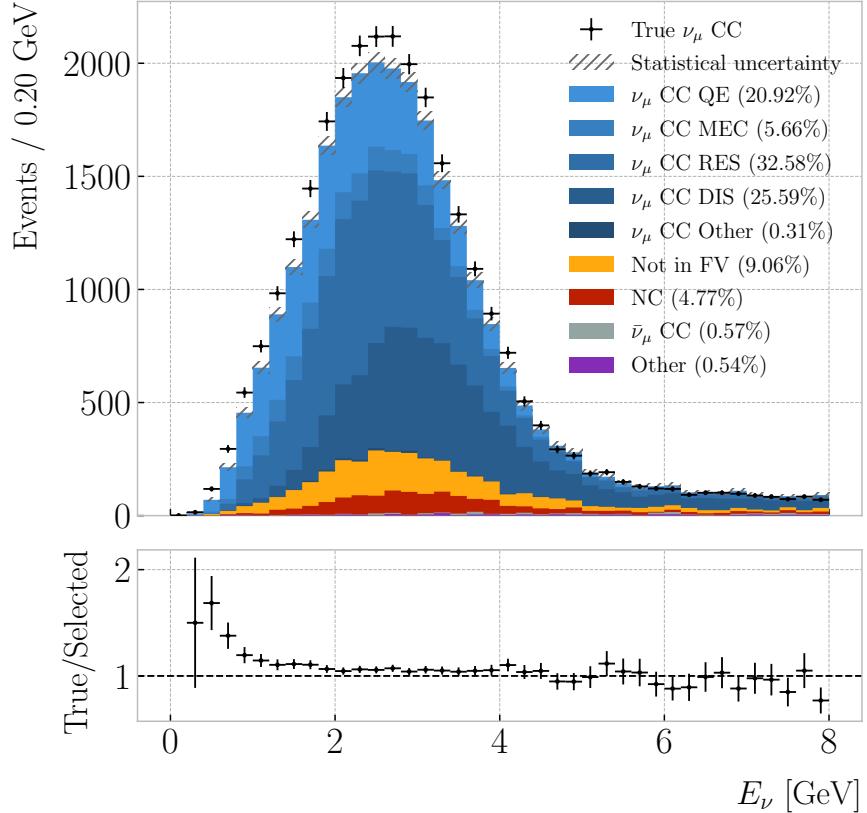


Figure 7.7: True neutrino energy spectra for the ν_μ CC selection. The selected events correspond to the coloured stacked histogram, broken down by signal and background subcategories. The statistical uncertainty is drawn in hatched gray. The true distribution is also shown with the black data points. The bottom panel shows the ratio between the number of true and selected ν_μ CC events per bin.

3734 with a significance of 138 ± 11 . Hereafter, I use this optimised selection cuts, unless
 3735 specified otherwise.

3736 A summary of the selection can be found in Tab. 7.2. It shows the number of
 3737 events in the selected sample after each selection cut, as well as the absolute and relative
 3738 passing rates. Figure 7.6 shows the overall efficiencies (blue) and purities (red) after
 3739 each cut in the event selection is applied. As expected, the efficiency drops while the
 3740 purity increases with the successive cuts.

3741 Notice how, out of the cuts prior to the FV constraint, the sign selection produces
 3742 the highest increase in purity. This is one of the advantages of having a magnetised
 3743 TPC, and can also be used for a $\bar{\nu}_\mu$ CC selection when running in RHC mode.

CHAPTER 7. EVENT SELECTION IN ND-GAR

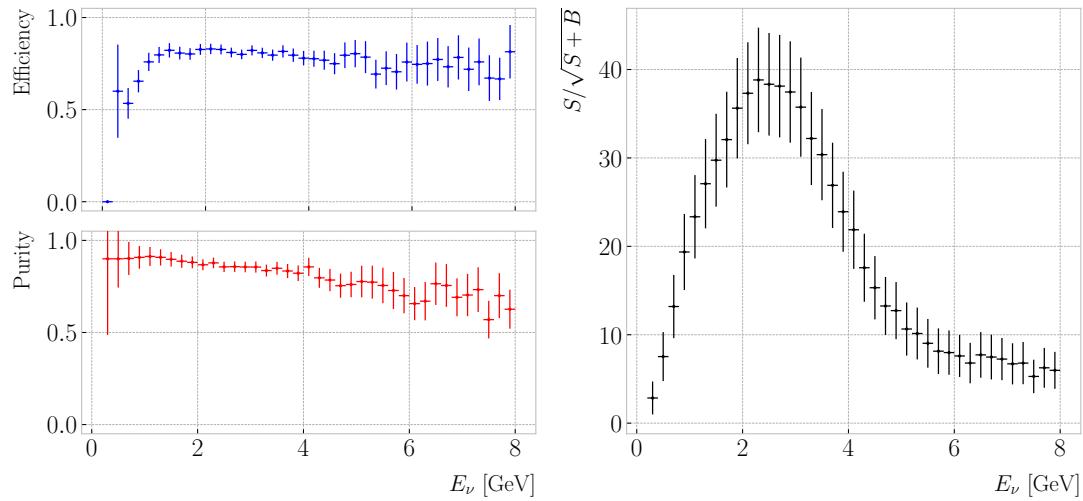


Figure 7.8: Left panel: efficiency (top panel) and purity (bottom panel) for the ν_μ CC selection as a function of the true neutrino energy. Right panel: significance for the ν_μ CC selection as a function of the true neutrino energy

3744 7.2.2 Selection performance

3745 Using the stored spectra discussed above, the true neutrino energy distribution for the
 3746 selected events can be recovered doing TP + FP. Similarly, the combination TP + FN
 3747 gives the true spectrum. Figure 7.7 shows the true (black data points) and selected
 3748 (coloured stacked histogram) E_ν distributions for the optimised ν_μ CC selection. The
 3749 colours in the selected spectrum indicate the different signal categories and backgrounds,
 3750 with the overall statistical uncertainty represented by the gray hatched mess. The ratio
 3751 between the true and selected events is also shown. One can see that it sits around 1 for
 3752 most of the energy range. However, for energies ≤ 1 GeV there is a significant deficit of
 3753 selected events.

3754 These spectra also allow to compute the efficiency and purity of the selection as
 3755 a function of the true neutrino energy, as shown in Fig. 7.8 (left panel). As it could
 3756 be expected from the previous ratio plot, the efficiency is low at low neutrino energies.
 3757 Nonetheless, it raises quickly with the energy, until it stabilises around a value of 0.80.
 3758 Looking at the purity, one may notice that, although it starts at around 0.90, there is a
 3759 significant decrease towards the high end of the spectrum. Figure 7.8 (right panel) also

7.2. ν_μ CC SELECTION

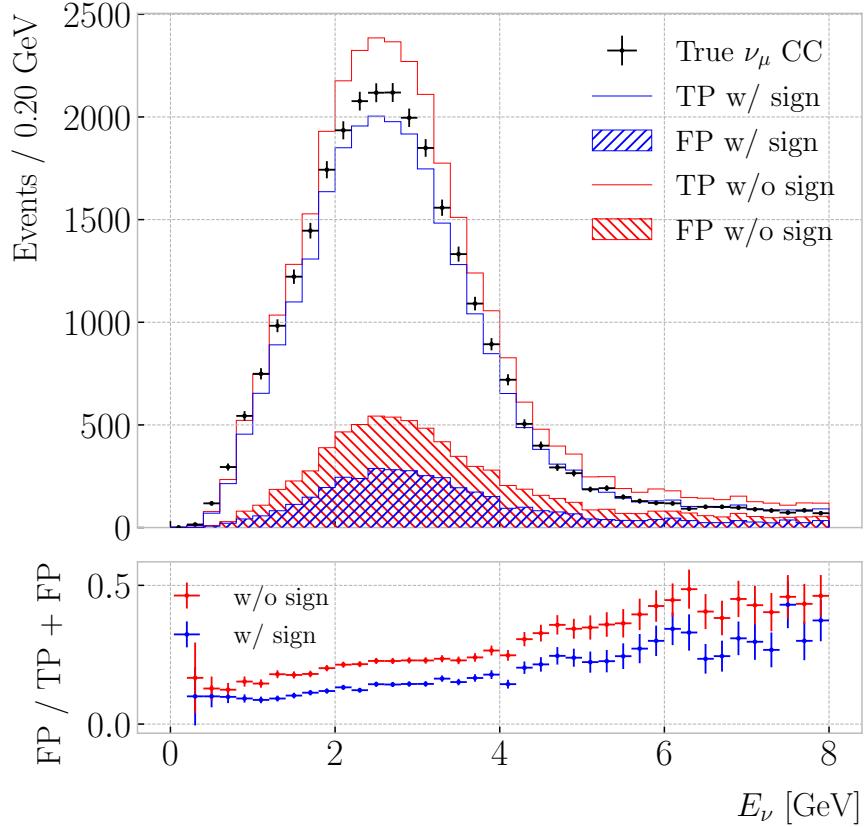


Figure 7.9: True neutrino energy spectra for the ν_μ CC selection with (blue) and without (red) sign selection. The selected events are broken down by true positives (signal) and false positives (background). The true distribution is also shown (black data points). The bottom panel shows the ratios between the number of false positives and total selected events per bin.

3760 shows the significance as a function of the energy. In this case, the highest $S/\sqrt{S+B}$ is
 3761 achieved around the energies where the spectrum peaks.

3762 A variation of the ν_μ CC selection one can try is to apply it without the reconstructed
 3763 charge cut. Figure 7.9 (top panel) shows the E_ν distributions corresponding to the
 3764 selection with (blue stacked histogram) and without (red stacked histogram) the sign
 3765 selection. In the former case, the out of FV contamination amounts to 9.06% of the
 3766 total, while the NC contamination results 4.77% and the wrong-sign contamination
 3767 0.57%. For the later, these backgrounds account for the 10.01%, 10.82%, and 2.18%
 3768 of the selected events, respectively. As expected, removing the positive particles does
 3769 not change the FV-related effects noticeably. However, the sign selection proves its

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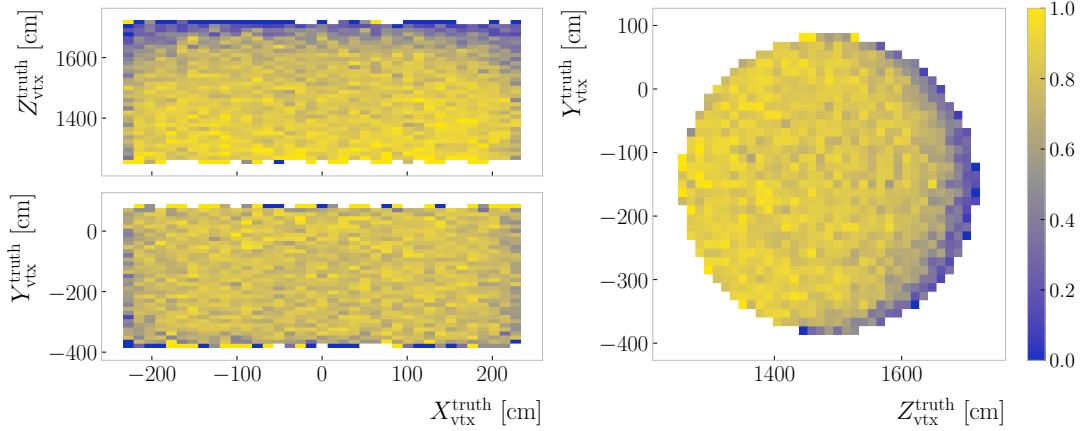


Figure 7.10: Efficiency 2D distributions for the ν_μ CC selection given the true position of the interaction vertex.

3770 worth in the rejection of $\bar{\nu}_\mu$ CC events, which drop almost by one order of magnitude.

3771 Additionally, the charge selection cuts the NC events in half, as it reduces the chances

3772 of misidentifying a positively charged hadron for a muon.

3773 As an additional check, I explored how the performance of the ν_μ CC selection
 3774 depends on the position of the neutrino interaction within the HPgTPC. Maps of the
 3775 selection efficiency for the X, Z (top left panel), X, Y (bottom left panel), and Z, Y
 3776 (right panel) true vertex position pairs are given in Fig. 7.10. It can be seen that the
 3777 efficiency remains stable along the drift direction, only slightly degrading close to the
 3778 edges of the FV. Regarding the radial direction, it is clear that an important number of
 3779 events with high $Z_{\text{vtx}}^{\text{truth}}$ are not being selected. Intuitively, the muons arising from these
 3780 interactions will leave short tracks. As their directions are typically aligned with the
 3781 beam direction, they enter the ECal shortly after production. This is likely to affect
 3782 the tracking, and therefore their identification. As a result, the regions with the lowest
 3783 efficiency are the downstream corners of the HPgTPC, i.e. the areas with high $|X_{\text{vtx}}^{\text{truth}}|$
 3784 and $Z_{\text{vtx}}^{\text{truth}}$.

3785 7.2.3 Primary muon kinematics

3786 This ν_μ CC selection relies on the identification of the a primary muon, meaning that
 3787 for each selected event a particle is picked out as the muon candidate. It is because of

7.2. ν_μ CC SELECTION

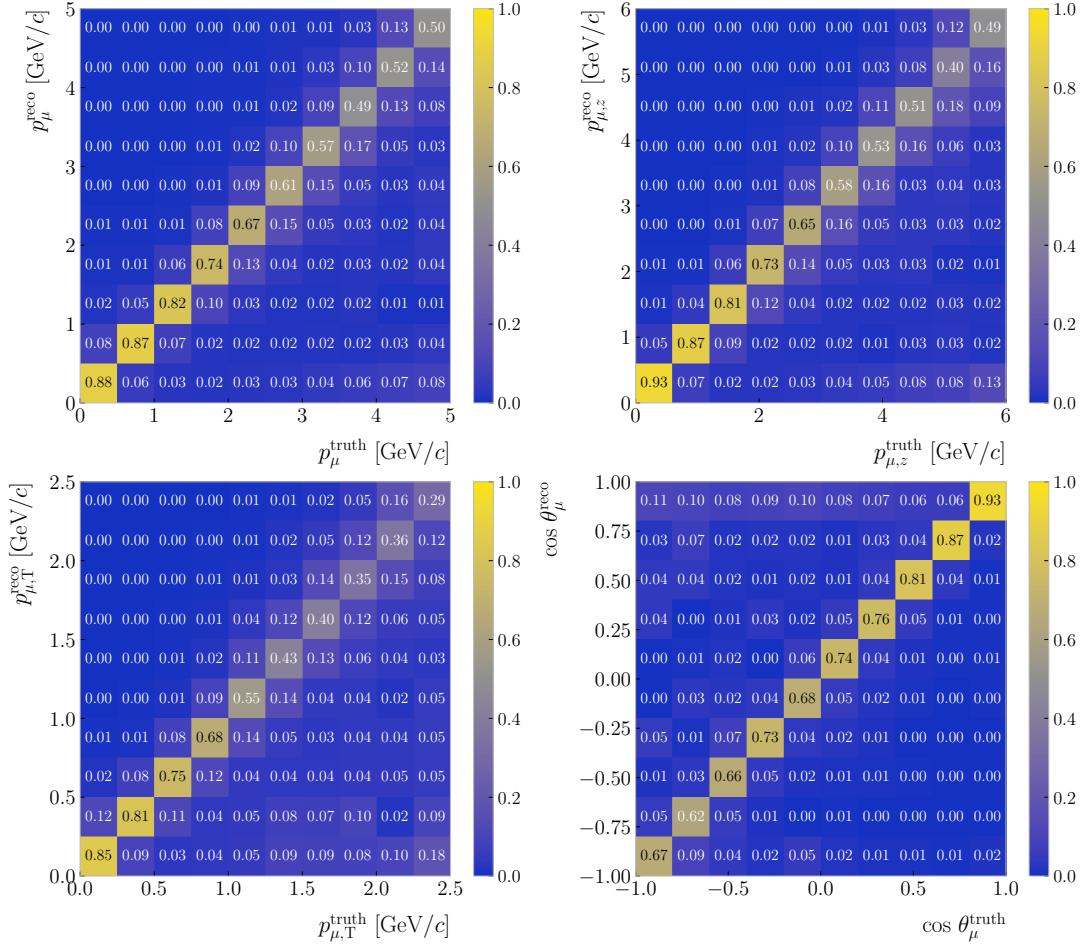


Figure 7.11: Distributions for the reconstructed versus truth generated primary muon momentum (top left panel), longitudinal momentum (top right panel), transverse momentum (bottom left panel), and beam angle (bottom right panel). The reconstructed values correspond to the selected primary muon candidate, whereas the truth values come from the true primary muon in the event.

3788 this that one can study the kinematics of these selected primary muons.

3789 Figure 7.11 shows a comparison between some of the reconstructed and truth primary
 3790 muon kinematic variables. From top to bottom, left to right, we have muon momentum,
 3791 longitudinal momentum, transverse momentum and beam angle. The histograms are
 3792 column-normalised, and so the diagonal entries give an idea of the resolution for the
 3793 different variables. The match between truth and reconstructed values can only be done
 3794 for the selected true ν_μ CC events, as the others do not have a primary muon. However,
 3795 for this comparison I do not require the events to start inside the FV.

CHAPTER 7. EVENT SELECTION IN ND-GAR

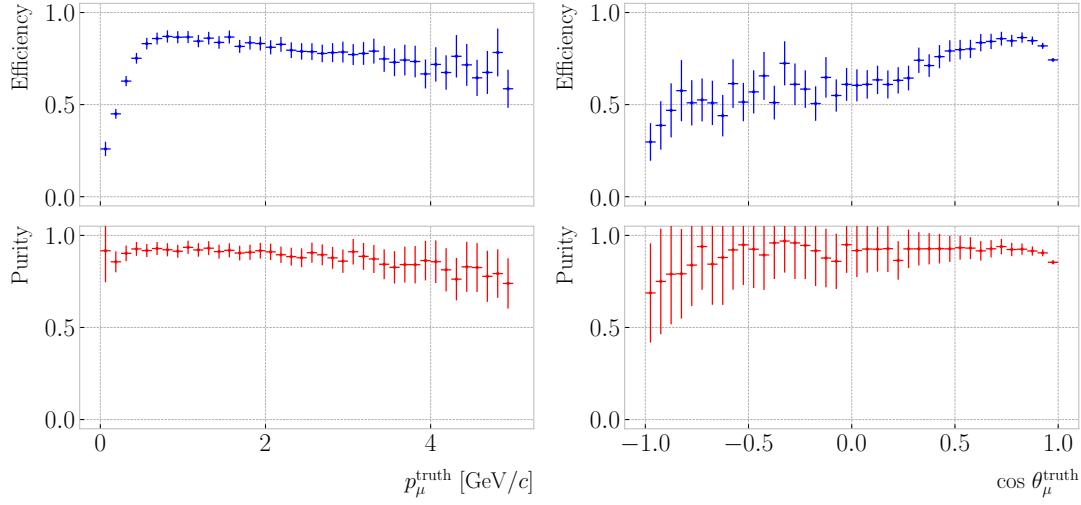


Figure 7.12: Efficiency (blue) and purity (red) of the ν_μ CC selection as a function of the primary muon true momentum (left panel) and beam angle (right panel).

3796 Notice that, for the reconstructed values, the variables do not necessarily come
 3797 from a reconstructed particle that matches the true primary muon. In other words,
 3798 sometimes, even though the event was correctly identified, the primary muon may have
 3799 been confused with another particle. That means that in these distributions include
 3800 both reconstruction and selection deficiencies.

3801 I also studied the performance of the ν_μ CC selection as a function of the kinematic
 3802 variables of the primary muon. As before, these metrics are only possible to compute for
 3803 true ν_μ CC events. The efficiency (top panels) and purity (bottom panels) as a function
 3804 of the truth muon momentum (left) and beam angle (right) are shown in Fig. 7.12. One
 3805 can see that there are some similarities in the behaviour of both metrics between the
 3806 true neutrino energy and the muon momentum cases. This is to be expected, as these
 3807 two variables are highly correlated. For the efficiency, there is a rapid increase at low
 3808 momentum values until it peaks at around 1 GeV/c, after which it starts decreasing
 3809 slowly. The purity remains relatively constant, with a slight drop towards high p_μ^{truth}
 3810 values. In the case of the muon angle, the decrease in efficiency at high $\theta_\mu^{\text{truth}}$ is more
 3811 noticeable. However, note that the number of events with backward-going muons is
 3812 much smaller than those aimed towards the forward direction, as can be seen from the

7.2. ν_μ CC SELECTION

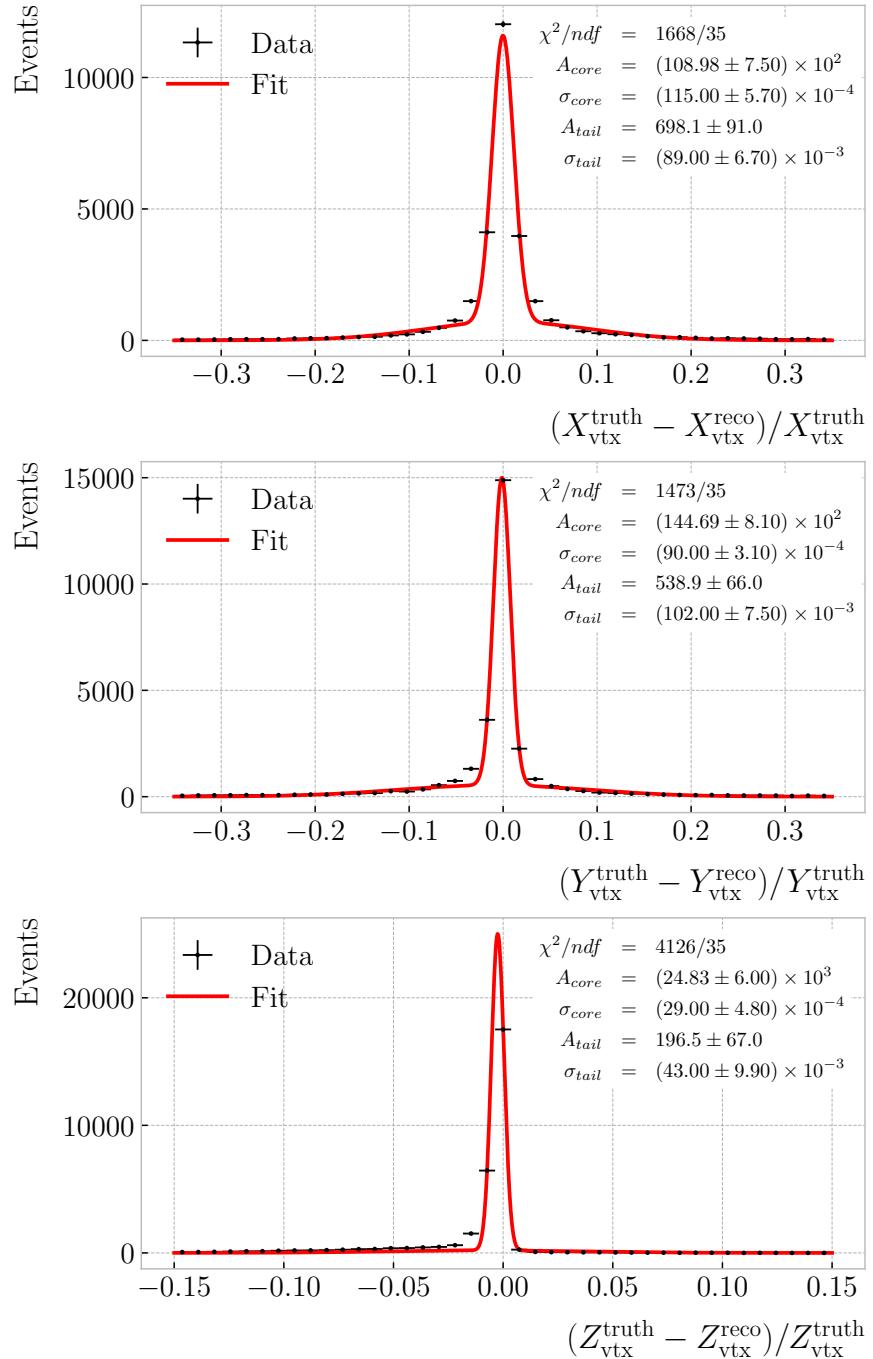


Figure 7.13: Fractional residual distributions for the position of the primary vertex in the ν_μ CC selection. The best fits to a double Gaussian function are also shown (red lines).

CHAPTER 7. EVENT SELECTION IN ND-GAR

3813 size of the vertical error bars. There is also a decline in the purity with the beam angle,
3814 but this effect is much smaller.

3815 A byproduct of selecting the primary lepton in the interaction is the position
3816 of the reconstructed neutrino vertex candidate. Checking how the position of the
3817 selected reconstructed primary vertex and the true vertex position compare is needed to
3818 understand the validity of our method. Figure 7.13 shows the distributions of fractional
3819 residuals between the truth and reconstructed vertex positions in the X (top panel),
3820 Y (middle panel), and Z (bottom panel) directions. Performing a double Gaussian fit
3821 to the distributions (red lines), I estimate the reconstructed vertex resolution achieved
3822 with this method to be $1.62 \pm 0.08\%$, $1.23 \pm 0.05\%$, and $0.32 \pm 0.05\%$ for the X , Y ,
3823 and Z directions, respectively. As expected, the resolution along the drift direction.
3824 However, the significant difference in resolution between the two transverse directions is
3825 worth noting. Not only the resolution is better for the Z direction, but the layout of the
3826 residual distribution is highly asymmetrical. This may be related to the variability in
3827 the selection efficiency along that direction.

3828 7.3 Charged pion identification

3829 Now that I have checked the robustness of the proposed ν_μ CC selection, it can be
3830 used as a starting point for other, more convoluted, selections. One of the priorities
3831 of ND-GAr, as mentioned previously, is the identification of pions. With its lower
3832 tracking thresholds, ND-GAr is expected to do better regarding π^\pm identification than
3833 the traditional LArTPCs, like ND-LAr. Moreover, it can make use of the different
3834 detector subcomponents to tag the charged pions.

3835 The ν_μ CC selection provides a starting point for the pion identification. The first
3836 thing one can do is rule out the selected primary muon candidate. Then, by looking at
3837 the properties of the rest of the reconstructed particles, one can start the counting of
3838 the charged pions.

3839 The two proton scores, the one based on the dE/dx in the HPgTPC and the one

7.3. CHARGED PION IDENTIFICATION

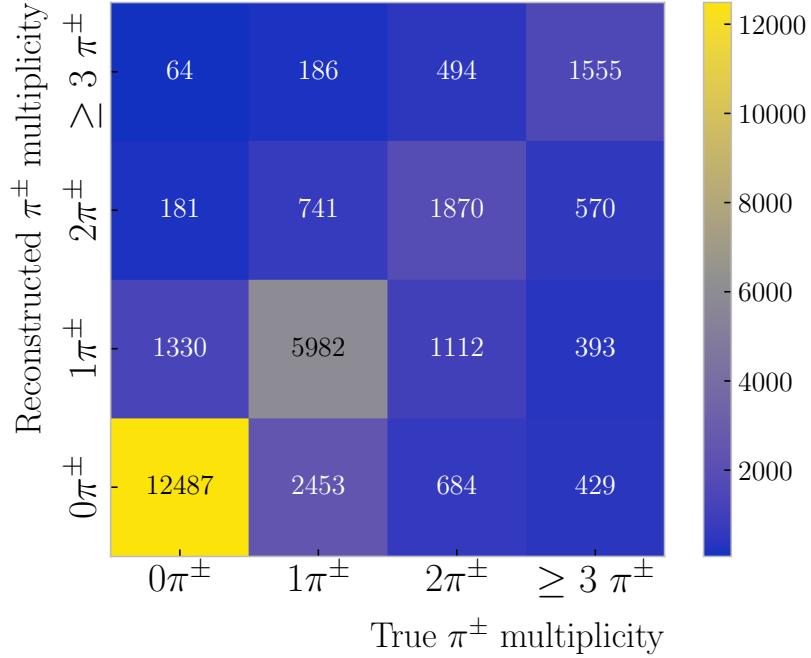


Figure 7.14: Distribution of events given their true and reconstructed π^\pm multiplicity, for the selection given by $p_{dE/dx}^{\text{cut}} = p_{\text{ToF}}^{\text{cut}} = 0.50$, $\Delta_{dE/dx}^{\pi^\pm} = 0.20$, and $d_\mu^{\text{cut}} = 50.0$ cm.

3840 obtained from the ToF measurement in the ECal, can be used to separate the protons
 3841 from the sample of charged pions. By providing appropriate cuts for these, a good
 3842 separation can be achieved.

3843 Another source of information available is the dE/dx of the track associated to the
 3844 reconstructed particle. To select the charged pions, we can require that the measured
 3845 mean dE/dx is compatible with the expectation for a true π^\pm , in other words:

$$\left\langle \frac{dE}{dx} \right\rangle_{\pi^\pm} \left(1 - \Delta_{dE/dx}^{\pi^\pm} \right) \leq \left\langle \frac{dE}{dx} \right\rangle_{\text{meas.}} < \left\langle \frac{dE}{dx} \right\rangle_{\pi^\pm} \left(1 + \Delta_{dE/dx}^{\pi^\pm} \right), \quad (7.6)$$

3846 where the parameter $\Delta_{dE/dx}^{\pi^\pm}$ measures the fractional variation one allows around the
 3847 theoretical expectation. To obtain the expected mean dE/dx of a charged pion with a
 3848 given momentum, I use the ALEPH parametrisation with the parameter values obtained
 3849 previously.

3850 Also, as we are only interested in the primary pions, and because these are by
 3851 definition close to the interaction vertex, one can apply an additional distance cut. Using

CHAPTER 7. EVENT SELECTION IN ND-GAR

3852 the start position of the muon candidate, we can restrict the starting point of pions to a
3853 certain volume around the vertex.

3854 Combining all these ideas, I propose the following procedure to identify the charged
3855 pions in an event:

- 3856 1. Apply ν_μ CC selection.
- 3857 2. Disregard particle selected as primary muon.
- 3858 3. Remove particles with momentum below threshold.
- 3859 4. Select particles with proton dE/dx score below threshold.
- 3860 5. Select particles with proton ToF score below threshold.
- 3861 6. Select particles with mean dE/dx around the expected value for a pion.
- 3862 7. Remove particles with a distance between the start of the track and the primary
3863 vertex greater than the cut.

3864 The remaining particles after all these cuts are taken to be charged pion candidates.

3865 This counting method depends on four cuts, denoted by $p_{dE/dx}^{\text{cut}}$, $p_{\text{ToF}}^{\text{cut}}$, $\Delta_{dE/dx}^{\pi^\pm}$, and
3866 d_μ^{cut} in order of appearance. The momentum threshold is necessary to compare with
3867 the true multiplicity. For values of the kinetic energy lower than 10 – 20 MeV, we
3868 do not expect to be able to tag individual pions. Such low energy particles just leave
3869 small traces in the TPC which, together with the busy environment of the neutrino
3870 interaction vertex, leaves one with no other option but to only account for their energy
3871 calorimetrically. As such, the true pion counting also features this momentum threshold.

3872 I performed an optimisation of the charged pion counting by scanning the space of
3873 possible cut configurations. For the two proton scores, I let them vary between 0.10 to
3874 0.90, in increments of 0.10. Similarly, the parameter $\Delta_{dE/dx}^{\pi^\pm}$ takes values in the range
3875 0.05 – 0.25, with a step size of 0.05. Finally, the distance cut changes in 10 cm steps,
3876 from 10 to 120 cm.

7.3. CHARGED PION IDENTIFICATION

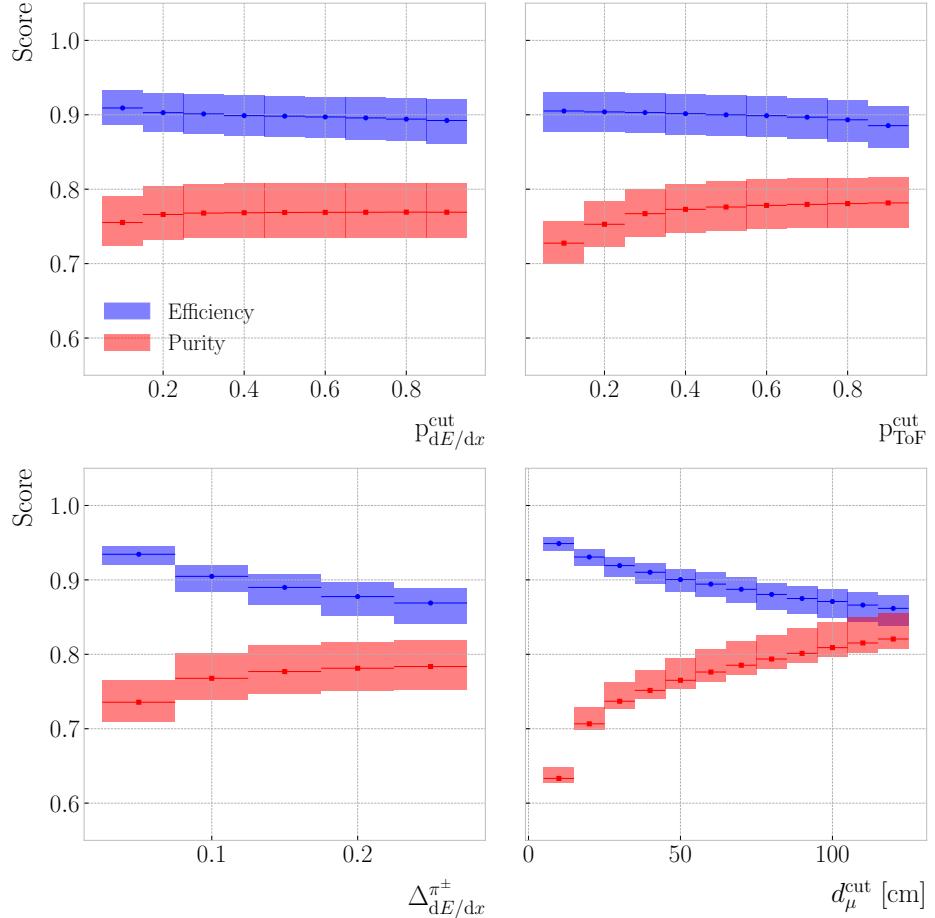


Figure 7.15: Efficiency (blue) and purity (red) for the ν_μ CC $0\pi^\pm$ selection as a function of the proton dE/dx score cut (top left panel), proton ToF score cut (top right panel), pion dE/dx cut (bottom left panel), and distance to muon cut (bottom right panel). The height of the boxes represents the IQR of the conditional distributions, whereas the line corresponds to the median.

3877 For each combination of selection cuts, I compare the true charged pion multiplicity
 3878 given by GENIE with the number of charged pion candidates I count with this method,
 3879 hereafter referred to as the reconstructed π^\pm multiplicity. The result of this comparison
 3880 is a matrix, with columns and rows indicating true and reconstructed charged pion
 3881 multiplicity, respectively. An example of one of these matrices, obtained for a certain
 3882 configuration of cuts, can be seen in Fig. 7.14. From these multiplicity matrices one can
 3883 extract performance metrics, like efficiency, purity, and significance.

3884 Given a multiplicity matrix \mathbf{M} , the efficiency for the i -th multiplicity value can be

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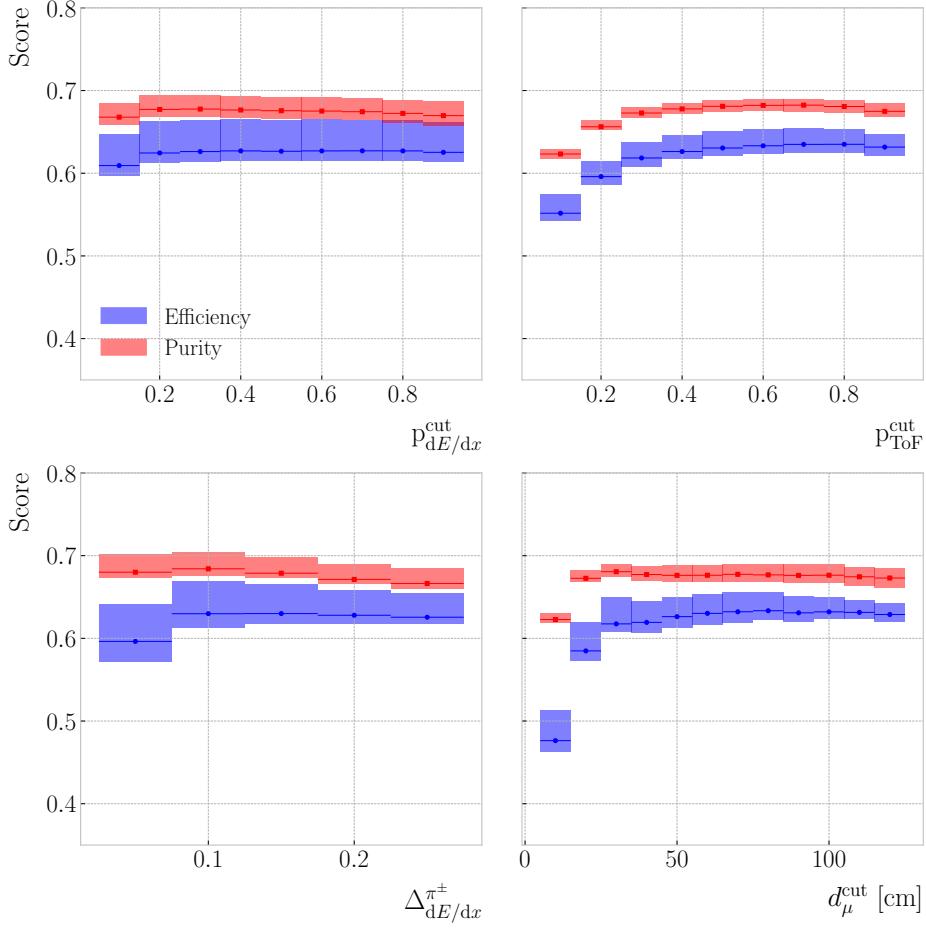


Figure 7.16: Efficiency (blue) and purity (red) for the ν_μ CC $1\pi^\pm$ selection as a function of the proton dE/dx score cut (top left panel), proton ToF score cut (top right panel), pion dE/dx cut (bottom left panel), and distance to muon cut (bottom right panel). The height of the boxes represents the IQR of the conditional distributions, whereas the line corresponds to the median.

3885 computed as:

$$\text{Efficiency}|_i = \frac{M_{ii}}{\sum_j M_{ij}}, \quad (7.7)$$

3886 or in other words, dividing the corresponding diagonal entry by the sum of all the entries

3887 in the same column. On the other hand, the purity is given by:

$$\text{Purity}|_i = \frac{M_{ii}}{\sum_j M_{ji}}, \quad (7.8)$$

3888 which is just the ratio between the diagonal entry and the sum of the entries in the

7.3. CHARGED PION IDENTIFICATION

3889 corresponding row. Similarly, the significance is obtained by taking the square root of
 3890 the denominator in the previous expression:

$$\text{Significance}|_i = \frac{S}{\sqrt{S+B}}|_i = \frac{M_{ii}}{\sqrt{\sum_j M_{ji}}}. \quad (7.9)$$

3891 Figures 7.15 and 7.16 show the efficiency (blue) and the purity (red) for the ν_μ
 3892 CC $0\pi^\pm$ and $1\pi^\pm$ selections, respectively, as a function of the different cut values. In
 3893 the figures, each box represents the IQR of the conditional distribution for the fixed
 3894 value of the corresponding cut, and the horizontal lines correspond to the medians. The
 3895 first thing one notices is that the efficiency is always higher than the purity in the $0\pi^\pm$
 3896 selection, while the opposite is true for the $1\pi^\pm$ selection. Also, it is clear that the range
 3897 within these metrics fluctuate in the $0\pi^\pm$ selection is significantly higher than it is for
 3898 the $1\pi^\pm$ case. This shows that it is easier to assess that no charged pions are present in
 3899 the event than actually tagging them.

3900 For the ν_μ CC $0\pi^\pm$ selection, the performance metrics follow the expected tendency.
 3901 As the purity grows with a cut value, the efficiency decreases. Interestingly, this is not
 3902 the case for the $1\pi^\pm$ selection, where both efficiency and purity follow roughly the same
 3903 trends along the different cuts. This makes sense when one comprehends that this is not
 3904 a traditional cut-based selection, but more of a counting exercise. Some restrictive cut
 3905 configurations will not tag any particles as pions. On the contrary, loose cuts will render
 3906 every particle as a π^\pm . Therefore, when looking at a specific multiplicity, the relation
 3907 between the cut value and the performance metrics is not obvious. Thus, sometimes
 3908 efficiency and purity can both increase, as the cuts refine the definition of a reconstructed
 3909 pion.

3910 To have a working point for our studies, I chose the cut configuration that yields
 3911 the maximum significance for the ν_μ CC $1\pi^\pm$ selection. Of course, other cuts would be
 3912 more appropriate in certain scenarios. However, this provides us with a starting point
 3913 to understand the performance of the selection. A significance of 66 ± 7 for the $1\pi^\pm$
 3914 selection is achieved for the cut values $p_{dE/dx}^{\text{cut}} = 0.30$, $p_{\text{ToF}}^{\text{cut}} = 0.70$, $\Delta_{dE/dx}^{\pi^\pm} = 0.10$, and

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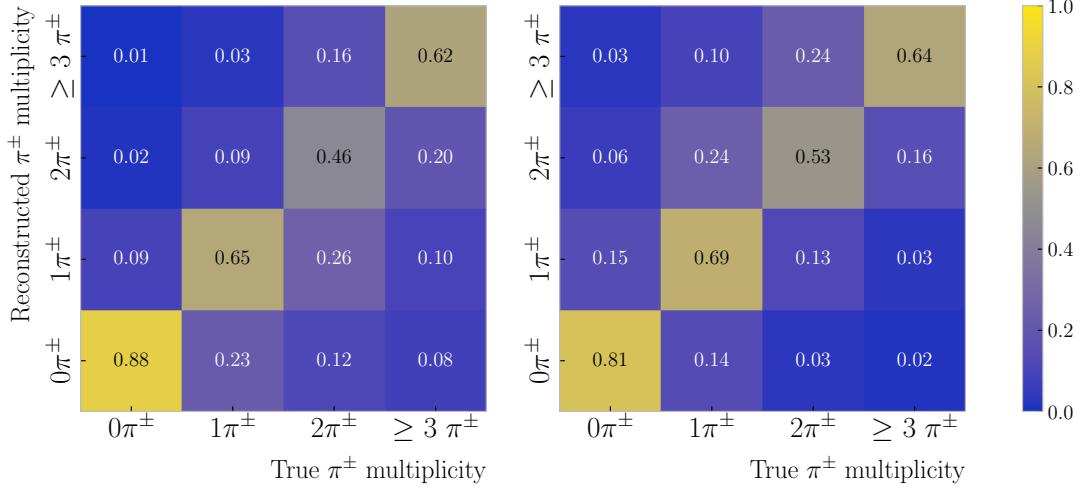


Figure 7.17: Distribution of events given their true and reconstructed π^\pm multiplicity, both column-wise (left panel) and row-wise (right panel) normalised, for the selection that maximises the significance of the ν_μ CC $1\pi^\pm$ selection. The column normalisation yields the efficiency in the diagonal entries, whereas the row normalisation reveals the purity.

3915 $d_\mu^{\text{cut}} = 110.0$ cm.

3916 Figure 7.17 shows the multiplicity matrices resulting from this optimised ν_μ CC $1\pi^\pm$
 3917 selection. Although both matrices are produced with the same selection cuts, one is
 3918 column normalised (left panel), whereas the other is row normalised (right panel). It
 3919 follows from the definitions in Eqs. (7.7) and ((7.8)) that the diagonal entries of these
 3920 matrices correspond to the efficiencies and the purities, respectively, for each of the
 3921 possible charged pion multiplicity selections.

3922 An additional check to make is understand how this configuration performs when
 3923 applied to the other selections, like ν_μ CC $0\pi^\pm$, and how it compares to the other
 3924 possible configurations. A comparison between the different pion multiplicity selections,
 3925 indicated with colours, in the purity versus efficiency space is shown in Fig. 7.18. For
 3926 each of the possible multiplicity choices, the performance obtained for the $1\pi^\pm$ optimised
 3927 selection is indicated by an outlined point. From this, one can see that the selected
 3928 configuration performs reasonably well, within the limits of what can be achieved in
 3929 each case, across the different multiplicities.

3930 At this point, one can study the charged pion selection performance as a function of

7.3. CHARGED PION IDENTIFICATION

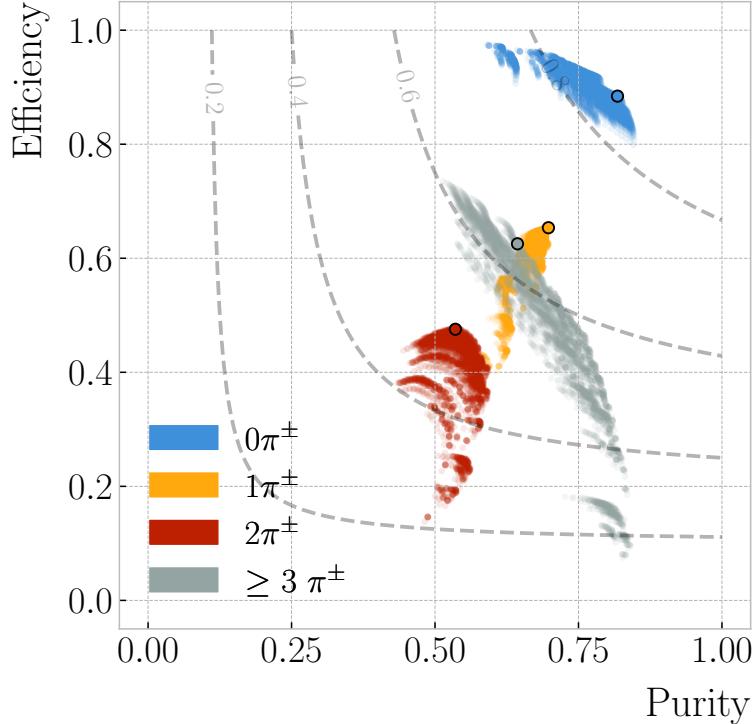


Figure 7.18: Purity versus efficiency achieved for the different cut configurations explored separated by the various ν_μ CC $N\pi^\pm$ selections. The outlined points indicate the state for each possible multiplicity when using the configuration that maximises the significance of the ν_μ CC $1\pi^\pm$ selection. The contours indicate the surfaces of equal F_1 -score.

3931 other quantities of interest. A natural variable to check is the hadronic invariant mass.

3932 It is defined as:

$$W = \sqrt{-Q^2 + 2m_n q_0 + m_n^2} \quad (7.10)$$

3933 where Q^2 is the momentum transfer from the neutrino to the primary muon, q_0 the
 3934 energy transfer, and m_n the mass of the nucleon. This quantity is related to the elasticity
 3935 of the neutrino interaction, and defines the transitions between the QEL, RES and DIS
 3936 regions. An interesting invariant mass range for DUNE is the one that extends between
 3937 the mass of the Δ resonance, even though it is typically extended down to $m_p + m_{\pi^\pm}$,
 3938 and 2.0 GeV. It is estimated that roughly 7 in every 10 events in our ND will take
 3939 place in this region. Although the RES production dominates at these W values, this
 3940 range also includes the transition to the DIS regime. Thus, it is often called the shallow

CHAPTER 7. EVENT SELECTION IN ND-GAR

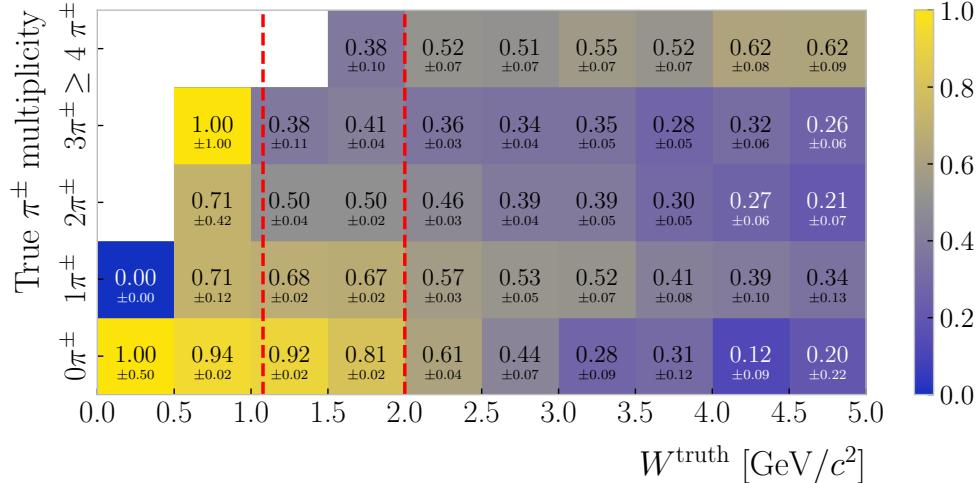


Figure 7.19: Efficiency of the various ν_μ CC $N\pi^\pm$ selections as a function of the true hadronic invariant mass. The dashed vertical lines correspond (from left to right) to the values $m_p + m_{\pi^\pm}$ and 2.0 GeV/ c^2 , which define the shallow inelastic scattering region.

3941 inelastic scattering (SIS) region.

3942 Within these boundaries, the resonant events produce either 1 or 2 charged pions,
 3943 whereas the multipion events are typically associated to non-resonant production.
 3944 Therefore, our ability of correctly select events with $\geq 2\pi^\pm$ in the SIS region will
 3945 impact our ability of constraining this poorly understood regime. Figure 7.19 shows the
 3946 efficiency of the various charged pion multiplicity selections in a number of hadronic
 3947 invariant mass bins. The two red dashed lines indicate the boundaries of the SIS region.
 3948 One can see that, although not as good as the single pion selection, the efficiency for the
 3949 multipion events is reasonable in the relevant invariant mass range. The total efficiency
 3950 for the ν_μ CC $\geq 2\pi^\pm$ selection in the SIS regime is estimated to be 0.65 ± 0.02 .

3951 7.3.1 ν_μ CC $1\pi^\pm$ selection

3952 By focusing on the $1\pi^\pm$ selection, one can study the kinematics of the selected pion.
 3953 This allows one to understand how well the charged pions are tagged. This is difficult
 3954 to do only using the multiplicity matrices, as with them one can only check that the
 3955 number of charged pions is the same as in the truth. Sometime, even if the estimated
 3956 pion multiplicity is correct, the identified particles may not be true pions.

7.3. CHARGED PION IDENTIFICATION

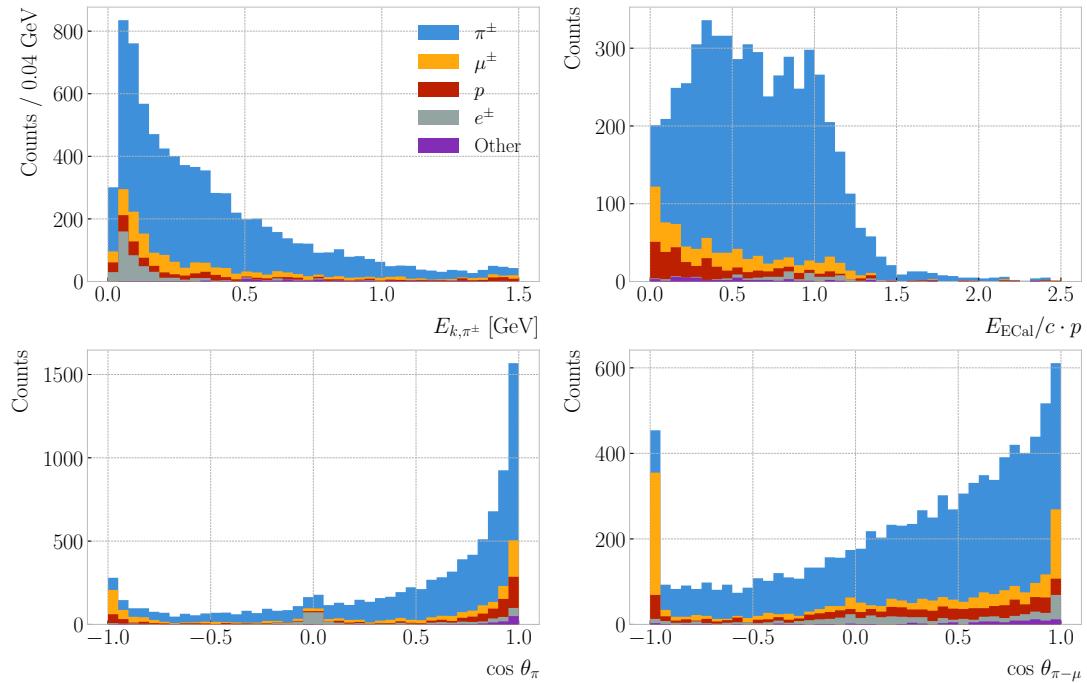


Figure 7.20: Reconstructed kinematic distributions for the pion candidate in the ν_μ CC $1\pi^\pm$ selection, broken down by true ID of the particle. From left to right, top to bottom, we have the kinetic energy given the pion hypothesis, the ratio between the energy deposited in the ECal and the momentum, the pion angle, and the angle between the muon and pion candidates.

3957 Figure 7.20 displays the distributions of various reconstructed kinematic variables
 3958 for the selected pion candidate. The different colours indicate the ID of the true particle
 3959 associated to the reconstructed pion.

3960 First, we have the kinetic energy distribution. For this set of reconstructed particles,
 3961 because they have been tagged as charged pions, the kinetic energy is computed using their
 3962 momentum assuming the pion hypothesis. One can see that most of the contaminants
 3963 sit in low energy range, up to around 0.2 GeV.

3964 The next distribution presents the ratio between the energy deposited in the ECal
 3965 associated to the particle over the momentum measured in the HPgTPC. This variable is
 3966 restricted to particles with at least one associated hit in the ECal. It is interesting to see
 3967 two peak structure in the true pion distribution. The first one presumably corresponds
 3968 to the pions punching-through the ECal, while the latter is probably due to the ones

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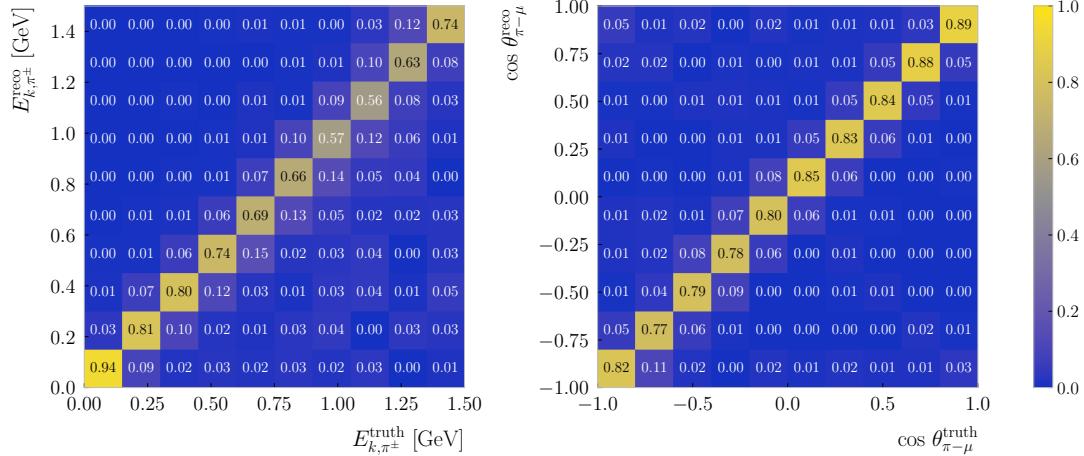


Figure 7.21: Distributions for the reconstructed versus truth generated pion kinetic energy (left panel) and cosine of the angle between the pion and muon (right panel). The reconstructed values correspond to the selected primary muon and pion candidates in the ν_μ CC $1\pi^\pm$ selection, whereas the truth values come from the true primary muon and pion in the events.

3969 stopping in it. On the other hand, the misidentified particles, other than the electrons,
 3970 tend to lower ratios. This is expected for protons, as this could not be higher than 0.5
 3971 for momenta ≤ 1 GeV/ c even if they stopped, but for the muons it may point to a
 3972 misreconstruction.

3973 The following distribution shows the angle of the pion candidates with respect to the
 3974 beam direction. Although most of them are aimed in the forward direction, it can be
 3975 noted that an important number of the misidentified muons seem to be backward-going.
 3976 This is likely a reconstruction artifact, produced by broken tracks that got assigned the
 3977 wrong propagation direction. Also, there is a sizeable number of true electrons with
 3978 directions perpendicular to the beam, probably delta electrons from the primary muon.

3979 Finally, I included the reconstructed pion-muon angular distribution. Even though
 3980 it shares some similarities with the previous distribution, as the primary muon typically
 3981 goes forward, the pion distribution is not as prominently forward-going in this case.
 3982 Also, it may be noted that approximately 25% of the muons misidentified as pions have
 3983 $\cos \theta_{\pi-\mu} \leq -0.95$. Therefore, putting an additional angular cut improves the purity of
 3984 the charged pion selection from 0.74 ± 0.01 to 0.77 ± 0.01 , while not loosing a substantial

7.4. NEUTRAL PION IDENTIFICATION

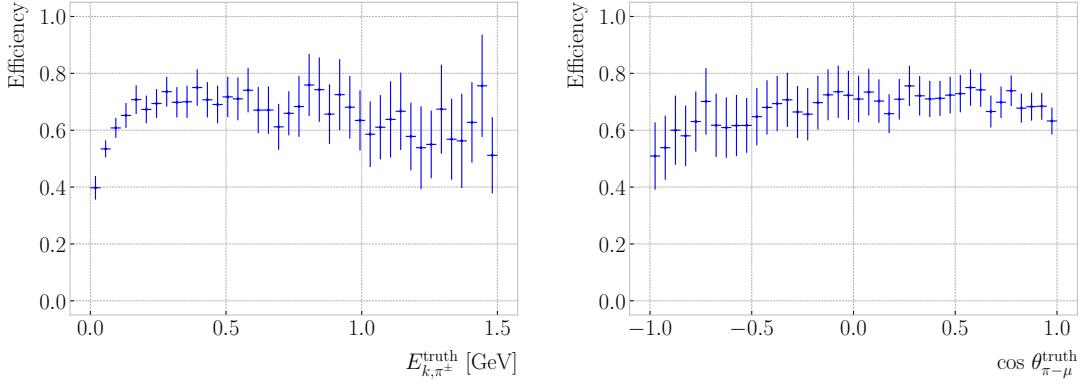


Figure 7.22: Efficiency of the ν_μ CC $1\pi^\pm$ selection as a function of the true pion kinetic energy (left panel) and pion-muon angle (right panel).

3985 amount of true pions.

3986 A comparison between the true and the reconstructed values of the pion kinetic
 3987 energy (left panel) and pion-muon angle (right panel) is shown in Fig. 7.21. The
 3988 distributions are column normalised, which allows to see the fraction of events in the
 3989 correct bins. For this, I selected the events where only one reconstructed pion and
 3990 one true pion were identified, as that is the only case where a pairing of the variables is
 3991 possible. It showcases the excellent agreement between the reconstruction and the truth
 3992 information.

3993 One can also study the performance of the pion selection as a function of the
 3994 truth pion kinematics. Fig. 7.22 shows the selection efficiency versus the true kinetic
 3995 energy (left panel) and the angle between the true primary pion and muon (right panel).
 3996 The efficiency is computed from the events with a single true and reconstructed pion,
 3997 comparing their number to the total of events with one true pion. Notice how the
 3998 efficiency, although it starts with relatively low values, plateaus around 0.70 quickly
 3999 after 0.20 GeV. In terms of the pion-muon angle, the efficiency looks relatively flat, only
 4000 dropping slightly towards the back-to-back case.

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4001 7.4 Neutral pion identification

4002 The ν_μ CC selection can also be used as a stepping stone for the identification of
4003 neutral pions. Although these particles do not leave any traces in the HPgTPC, using a
4004 combination of the different detectors within ND-GAr. Being able to tag the neutral
4005 pions is a valuable asset for the estimation of the reconstructed neutrino energy, as both
4006 their kinetic and mass components can then be added in the calculation.

4007 In the case that both photons from the π^0 decay do not undergo pair production
4008 of a e^+e^- pair, they will reach the ECal where they will produce an electromagnetic
4009 shower. This activity inside the ECal will not be associated to any charged particle track
4010 inside the HPgTPC, unless there is a reconstruction failure. Thus, having a neutrino
4011 interaction vertex candidate from the ν_μ CC selection, one can reconstruct the mass of
4012 the π^0 using the energy and position of the photons. I already used this same technique
4013 in section 6.6 for a single π^0 sample. However, here I apply it to neutrino interaction
4014 events, and the vertex position is not cheated but selected from the reconstruction
4015 products.

4016 The idea is to look for all the ECal clusters that were not associated to tracks in
4017 each event. Then, if two or more were identified, compute the invariant mass for all
4018 possible combinations. At this point, I select the pair whose invariant mass is closest to
4019 m_{π^0} , remove the pairs containing any of the two selected clusters from the collection,
4020 and iterate until no more pairs can be formed.

4021 I repeat this procedure for the events with 0, 1, 2 and 3 or more true neutral pions.
4022 For each of them, I extract the invariant mass of the first three cluster pair candidates
4023 (in order of proximity to m_{π^0}), in case they can be formed. If the number of the cluster
4024 pair is lower than the true neutral pion multiplicity of the event, that entry will be
4025 counted as signal. The additional candidates for an event of a given multiplicity are
4026 considered background. The resulting distribution is shown in Fig. 7.23 (black data
4027 points).

7.4. NEUTRAL PION IDENTIFICATION

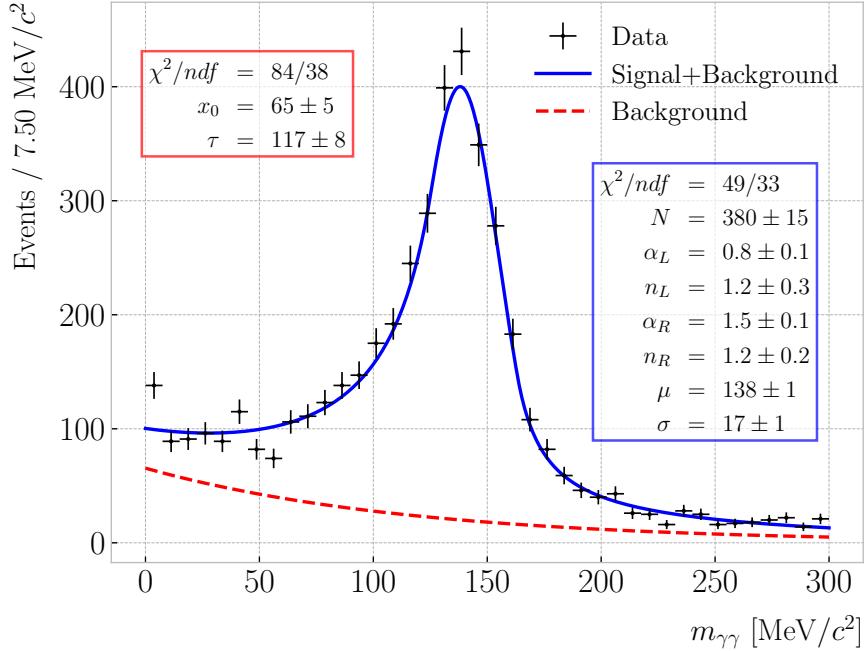


Figure 7.23: Invariant mass distribution obtained for the unassociated ECal cluster pair in the event with the value closest to the true π^0 mass. The best fits for signal plus background (solid blue line) and background only (dashed red line) are also shown.

4028 I fit the signal distribution to a double-sided Crystal Ball function:

$$f_s(x; \alpha_{L,R}, n_{L,R}, \mu, \sigma, N) = N \begin{cases} A_L \left(B_L - \frac{x-\mu}{\sigma} \right)^{-n_L}, & \text{for } \frac{x-\mu}{\sigma} < -\alpha_L, \\ e^{-\frac{(x-\mu)^2}{2\sigma^2}}, & \text{for } -\alpha_L \leq \frac{x-\mu}{\sigma} \leq \alpha_R, \\ A_R \left(B_R + \frac{x-\mu}{\sigma} \right)^{-n_R}, & \text{for } \frac{x-\mu}{\sigma} > \alpha_R, \end{cases} \quad (7.11)$$

4029 where $A_{L,R}$ and $B_{L,R}$ are given by:

$$A_{L,R} = \left(\frac{n_{L,R}}{|\alpha_{L,R}|} \right)^{n_{L,R}} e^{-\frac{|\alpha_{L,R}|^2}{2}}, \quad (7.12)$$

$$B_{L,R} = \frac{n_{L,R}}{|\alpha_{L,R}|} - |\alpha_{L,R}|.$$

4030 The tails of this distribution accommodate the asymmetric shape of the misreconstruction
 4031 effects. The values obtained for the best fit parameters are indicated in Fig. 7.23 (blue
 4032 box).

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4033 The background is characterised by an exponential function of the form:

$$f_b(x; x_0, \tau) = x_0 e^{-x/\tau}. \quad (7.13)$$

4034 Similarly, the best fit values can be seen in Fig. 7.23 (red box).

4035 Figure 7.23 also shows the results of the fits for the signal plus background (blue line)
 4036 and the background only (dashed red line) cases. Using these, I estimate the tagging
 4037 efficiency of this method to be 0.90 ± 0.01 with a purity of 0.85 ± 0.01 , when selecting
 4038 the candidates with an invariant mass in the range $54.0 - 288.0 \text{ GeV}/c^2$.

4039 This is a robust method to identify the photon pair from the π^0 decay. However,
 4040 this approach is not enough to efficiently identify all the events containing neutral pions
 4041 in the sample. A quick calculation reveals that only 20% of the ν_μ CC $1\pi^0$ events can
 4042 be correctly identified with it.

4043 This approach can be complemented with the identification of the secondary vertices
 4044 from the e^+e^- conversions. This will make it possible to cover the cases when either
 4045 one or both photons convert in the HPgTPC. In those cases, one can try pairing the
 4046 e^+e^- with unassociated activities in the ECal, or matching pairs of secondary vertices.
 4047 However, this will require further work on the reconstruction, and thus falls out of the
 4048 scope of this analysis.

4049 7.5 Neutrino energy reconstruction

4050 In a neutrino-nucleus CC interaction, where alongside the charged lepton N nucleons
 4051 where knocked out and M mesons produced, the reconstructed neutrino energy can be
 4052 computed as:

$$E_{\text{rec}} = S_n + E_\ell + \sum_{i=0}^N E_{k,n_i} + \sum_{j=0}^M E_{m_j}, \quad (7.14)$$

4053 where S_n is the average single-nucleon separation energy, E_ℓ the energy of the primary
 4054 lepton, E_{k,n_i} is the kinetic energy of the i -th knocked-out nucleon and E_{m_j} the total
 4055 energy of the j -th produced meson.

7.5. NEUTRINO ENERGY RECONSTRUCTION

4056 This represents the ideal scenario, where all the kinetic energy of the nucleons is
 4057 visible in the detector and one can identify all mesons produced in the interaction. In a
 4058 real experiment, some of these energy components will not be , and this needs to be
 4059 accounted for in any estimation of the reconstructed energy.

4060 For instance, in ND-GAr neutrons are complicated to account for, as they do not
 4061 produce tracks in the TPC. They may be identified either from scatterings off Ar nuclei
 4062 in the HPgTPC, or performing a ToF measurement in the ECal. However, these methods
 4063 are not fully mature in the current reconstruction, and their development is beyond the
 4064 scope of this study. So, in the following, I will completely ignore the contribution of
 4065 neutrons.

4066 Also, with a real detector we can not expect to tag all the charged pions irrespective
 4067 of their energy. This is why one has to introduce detection thresholds in the energy
 4068 estimation. Thus, in the reconstructed energy calculation I will add only the kinetic
 4069 energy for the charged pions below the threshold, and the total energy for the pions
 4070 above the threshold.

4071 Likewise, the identification of all neutral pions in the sample is challenging. As
 4072 discussed in the previous section, with our ECal we are able to identify the photons
 4073 from the π^0 decays, but that selection still needs to be completed with other methods.
 4074 Therefore, for this first study I do not take into account the energy contribution of the
 4075 neutral pions.

4076 With all this in mind, using the truth information from the events I compute the
 4077 reconstructed neutrino energy as:

$$E_{\text{rec}}^{\text{truth}} = S_n + E_\ell + \sum_{i=0}^{N_p} E_{k,p_i} + \sum_{j=0}^{M_{\pi^\pm}^<} E_{k,\pi_j^\pm} + \sum_{k=0}^{M_{\pi^\pm}^>} E_{\pi_k^\pm}, \quad (7.15)$$

4078 where N_p is the number of protons, and $M_{\pi^\pm}^<$ and $M_{\pi^\pm}^>$ the number of charged pions
 4079 below and above the threshold, respectively. As before, I assume a kinetic energy
 4080 threshold of 20 MeV for the charged pions.

4081 At the reconstruction level, I use the energy of the primary muon candidate, computed

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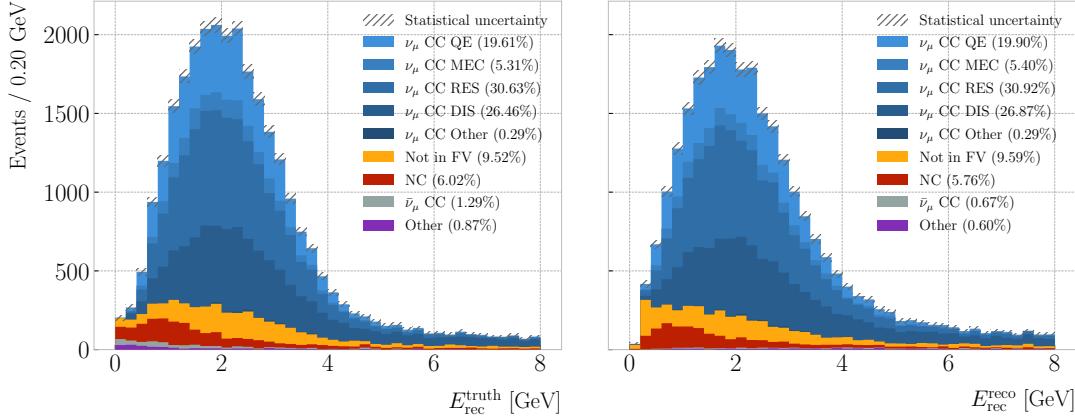


Figure 7.24: Reconstructed neutrino energy spectra for the ν_μ CC selection obtained using the truth (left panel) and reconstructed (right panel) information. The selected events are broken down by signal and background subcategories. The statistical uncertainty is drawn in hatched gray.

from its momentum, as the starting point for the neutrino energy calculation. Then, I add the total energy contributions from the identified charged pions, again using their momenta. After that, I try to identify the protons by looking at the two proton scores. If any of them are above threshold (here the thresholds used are the same as for the pion identification), the kinetic energy of the particle is added to the total. Finally, I check if any of the remaining particles are fully contained within the FV. I add their kinetic contributions using the total energy they deposited in the HPgTPC.

Figure 7.24 shows the resulting distributions of reconstructed neutrino energy obtained from the truth (left panel) and reconstructed (right panel) particle collections. The overall shape of the distributions is similar, with the reconstructed one having a slightly larger high energy tail. Note also that the background events from outside the FV tend to have a smaller energy in the reconstructed case. This is likely due to a misreconstruction of the primary muon, which clearly does not affect the other computation.

I also compared the reconstructed energies to the true energy of the neutrino. Figure 7.25 displays the ratio of the energy residuals to the true energy for the truth (left panel) and reconstructed (right panel) cases. As expected, using the true particles one never overestimates the neutrino energy. Also, using the reconstructed objects one is more

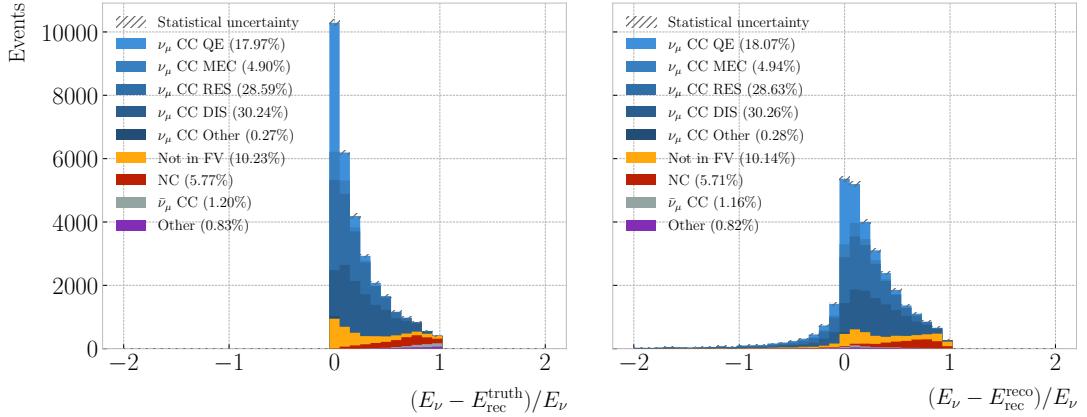


Figure 7.25: Neutrino energy residuals distributions for the ν_μ CC selection obtained using the truth (left panel) and reconstructed (right panel) information. The selected events are broken down by signal and background subcategories. The statistical uncertainty is drawn in hatched gray.

4100 prone to underestimate the neutrino energy, due to deficiencies in the reconstruction.

4101 7.6 Systematic uncertainties

4102 Although the implementation and study of the systematic uncertainties relevant for
 4103 ND-GAr is out of the scope of this preliminary analysis, in this section I give an extended
 4104 overview of the topic. can be classified in three categories: neutrino flux uncertainties,
 4105 neutrino-nucleus interaction model uncertainties, and detector response uncertainties.

4106 7.6.1 Flux uncertainties

4107 The neutrino flux prediction is affected by systematic uncertainties arising from two
 4108 sources: the uncertainties in the production of hadrons in the target and the uncertainties
 4109 in the design parameters of the beamline itself. These fluxes and their uncertainties are
 4110 generated with the G4LBNF simulation [83], a Geant4 implementation of the LBNF
 4111 beamline, and the Package to Predict the FluX (PPFX) framework, originally developed
 4112 for MINERvA [185].

4113 The hadron production uncertainties are associated to the kinematic distributions
 4114 of the hadrons produced when the protons interact with the carbon target, as well

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as the possible interactions of the hadrons with the beamline materials. The PPFX package estimates these uncertainties by performing a number of random throws of the production model parameters [186]. This way, different predictions of the LBNF flux are generated, which can be compared to the nominal prediction to build a matrix of the covariances between neutrino energies, flavours and running modes (either FHC or RHC). The resulting hadron production uncertainties are described by the eigenvectors associated to the largest eigenvalues in this matrix, obtained performing a PCA analysis.

The other set of uncertainties affecting the neutrino flux prediction come from the limited precision with which we know the parameters of the different components in the beamline. These include the specifications of the target, the dimensions of the decay pipe, and the current and alignment of the magnetic horns. The effects on the flux predictions of these uncertainties are estimated using the G4LBNF simulation. For each of the parameters, the simulation runs with said parameter shifted by $\pm 1\sigma$ from the nominal value, and the resulting flux prediction is compared to the nominal one.

7.6.2 Cross section uncertainties

As discussed previously in section 2.6, the neutrino-nucleus interaction model is of great importance for neutrino experiments, as it maps the true neutrino energy to the kinematics of the final state particles. The uncertainties on the cross section model are implemented in three ways: varying the parameters used in the GENIE simulation, using weights that parametrise cross section effects not accounted for in GENIE, and comparing the GENIE predictions to other interaction models.

Within the DUNE TDR LBL analysis, the default interaction model was that implemented in GENIE v2_12_10 [119]. A summary of the cross section systematic parameters present in GENIE used in that analysis is presented in Tab. 7.3. The additional systematic parameters used in the analysis are described in Tab. 7.4.

In this default GENIE configuration, the initial state of the nucleons is described by the Bodek-Ritchie global Fermi gas model [187]. The model is known give a poor agreement whe compared to neutrino-nucleon data [188]. Because of the limitations of

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Table 7.3: Neutrino interaction systematic parameters implemented in GENIE used in the DUNE TDR LBL analysis. Events with low W that are not QE are mainly RES, whereas DIS events dominate at high W . The initials BY refer to the Bodek-Yang model. Table adapted from Ref. [119].

Systematic	1σ value
Quasielastic	
Axial mass for CCQE	$+0.25_{-0.15}$ GeV
CCQE vector form factor shape	N/A
Fermi surface momentum for Pauli blocking	$\pm 30\%$
Low W	
Axial mass for CC resonance	± 0.05 GeV
Vector mass for CC resonance	$\pm 10\%$
θ_π distribution for Δ decay	N/A
High W (BY model)	
A_{HT}	$\pm 25\%$
B_{HT}	$\pm 25\%$
C_{v1u}	$\pm 30\%$
C_{v2u}	$\pm 40\%$
Other neutral current	
Axial mass for NC resonance	$\pm 10\%$
Vector mass for NC resonance	$\pm 5\%$
Intra-nuclear	
Nucleon charge exchange	$\pm 50\%$
Nucleon elastic reaction	$\pm 30\%$
Nucleon inelastic reaction	$\pm 40\%$
Nucleon absorption	$\pm 20\%$
Nucleon π -production	$\pm 20\%$
π charge exchange	$\pm 50\%$
π elastic reaction	$\pm 10\%$
π inelastic reaction	$\pm 40\%$
π absorption	$\pm 20\%$
π π -production	$\pm 20\%$

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Table 7.4: Neutrino interaction systematic parameters used in the DUNE TDR LBL analysis not present in **GENIE**. I have omitted the parameters only relevant for the FD. Table adapted from Ref. [119].

Systematic	Mode	Description
BeRPA	$1p1h/\text{QE}$	Nuclear model suppression
ArC2p2h	$2p2h \text{ Ar/C}$	Electron scattering SRC pairs
E_{2p2h}	$2p2h$	$2p2h$ energy dependence
CC non-resonant	CC DIS 1π	$\nu + n/p \rightarrow \ell + 1\pi$
Other non-resonant	DIS $N\pi$	$1 < W < 5 \text{ GeV}/c^2$
NC normalisation	NC	$\pm 20\%$ to all NC events at the ND

4143 the model, the current versions of **GENIE** use the local Fermi gas approach, which takes
 4144 into account the correlation between the momentum of the nucleons and their location
 4145 within the nucleus.

4146 For the CCQE events, the dominant model uncertainties arise from the axial form
 4147 factor of the nucleon, for which a dipole parametrisation is used, and the nuclear
 4148 correlation effects computed using the random phase approximation (RPA). In the
 4149 analysis, a parametrisation of the Valencia RPA effect [181] is used. This consists of
 4150 a third-order Bernstein polynomial up to $Q^2 = 1.2 \text{ GeV}^2$ followed by an exponential
 4151 decay (BeRPA), originally proposed by the T2K collaboration [189].

4152 The $2p2h$ interactions are included using the Valencia model [181], with an additional
 4153 correction following the observation of an underprediction of these events in MINERvA
 4154 [190]. Additional uncertainties for the energy dependence of the missing strength were
 4155 added. Also, the uncertainties in the scaling from carbon to argon are included, based
 4156 on measurements of electron scattering off short-range correlated (SRC) nucleon pairs
 4157 on multiple targets [191].

4158 In this version of **GENIE**, the Rein-Sehgal model describes the single pion resonant
 4159 production events [192]. It includes 16 different resonances, with no interference between
 4160 them. Two parameters account for the uncertainties on the axial and vector masses of
 4161 the resonances. In subsequent **GENIE** tunes, like the one used in the studies presented in
 4162 this Chapter, the Berger-Sehgal model is used [182]. This is an improved version of the

7.6. SYSTEMATIC UNCERTAINTIES

4163 Rein-Sehgal model, which includes the lepton mass effects in the calculations.

4164 The Bodek-Yang parametrisation is used to describe the DIS events [184]. The
4165 parameters A_{HT} and B_{HT} account for higher twist effects in the scaling variable, while
4166 C_{v1u} and C_{v2u} control the form of the valence quark K factors. For the analysis, the
4167 uncertainties on the values of these parameters are taken into consideration. Also, due to
4168 the difficulties of GENIE at describing the transition region between RES and DIS events,
4169 a set of systematic parameters affecting the different non-resonant pion production
4170 channels were developed, following the example of NOvA [193]. There are independent
4171 parameters for the interactions on protons and neutrons, except for the CC DIS 1π case
4172 where they are merged. All start with an uncertainty of 50% for $W \leq 3 \text{ GeV}/c^2$, which
4173 linearly decreases until reaching a 5% at $W = 5 \text{ GeV}/c^2$.

4174 For the TDR analysis, an additional 20% normalisation uncertainty was added to all
4175 NC events in the ND. It was implemented to understand if the NC events passing the
4176 selection cuts affected the results of the analysis [119].

4177 Finally, the effective intranuclear transport model (often denoted as hA) is a part
4178 of GENIE, implemented in the INTRANUKE module. GENIE features a large number of
4179 parameters for the uncertainties on the intranuclear cascade model, which are summarised
4180 in the last portion of Tab. 7.3. In following GENIE releases, updated versions of the
4181 INTRANUKE model are used.

4182 Although part of this cross section systematic treatment is outdated, as the tunes
4183 currently used feature different models, it gives a good idea of what systematic effects
4184 are relevant for the different measurements we may want to perform in the future. At
4185 the moment, a significant effort is channeled to the creation of new tunes specifically
4186 tailored for DUNE, including the development of parametrisations particularly relevant
4187 for ND-GAr.

4188 7.6.3 Detector uncertainties

4189 The DUNE ND CDR [89] presents a number of studies on the performance of ND-GAr.
4190 These were based on the reference design described in section 3.5. Because the detector

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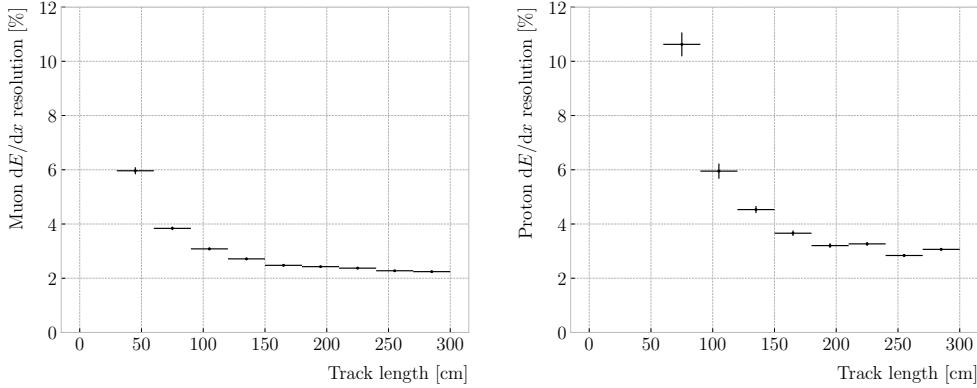


Figure 7.26: Estimated dE/dx resolution as a function of the track length for true muons (left panel) and protons (right panel) in a ν_μ CC sample.

is still in an R&D stage, with the design continually evolving, these performance metrics will need to be revisited in the future. However, they still provide valuable information. These studies help understand what detector requirements are needed to achieve the physics goals of the experiment, and on what design aspects we need to improve.

Since the reference design of ND-GAr repurposes the ALICE MWPCs and other hardware components, the ALICE TPC operation experience point of reference for the spatial resolution performance. They reported a single hit resolution of 0.25 mm and 1.50 mm in the directions perpendicular and parallel to the drift direction, respectively [194]. Nevertheless, the MWPCs are not the leading option for the charge readout anymore. Current efforts focus on the study of the effects of different pixelisation choices. of the GEMs setups.

For other performance metrics, a fairer comparison for the ND-GAr HPgTPC could be the PEP-4. It operated with a 80:20 Ar:CH₄ mixture at 8.5 bar, achieving a two-track separation of 1 cm [195, 196]. This metric is particularly relevant in our case, as the neutrino interaction vertex can be an area of very high track multiplicity. Thus, our track separation capabilities will have a direct impact on the primary vertex identification and resolution. There are several difference between our HPgTPC and PEP-4. The operating pressure of ND-GAr will be higher, and the gas mixture likely to contain a higher fraction of Ar.

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4210 In terms of the ionisation measurement, both the experience from ALICE and PEP-4
4211 are relevant, as this depends on the readout and the running conditions (pressure and
4212 gas mixture). They obtained resolutions of 4.5% and 3.0% for typical track lengths of
4213 160 and 75 cm, respectively. According to previous studies on the dE/dx resolution in
4214 gaseous detectors [197], ND-GAr can achieve a 2% resolution for a typical track length of
4215 200 cm. Figure 7.26 shows the values of the resolution I estimate for muons (left panel)
4216 and proton (right panel) tracks with different lengths, using the procedure described in
4217 section 6.2.

4218 The tracking capabilities of ND-GAr were studied in the context of ν_μ CC interactions.
4219 Using a sample of reconstructed tracks from true muons and charged pions, the tracking
4220 efficiency was estimated to be above 90% for momenta $\geq 40 \text{ MeV}/c$, with it steadily
4221 rising with the momentum. As a function of the angle with respect to the beam direction,
4222 the efficiency was almost flat for particles with $p \geq 200 \text{ MeV}/c$. In the case of protons,
4223 the tracking performs for kinetic energies $\geq 20 \text{ MeV}$. A machine learning algorithm is
4224 being developed for low energy proton track identification near the interaction vertex.
4225 Preliminary results show an efficiency of 30% at 5 MeV for this method.

4226 The same samples used for the tracking studies were employed to estimate the
4227 momentum resolution. The momentum is computed from the curvature of the tracks
4228 in the magnetic field, and is therefore limited by the track length in the direction
4229 perpendicular to the field. Focusing on the tracks associated to true muons, a double
4230 Gaussian fit revealed a width of 2.7% and 12% for the core and tails of the momentum
4231 distribution. This same study determined the 3D angular resolution in the HPgTPC to
4232 be 0.80° .

4233 The main source of uncertainty in the momentum measurement is the value of the
4234 magnetic field. The magnetic field simulations indicate that the overall uncertainty on
4235 the central field value is $< 0.05\%$. A preliminary study investigated the use of K_s^0 decays
4236 in the HPgTPC to measure any deviations of the magnetic field from its nominal 0.5 T
4237 value. This showed that even a magnetic field bias of 1% will shift the reconstructed
4238 invariant mass distribution significantly.

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4239 The results presented for the ECal in Ref. [89] use an outdated version of the
4240 geometry, where the entire ECal sits outside of the pressure vessel and the layers consist
4241 of 5 mm of scintillator and 2 mm of Cu. The sample used consists of single photons in
4242 a 20° cone aligned with the beam direction. In the simulation, an energy threshold of
4243 200 keV and a time resolution of 0.25 ns are assumed.

4244 The energy resolution of the photons is obtained from a Gaussian fit. The resulting
4245 resolutions are then fitted to a function of the form:

$$\frac{\sigma_E}{E} = \frac{A}{\sqrt{E}} \oplus \frac{B}{E} \oplus C, \quad (7.16)$$

4246 where A is the stochastic term, B the noise term and C the constant term. The best fit
4247 finds the values $A = 6.1\%$, $B = 1.6\%$, and $C = 4.5\%$. The photon angle is estimated
4248 using a PCA analysis of the associated ECal cluster, taken to be the direction of the
4249 first principal component. The angular resolution is computed from a Gaussian fit to
4250 the core of the distribution. As a function of the photon energy, the values obtained are
4251 $\frac{8.17^\circ}{\sqrt{E}} + 4.18^\circ$. Different arrangements of the layers and alternative absorber choices may
4252 improve these results.

Conclusion and outlook

4255 *Our plans miscarry because they have no aim. When a man does not know
4256 what harbour he is making for, no wind is the right wind.*

4257 – Lucio Anneo Seneca, *Epistulae morales ad Lucilium*

4258 This thesis is a compilation of three different projects within DUNE. However,
4259 the idea behind each one of them is the same. The common theme is the prospect
4260 of improving or extending the physics of DUNE. In the first case, by enhancing the
4261 production of TPs in the induction channels what I seek is to provide more useful
4262 information to the FD data selection. The investigations with both data and MC, as
4263 well as the opportunity to run with a live detector, showed that such an enhancement
4264 is possible and should be pursued. Next, the solar DM analysis adds to the already
4265 rich BSM programme of DUNE. With the results of these preliminary studies, I want
4266 to show that DUNE can be complementary to the large-volume neutrino detectors in
4267 this kind of searches. Finally, the goal of the ND-GAr reconstruction improvements
4268 was the development of the PID strategy of the detector. For this, I tried to extract all
4269 the possible information from its different subcomponents. With the PID at hand, it
4270 is possible to form the selections of the different ND-GAr samples, as I have shown in
4271 this work. These will help understand how the detector is going to further constrain the
4272 neutrino interaction uncertainties in DUNE Phase II, which will eventually allow DUNE
4273 to reach its ultimate physics goals.

4274 The DAQ system of the DUNE FD relies on the online identification of hits on

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4275 channels, the so-called TPs, to form decisions data to store. The goal of Chapter 4
4276 is to motivate a method to enhance the production of TPs in the induction channels
4277 of the detectors. Forming TPs from all the charge readout planes will improve the
4278 redundancy of the trigger algorithms. Not only that, but this may be the key to have
4279 more complex trigger logic that requires directional information. The aspect I focused on
4280 to improve the hit finding is the filtering of the waveforms. In section 4.3 I use a sample
4281 of ProtoDUNE-SP cosmic data to show how different low-pass FIR filters affect the S/N
4282 in the collection and induction planes. Then, I introduce the concept of the matched
4283 filter in section 4.4. Using the same dataset, I demonstrate that the improvement in the
4284 S/N of the induction channels achieved with these filters can be significantly higher than
4285 with the standard filter approach. A series of studies using MC samples are presented in
4286 section 4.5. These allow to study the dependence of the filtering on the orientation and
4287 the energy of the tracks. I also use them to assess the impact of this method on the hit
4288 sensitivity. Finally, in section 4.6 I briefly summarise the results from the VD ColdBox
4289 runs which featured the matched filter.

4290 With these studies, I showed that the matched filter puts the production of TPs in
4291 the induction and collection planes on the same level. The natural next step will be to
4292 understand the impact that this has in the context of the current trigger algorithms.
4293 Then, explore the development of new trigger routines, like triggers based on coincidence
4294 across planes. At the same time, these alternative hit finder chains should be implemented
4295 in the trigger simulations currently under development.

4296 The solar DM analysis is covered in Chapter 5. There I explain how the DUNE
4297 FD can be used to probe DM interactions by measuring the neutrino flux coming from
4298 DM annihilations in the core of the Sun. After introducing the topic of DM capture
4299 and annihilation in a massive object like the Sun, I describe what kind of neutrino
4300 signals one can expect from such events in section 5.2. Later, I comment on how
4301 DUNE could constrain the DM parameter space by performing counting experiments.
4302 In section 5.5 I study the selection efficiency for the $\tau^+\tau^-$ and $b\bar{b}$ channels. I focus
4303 on two different kinematic regimes: the high energy neutrinos where DIS interactions

4304 with argon dominate, and the low energy part of the spectrum where neutrinos mainly
4305 undergo QEL interactions. This allows me to compute the projected generator-level DM
4306 cross section sensitivities, showing how DUNE can be complementary to other indirect
4307 DM searches. Additionally, I explore two specific realisations of the DM interactions,
4308 namely Kaluza-Klein and leptophilic DM.

4309 At this stage, this analysis already shows the potential of DUNE to explore these
4310 scenarios. However, including the full simulation and reconstruction of the events will
4311 be necessary moving forward. At the moment, a significant effort is aimed towards the
4312 reconstruction of atmospheric neutrinos in the DUNE FD, which could be relevant for
4313 the case at hand. Also, following iterations of the analysis should include all the relevant
4314 systematic uncertainties. A summary of these is presented in section 5.7.

4315 Chapter 6 reviews my work on the reconstruction for ND-GAr. In section 6.2 I try
4316 to establish the relation between the measured charge in the readout and the deposited
4317 energy from a stopping proton sample, using the residual range of the tracks. This
4318 calibration allows to compute the mean dE/dx for the particles. I finish the section
4319 providing a parametrisation for how this depends on the momentum. The problem of the
4320 muon and pion separation is the topic of section 6.3. I propose to use the information
4321 from the ECal to achieve this classification. In this section, I describe the features and
4322 the procedure I follow to train the classifier, showing its performance as a function of
4323 the particle momentum. In section 6.4 I explore the possibility of performing a ToF
4324 measurement with the ECal. With this, I achieve a separation between pions and protons
4325 in a momentum range beyond the reach of the HPgTPC alone. Section 6.5 is devoted to
4326 the identification of charged particle decays inside the HPgTPC where the parent plus
4327 (charged) daughter system is reconstructed as a single track. I use the information from
4328 the track fit to construct a series of variables which can identify the tracks containing
4329 decays, as well as locate their position. I finish the Chapter introducing a new clustering
4330 algorithm for the ECal hits in section 6.6. It aims at having a one-to-one correspondence
4331 between particles and clusters, which will facilitate the reconstruction of neutral particles
4332 in the ECal.

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4333 The goal of these developments was establishing a robust PID strategy for ND-GAr,
4334 that allows to reconstruct the multiplicity of pions and other hadrons in the neutrino
4335 interactions final states. In section 6.7 I describe the status of the integration of the
4336 different additions to the reconstruction chain.

4337 Finally, in Chapter 7 I apply to the event selection in ND-GAr. I start by describing
4338 a method for selecting ν_μ CC events in section 7.2. This is mainly based on the muon
4339 score derived from the muon/pion classification I developed. Additionally, I perform
4340 an optimisation of the FV. As part of this study, I also examined the kinematics of
4341 the selected primary muon and the reconstructed interaction vertex. Next, in section
4342 7.3 I explore the capabilities of ND-GAr and its reconstruction at identifying charged
4343 pions. I optimise a selection based on the reconstructed charged pion multiplicity, for
4344 events with 0, 1, 2, and $\geq 3\pi^\pm$ in the final state. I the performance of the selection as a
4345 function of the truth hadronic invariant mass, as well as the true pion kinematics for the
4346 ν_μ CC $1\pi^\pm$ case. I briefly discuss the possibility of tagging events with neutral pions
4347 by reconstructing the invariant mass of the photon pairs from their decay in section
4348 7.4. Lastly, in section 7.5 I study the neutrino energy reconstruction of the selected ν_μ
4349 CC events using a calorimetric approach. For this, I compare the values obtained using
4350 generator-level and reconstructed information.

4351 These studies constitute the first try at an event selection in ND-GAr using full
4352 simulation and reconstruction. It will serve as a stepping stone for the development
4353 of other selections and analyses. Ultimately, the goal is to quantify the impact of
4354 ND-GAr on the LBL analysis in DUNE. For this, including the effect of the systematic
4355 uncertainties outlined in section 7.6 will be necessary.

4356 In summary, this thesis provides an overview of three novel topics within DUNE. As
4357 a single sentence, in this work I investigate the enhancement of the triggering capabilities
4358 of the FD, study the sensitivity of the FD to solar DM signatures, and develop the
4359 particle identification and event selection strategies for the Phase II ND. Each Chapter
4360 aims to be a comprehensive summary of the status of the different studies. I hope they
4361 can be helpful guides for future work both in the ND and FD.

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