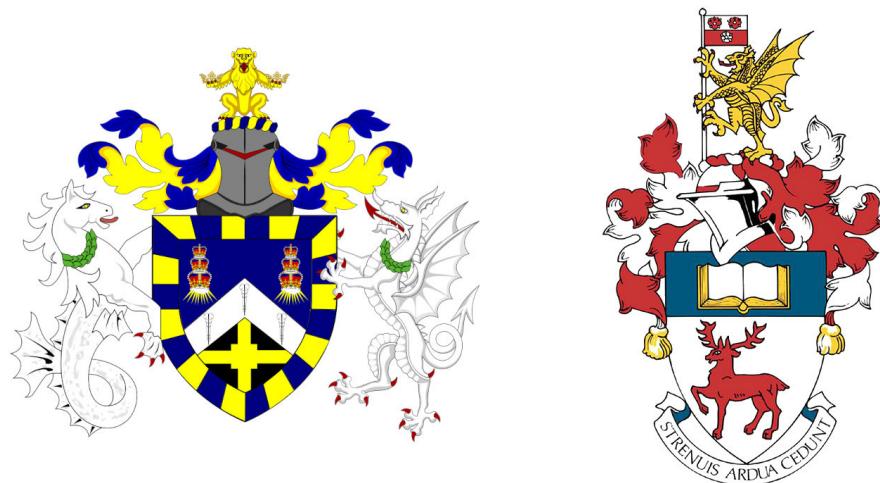


<sup>1</sup> ADVANCING NEUTRINO  
<sup>2</sup> DETECTION AND TRIGGERING IN  
<sup>3</sup> DUNE



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<sup>6</sup> *Submitted in partial fulfillment of the requirements*  
<sup>7</sup> *of the Degree of Doctor of Philosophy*

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<sup>12</sup> December 2024



## <sup>13</sup> Statement of originality

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# <sup>31</sup> Abstract

<sup>32</sup> Work in progress . . .



*¡Oh memoria, enemiga mortal de mi descanso!*

---

*El ingenioso hidalgo don Quijote de la Mancha*

MIGUEL DE CERVANTES SAAVEDRA



## <sup>33</sup> Acknowledgements

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## <sup>509</sup> List of Abbreviations

**ADC** Analog to Digital Converter.

**ALEPH** Apparatus for LEP PHysics.

**ALICE** A Large Ion Collider Experiment.

**BDT** Boosted Decision Tree.

**CC** Charged Current.

**DM** Dark Matter.

**DUNE** Deep Underground Neutrino Experiment.

**ECal** Electromagnetic Calorimeter.

**FD** Far Detector.

**FHC** Forward Horn Current.

**HPgTPC** High Pressure gaseous Time Projection Chamber.

**LBL** Long BaseLine.

## List of Abbreviations

|               |                              |
|---------------|------------------------------|
| <b>MuID</b>   | Muon IDentification system.  |
| <b>NC</b>     | Neutral Current.             |
| <b>ND</b>     | Near Detector.               |
| <b>ND-GAr</b> | Near Detector Gaseous Argon. |
| <b>ND-LAr</b> | Near Detector Liquid Argon.  |
| <b>PDG</b>    | Particle Data Group.         |
| <b>RHC</b>    | Reverse Horn Current.        |

510 Chapter 1

511 Introduction



512 **Chapter 2**

513 **Neutrino physics**

514 Ever since they were postulated in 1930 by Wolfgang Pauli to explain the continuous  
515  $\beta$  decay spectrum [17] and later found by Reines and Cowan at the Savannah River  
516 reactor in 1953 [18], neutrinos have had a special place among all other elementary  
517 particles. They provide a unique way to probe a wide range of quite different physics,  
518 from nuclear physics to cosmology, from astrophysics to colliders. Moreover, there is  
519 compelling evidence to believe that the study of neutrinos may be key to unveil different  
520 aspects of physics beyond the SM, difficult to test elsewhere.

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

524 **2.1 Neutrinos in the SM**

525 By definition, in the SM there are no right-handed neutrino fields. A direct implication  
526 of this fact is that neutrinos are strictly massless within the SM. This follows from the  
527 experimental observation that all neutrinos produced via weak interactions are pure  
528 left-handed helicity states (and similarly antineutrinos are pure right-handed states).  
529 The hypothetical existence of right-handed neutrinos could be indirectly inferred from  
530 the observation of non-zero neutrino masses, nevertheless the existence neutrino masses

## Chapter 2. Neutrino physics

531 is not a sufficient condition for the existence of such fields.

532 In the SM neutrinos appear in three flavours, namely  $\nu_e$ ,  $\nu_\mu$  and  $\nu_\tau$ . These are  
533 associated with the corresponding charged leptons  $e$ ,  $\mu$  and  $\tau$ , in such a way that the  
534 charged current part of the Lagrangian coupling them is diagonal. As in the electroweak  
535 theory neutrinos are coupled to the Z boson in a universal way, by measuring the so-called  
536 invisible decay width of the Z we have an estimate of the number of light (i.e. lighter  
537 than the Z boson) neutrino flavours. This number was measured by LEP in a combined  
538 analysis of  $e^+e^- \rightarrow \mu^+\mu^-$  and  $e^+e^- \rightarrow$  hadrons to be  $N_\nu = 2.9840 \pm 0.0082$  [19].

## 539 2.2 Neutrino oscillations

540 The evidence for neutrino oscillation [20], and therefore the existence of non-zero neutrino  
541 masses, constitutes one of the groundbreaking discoveries of modern Physics and has  
542 acted as driving force for Beyond the Standard Model (BSM) Physics. The minimal  
543 extension of the Standard Model (SM) we can do to address these phenomena is  
544 introducing distinct masses for at least two of the neutrinos. This way, we are left with  
545 three neutrino mass eigenstates  $\nu_1$ ,  $\nu_2$  and  $\nu_3$ , with masses  $m_1$ ,  $m_2$  and  $m_3$  respectively,  
546 which in general will not coincide with the flavour eigenstates  $\nu_e$ ,  $\nu_\mu$  and  $\nu_\tau$ .

547 The way to relate these two sets of neutrino eigenstates is via a  $3 \times 3$  unitary matrix,  
548 called the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix [21, 22], as:

$$|\nu_\alpha\rangle = \sum_{i=1}^3 U_{\alpha i}^* |\nu_i\rangle, \quad (2.1)$$

549 where the Greek index  $\alpha$  denotes the flavour  $\{e, \mu, \tau\}$  and the Latin index  $i$  the associated  
550 masses  $\{1, 2, 3\}$ . This leptonic mixing matrix may be parametrized in terms of 6  
551 parameters, 3 of which are mixing angles  $\theta_{12}$ ,  $\theta_{13}$  and  $\theta_{23}$ , one CP-violating phase  $\delta_{CP}$

## 2.2. Neutrino oscillations

552 and 2 Majorana phases  $\alpha$  and  $\beta$ :

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta_{CP}} \\ 0 & 1 & 0 \\ -s_{13}e^{-i\delta_{CP}} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\alpha} & 0 \\ 0 & 0 & e^{i\beta} \end{pmatrix}, \quad (2.2)$$

553 where  $c_{ij} \equiv \cos \theta_{ij}$  and  $s_{ij} \equiv \sin \theta_{ij}$ . This matrix is analogous to the Cabibbo-Kobayashi-  
554 Maskawa (CKM) matrix in the quark sector. If neutrinos are Dirac fermions, we can  
555 drop the Majorana phases in the PMNS matrix. But, in any case, these phases play no  
556 role on the neutrino oscillations.

### 557 2.2.1 Oscillations in vacuum

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

$$|\nu_\alpha(t)\rangle = \sum_{i=1}^3 U_{\alpha i}^* e^{-iE_i t} |\nu_i(t=0)\rangle, \quad (2.3)$$

560 as the mass eigenstates are also eigenstates of the free Hamiltonian. Now, if we express  
561 the mass eigenstates as a superposition of flavour eigenstates, the last expression can be  
562 rewritten as:

$$|\nu_\alpha(t)\rangle = \sum_{i=1}^3 U_{\beta i} e^{-iE_i t} U_{\alpha i}^* |\nu_\beta\rangle. \quad (2.4)$$

563 This way, the probability for the neutrino to transition from flavour  $\alpha$  to flavour  $\beta$   
564 will be given by:

$$P(\nu_\alpha \rightarrow \nu_\beta) = |\langle \nu_\beta | \nu_\alpha(t) \rangle|^2 = \left| \sum_{i=1}^3 U_{\beta i} e^{-iE_i t} U_{\alpha i}^* \right|^2. \quad (2.5)$$

565 A usual approximation to take at this point is to consider ultra-relativistic neutrinos,  
566 i.e.  $E \approx |\vec{p}|$ , so we can write the dispersion relations as:

$$E_i = \sqrt{p^2 + m_i^2} \approx E + \frac{m_i^2}{2E}, \quad (2.6)$$

## Chapter 2. Neutrino physics

567 so we can write the oscillation probability as:

$$\begin{aligned} P(\nu_\alpha \rightarrow \nu_\beta) &= \sum_{i,j} U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^* e^{-i \frac{\Delta m_{ij}^2}{2E} t} \\ &= \delta_{\alpha\beta} - 4 \sum_{i < j} \Re [U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^*] \sin^2 \left( \frac{\Delta m_{ij}^2}{4E} t \right) \\ &\quad + 2 \sum_{i < j} \Im [U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^*] \sin \left( \frac{\Delta m_{ij}^2}{2E} t \right), \end{aligned} \quad (2.7)$$

568 where  $\Delta m_{ij}^2$  is the difference of the squared masses of the  $j$ th and  $i$ th neutrino mass  
 569 eigenvalues. At this point, it is usual to write the phase responsible for the oscillations  
 570 as (under the approximate assumption  $t \approx L$ ):

$$\Delta_{ij} \equiv \frac{\Delta m_{ij}^2}{4E} L \simeq 1.27 \frac{\Delta m_{ij}^2}{(\text{eV}^2)} \frac{L}{(\text{km})} \frac{(\text{GeV})}{E}. \quad (2.8)$$

571 Notice that, in the case of antineutrinos the only difference would be the sign of the  
 572 last term in the oscillation probability. This way, one can write the CP asymmetry as:

$$\begin{aligned} A_{CP}^{\alpha\beta} &= P(\nu_\alpha \rightarrow \nu_\beta) - P(\bar{\nu}_\alpha \rightarrow \bar{\nu}_\beta) \\ &= 4 \sum_{i < j} \Im [U_{\alpha i}^* U_{\beta i} U_{\alpha j} U_{\beta j}^*] \sin 2\Delta_{ij}. \end{aligned} \quad (2.9)$$

### 573 2.2.2 Oscillations in matter

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

580 The first proposed model to account for neutrino oscillations in matter was proposed  
 581 by Mikhaev, Smirnov and Wolfenstein (MSW) [23]. It relies on the fact that, as the  
 582 only charged lepton present in ordinary matter is the electron, electron neutrinos can

## 2.2. Neutrino oscillations

583 undergo both charged and neutral-current interactions with matter whereas for muon  
584 and tau neutrinos just neutral currents are possible.

### 585 2.2.3 Current status of neutrino oscillations

586 A wide range of neutrino experiments provide experimental input to the neutrino  
587 oscillation framework, both using natural or synthetic neutrino sources. The results  
588 from one of the neutrino global fit analyses, shown in Tab. 2.1<sup>1</sup>, summarise well our  
589 current understanding of the different oscillation parameters.

590 **Solar neutrino experiments** detect neutrinos produced in thermonuclear reactions  
591 inside the Sun, mainly from the so-called *pp* chain and the CNO cycle. These neutrinos  
592 have a typical energy in the range from 0.1 to 20 MeV. These experiments (Homestake  
593 [24], GALLEX [25], SAGE [26], Borexino [27], Super-Kamiokande [28] and SNO [29])  
594 provide the best sensitivities to  $\theta_{12}$  and  $\Delta m_{21}^2$ .

595 **Atmospheric neutrino experiments** detect the neutrino flux produced when  
596 cosmic rays scatter with particles in Earth's atmosphere. These collisions generate particle  
597 showers that eventually produce electron and muon neutrinos (and antineutrinos). Their  
598 energies range from few MeV to about  $10^9$  GeV. Experiments, like Super-Kamiokande  
599 [30] and IceCube [31] use atmospheric neutrinos to measure oscillations and are specially  
600 sensitive to  $\theta_{23}$  and  $\Delta m_{32}^2$ .

601 **Reactor neutrino experiments** look for the  $\bar{\nu}_e$  spectrum produced by nuclear  
602 reactors, with energies in the MeV scale. Depending on the distance to the source,  
603 long-baseline experiments like KamLAND [32] are sensitive to the solar mass splitting  
604  $\Delta m_{21}^2$  whereas much shorter baseline experiment such as RENO [33] or DayaBay [34]  
605 measure  $\theta_{13}$  and  $\Delta m_{31}^2$ .

606 **Accelerator experiments** measure neutrino fluxes generated in particle accelerators.  
607 Usually mesons are produced in the accelerator to be focused into a beam, then some  
608 decay to muon neutrinos and the rest are absorbed by a target. Depending on the

---

<sup>1</sup>These 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.

## Chapter 2. Neutrino physics

**Table 2.1:** Summary of neutrino oscillation parameters determined in the Neutrino Global Fit of 2020 [16].

| Parameter                                          | Best fit $\pm 1\sigma$ | $3\sigma$ range |
|----------------------------------------------------|------------------------|-----------------|
| $\Delta m_{21}^2$ [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     |
| $\sin^2 \theta_{12}/10^{-1}$                       | $3.04 \pm 0.16$        | 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     |
| $\delta_{CP}/\pi$ (NO)                             | $1.12^{+0.16}_{-0.12}$ | 0.76 – 2.00     |
| $\delta_{CP}/\pi$ (IO)                             | $1.50^{+0.13}_{-0.14}$ | 1.11 – 1.87     |

609 configuration one can obtain a beam made of mostly neutrinos or antineutrinos. The  
 610 typical energies of these neutrinos are in the GeV range. Experiments such as NOvA  
 611 [35], T2K [36], MINOS [37], OPERA [?] and K2K [38] (and in the future DUNE [39])  
 612 are primarily sensitive to  $\theta_{13}$ ,  $\theta_{23}$  and  $\Delta m_{32}^2$ . Also, in the coming years DUNE [39] and  
 613 Hyper-Kamiokande [40] will be sensitive to  $\delta_{CP}$ .

### 614 2.3 Open questions in the neutrino sector

615 A crucial question that remains open these days, and is of vital importance for oscillation  
 616 phenomena, is whether the mass eigenvalue  $\nu_3$  is the heaviest (what we call normal  
 617 ordering) or the lightest (referred to as inverted ordering) of the mass eigenstates. In  
 618 other words, this means that we do not know the sign of  $\Delta m_{32}^2$ , so we can either have  
 619  $m_1 < m_2 < m_3$  (NO) or  $m_3 < m_1 < m_2$  (IO).

620 Another big puzzle is related to the value of  $\delta_{CP}$ . Nowadays it is poorly constrained,  
 621 with all values between  $\pi$  and  $2\pi$  being consistent with data. A prospective measurement  
 622 different from  $\delta_{CP} = 0, \pi$  will predict CP-violation in the leptonic sector, and thus

### 2.3. Open questions in the neutrino sector

contribute along with the one measured in the quark sector to the total amount of CP-violation. Although it is true that these two contributions by themselves are not enough to explain the matter anti-matter asymmetry in our universe, the amount of CP-violation in the leptonic sector can be key to explain such imbalance.

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

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

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



642 Chapter 3

643 The Deep Underground Neutrino  
644 Experiment

645 The Deep Underground Neutrino Experiment (DUNE) is a next generation long-baseline  
646 neutrino experiment [1]. It will aim to address several questions in neutrino physics,  
647 study neutrinos from astrophysical sources and search for beyond the standard model  
648 physics.

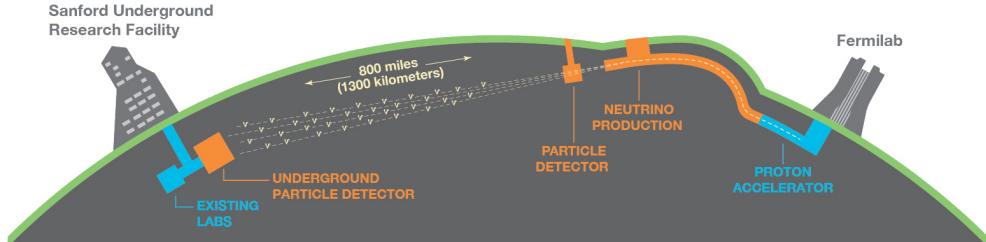
649 This chapter reviews the main goals of the DUNE experiment, the design of the far  
650 detector modules and their data acquisition (DAQ) system, and the role that the near  
651 detector plays in the physics program of DUNE.

652 3.1 Overview

653 The main physics goals of DUNE are:

- 654 • measure the neutrino mass hierarchy, the amount of CP violation in the leptonic  
655 sector and the  $\theta_{23}$  octant,
- 656 • detect rare low energy neutrino events, like neutrinos from supernova bursts, and
- 657 • 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 [1].

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 in 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. Fig. 3.1 shows a simplified view of the various components of DUNE (not to scale).

The beam neutrinos to be used in DUNE will be provided by the LBNF beamline, the multi-megawatt wide-band neutrino beam planned for Fermilab. First, an intense proton beam is extracted from the Fermilab Main Injector. Then, these protons with energies between 60 GeV and 120 GeV collide with a high-power production target and produce charged mesons. Two magnetic horns allow to focus the mesons and perform a sign selection (thus having the capability to switch between neutrino and antineutrino mode). Soon after that, the mesons decay and produce neutrinos (or antineutrinos) which are then aimed to SURF.

Before arriving to the FD, the neutrino beam meets the ND complex, which serves as the experiment's control. Its 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 in order to extract the oscillation parameters. Therefore, the design of the DUNE ND is mainly driven by the needs of the oscillation physics program.

The liquid Argon time projection chamber (LArTPC) technology has been chosen for

## 3.2. Physics goals of DUNE

**Table 3.1:** Summary of the two-phased plan for DUNE. Adapted from Ref. [41].

| 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,<br>SAND | ND-LAr,<br>ND-GAr, SAND | Systematic constraints |

the FD modules of DUNE. Its four modules will record neutrino interactions from the accelerator-produced beam arriving at predictable times. As it also aims at recording rare events, the FD requires trigger schemes which can deal with both kinds of physics, and also maximum uptime.

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

A summary of the DUNE science program can be found in the DUNE FD Technical Design Report (TDR) Volume I [1]. For a detailed discussion on the two-phased approach the reader is referred to the DUNE Snowmass 2021 report [41].

## 3.2 Physics goals of DUNE

As noted in the literature (see for instance Ref. [16] for a review), the parameter space of the neutrino oscillation phenomena within the three-flavour picture is quite constrained by current experimental data. However, there are still crucial open questions, like the mass ordering, the value of  $\delta_{CP}$  or the  $\theta_{13}$  octant. One of the main goals of DUNE is to shed some light on the values of these parameters [42].

To address these questions DUNE can look to the subdominant oscillation channel

### Chapter 3. The Deep Underground Neutrino Experiment

**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. [41].

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

701     $\nu_\mu \rightarrow \nu_e$  ( $\bar{\nu}_\mu \rightarrow \bar{\nu}_e$ ) and study the energy dependence of the  $\nu_e$  ( $\bar{\nu}_e$ ) appearance probability.

702    When we focus on the antineutrino channel  $\bar{\nu}_\mu \rightarrow \bar{\nu}_e$  there is a change in the sign of  $\delta_{CP}$ ,  
 703    thus introducing CP-violation. Moreover, due to the fact that there are no positrons in  
 704    the composition of Earth, there is a sign difference for the matter effect contribution  
 705    when looking to the antineutrino channel. This asymmetry is proportional to the baseline  
 706    length  $L$  and is sensitive to the sign of  $\Delta_{31}$ , and thus to the neutrino mass ordering.

707       Another of the main physics goals of DUNE is the search for baryon-number violating  
 708    processes. Specifically, it will try to answer the question of whether protons are stable  
 709    or not. There is no symmetry argument that forbids protons from decaying, but its  
 710    apparent stability seems to suggest that baryon number is conserved [43]. However,  
 711    proton decay is a usual feature of grand-unified theories, where electromagnetic, weak  
 712    and strong interactions are unified above a certain energy scale [44].

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

717       The last of the main objectives of DUNE is the detection of neutrinos originated in  
 718    supernovae explosions, what is called a supernova neutrino burst (SNB). These neutrinos  
 719    carry with them information about the core-collapse process, from the progenitor to the

### 3.3. Far Detector

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  $\bar{\nu}_e$  events from the 1987A supernova located in the Magellanic Cloud, 50 kpc away from Earth [45, 46].

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

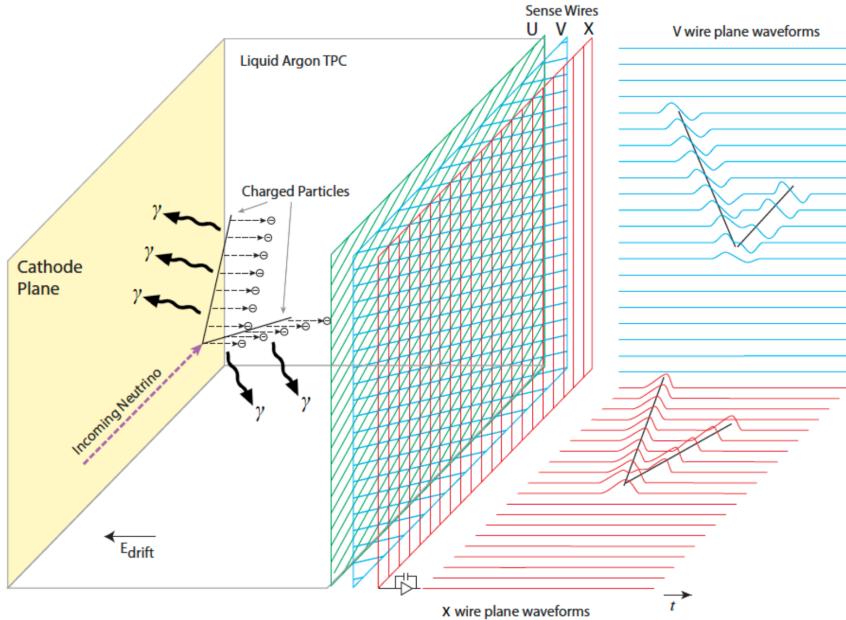
Moreover, due to the stringent requirements that the main physics goals set for DUNE, it will allow also to perform searches for all kind of BSM physics. Among others, DUNE will be able to look for: active-sterile neutrino mixing, non-unitarity of the PMNS matrix, non-standard interactions, Lorentz and CPT violations, neutrino trident production, light-mass DM, boosted DM and heavy neutral leptons. The reader is referred to the DUNE FD TDR Volume II [42] for a full discussion of the physics scope of DUNE.

### 3.3 Far Detector

The so-called DUNE FD complex will sit 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,

## Chapter 3. The Deep Underground Neutrino Experiment



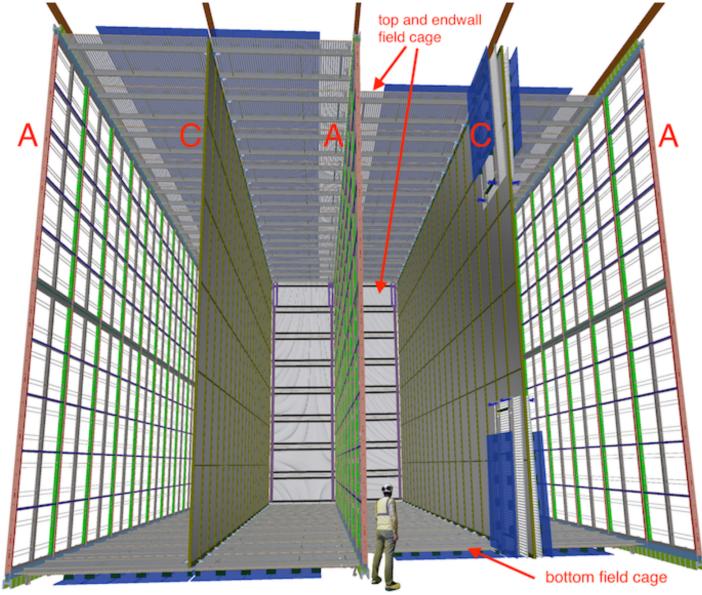
**Figure 3.2:** Schematic diagram showing the operating principle of a LArTPC with wire readout. Figure taken from Ref. [1].

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 start to drift, thus enabling reconstruction over the drift coordinate when compared to the time when the first ionisation electron arrives to the anode. Reconstruction of the topology in the transverse direction is achieved using the charge readout. Fig. 3.2 illustrates the detection principle described, for the case of a HD detector with a wire readout.

### 3.3.1 Horizontal Drift

Within the HD design the ionisation electrons produced as charged particles traverse the LAr drift horizontally towards the anode planes, made out of three layers of wire readout, due to the effect of an electric field. This design, previously known as single-phase (SP), was tested by the ProtoDUNE-SP detector at CERN. The prototype collected data from

### 3.3. Far Detector



**Figure 3.3:** Proposed design for the FD-1 and FD-2 modules following the HD principle. Figure taken from Ref. [1].

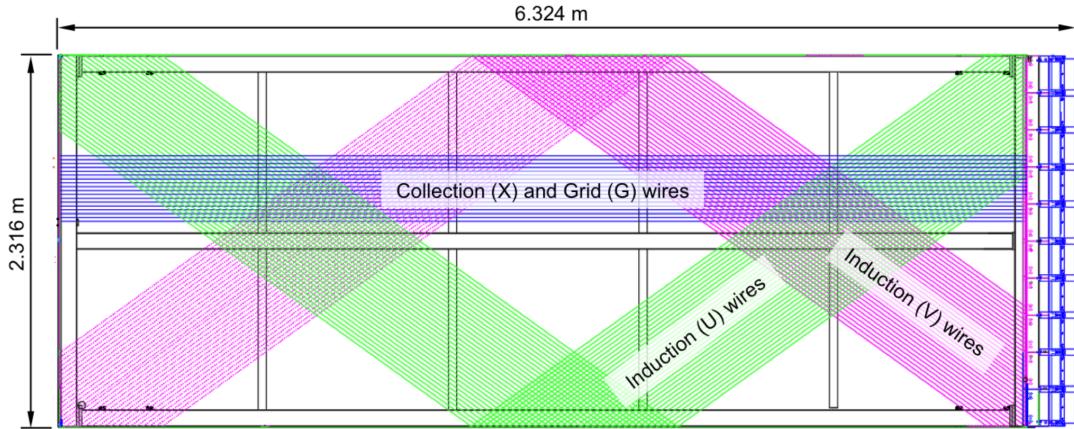
762 a hadron beam and cosmic rays, providing high-quality data sets for calibration studies  
763 and proving the excellent performance of this design.

764 Each FD HD detector module is divided in four drift regions, with a maximum drift  
765 length of 3.5 m, by alternating anode and cathode walls. The surrounding field cage  
766 ensures the uniformity of the 500 V/cm horizontal electric field across the drift volumes.  
767 The three anode walls, which constitute the charge readout of the detector, are built by  
768 stacking anode plane assemblies (APAs), 2 high times 25 wide. The design of the HD  
769 modules is shown in Fig. 3.3.

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

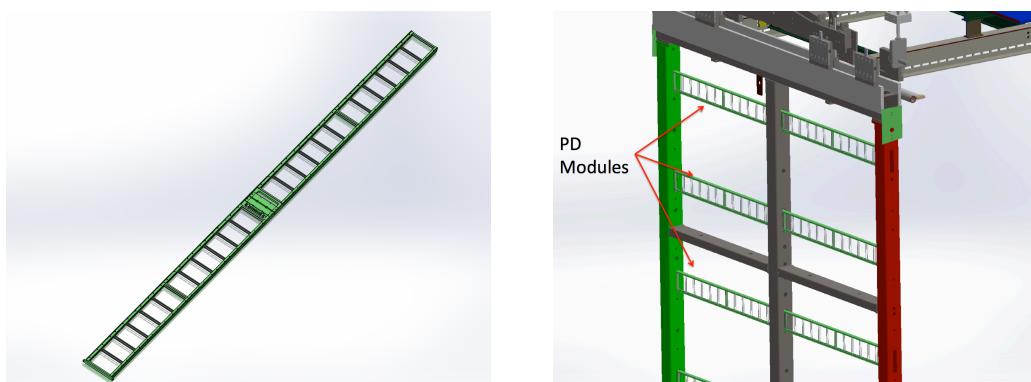
777 The front-end readout electronics, or cold electronics as they are immerse in the LAr,

### Chapter 3. The Deep Underground Neutrino Experiment



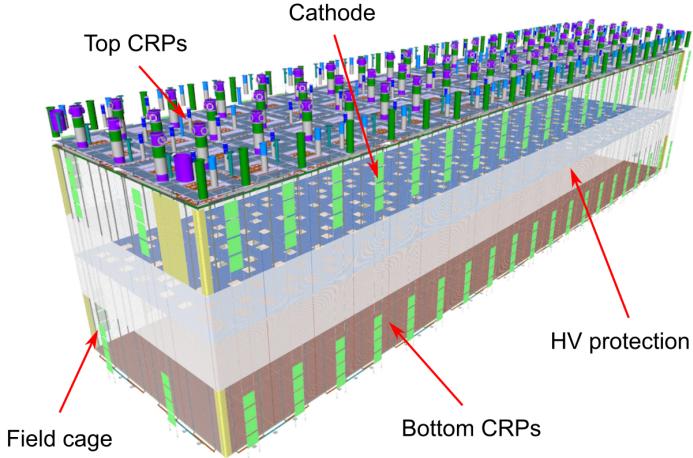
**Figure 3.4:** Schematic representation of an APA. The black lines represent the APA steel frame. The green and magenta lines correspond to the direction of the U and V induction wires respectively. The blue lines indicate the direction of the X collection wires and the wire shielding G. Figure taken from Ref. [1].

are attached to the top of the up APAs and the bottom of the down APAs. Mounted on the front-end mother boards we have a series of ASICs that digitize the signals from the collection and induction planes. Each wire signal goes to a charge-sensitive amplifier, then there is a pulse-shaping circuit and this is followed by the analogue-to-digital converter. This part of the process happens inside the LAr to minimise the number of cables penetrating the cryostat. The digitised signals come out finally via a series of high-speed serial links to the warm interface boards (WIBs), from where the data is sent to the back-end DAQ through optical fibers.



**Figure 3.5:** A PDS module containing 24 X-ARAPUCAs (left) and the location of the modules on the APAs (right). Figure taken from Ref. [1].

### 3.3. Far Detector



**Figure 3.6:** Proposed design for the FD-3 module following the VD principle. Figure adapted from Ref. [47].

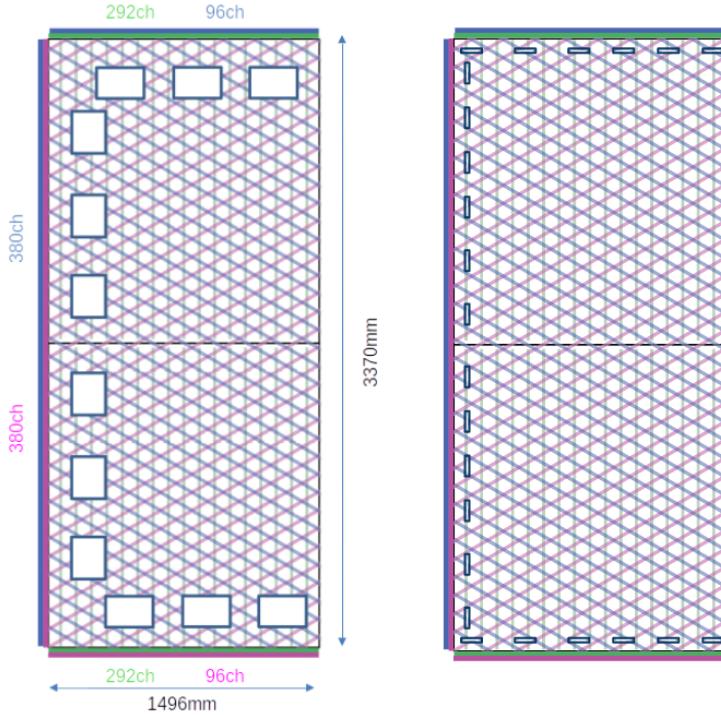
The PDS uses modules of X-ARAPUCA devices, mounted on the APA frames between the wire planes. Each X-ARAPUCA consists of layers of dichroic filter and wavelength-shifter. They shift the VUV scintillation light into the visible spectrum, sending then the visible photons to silicon photomultiplier (SiPM) devices. The PDS modules are  $209\text{ cm} \times 12\text{ cm} \times 2\text{ cm}$  bars, containing 24 X-ARAPUCAs. There are 10 of these PDS modules per APA. Fig. 3.5 shows a PDS module (left) and the placement of the modules on the APAs (right).

#### 3.3.2 Vertical Drift

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

The current design of the FD VD module counts with two drift chambers with a maximum drift distance of 6.5 cm. A cathode plane splits the detector volume along the

## Chapter 3. The Deep Underground Neutrino Experiment



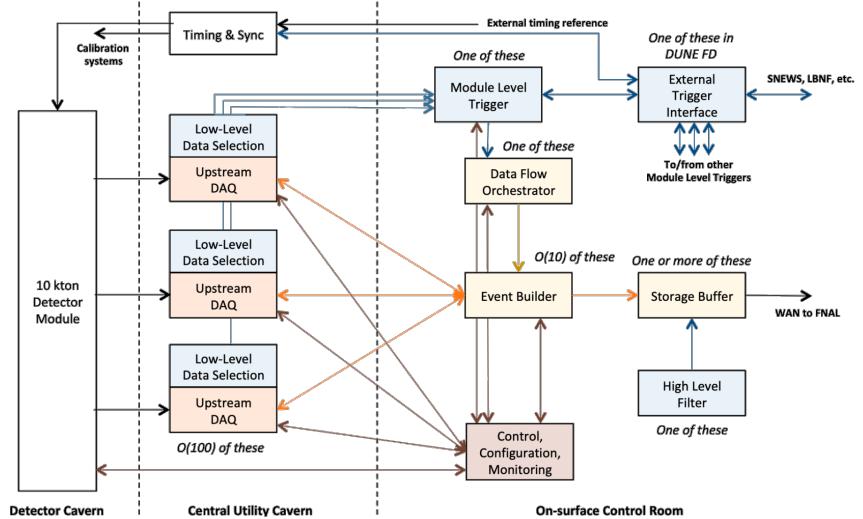
**Figure 3.7:** Schematic representation of the electrode strip configuration for a top (left) and bottom (right) CRU. Figure taken from Ref. [47].

802 drift direction while the two anode planes are connected to the bottom and top walls  
803 of the detector. The layout of the VD module is shown in Fig. 3.6. Compared with  
804 the HD design, the VD option offers a slightly larger instrumented volume and a more  
805 cost-effective solution for the charge readout.

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

811 The PCB face opposite to the cathode has a copper guard plane which acts as  
812 shielding, while its reverse face is etched with electrode strips forming the first induction  
813 plane. The outer PCB has electrode strips on both faces, the ones facing the inner PCB  
814 form the second induction plane while the outermost ones form the collection plane. Fig.  
815 3.7 shows the layout of the electrode strips for the top (left) and bottom (right) CRUs.

### 3.3. Far Detector



**Figure 3.8:** Detailed diagram of the DUNE FD DAQ system. Figure taken from Ref. [2].

816 The magenta and blue lines represent the first and second induction planes respectively,  
817 and the green lines correspond to the collection plane.

818 The PDS in the VD module will use the same X-ARAPUCA technology developed  
819 for the HD design. The plan is to place the PDS modules on the cryostat walls and on  
820 the cathode, in order to maximise the photon yield.

#### 821 3.3.3 FD Data Acquisition System

822 The task of the data acquisition (DAQ) system is to receive, process and store data from  
823 the detector modules. In the case of DUNE the DAQ architecture is designed to work  
824 for all FD modules interchangeably, except some aspects of the upstream part which  
825 may depend on the specific module technology.

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

### Chapter 3. The Deep Underground Neutrino Experiment

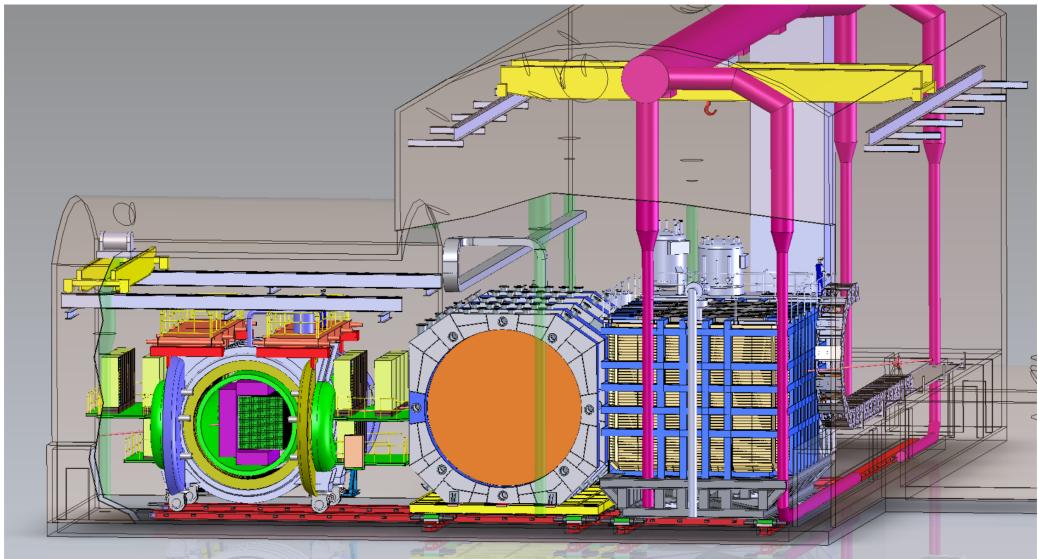
832        The DAQ system of the DUNE FD is composed of five different subsystems. The  
833        first one is the upstream DAQ, which receives the raw data from the detector, buffers it  
834        and perform some low-level pre-processing. The minimally processed data is then fed  
835        into a hierarchical data selection system, which then performs a module level trigger  
836        decision. In case of a positive decision a trigger command is produced and executed by  
837        the data flow orchestrator, located in the back-end (BE) DAQ subsystem. Subsequently  
838        the DAQ BE retrieves the relevant data from the buffers located in the upstream DAQ,  
839        adds all the data into a cohesive record and saves it to permanent storage. Watching  
840        over all the other subsystems we also have the control, configuration and monitoring  
841        subsystem and the time and synchronization subsystem. Fig. 3.8 shows a schematic  
842        diagram of the DAQ system, showing the different subsystems and their relations.

843        A notorious challenge for the DUNE DAQ system comes from its broad physics  
844        goals. We must be prepared to process events spanning a wide range of time windows  
845        (from 5 ms in the case of beam and cosmic neutrinos and nucleon decay to 100 s in the  
846        case of SNBs) and therefore this requires a continuous readout of the detector modules.  
847        Moreover, because of the off-beam measurements we need to ensure the capabilities  
848        of online data processing and self-triggering. Having this into account, together with  
849        the technical constraints, the DUNE FD DAQ faces a series of challenges: it needs to  
850        be fault tolerant and redundant to reduce downtime, accommodate new components  
851        while it keeps serving the operational modules, have large upstream buffers to handle  
852        SNB physics, be able to support a wide range of readout windows and last reduce the  
853        throughput of data to permanent storage to be at most 30 PB/year.

### 854        3.4 Near Detector

855        In order to estimate the oscillation parameters we measure the neutrino energy spectra  
856        at the FD. This reconstructed energy arises from a convolution of the neutrino flux, cross  
857        section, detector response and the oscillation probability. Using theoretical and empirical  
858        models to account for the other effects, one can extract the oscillation probability using

### 3.4. Near Detector



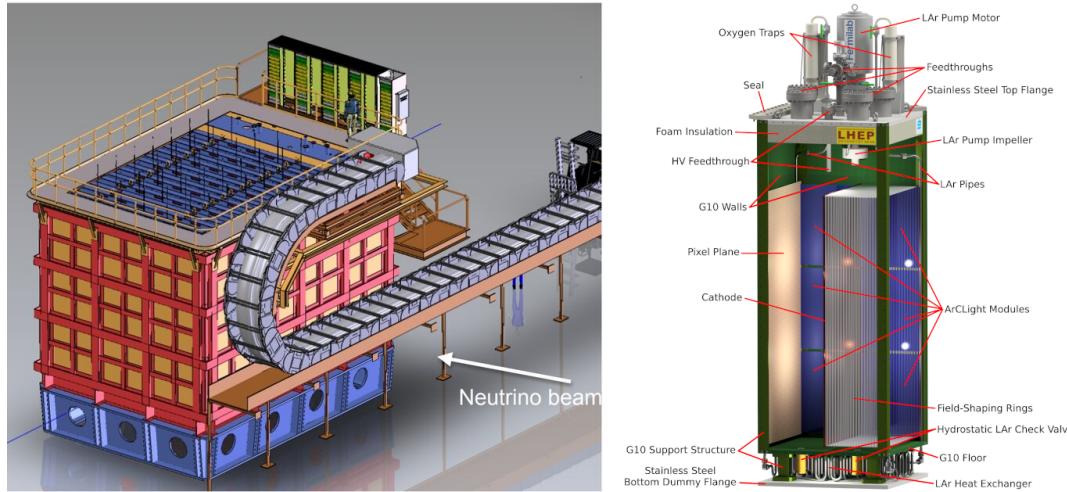
**Figure 3.9:** Representation of the ND hall in Phase II, showing the different subcomponents. From right to left, in the direction of the beam, we have ND-LAr, ND-GAr and SAND. Figure taken from Ref. [48].

859 the measurement. However, these models have associated a number of uncertainties that  
 860 are then propagated to the oscillation parameters.

861 One of the main roles of the ND is to measure the neutrino interaction rates before  
 862 the oscillation effects become relevant, i.e. close to the production point. By measuring  
 863 the  $\nu_\mu$  and  $\nu_e$  energy spectra, and that of their corresponding antineutrinos, at the ND  
 864 we can constrain the model uncertainties. A complete cancellation of the uncertainties  
 865 when taking the ratio between the FD and ND measurements is not possible, as that  
 866 would require both detectors to have identical designs and the neutrino fluxes to be  
 867 the same. Because of the distance, the flux probed by the FD will have a different  
 868 energy and flavour composition than that at the ND, as neutrinos oscillate and the beam  
 869 spreads. The differences in the flux also determine the design of the detectors, therefore  
 870 the ND is limited in its capability to match the FD design.

871 Nevertheless, having a highly capable ND DUNE can minimise the systematic  
 872 uncertainties affecting the observed neutrino energy. The ND data can be used to  
 873 tune the model parameters by comparison with the prediction. Then, one uses the  
 874 tuned model to predict the unoscillated FD spectra. Comparing the prediction with the

## Chapter 3. The Deep Underground Neutrino Experiment



**Figure 3.10:** 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. [1].

875 measured spectra it is possible to extract the oscillation parameters.

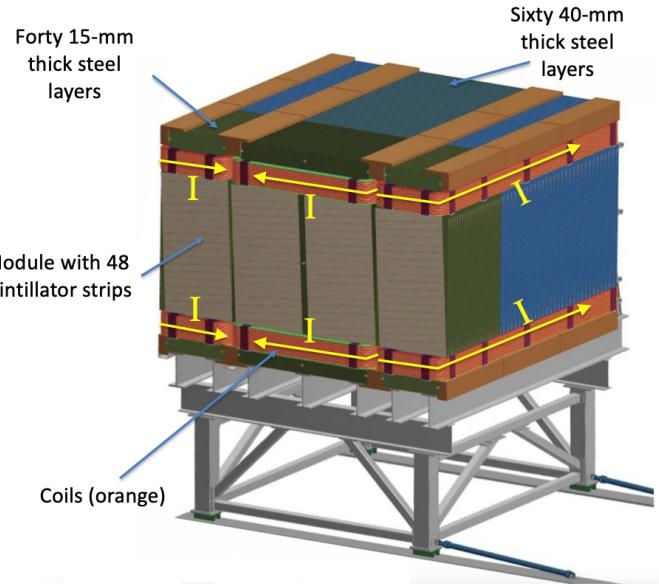
876     Additionally, the ND will have a physics program of its own. In particular, it will  
 877     measure neutrino cross sections that will then be used to constrain the model used in  
 878     the long-baseline oscillation analysis. It will also be used to search for BSM phenomena  
 879     such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

880     The DUNE ND can be divided in three main components, a LArTPC known as ND-  
 881     LAr, a magnetised muon spectrometer, which will be the Temporary Muon Spectrometer  
 882     (TMS) in Phase I and ND-GAr in Phase II, and the System for on-Axis Neutrino  
 883     Detection (SAND). The layout of the Phase II DUNE ND can be seen in Fig. 3.9. The  
 884     first two components of the ND will be able to move off-axis, in what is called the  
 885     Precision Reaction-Independent Spectrum Measurement (PRISM) concept. More details  
 886     on the purpose and design of the ND can be found in the DUNE ND Conceptual Design  
 887     Report (CDR) [48].

### 888 3.4.1 ND-LAr

889     ND-LAr is a LArTPC, as the ND needs a LAr component in order to reduce cross  
 890     section and detector systematic uncertainties in the oscillation analysis. However, its

### 3.4. Near Detector



**Figure 3.11:** Schematic view of the TMS detector, highlighting its main parts. Figure adapted from Ref. [1].

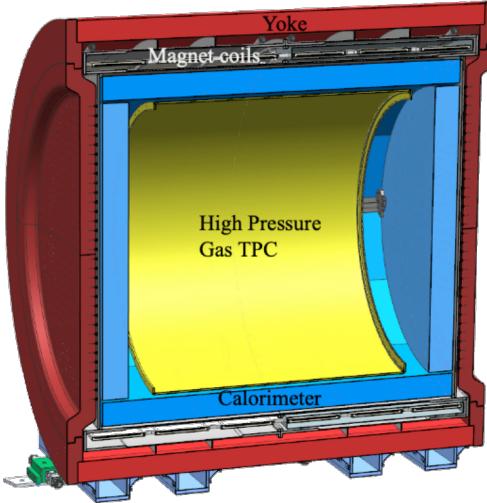
891 design differs significantly from those proposed for the FD modules. Because of the  
 892 high event rates at the ND, approximately 55 neutrino interaction events per  $10 \mu\text{s}$  spill,  
 893 ND-LAr will be built in a modular way. Each of the modules, based on the ArgonCube  
 894 technology, is a fully instrumented, optically isolated TPC with a pixelated readout.  
 895 The pixelisation allows for a fully 3D reconstruction and the optical isolation reduces  
 896 the problems due to overlapping interactions. Fig. 3.10 shows a representation of the  
 897 external parts of ND-LAr (left) and a detailed diagram of an ArgonCube module (right).

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

#### 902 3.4.2 TMS/ND-GAr

903 In order to accurately estimate the neutrino energy, the momentum of the outgoing  
 904 muons needs to be determined. That is the reason why a muon spectrometer is needed  
 905 downstream of ND-LAr.

## Chapter 3. The Deep Underground Neutrino Experiment



**Figure 3.12:** Cross section of the ND-GAr geometry, showing the HPgTPC, ECal and magnet. Figure adapted from Ref. [1].

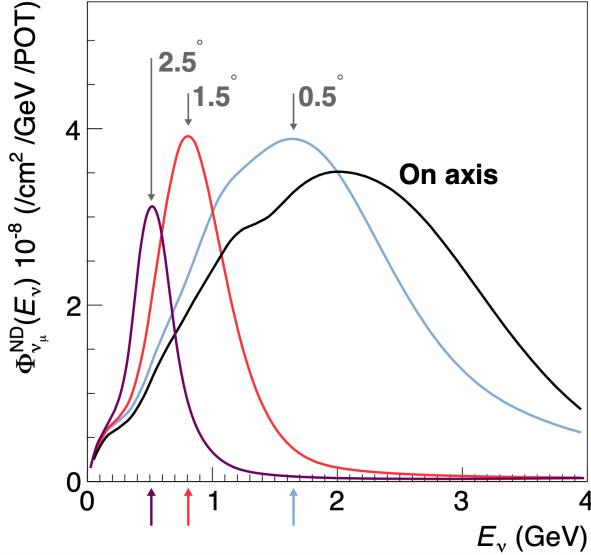
906 In Phase I that role will be fulfilled by TMS. It is a magnetised sampling calorimeter,  
907 with alternating steel and plastic scintillator layers. Fig. 3.11 shows a schematic view of  
908 the TMS detector. The magnetic field allows a precise measurement of the sign of the  
909 muon, so one can distinguish between neutrino and antineutrino interactions.

910 After the Phase II upgrade, TMS will be replaced with ND-GAr. This detector is  
911 a magnetised, high-pressure GAr TPC (often denoted as HPgTPC) surrounded by an  
912 electromagnetic calorimeter (ECal) and a muon tagger. A cross section of its geometry  
913 can be seen in Fig. 3.12. ND-GAr will be able to measure the momenta of the outgoing  
914 muons while also detect neutrino interactions inside the GAr volume. This allows  
915 ND-GAr to constrain the systematic uncertainties even further, as it will be able to  
916 accurately measure neutrino interactions at low energies thanks to the lower tracking  
917 thresholds of GAr.

### 918 3.4.3 PRISM

919 In general, the observed peak neutrino energy of a neutrino beam decreases as the  
920 observation angle with respect to the beam direction increases. This feature has been  
921 used in other long-baseline neutrino experiments, like T2K ( $2.5^\circ$  off-axis) and NOvA

### 3.4. Near Detector



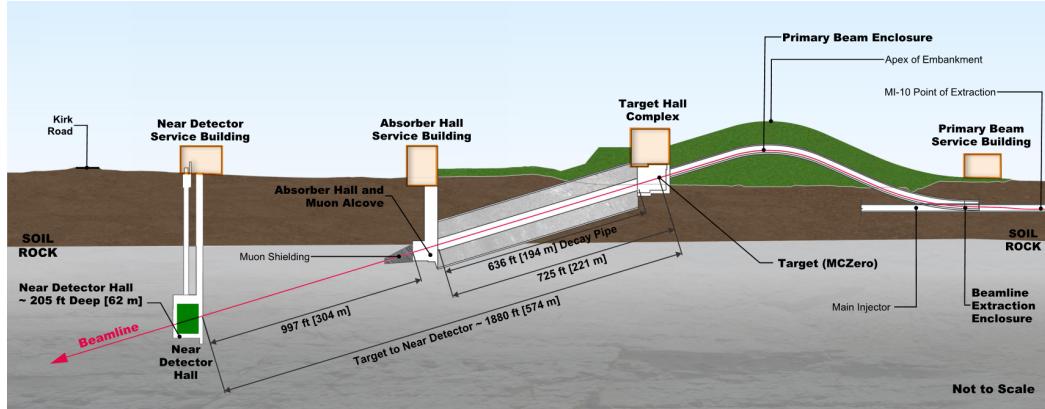
**Figure 3.13:** Predicted beam muon neutrino flux at the ND location for different off-axis positions. Figure taken from Ref. [48].

(0.8° off-axis), in order to achieve narrower energy distributions. The DUNE PRISM concept exploits this effect using a movable ND. Within PRISM both ND-LAr and the muon spectrometer (TMS in Phase I and ND-GAr in Phase II) can be moved up to 3.2° off-axis, equivalent to move the detectors 30.5 m laterally through the ND hall.

This allows to record additional data samples with different energy compositions. Fig. 3.13 compares the on-axis muon neutrino flux at the ND with the fluxes at different off-axis positions. As the off-axis position increases the neutrino flux becomes closer to a monoenergetic beam with a lower peak energy. These samples can be used to perform a data-driven determination of the relation between true and reconstructed neutrino energy, in order to reduce the dependence on the interaction model. The off-axis samples are linearly combined to produce a narrow Gaussian energy distribution centered on a target true energy. From the combination coefficients one can build a sample of reconstructed neutrino events that will determine the energy mapping.

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

## Chapter 3. The Deep Underground Neutrino Experiment



**Figure 3.14:** Schematic longitudinal section of the LBNF beamline at Fermilab (not to scale). Figure taken from Ref. [49].

### 938 3.4.4 SAND

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

945 The SAND detector is magnetised, and it counts with an inner low density tracker,  
 946 a LAr target with optical readout and surrounding sampling calorimeter.

## 947 3.5 LBNF beamline

948 The Long-Baseline Neutrino Facility (LBNF) project is responsible for producing the  
 949 neutrino beam for the DUNE detectors. A detailed discussion of the LBNF program  
 950 can be found in the DUNE/LBNF CDR Volume III [49].

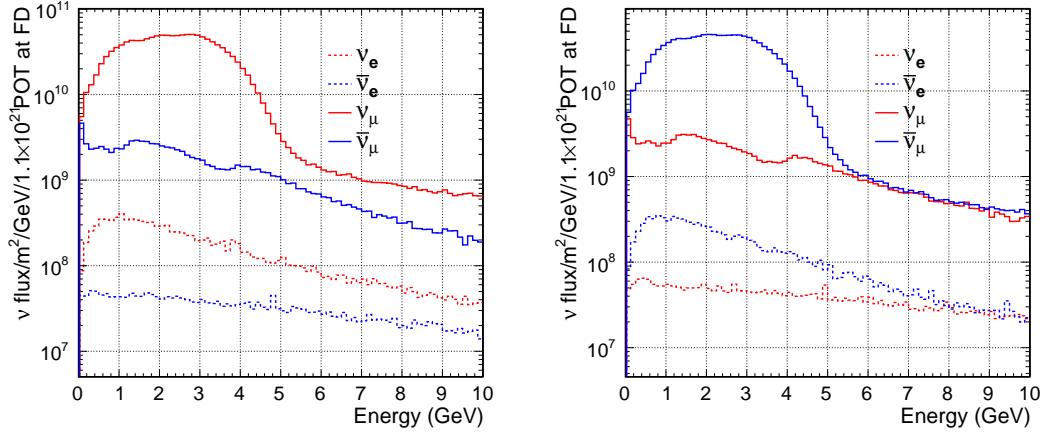
951 The LBNF beamline will provide a high-intensity neutrino beam within the adequate  
 952 energy range in order to meet the long-baseline oscillation physics goals of DUNE. A  
 953 schematic diagram of the longitudinal section of the LBNF beamline is shown in Fig.  
 954 3.14. First, a beam of  $60 - 120$  GeV protons is extracted from the Fermilab Main

### 3.5. LBNF beamline

955 Injector. This beam is aimed towards the target area, where it collides with a cylindrical  
 956 graphite target to produce pions and kaons.

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

963 At the end of the decay pipe a hadron absorber removes the undecayed hadrons and  
 964 muons from the beam, which reduces the  $\nu_e$  ( $\bar{\nu}_e$ ) and  $\bar{\nu}_\mu$  ( $\nu_\mu$ ) contamination coming  
 965 from the  $\mu^+$  ( $\mu^-$ ) decays. The resulting neutrino flux at the FD is shown in Fig. 3.15,  
 966 both for FHC (left) and RHC (right) modes. These predictions show the intrinsic  $(\bar{\nu}_e)$   
 967 contamination and wrong sign component from wrong sign and neutral meson decays,  
 968 as well as muons decaying before reaching the absorber.



**Figure 3.15:** Predicted neutrino fluxes at the FD in FHC mode (left panel) and RHC mode (right panel). Figures taken from Ref. [42].



969 **Chapter 4**

970 **ND-GAr**

971 ND-GAr is a magnetised, high-pressure gaseous argon TPC (HPgTPC), surrounded by  
972 an electromagnetic calorimeter (ECal) and a muon detector (commonly refer to as  $\mu$ ID).  
973 A detailed discussion on the requirements, design, performance and physics of ND-GAr  
974 can be found in the DUNE ND CDR [48] and the ND-GAr whitepaper (cite).

975 In DUNE Phase II ND-GAr will fulfill the role of TMS, measuring the momentum  
976 and sign of the charged particles exiting ND-LAr. Additionally, it will be able to measure  
977 neutrino interactions inside the HPgTPC, achieving lower energy thresholds than those  
978 of the ND and FD LArTPCs. By doing so ND-GAr will allow to constrain the relevant  
979 systematic uncertainties for the LBL analysis even further.

980 The goal of the present chapter is to review the requirements that the physics program  
981 of DUNE impose on ND-GAr, present the current status of its design and describe the  
982 GArSoft package, its simulation and reconstruction software.

983 **4.1 Requirements**

984 The primary requirement for ND-GAr is to the measure the momentum and charge of  
985 muons from  $\nu_\mu$  and  $\bar{\nu}_\mu$  CC interactions in ND-LAr, in order to measure their energy  
986 spectrum. To achieve the sensitivity to the neutrino oscillation parameters described  
987 in the DUNE FD TDR Volume II [42] ND-GAr should be able to constrain the muon

## Chapter 4. ND-GAr

988 energy within a 1% uncertainty or better. The main constraint will come from the  
989 calibration of the magnetic field, performed using neutral kaon decays in the HPgTPC.

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

995 ND-GAr should also be able to the relationship between true and reconstructed energy  
996 from neutrino interactions on argon with low thresholds, being sensitive to particles that  
997 are not observed or may be misidentified in ND-LAr. In particular, ND-GAr needs to  
998 have low tracking thresholds in order to measure the spectrum of pions and protons  
999 produced in final-state interactions (FSI). It also must be able to accurately measure  
1000 the pion multiplicity in 1, 2 and 3 pions final states, to inform the pion mass correction  
1001 in the LArTPCs.

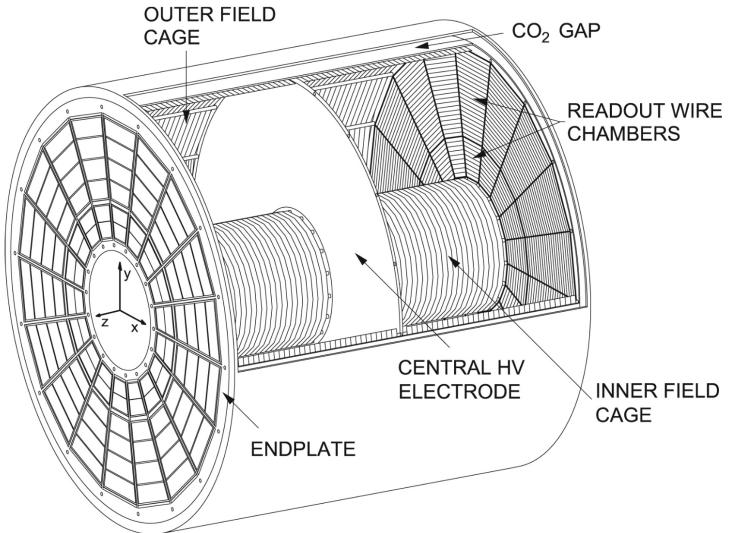
### 1002 4.2 Reference design

1003 The final design of ND-GAr is still under preparation. However, a preliminary baseline  
1004 design was in place at the time of the ND CDR. This section summarises the main  
1005 features of that design, as it is also the one used for the default geometry in our simulation.  
1006 A DUNE Phase II whitepaper, discussing the different options under consideration for  
1007 the ND-GAr design, is in progress.

#### 1008 4.2.1 HPgTPC

1009 The reference design for the ND-GAr HPgTPC follow closely that of the ALICE TPC.  
1010 It is a cylinder with a central high-voltage cathode, generating the electric field for  
1011 the two drift volumes, with a maximum drift distance of 2.5 m each. The anodes will  
1012 be instrumented with charge readout chambers. The original design repurposed the  
1013 multi-wire proportional readout chambers of ALICE, however the current R&D efforts

## 4.2. Reference design



**Figure 4.1:** Diagram of the ALICE TPC, showing the two drift chambers, inner and outer field cages and readout chambers. Figure taken from Ref. [1].

1014 focus on a gas electron multiplier option instead. Fig. 4.1 shows a schematic diagram of  
 1015 the ALICE TPC design. The basic ND-GAr geometry will resemble this, except for the  
 1016 inner field cage.

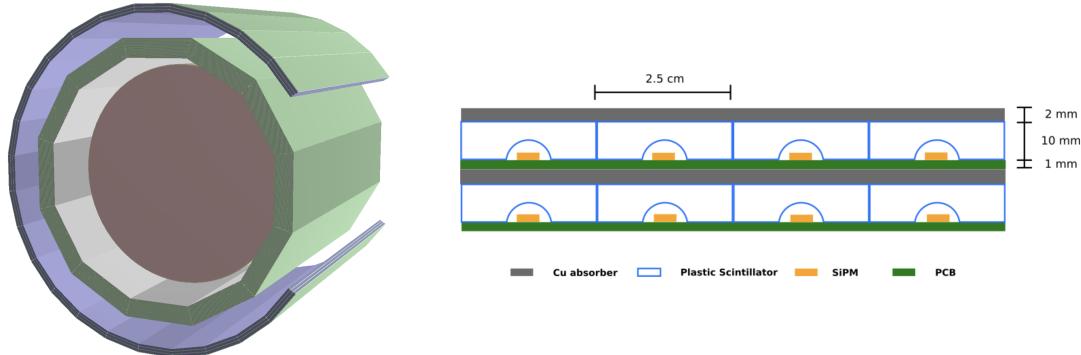
1017 It will use a 90-10 molar fraction argon-CH<sub>4</sub> mixture at 10 bar. With this baseline  
 1018 gas mixture light collection is not possible, as the quenching gas absorbs most of the  
 1019 VUV photons. Additional R&D efforts are underway, to understand if different mixtures  
 1020 allow for the light signal to be used to provide a  $t_0$  while maintaining stable charge gain.

### 1021 4.2.2 ECal

1022 The main role of the ND-GAr ECal is the calorimetric measurement of the electron  
 1023 energies and the reconstruction of photons, in particular those from neutral pion decays.  
 1024 Also, the ECal is able to provide a  $t_0$  timestamp for neutrino interactions, by associating  
 1025 its activity to the tracks in the HPgTPC. The ECal will also be able to perform  
 1026 neutron reconstruction using time of flight and reject external backgrounds, thanks to  
 1027 its sub-nanosecond time resolution.

1028 The ECal design features three independent subdetectors, two end caps at each side  
 1029 and a barrel surrounding the HPgTPC. Each of the detectors is divided in modules,

## Chapter 4. ND-GAr



**Figure 4.2:** 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. [1].

1030 which combine alternating layers of plastic scintillator and absorber material readout  
 1031 by SiPMs. The inner scintillator layers consist of  $2.5 \times 2.5 \text{ cm}^2$  high-granularity tiles,  
 1032 whereas the outer ones are made out of 4 cm wide cross-strips spanning the whole  
 1033 module length. The current barrel geometry consists of 8 tile layers and 34 strip layers,  
 1034 while the end caps feature 6 and 36 respectively. The thickness of the scintillator layers  
 1035 is 7 mm and 5 mm for the Pb absorber layers. The 12-sided geometry of the ECal barrel  
 1036 (left) and the layout of the tile layers (left)<sup>1</sup> can be seen in Fig. 4.2.

### 1037 4.2.3 Magnet

1038 The ND-GAr magnet design, known as the Solenoid with Partial Yoke (SPY), consists of  
 1039 two coupled solenoids with an iron return yoke. The idea behind the design is to have a  
 1040 solenoid as thin as possible, as well as a return yoke mass distribution that minimises  
 1041 the material budget between ND-LAr and ND-GAr. The magnet needs to provide a  
 1042 0.5 T field in the direction perpendicular to the beam, parallel to the drift electric field.  
 1043 It needs to host the pressure vessel and the surrounding ECal, which points to an inner  
 1044 diameter of  $\sim 6.4$  m.

1045 The solenoid is a single layer coil, based on niobium titanium superconducting

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<sup>1</sup>The 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.

### 4.3. GArSoft

1046 Rutherford cable. The total length of the coil is 7.5 m. The bobbin will be split in four  
1047 segments grouped in pairs with two identical cryostats, connected in series. The iron  
1048 yoke features an aperture in the upstream side to allow the muons coming from ND-LAr.  
1049 Still, its material will be enough to reduce the magnetic field reaching SAND, and also  
1050 stop the charged pions produced inside the HPgTPC.

#### 1051 4.2.4 Muon system

1052 The design of the ND-GAr muon system is still in a preliminary stage. Its role is to  
1053 distinguish between muons and pions punching through the ECal. This is especially  
1054 important for wrong-sign determination, to separate these from neutral current events.

1055 In its current form, the muon system consists of three layers of longitudinal sampling  
1056 structures. It alternates 10 cm Fe absorber slabs with 2 cm plastic scintillator strips.

1057 The transverse granularity required is still under study.

### 1058 4.3 GArSoft

1059 GArSoft is a software package developed for the simulation and reconstruction of events  
1060 in ND-GAr. It is inspired by the LArSoft toolkit used for the simulation of LArTPC  
1061 experiments, like the DUNE FD modules. It is based on `art`, the framework for event  
1062 processing in particle physics experiments [?]. Other of its main dependencies are `ROOT`,  
1063 `NuTools`, `GENIE` and `Geant4`. It allows the user to run all the steps of a generation-  
1064 simulation-reconstruction workflow using FHiCL configuration files.

#### 1065 4.3.1 Event generation

1066 The standard generator FHiCLs in GArSoft run the event generation and particle  
1067 propagation simulation (i.e. Geant4) in the same job by default. However, it is possible  
1068 to split them up if needed. The current version of GArSoft provides five different event  
1069 generators, each of them producing `simb::MCTruth` products defined in `NuTools`. The  
1070 available modules are:

## Chapter 4. ND-GAr

- 1071     • **SingleGen**: particle gun generator. It produces the specified particles with a given  
1072         distribution of momenta, initial positions and angles.
  - 1073     • **TextGen**: text file generator. The input file must follow the `hepevt` format<sup>2</sup>, the  
1074         module simply copies this to `simb::MCTruth` data products.
  - 1075     • **GENIEGen**: GENIE neutrino event generator. The module runs the neutrino-nucleus  
1076         interaction generator using the options specified in the driver FHiCL file (flux file,  
1077         flavour composition, number of interactions per event,  $t_0$  distribution, ...). Current  
1078         default version is `v3_04_00`.
  - 1079     • **RadioGen**: radiological generator. It produces a set list of particles to model  
1080         radiological decays. Not tested.
  - 1081     • **CRYGen**: cosmic ray generator. The module runs the CRY event generator with a  
1082         configuration specified in the FHiCL file (latitude and altitude of detector, energy  
1083         threshold, ...). Not tested.
- 1084     The module `GArG4` searches for all the generated `simb::MCTruth` data products, using  
1085     them as inputs to the Geant4 simulation with the specified detector geometry. A constant  
1086     0.5 T magnetic field along the drift coordinate is assumed. The main outputs of this step  
1087     are `simb::MCParticle` objects for the generated Geant4 particles, `gar::EnergyDeposit`  
1088     data products for the energy deposits in the HPgTPC and `gar::CaloDeposit` data  
1089     products for the energy deposits in the ECal and muon system.

### 1090 4.3.2 Detector simulation

- 1091     The standard detector simulation step in GArSoft is all run with a single FHiCL, but  
1092     the different modules can be run independently as well. First the `IonizationReadout`

<sup>2</sup>In 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.

### 4.3. GArSoft

1093 module simulates the charge readout of the HPgTPC, and later the `SiPMReadout` module  
1094 runs twice, once for the ECal and then for the muon system, with different configurations.

1095 The `IonizationAndScintillation` module collects all the `gar::EnergyDeposit`  
1096 data products, to compute the equivalent number of ionization electrons for each energy  
1097 deposit. The `ElectronDriftAlg` module simulates the electron diffusion numerically  
1098 both in the longitudinal and transverse directions and applies an electron lifetime  
1099 correction factor. The induced charge on the nearest and neighbouring readout pads  
1100 is modeled using the provided pad response functions. The digitisation of the data is  
1101 then simulated with the `TPCReadoutSimAlg` module. By default, the ADC sampling  
1102 rate used is 50.505 MHz. The resulting raw waveforms for each channel are stored with  
1103 zero-suppression, in order to save memory and CPU time. The algorithms keep blocks  
1104 of ADC values above a certain threshold, plus some adjustable additional early and late  
1105 tick counts. The results of these three steps are `gar::raw::RawDigit` data products.

1106 For the ECal and the muon system the `SiPMReadout` module calls either the  
1107 `ECALReadoutSimStandardAlg` or `MuIDReadoutSimStandardAlg` modules. These take  
1108 all the `gar::CaloDeposit` data products in the corresponding detector and do the  
1109 digitisation depending on whether the hit was in a tile or strip layer. They include single  
1110 photon statistics, electronic noise, SiPM saturation and time smearing. The resulting  
1111 objects are `gar::raw::CaloRawDigit` data products.

#### 1112 4.3.3 Reconstruction

1113 The reconstruction in GArSoft is also run as a single job by default. It first runs the hit  
1114 finding, clustering, track fitting and vertex identification in the HPgTPC, followed by  
1115 the hit finding and clustering in the ECal and muon system. After those it produces the  
1116 associations between the associations between the tracks and the ECal clusters.

1117 Focusing first on the HPgTPC reconstruction, the `CompressedHitFinder` module  
1118 takes the zero-suppressed ADCs from the `gar::raw::RawDigit` data products. The  
1119 reconstructed hits largely correspond to the above threshold blocks, however the hit  
1120 finder identifies waveforms with more than one maximum, diving them in multiple hits

## Chapter 4. ND-GAr

1121 if they dip below a certain threshold. The data products produced are of the form  
1122 `gar::rec::Hit`. These are the inputs to the clustering of hits in the `TPCHitCluster`  
1123 module. Hits close in space and time are merged, and the resulting centroids are found.  
1124 This module outputs `gar::rec::TPCClusters` objects and associations to the input  
1125 hits.

1126 The following step prior to the track fitting is pattern recognition. The module  
1127 called `tpcvecchitfinder2` uses the `gar::rec::TPCClusters` data products to find track  
1128 segments, typically called vector hits. They are identified by performing linear 2D fits  
1129 to the positions of the clusters in a 10 cm radius, one fit for each coordinate pair. A  
1130 3D fit defines the line segment of the vector hit, using as independent variable the one  
1131 whose sum of (absolute value) slopes in the 2D fits is the smallest. The clusters are  
1132 merged to a given vector hit if they are less than 2 cm away from the line segment. The  
1133 outputs are `gar::rec::VecHit` data products, as well as associations to the clusters. The  
1134 `tpcpatrec2` module takes the `gar::rec::VecHit` objects to form the track candidates.  
1135 The vector hits are merged together if their direction matches, their centers are within  
1136 60 cm and their direction vectors point roughly to their respective centers. Once  
1137 the clusters of vector hits are formed they are used to make a first estimation of the  
1138 track parameters, simply taking three clusters along the track. The module produces  
1139 `gar::rec::Track` data products and associations between these tracks and the clusters  
1140 and vector hits.

1141 The track is fitted by means of a Kalman filter in the `tpctrackfit2` module, using  
1142 the position along the drift direction as the independent variable. Two different fits are  
1143 performed per track, a forward and a backwards fit, each starting from one of the track  
1144 ends. The Kalman filter state vector ( $y, z, R, \phi, \tan\lambda$ ) is estimated at each point along  
1145 the track using a Bayesian update. The track parameters reported in the forward and  
1146 backwards fits are the ones computed at the opposite end where the fit started. The  
1147 main outputs of the track fit are the `gar::rec::Track` objects. Additionally, the module  
1148 stores the fitted 3D positions along the track in the `gar::rec::TrackTrajectory` data  
1149 products and the total charge and step sizes for each point also get stored in the form of

### 4.3. GArSoft

1150    `gar::rec::TrackIonization` objects.

1151    After the tracking step, the `vertexfinder1` module looks at the reconstructed  
1152    `gar::rec::Track` products, creating vertex candidates with the track ends that are  
1153    within 12 cm of each other. The vertices are then fitted using linear extrapolations from  
1154    the different track ends associated. The results are `gar::rec::Vertex` data products,  
1155    and associations to the tracks and corresponding track ends.

1156    For the ECal and muon tagger, the `SiPMHitFinder` module runs twice with different  
1157    configurations, adapted to the particular capabilities of both. The module simply takes  
1158    the `gar::raw::CaloRawDigit` products, applies a calibration factor to convert the ADC  
1159    counts to MeV and for the strip layer hits it calculates the position along the strip using  
1160    the times recorded of both SiPMs. This module produces `gar::rec::CaloHit` data  
1161    products. Next, these objects are used as inputs to the `CaloClustering` module. It  
1162    merges the hits based on a simple nearest neighbours (NN) algorithm. For the resulting  
1163    clusters it also computes the total energy and position of the centroid. The results are  
1164    stored as `gar::rec::Cluster` data products, with associations to the hits.

1165    The last step in the reconstruction is associating the reconstructed tracks in the  
1166    HPgTPC to the clusters formed in the ECal and muon system. The `TPCECALAssociation`  
1167    module checks first the position of the track end points, considering only the points  
1168    that are at least 215 cm away from the cathode or have a radial distance to the center  
1169    greater than 230 cm. The candidates are propagated up to the radial position, in the  
1170    case of clusters in the barrel, or the drift coordinate position, for the end cap cluster, of  
1171    the different clusters in the collection using the track parameters computed at the end  
1172    point. The end point is associated to the cluster if certain proximity criteria are met.  
1173    This module creates associations between the tracks, the end points and the clusters.  
1174    The criteria for the associations are slightly different for the ECal and the muon tagger.



<sub>1175</sub> Chapter 5

<sub>1176</sub> FWTPG offline software



<sub>1177</sub> **Chapter 6**

<sub>1178</sub> **Matched Filter approach to**  
<sub>1179</sub> **induction wire Trigger Primitives**

<sub>1180</sub> **6.1 Motivation**

<sub>1181</sub> The filter implemented in the firmware of the upstream DUNE FD DAQ is a 32nd-order  
<sub>1182</sub> low-pass finite impulse-response (FIR) filter. The output of such filter for a discrete  
<sub>1183</sub> system can be written as:

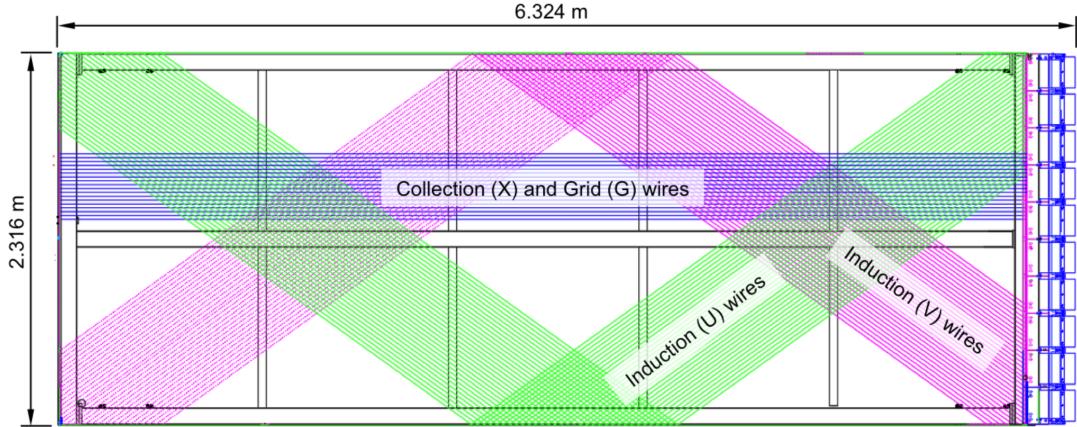
$$y[i] = \sum_{j=0}^N h[j]x[i-j], \quad (6.1)$$

<sub>1184</sub> where  $N$  is the order of the filter,  $y$  is the output sequence,  $x$  is the input sequence and  $h$   
<sub>1185</sub> is the set of coefficients of the filter. The current implementation within `dtp-firmware`  
<sub>1186</sub> [50] uses a set of 16 non-zero integer coefficients.

<sub>1187</sub> Filtering is a vital step in the hit finder chain. It helps to suppress the noise and  
<sub>1188</sub> enhance the signal peaks with respect to the noiseless baseline. A good filtering strategy  
<sub>1189</sub> allows us to use lower thresholds when forming the trigger primitives (TPs) and thus  
<sub>1190</sub> increasing the sensitivity of our detector to low energy physics events. In such events,  
<sub>1191</sub> the hits produced by the ionisation electrons tend to have lower amplitudes than those  
<sub>1192</sub> of interest to the baseline physics programme of the DUNE experiment.

<sub>1193</sub> This is particularly important for the induction planes. In general, signal peaks in

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives



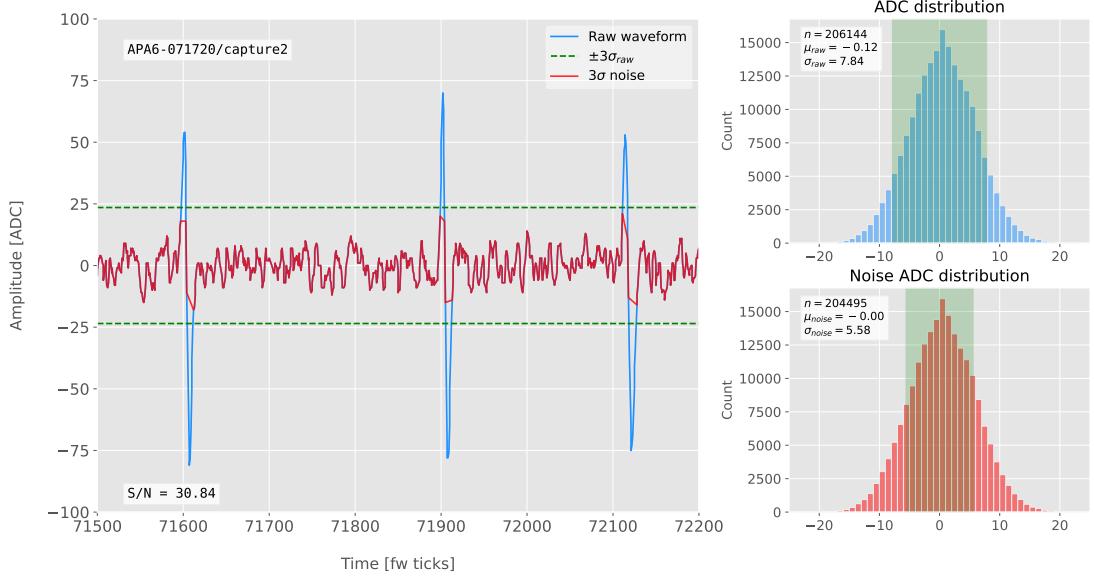
**Figure 6.1:** Schematic representation of an APA. The black lines represent the APA steel frame. The green and magenta lines correspond to the direction of the U and V induction wires respectively. The blue lines indicate the direction of the X collection wires and the wire shielding G.

the induction wires have smaller amplitude than the ones in the induction plane. This, together with the fact that the pulse shapes are bipolar, reduces our capacity to detect the hits on these channels. The inefficiency of detecting TPs in the induction planes (denoted as U and V planes) lead trigger algorithms to focus mainly on the TPs from the collection plane (so-called X plane). As a result, the possibility of making trigger decisions based on the coincidence of TPs across the three wire planes remains nowadays unexploited in DUNE. Fig. 6.1 shows a schematic view of an anode plane assembly (APA), with the different wire plane orientations highlighted.

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

The goal is to implement a better finite-impulse response filter design and to evaluate its performance relative to the current filter. To do so, we need to take into account the limitations of the firmware: the FIR filter shall have maximum 32 coefficients (so-called taps) whose values are 12-bit unsigned integers. Although it is technically possible to include non-integer coefficients, it would be a technical challenge as we have 40 FIR

## 6.2. Signal-to-noise ratio definition



**Figure 6.2:** 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  $\pm 3\sigma_{\text{raw}}$ . The resulting noise waveform is also shown (red line). Top right panel: ADC distribution for channel 7840, where the green shaded region represents  $\pm \sigma_{\text{raw}}$ . Bottom right panel: noise ADC distribution for channel 7840, where the green shaded region represents  $\pm \sigma_{\text{noise}}$ .

1211 instances per APA, as there are 4 FIR per optical link and 10 optical links per APA.  
 1212 With these restrictions, the task is to provide a set of 32 coefficients which yield an  
 1213 optimal filter performance for the induction wires.

## 1214 6.2 Signal-to-noise ratio definition

1215 I introduce the signal to noise ratio (S/N) as a measure of the FIR filter performance  
 1216 and demonstrate how to extract its value for a set of ProtoDUNE-SP data. The S/N  
 1217 metrics allow us to compare different filter implementations and serve as a basis for more  
 1218 detailed studies presented later in this document. Specifically, I use the ADC capture  
 1219 `felix-2020-07-17-21:31:44` (data capture taken for firmware validation purposes). I  
 1220 defined S/N as the height of the signal peaks relative to the size of the noise peaks.  
 1221 To quantify this quantity channel by channel one first need to estimate the standard  
 1222 deviation of the ADC data for each channel,  $\sigma_{\text{ADC}}$ . Then, I define the corresponding

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

noise waveform to be the ADC values in the range  $\pm 3\sigma_{ADC}$ . From this new noise data one can estimate again the mean and standard deviation,  $\mu_{noise}$  and  $\sigma_{noise}$ , so I can write the S/N for any given channel as:

$$S/N = \frac{\max [ADC] - \mu_{noise}}{\sigma_{noise}}, \quad (6.2)$$

where  $\max [ADC]$  is simply the maximum ADC value found in the corresponding channel.

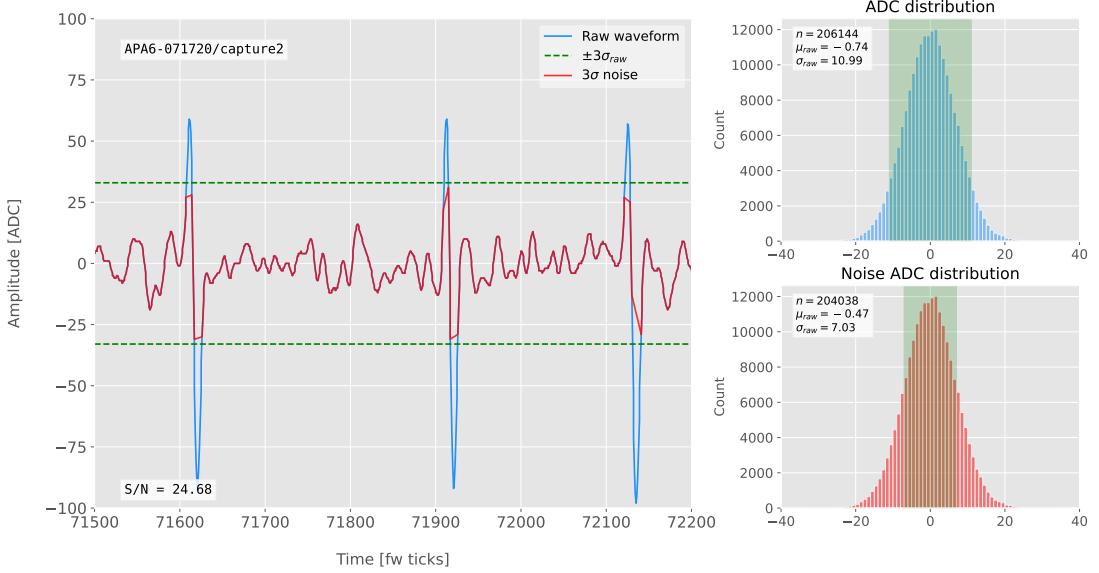
One can apply this definition of the S/N with a waveform from one of the channels of the data capture<sup>1</sup>. Fig. 6.2 shows a zoomed region of the waveform corresponding to channel 7840 (blue line), where one can clearly see three signal peaks and continuous additive noise (we actually see 6 peaks, 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  $\pm 23.52$  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). In Fig. 6.3 I plotted 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 resulting noise waveform (red line) results from selection the ADC values in the range  $\pm 32.91$  ADC, giving now  $\mu_{noise} = -0.47$  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.

---

<sup>1</sup>All the original work was done within the `dtp-simulation` package [51], 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 [52]. Its main purpose is the emulation of the TPG block and, in the same way as its predecessor, it has been cross-checked against the current firmware implementation.

### 6.3. Low-pass FIR filter design



**Figure 6.3:** 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  $\pm 3\sigma_{raw}$ . 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  $\pm \sigma_{raw}$ . Bottom right panel: noise ADC distribution for channel 7840 after filtering, where the green shaded region represents  $\pm \sigma_{noise}$

## 1246 6.3 Low-pass FIR filter design

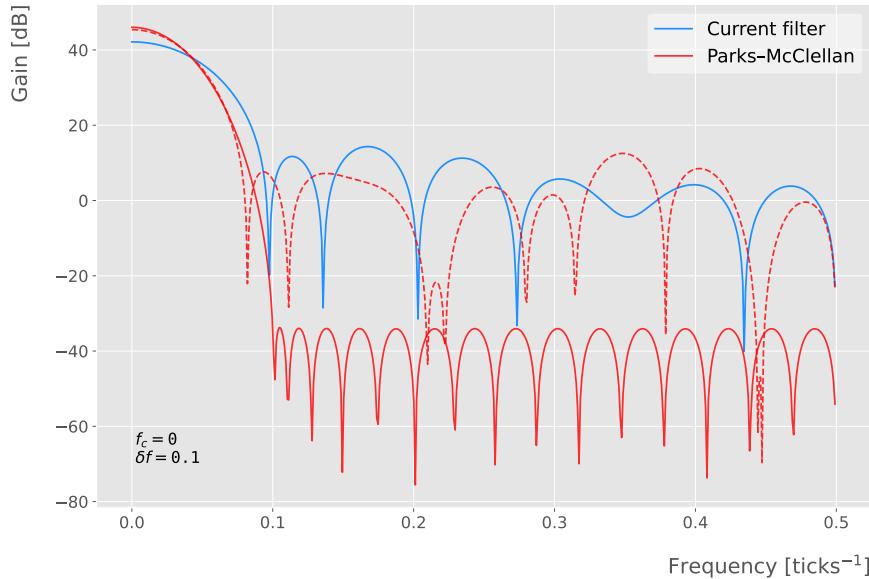
1247 In general, when one uses a method to optimize the frequency response of a digital filter,  
 1248 such as the Parks-McClellan algorithm, one finds a set of  $N$  real coefficients that give  
 1249 the best response for the specified pass-band and order of the filter [53].

1250 In our case, as the sampling frequency is defined as  $1 \text{ ticks}^{-1}$ , the Nyquist frequency  
 1251 will simply be  $1/2 \text{ ticks}^{-1}$ . The current implementation of the filter seems to have as  
 1252 pass-band the range  $[0, 0.1] \text{ ticks}^{-1}$ . This can be seen in Fig. 6.4, where I show the  
 1253 power spectrum, in decibels, of such filter implementation (blue solid line). For instance,  
 1254 the Park-McClellan algorithm finds the optimal Chebyshev FIR filter taking as input  
 1255 the boundaries of the target pass-band and stop-band, which can be written in the form:

$$\left\{ \begin{array}{l} [0, f_c] \\ [f_c + \delta f, f_N] \end{array} \right. , \quad (6.3)$$

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

where  $f_c$  is the cut-off frequency,  $\delta f$  is the transition width and  $f_N$  is the aforementioned Nyquist frequency. A similar behaviour to the one in the current filter can be obtained by setting  $f_c = 0$  and  $\delta f = 0.1 \text{ ticks}^{-1}$ . The response of the resulting filter is also shown in Fig. 6.4 (blue solid line). Notice that the suppression of the stop-band is enhanced for this optimal filter. For comparison I included the power response of the filter obtained by taking the integer part of the coefficients resulting from the Parks-McClellan method (red dashed line). One can see that it does not suppress that much the stop-band, in a similar way to the current implementation of the filter.

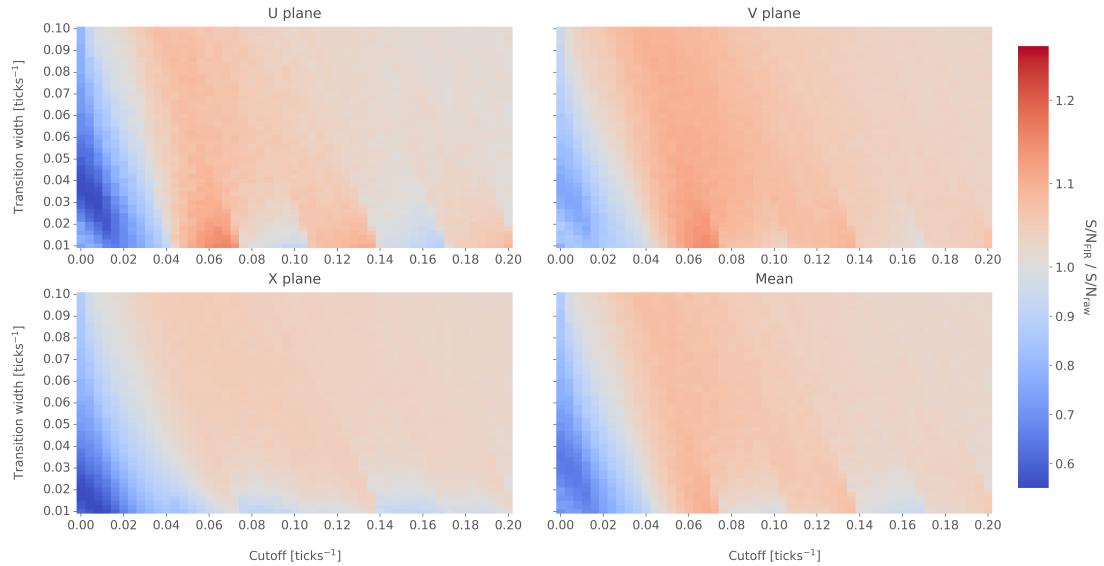


**Figure 6.4:** Power spectrum in decibels for the current implementation of the low-pass FIR filter in `dtp-firmware` (blue line), compared to the response of an optimal filter obtained using the Parks-McClellan algorithm for the same pass-band (red line). Also for comparison I include the spectrum of the optimal filter when taking only the integer part of the coefficients (red dashed line).

At this point, I tried to improve the performance of the FIR filter using the Parks-McClellan method, i.e. maximize the overall S/N, using the available data captures. I did so by varying the values of the two quantities that parametrize the pass-band and stop-band, the cut-off frequency  $f_c$  and the transition width  $\delta f$ .

Fig. 6.5 shows the average relative change in the S/N (i.e. the ratio between the value of the S/N after and before the filtering) for capture `felix-2020-07-17-21:31:44`,

### 6.3. Low-pass FIR filter design

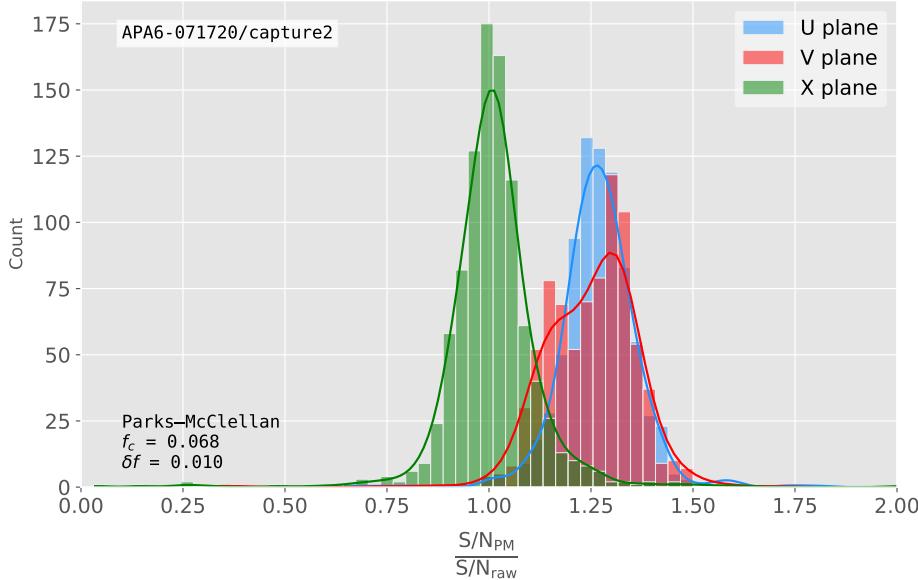


**Figure 6.5:** Relative change in the S/N for the ProtoDUNE-SP raw data capture `felix-2020-07-17-21:31:44`, using different values of the cutoff frequency  $f_c$  and the transition width  $\delta f$ . The optimal Chebyshev filters were applied using just the integer part of the coefficients given by the Parks-McClellan algorithm.

when using filters designed with the Parks-McClellan algorithm for the specified values of the cut-off frequency  $f_c$  and the transition width  $\delta f$ , restricted to integer values for the filter coefficients. One can clearly distinguish different regions where we get an improvement of up to a factor of 1.35 for the U plane. For large values of  $f_c + \delta f$  the ratio tends to 1, as expected (in that limit the width of the stop-band goes to 0, meaning that no frequencies are filtered out and thus the waveform remains the same).

Using the configuration which gives the best mean performance for the three planes (see bottom right panel of Fig. 6.5), i.e.  $f_c = 0.068 \text{ ticks}^{-1}$  and  $\delta f = 0.010 \text{ ticks}^{-1}$ , we can see how such filter affects the different channels. Fig. 6.6 shows the distribution of the S/N improvement values for all the channels in the raw ADC capture `felix-2020-07-17-21:31:44`, separated by wire plane, after the optimal Chebyshev filter was applied. One can see that there is a clear improvement for both U and V induction wire planes, obtaining a mean change of 1.25 and 1.30 for them respectively. However, in the case of the collection plane X the mean of this distribution is roughly 1, meaning that a good fraction of channels in that plane get a slightly worse S/N after the

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives



**Figure 6.6:** 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  $\delta f = 0.010 \text{ ticks}^{-1}$ .

filter is applied. In any case, this is not a big issue as the S/N for collection channels is usually much higher than the one for induction channels.

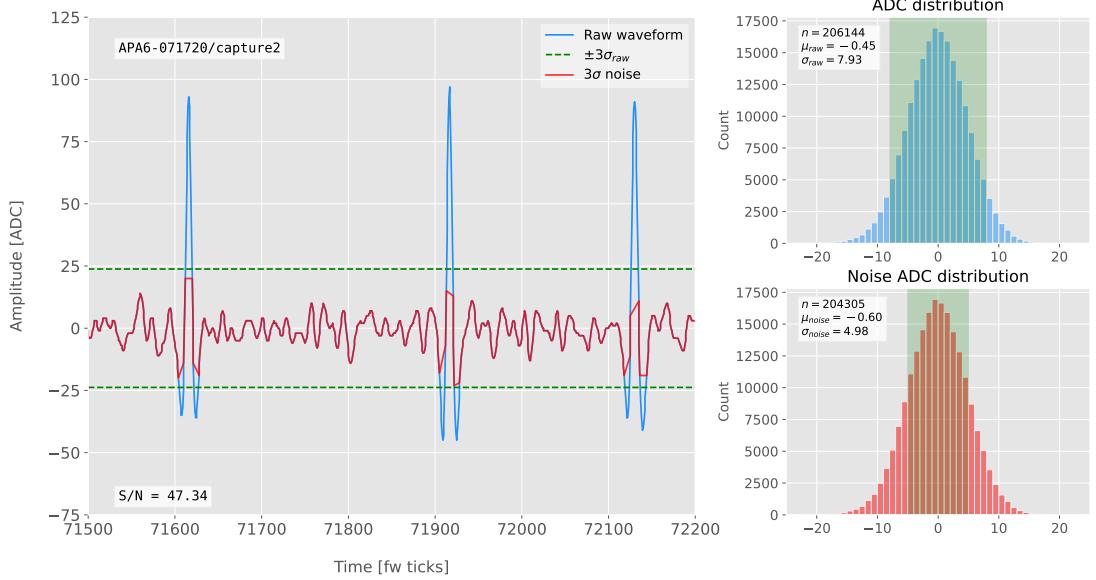
The results I obtained optimising the low pass filter with the Parks-McClellan method are promising. Nonetheless, the improvement found is rather marginal so I wondered if there could be an alternative approach to the filtering problem which yields better outputs. At this point, I found a possible alternative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

## 6.4 Matched filters

In the context of signal processing, a matched filter is the optimal linear filter for maximising the signal-to-noise ratio (S/N) in the presence of additive noise, obtained by convolving a conjugated time-reversed known template with an unknown signal to detect the presence of the template in the signal [54].

Given a known signal sequence  $s(t)$  and another (a priori unknown) noise sequence

## 6.4. Matched filters



**Figure 6.7:** 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  $\pm \sigma_{\text{noise}}$

1298  $n(t)$ , the input signal can be written as:

$$x(t) = s(t) + n(t). \quad (6.4)$$

1299 Now, considering a linear time-invariant filter, whose impulse-response function I  
1300 will refer to as  $h(t)$ , one can write the output signal as:

$$\begin{aligned} y(t) &= x(t) * h(t) \\ &= (s(t) + n(t)) * h(t) \\ &= y_s(t) + y_n(t), \end{aligned} \quad (6.5)$$

1301 where  $y_s(t)$  and  $y_n(t)$  are simply the outputs of the filter due to the signal and the noise  
1302 components respectively.

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

1303     The goal of the matched filter is to detect the presence of the signal  $s(t)$  in the input  
 1304   sample  $x(t)$  at a certain time  $t_0$ , which effectively means we need to maximise the S/N.  
 1305   This way, what one wants is to have a filter which gives a much bigger output when the  
 1306   known signal is present than when it is not. Putting it in other words, the instantaneous  
 1307   power of the signal output  $y_s(t)$  should be much larger than the average power of the  
 1308   noise output  $y_n(t)$  at some time  $t_0$ .

1309     For the case of the filtered signal, one can easily re-write it as an inverse Fourier  
 1310   transform:

$$y_s(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega H(\omega)S(\omega)e^{i\omega t}, \quad (6.6)$$

1311   where  $H(\omega)$  and  $S(\omega)$  are the Fourier transforms of the impulse-response function (i.e.  
 1312   the transfer function of the filter) and of the input signal, respectively.

1313     Now focusing on the noise, we can use the Wiener-Khinchin theorem [55] to write  
 1314   the mean power of the noise after filtering as:

$$E|y_n(t)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega |H(\omega)|^2 S_n(\omega), \quad (6.7)$$

1315   where  $S_n(\omega)$  is the power spectral density of the noise.

1316     Having these, one can write the instantaneous S/N at time  $t_0$  as:

$$\begin{aligned} \left( \frac{S}{N} \right)_{t_0} &= \frac{|y_s|^2}{E|y_n(t)|^2} \\ &= \frac{1}{2\pi} \frac{\left| \int_{-\infty}^{\infty} d\omega H(\omega)S(\omega)e^{i\omega t_0} \right|^2}{\int_{-\infty}^{\infty} d\omega |H(\omega)|^2 S_n(\omega)}. \end{aligned} \quad (6.8)$$

1317     Once we have this expression, we need to find the upper limit of it to determine what  
 1318   would be the optimal choice for the transfer function. One can use the Cauchy-Schwarz  
 1319   inequality, which in the present case takes the form:

$$\left| \int_{-\infty}^{\infty} dx f(x)g(x) \right|^2 \leq \int_{-\infty}^{\infty} dx |f(x)|^2 + \int_{-\infty}^{\infty} dx |g(x)|^2, \quad (6.9)$$

## 6.4. Matched filters

1320 for any two analytical functions  $f(x)$  and  $g(x)$ . One can prove that making the choice:

$$\begin{aligned} f(x) &= H(\omega) \sqrt{S_n(\omega)} e^{i\omega t_0}, \\ g(x) &= \frac{S(\omega)}{\sqrt{S_n(\omega)}}, \end{aligned} \quad (6.10)$$

1321 leads to the following upper bound for the S/N:

$$\left( \frac{S}{N} \right)_{t_0} \leq \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{|S(\omega)|^2}{S_n(\omega)}. \quad (6.11)$$

1322 From Eqs. (6.8), (6.9) and (6.10) one can also derive the form of the transfer function  
1323 such that the upper bound is exactly reached [56]:

$$H(\omega) \propto \frac{S^*(\omega) e^{-i\omega t_0}}{S_n(\omega)}. \quad (6.12)$$

1324 From this last expression we can clearly see the way the matched filter acts. As the  
1325 transfer function is proportional to the Fourier transform of the signal it will try to only  
1326 pick the frequencies present in the signal [57].

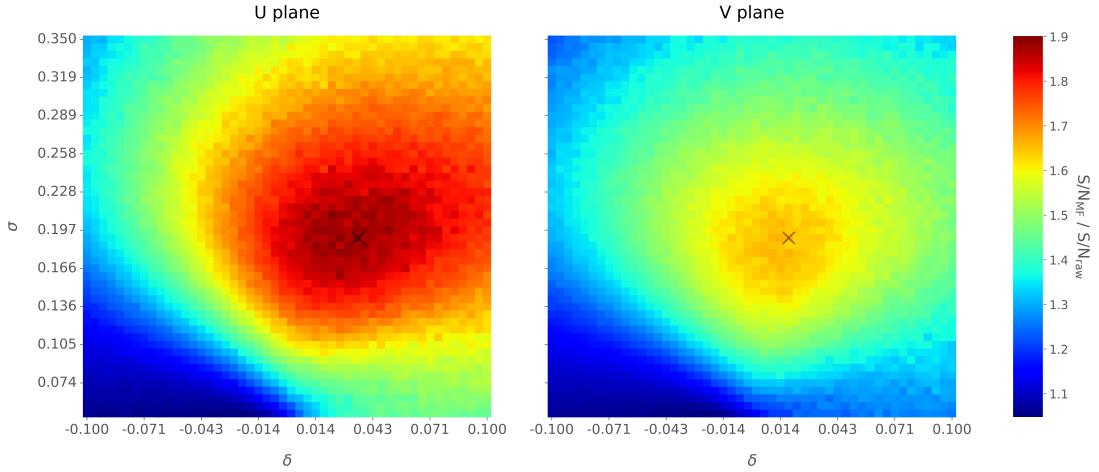
1327 The matched filter transfer function can be greatly simplified if the input noise is  
1328 Gaussian. In that case, the power spectral density of the noise is a constant, so it can be  
1329 re-absorbed in the overall normalisation of the transfer function. Moreover, considering  
1330 that the input signal is a real function, one can simply set  $S^*(\omega) = S(-\omega)$ , which gives:

$$H(\omega) \propto S(-\omega) e^{-i\omega t_0}. \quad (6.13)$$

1331 For a discrete signal, one can think of the input and impulse-response sequences as  
1332 vectors of  $\mathbb{R}^N$ . Then, the matched filter tries to maximise the inner product of the signal  
1333 and the filter while minimising the output due to the noise by choosing a filter vector  
1334 orthogonal to the later. In the case of additive noise, that leads to the impulse-response  
1335 vector:

$$h = \frac{1}{\sqrt{s^\dagger R_n^{-1} s}} R_n^{-1} s, \quad (6.14)$$

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives



**Figure 6.8:** Relative improvement in the S/N for the raw data capture `felix-2020-07-17-21:31:44`, using the matched filter following the parametrisation in Eq. (6.17). The black crosses in both panels denote the location of the maximum ratio value.

1336 where  $s$  is a reversed signal template sequence of length  $N$  equal to the order of the filter  
 1337 and  $R_n$  is the covariance matrix associated with the noise sequence  $n$ . For the Gaussian  
 1338 noise case, the covariance matrix is simply the unit matrix, so the above expression  
 1339 simplifies again to:

$$h = \frac{s}{|s|}. \quad (6.15)$$

1340 For this first stage of the study, I use a definition of the S/N per channel given by:

$$\text{S/N} = \frac{\max [ADC] - \mu_{noise}}{\sigma_{noise}}, \quad (6.16)$$

1341 where the subscript *noise* refers to a subset of the data obtained by only taking into  
 1342 account waveform values within a  $\pm 3\sigma$  range around the mean of the data and  $\max [ADC]$   
 1343 is the maximum of the original waveform. This definition is further discussed in App.  
 1344 6.2, where I also show examples of its application to raw data and to a waveform filtered  
 1345 with the current low-pass FIR filter.

1346 To test whether this choice of filter is appropriate one needs to choose a signal  
 1347 template. As an example of how a matched filter would affect our signal, I simply took  
 1348 the filter coefficients to be the 32 ADC values around a signal peak present in the data.

## 6.4. Matched filters

1349 In Fig. 6.7 (left panel) I plotted a zoomed region for channel 7840 in the raw data capture  
1350 `felix-2020-07-17-21:31:44`, after applying the matched filter described before (blue  
1351 line). When compared to the raw and FIR filtered case (see App. 6.2), after applying  
1352 the match filter the standard deviation of the noise waveform (red line) decreases and at  
1353 the same time the signal peaks are enhanced. This leads to an improvement of the S/N  
1354 by a factor of 1.92 when compared to the raw waveform.

1355 In order to obtain the matched filter that is more suitable for our data, I explored  
1356 different configurations of signal templates. In order to perform this exploration, I  
1357 parametrised the signal using the bipolar function:

$$f(x) = -A(x + \delta) e^{-x^2/\sigma^2}, \quad (6.17)$$

1358 where the parameter  $\delta$  controls the asymmetry between the positive and negative peaks  
1359 and  $\sigma$  controls their width. The amplitude parameter  $A$  is set such that it keeps the  
1360 height of the biggest peak to be less than 200 ADC in absolute value.

1361 As this parametrisation is only adequate for bipolar signals I will focus exclusively  
1362 on the induction channels. Also, the optimal configurations I found for the U and V  
1363 plane will be kept separate, i.e. I will have two sets of coefficients that will be applied to  
1364 either the U and V planes of wires. I do so as I found this was the choice giving the  
1365 best performance. Even so, as I will discuss, the differences are not very pronounced. In  
1366 case it is not technically possible to separate channels in the firmware according to the  
1367 wire plane they come from and use different sets of filter coefficients for them, we can  
1368 just find a common unique set of coefficients. In such case, I do not expect our results  
1369 to change dramatically.

1370 In Fig. 6.8 I present the results of our parameter scan, for channels in the induction  
1371 planes U (left panel) and V (right panel). For each configuration of  $\sigma$  and  $\delta$  the resulting  
1372 matched filter was applied to all channels in the corresponding plane within the data  
1373 capture `felix-2020-07-17-21:31:44`, the S/N improvement was computed with respect  
1374 to the raw waveforms and then the S/N mean value was kept as a score for such filter.

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

1375 One can see that the improvement obtained for the U plane is in general higher than the  
1376 one for the V plane. In any case, I got substantially higher ratios than the ones obtained  
1377 for the low-pass FIR filters. For the optimal configurations I attained improvements up  
1378 to a factor of 1.85 for the U plane and 1.65 for the V plane.

1379 The sets of optimal matched filter coefficients were obtained for the parameters  
1380  $\delta = 0.035$ ,  $\sigma = 0.191$  for the U plane and  $\delta = 0.018$ ,  $\sigma = 0.191$  for the V plane. I  
1381 show these two sets of coefficients in Fig. 6.9 (left panel). Also in Fig. 6.9 (right  
1382 panel) I plot the distribution of the S/N improvement after the optimal match filters  
1383 for the U and V were applied to the corresponding channels in the raw data capture  
1384 `felix-2020-07-17-21:31:44`. As mentioned before, the mean improvement achieved  
1385 for the U plane channels is slightly bigger than the one for the V channels. Note, however,  
1386 that the spread of the distribution for the V plane is also smaller than the one for the U  
1387 plane.

1388 I also performed a similar scan for the case of a low-pass FIR filter using the Parks-  
1389 McClellan algorithm. In that case, the parameters to check were the cutoff frequency  
1390 and the transition width of the filter. A summary of the results is given in App. 6.3.

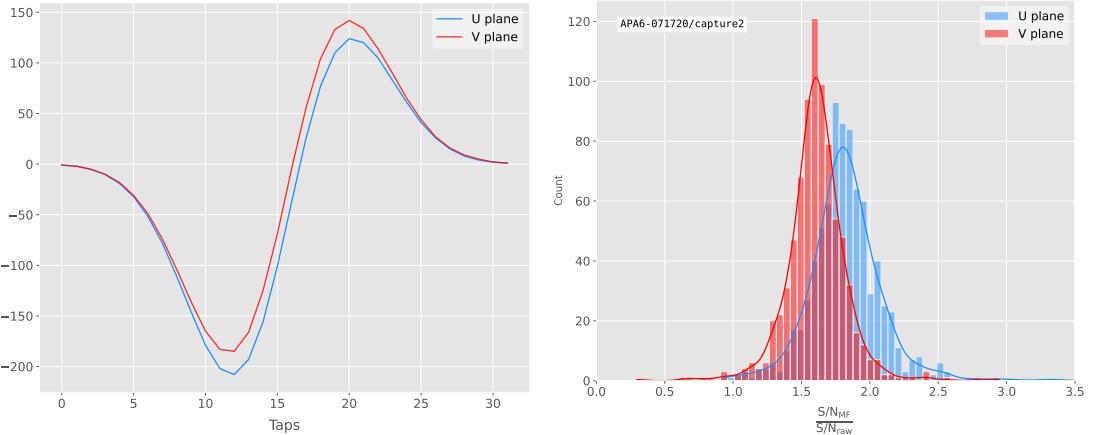
1391 Overall, one can see that the improvements on the S/N are much more significant in  
1392 the case of the matched filter than it is for the low-pass FIR filters. The analysis of this  
1393 and other raw data captures from ProtoDUNE-SP suggest that matched filters increase  
1394 the S/N of induction channels by a factor of 1.5 more than the optimal low-pass FIR  
1395 filters.

1396 Although these results are by themselves great points in favour of the matched  
1397 filter, more studies are needed to completely assess the robustness of this approach. I  
1398 proceeded then to test the matched filter with simulated data samples.

### 1399 6.5 Using simulated samples

1400 In order to further test the matched filter, the next step was to generate and process  
1401 data samples using *LArSoft* [58]. In this way, one can control the particle content of

## 6.5. Using simulated samples



**Figure 6.9:** 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. (6.17) 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.

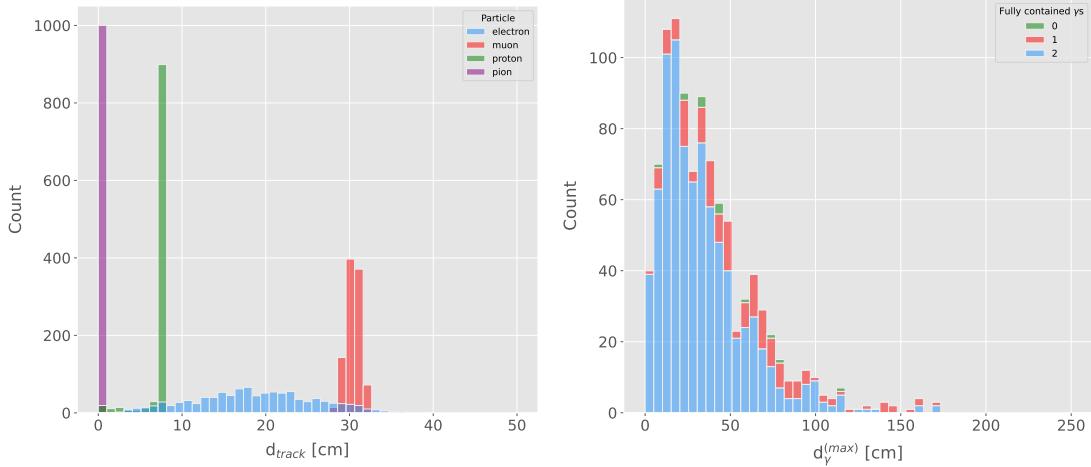
1402 the samples, the orientation of the tracks and their energy, and therefore see how the  
1403 matched filter behaves in various situations.

1404 To begin with, I prepared different monoenergetic and isotropic samples containing  
1405 a single particle per event. Each sample contains a different particle species, namely  
1406 electrons, muons, protons and neutral pions all with a kinetic energy of  $E_k = 100$  MeV.  
1407 I chose these because of the fairly different topologies they generate in the liquid argon,  
1408 ranging from shower-like to track-like. The procedure I followed to generate the samples  
1409 and process them is discussed in detail in App. ??.

1410 These were generated with the single particle gun and the Geant4 stage of the  
1411 *LArSoft* simulation [58] was performed with the standard configuration for the DUNE  
1412 FD 10kt module.

1413 For simplicity, I restricted the particles to start drifting in a single TPC volume  
1414 (in this case TPC 0), so I can focus exclusively on the signals coming from one APA.  
1415 The chosen kinetic energy for all the particles in my first trial is  $E_k = 100$  MeV, so a  
1416 necessary check is to see if all our tracks will be typically contained in one TPC volume.  
1417 Fig. 6.10 (left panel) shows the distributions of the track lengths in the liquid argon

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**Figure 6.10:** 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  $\pi^0 \rightarrow \gamma\gamma$ .

of all generated particles with  $E_k = 100$  MeV. One can see that, in the case of the track-like particles (i.e. muons and protons), their length distributions are quite sharp and centered at relatively low distances (30 and 8 cm, respectively). For electrons, the distribution is quite broad but it does not extend past  $\sim 30$  cm. The case of neutral pions can be misleading, as they decay promptly the track length associated with the true Monte Carlo particle is always  $< 1$  cm. In Fig. 6.10 (right panel) I show the effective length distribution of the longest photon after the pion decays as  $\pi^0 \rightarrow \gamma\gamma$ , highlighting the number of fully contained photons in the TPC volume per event (either zero, one or both). One can see that the vast majority of events has both photons contained and that just a negligible number of them has none of them contained in the TPC volume. In any case, for the sake of caution, I will only keep the pion events with both photons contained.

Once I have prepared a sample at the Geant4 level, I need to process it through the detector simulation. In order to make adequate estimations of the noise levels and run the filtering and hit finder as I did with the ProtoDUNE data, one needs to turn off the default zero-suppression of the waveforms produced by the simulation. At this first stage I am only concerned with the waveforms with the noise added, so I keep the noise

## 6.5. Using simulated samples

addition option as true in the configuration. However, for studies related to the hit finder performance one will also need to store the noiseless waveforms in order to retrieve the truth information of the hits. I will discuss this approach next.

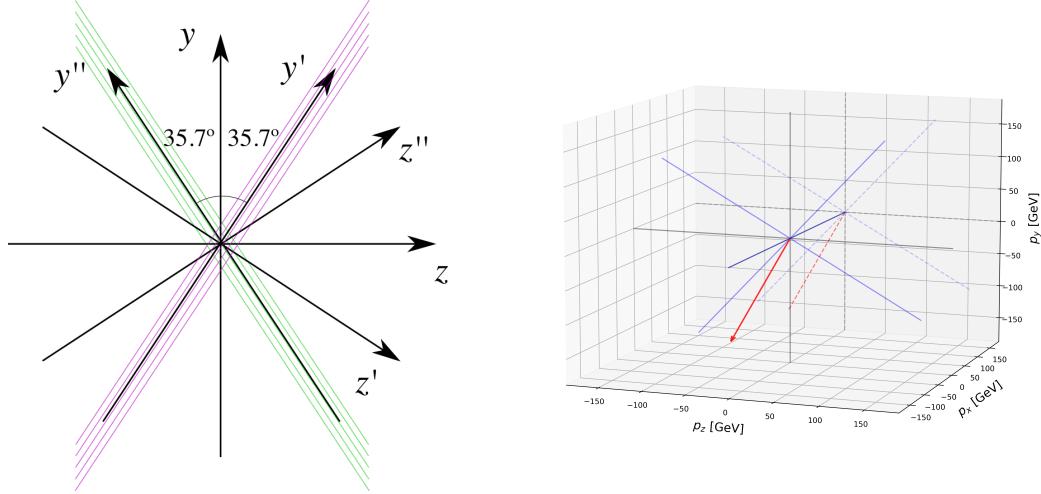
After the detector simulation stage, one needs to extract the no zero-suppressed noisy waveforms, along with their offline channel numbers, and store them in a certain format to be analysed later. To reduce the amount of data that will go for processing, I used the information from the Geant4 step of the simulation to select only the active channels, i.e. the channels where some ionisation electrons arrive. Moreover, as said previously, I only extract the waveforms from APA 0 and exclusively the ones coming from induction channels. The resulting ROOT file contains a tree with two branches, one containing the waveforms for each event and channel and the other with the corresponding offline channel numbers.

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

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

Additionally, for the analysis of the samples it was necessary to use two different reference frames, to study separately the signals coming from the U and V induction wire planes. As I am focussing on a single APA, the U and V wires have a different orientation in the  $yz$  plane. In the case of U wires, these are tilted  $35.7^\circ$  clockwise from the vertical ( $y$  direction), whereas the V wires are at the same angle but in the counter clockwise direction. Because of this, the best option is to deal with two new coordinate systems rotated by  $\pm 35.7^\circ$  along the  $x$  axis, so the new  $y'$  and  $y''$  directions are aligned with the

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

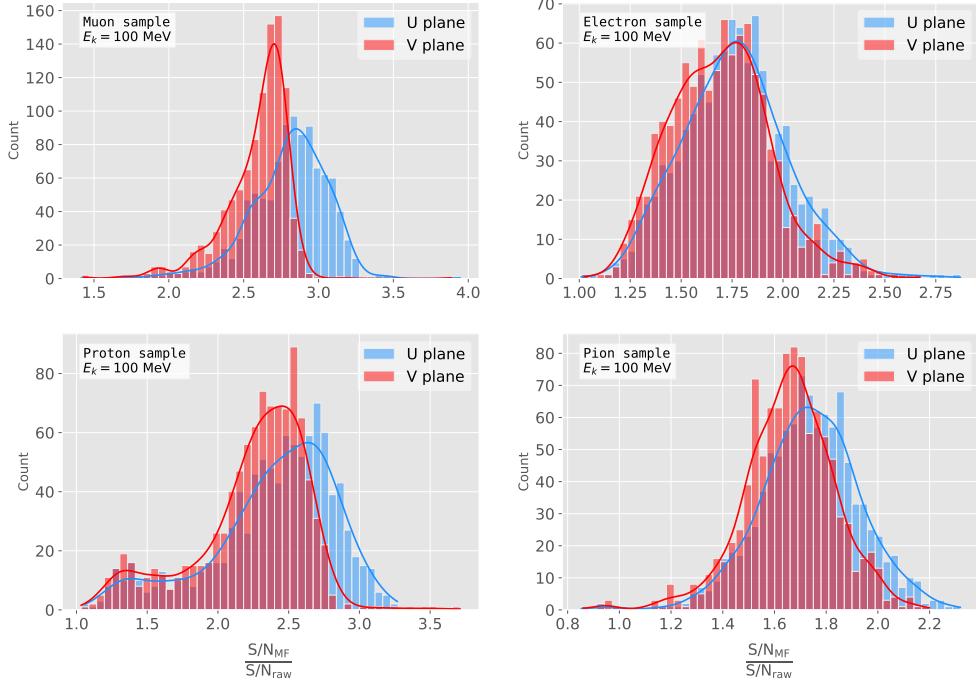


**Figure 6.11:** Left panel: schematic representation of the two new rotated reference frames used in this analysis (denoted as prime and double prime), viewed from the  $yz$  plane. The magenta stack of lines represent the wires in the  $U$  plane, whereas the green lines correspond to the wires in 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.

1464 U and V induction wires. Fig. 6.11 (left panel) shows a schematic representation of  
 1465 the original reference frame together with the two rotated ones (denoted by primed and  
 1466 double primed). This way, one can easily understand how parallel was a track to the  
 1467 wires in the two induction planes. Fig. 6.11 (right panel) shows a 3D representation of  
 1468 the momentum of a track (red arrow) in the original reference frame (black lines), along  
 1469 with the new reference frame for  $U$  wires (blue lines). I added the projection in the  $yz$   
 1470 plane of this three, to show the usefulness of the new reference frame to tell whether a  
 1471 track is parallel or normal to the wires in the induction plane.

1472 Fig. 6.12 shows the distribution of the average S/N improvement per event when one  
 1473 applies the optimal matched filters. I produced separate distributions for the channels  
 1474 in the  $U$  (red) and  $V$  (blue) induction wire planes. Notice that the S/N distributions  
 1475 for the track-like particles, i.e. muons (top left panel) and protons (bottom left panel),  
 1476 have significantly larger mean values than the distributions of the shower like particles,  
 1477 i.e. electrons (top right panel) and neutral pions (bottom right panel). An important

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**Figure 6.12:** Distributions of the mean  $S/N$  improvement per event for the corresponding sample 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  $E_k = 100 \text{ MeV}$ .

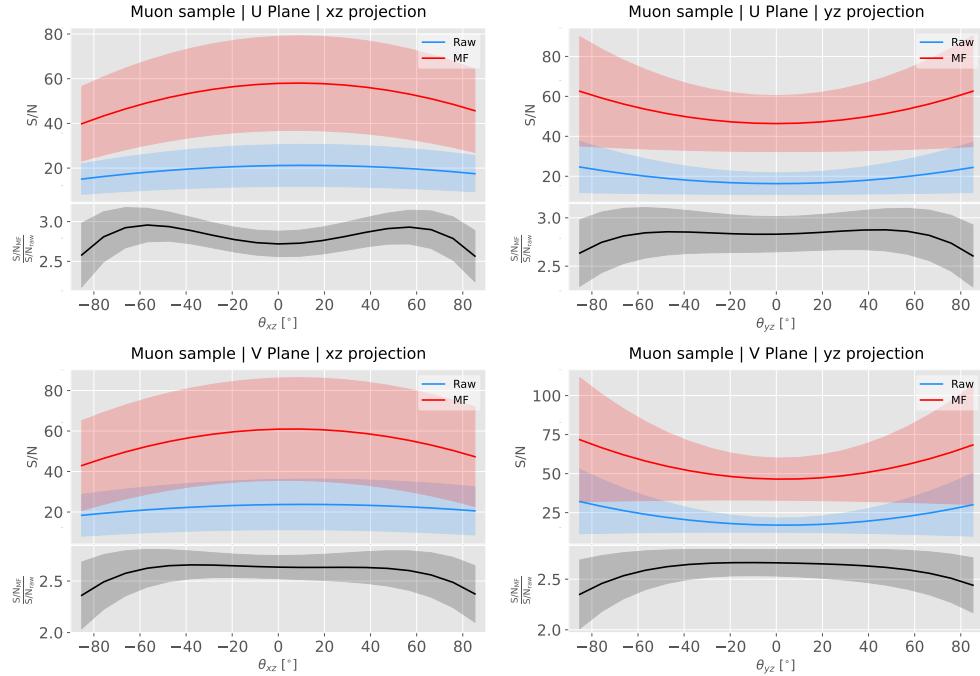
difference between these results and the ones seen before for ProtoDUNE data is that, overall, the improvements that I get for simulated data are bigger. This could be due either to the default noise model used in the *LArSoft* simulation or to the simulated hits having higher energy than the ones in the recorded data. Nonetheless, the concluding message is that the previously optimised matched filters give an overall significant 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:

$$(S/N_{fir})_{event} = \frac{\sum_{i=0}^{N_{chan}} (S/N_{fir})_i}{N_{chan}}, \quad (6.18)$$

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

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**Figure 6.13:** Angular dependence of the mean S/N and the S/N improvement, for the different monoenergetic samples considered (from top to bottom: electrons, muons, protons and neutral pions). The two columns on the left represent the values for the U plane waveforms. The top subplots show the mean S/N for raw (green) and filtered (red) waveforms whereas the bottom subplots depict the averaged S/N improvement (black).

1488 However, for the ratio of the raw and filtered S/N (what I called the S/N improvement)  
 1489 per event I am not just taking the ratio of the previous two quantities but computing  
 1490 the average of the individual ratios per channel in the event:

$$\left( \frac{S/N_{fir}}{S/N_{raw}} \right)_{event} = \frac{\sum_{i=0}^{N_{chan}} \left( \frac{S/N_{fir}}{S/N_{raw}} \right)_i}{N_{chan}}, \quad (6.19)$$

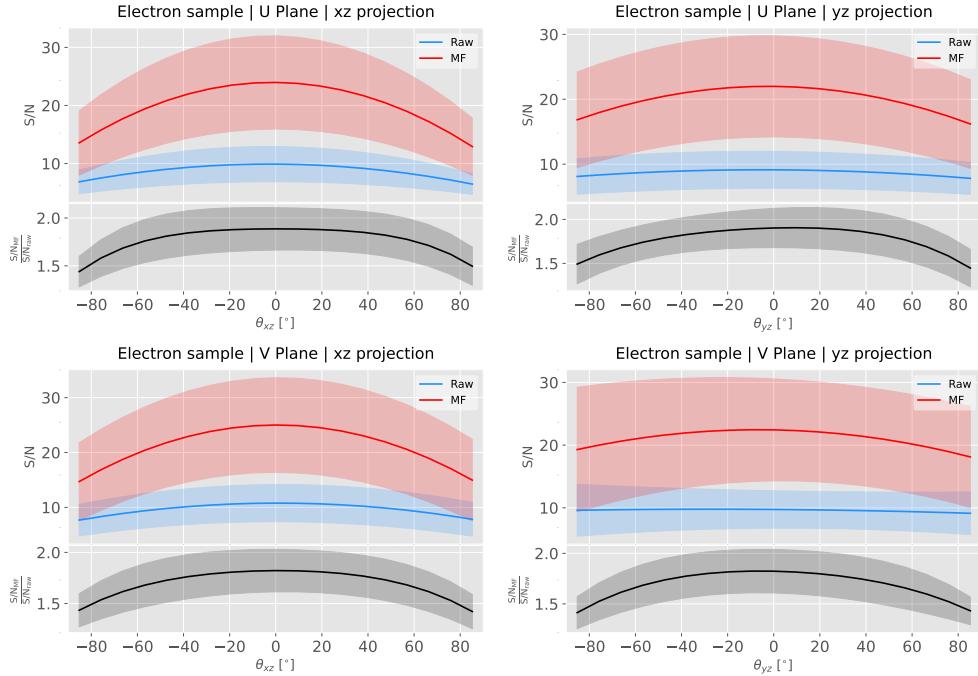
1491 and so:

$$\left( \frac{S/N_{fir}}{S/N_{raw}} \right)_{event} \neq \frac{(S/N_{fir})_{event}}{(S/N_{raw})_{event}}. \quad (6.20)$$

### 1492 6.5.1 Angular dependence

1493 Having these monoenergetic samples, one can also study the angular dependence of the  
 1494 performance of the matched filter. This is an important point, as it is a well established  
 1495 fact that for certain configurations (an extreme case configuration being signals normal

## 6.5. Using simulated samples



**Figure 6.14:** Angular dependence of the mean S/N and the S/N improvement, for the different monoenergetic samples considered (from top to bottom: electrons, muons, protons and neutral pions). The two columns on the left represent the values for the U plane waveforms. The top subplots show the mean S/N for raw (green) and filtered (red) waveforms whereas the bottom subplots depict the averaged S/N improvement (black).

1496 to the wire plane and perpendicular to the induction wires at the same time) the S/N is  
 1497 much lower than average as the corresponding waveforms are severely distorted. In this  
 1498 sense, I am interested to see how the matched filter behaves for these cases and how the  
 1499 S/N improvement on those compare to the average.

1500 Fig. 6.13 shows the angular dependence of the S/N for the monoenergetic  $E_k =$   
 1501 100 MeV isotropic muons, for the different induction wire planes and projections. The  
 1502 angles for each event are given by the components of the initial value of the momentum  
 1503 of the particles, taking the angles of the projections on the  $xz$  and  $yz$  planes with respect  
 1504 to the  $z$  axis (more accurately, one needs to compute these angles twice for each event, a  
 1505 pair for the  $xy'z'$  coordinate system and the other for the  $xy''z''$ ). The top row shows the  
 1506 dependence on the angles corresponding to the U plane, i.e.  $\theta_{xz'}$  and  $\theta_{y'z'}$ , whereas the  
 1507 bottom row shows the angular dependence viewed from the V plane,  $\theta_{xz''}$  and  $\theta_{y''z''}$ . In  
 1508 each plot, the top subplot represents the mean values of the S/N for the raw (blue) and

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

1509 matched filtered (red) signals, and the bottom subplot the averaged S/N improvement  
1510 (black). The solid lines represent the mean value obtained for the corresponding angular  
1511 value, whereas the semitransparent bands represent one standard deviation around the  
1512 mean at each point.

1513 As expected, the S/N is in general higher when tracks are parallel to the APA (i.e.  
1514  $\theta_{xz} \sim 0$ ) and lower when it is normal to the plane ( $\theta_{xz} \sim \pm 90^\circ$ ). In the same way, tracks  
1515 parallel to the wires ( $\theta_{yz} \sim \pm 90^\circ$ ) tend to have higher S/N than those perpendicular to  
1516 these ( $\theta_{yz} \sim \pm 0$ ).

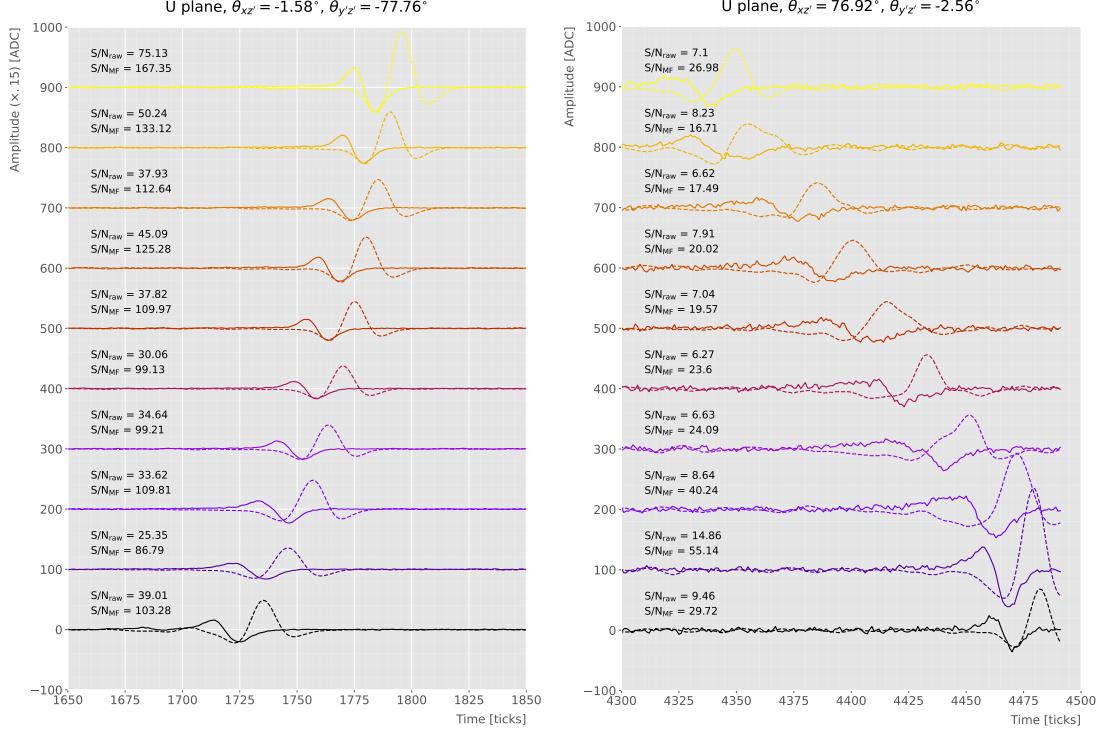
1517 Fig. 6.14 shows the corresponding angular dependence information for the  $E_k =$   
1518 100 MeV electrons sample. Notice that, in this case, the S/N behaviour discussed above  
1519 does not hold. A possible explanation can be that, because most hits in these events  
1520 are produced by the secondary particles generated in the EM shower, the signal peaks  
1521 whose S/N ratios were computed do not correspond to the directional information of  
1522 the primary electron.

### 1523 6.5.2 Distortion and peak asymmetry

1524 As a little case of study, I selected two of the simulated  $E_k = 100$  MeV monoenergetic  
1525 muon events. With respect to the U induction plane, one is parallel to the APA (low  
1526  $\theta_{xz'}$ ) and to the wires (high  $\theta_{y'z'}$ ) and the other is normal to the APA plane (high  $\theta_{xz'}$ )  
1527 and perpendicular to the wires (low  $\theta_{y'z'}$ ). As expected from the results on the angular  
1528 dependence discussed above, the former has a higher S/N (before and after the filtering)  
1529 when compared to the latter. An interesting thing to notice about these two samples  
1530 is that, even though one has a much bigger S/N than the other, it is the one with the  
1531 smallest S/N the one that got the biggest averaged S/N improvement. In Table 6.1  
1532 I included all the relevant parameters of these two  $E_k = 100$  MeV muon events I am  
1533 considering, namely, the angles with respect to the  $xy'z'$  reference frame, the values of  
1534 the S/N, the S/N improvement and also the so-called peak asymmetry  $\Delta_{peak}$  that I will  
1535 discuss next.

1536 One can try to understand better what is going on with these two events by looking

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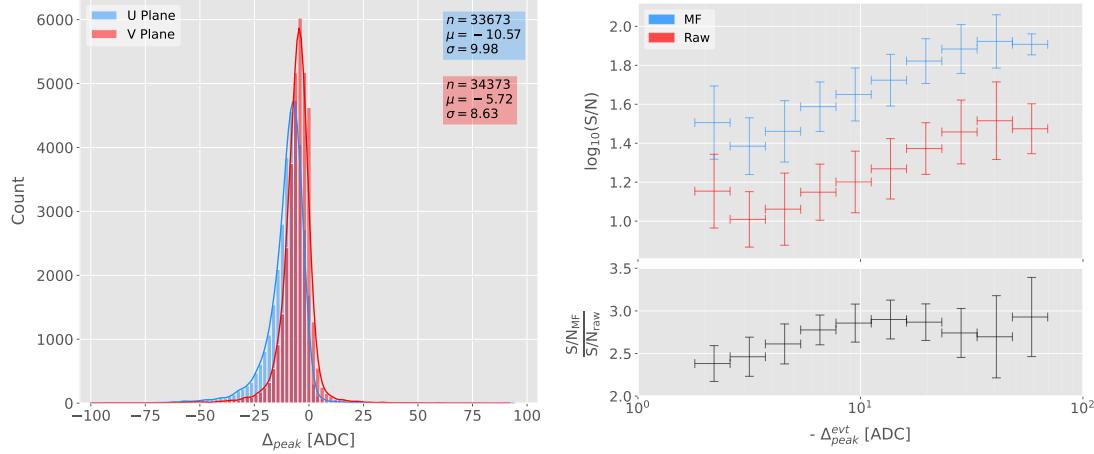
**Figure 6.15:** Selected consecutive waveforms corresponding to two monoenergetic  $E_k = 100$  MeV muon events, one is parallel to the APA and to the wires in the U plane (left panel) and the other is normal to the APA plane and perpendicular to the U plane wires (right panel). The solid lines represent 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.

**Table 6.1:** 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.

|                   | $\theta_{xz}'$ (°) | $\theta_{y'z}'$ (°) | S/N <sub>raw</sub> | S/N <sub>MF</sub> | $\frac{S/N_{MF}}{S/N_{raw}}$ | $\Delta_{peak}$ (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                |

at the raw and filtered data from some of their active channels. Fig. 6.15 shows a selection of consecutive raw and filtered U plane waveforms from the event with high S/N (left panel) and the one with low S/N (right panel). Notice that to show both collections of waveforms at a similar scale I had to apply a factor of 0.15 to the waveforms with high S/N. Additionally, next to each waveform I included the values of the raw and

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**Figure 6.16:** 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.

1542 matched filtered S/N for the corresponding channel. The first thing to notice in this plot  
 1543 is that the amplitude of the signal peaks from the normal track have a much smaller  
 1544 amplitude, and also appear quite distorted when compared to the others. On the other  
 1545 hand, although the matched filtered S/N is still smaller, the relative improvement is  
 1546 bigger than in the parallel case.

1547 A way I found to quantify the difference between the shapes within these two events  
 1548 is their different peak asymmetry. One can define the peak asymmetry as the (signed)  
 1549 difference between the positive and the negative peaks of the bipolar shape, i.e.:

$$\Delta_{peak} \equiv h_+ - h_-, \quad (6.21)$$

1550 where both heights  $h_+$  and  $h_-$  are positive defined. Fig. 6.16 (left panel) shows the  
 1551 distribution of this peak asymmetry for all the waveforms corresponding to channels  
 1552 in the U (blue) and V (red) planes for the monoenergetic muon sample. One can  
 1553 see that these distributions are clearly shifted to negative values (with mean values

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1554  $\mu_{\Delta}^U = -10.57$  ADC and  $\mu_{\Delta}^V = -5.72$  ADC respectively). It is interesting to notice  
1555 that the peak asymmetry value of the sample with high S/N sits at the left tail of the  
1556 distribution whereas the corresponding value of the sample with low S/N lies around  
1557 the mean.

1558 Now, one can try to correlate the peak asymmetry with the S/N and the S/N change  
1559 per event. Fig. 6.16 (right panel) shows the result of comparing (minus) the mean  
1560 peak asymmetry per event to the averaged raw (red) and matched filtered (blue) S/N  
1561 per event (top subplot). The horizontal lines sit at the mean value obtained in the fit  
1562 and represent the width of the  $-\Delta_{peak}$  bins used, while the vertical lines indicate one  
1563 standard deviation around that mean value. Notice that, when taking decimal logarithm  
1564 on both, there is an approximate linear relation between these quantities, except for  
1565 peak asymmetry values bigger than  $-5$  ADC where the S/N remains constant.

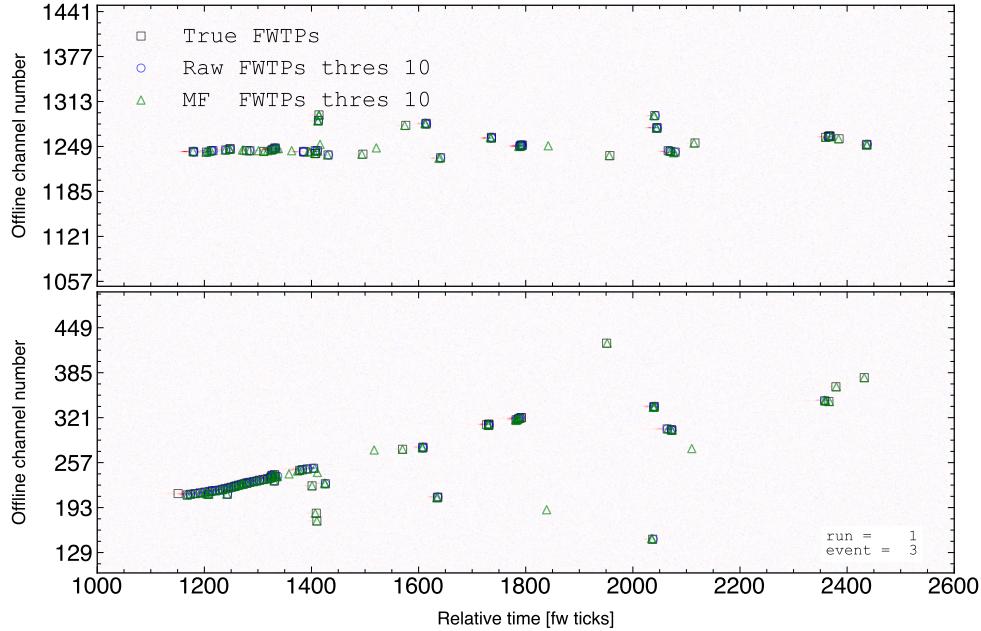
1566 Also, in the bottom subplot of Fig. 6.16 (right panel) I show the relation between  
1567 the peak asymmetry and the mean S/N improvement. In this case, one see that there is  
1568 a maximum at  $\Delta_{peak} \sim -10$  ADC. As mentioned previously, this is also the value of the  
1569 mean of the peak asymmetry distribution. In fact, it is expected that our filter favours  
1570 the signal peaks with the most common values of the peak asymmetry, as this was one  
1571 of the features I target in our filter coefficient optimisation through the parameter  $\delta$ .

1572 These results suggest that events with poorer values of the mean S/N, usually  
1573 associated to non-favourable track orientations, tend to have smaller values of the mean  
1574 peak asymmetry (in absolute value). Nonetheless, because our matched filters have  
1575 been optimised to account for these asymmetries, the improvement on the S/N for these  
1576 events is sizeable if not better than the one for events which already had a high S/N.

### 1577 6.5.3 Hit sensitivity

1578 One of the advantages of the matched filter, directly related to increasing the S/N, is  
1579 the capability of picking hits that before fell below the threshold. For instance, Fig. 6.17  
1580 shows the raw ADC data from an example event (electron,  $E_k = 100$  MeV) with the  
1581 produced true hits superimposed (black boxes), together with the hits produced by the

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**Figure 6.17:** Raw data display in the plane time (in firmware ticks) vs. offline channel number for an  $E_k = 100$  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).

standard hit finder chain (blue circles), i.e. using the current FIR filter, and the hits obtained using the matched filters (green triangles). Both the standard and the matched filter hit finders were run with a threshold of 10 ADC. Notice that the standard hits match well the true ones at the initial part of the event (where we have a track-like 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.

Notwithstanding that now I get more hits with this combination of matched filter and low threshold as a results of the enhancement of the signal peaks relative to the noise level, it is also true that I pick some spurious hits not related to any real activity if one lowers the thresholds too much. Therefore, some optimisation of the threshold is needed. Basically one will need to make 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.

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1596 By running the hit finders on our samples with different values of the threshold one  
1597 can understand, for instance, how low one can set the threshold without getting mostly  
1598 spurious hits and then evaluate the gains obtained from this.

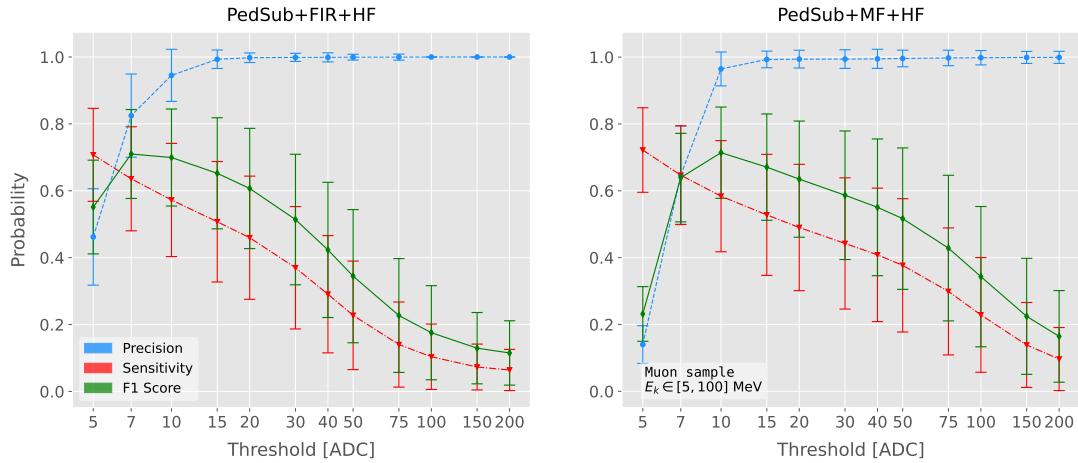
1599 Because now I am also interested in seeing how the hit sensitivity changes with the  
1600 energy, I prepared new isotropic samples with the same types of particles as before  
1601 (muons, electrons, protons and neutral pions) but with a flat kinetic energy distribution  
1602 ranging from 5 to 100 MeV.

1603 In order to estimate the hit sensitivity, given a certain sample, one needs to recover  
1604 the set of true hits to be able to compare these with the ones produced. To do so,  
1605 a modification in the procedure I was using to extract the raw waveforms is needed.  
1606 For this kind of study I run the detector simulation in two steps, first I produce the  
1607 waveforms without noise and extract them in the same format I used for the raw data,  
1608 then the noise is added and the noisy waveforms are then written to a file as well.

1609 To have a better comparison between the true hits and the ones produced from  
1610 the raw waveforms after applying the two filters, I applied also the FIR filter and the  
1611 matched filters to the noiseless waveforms and then I run the hit finder with a minimal  
1612 threshold (in this case I used 1 ADC) on these noiseless filtered waveforms. In this way  
1613 I generated two sets of true hits, I will refer to them as standard true hits (with the  
1614 current/default FIR filter) and matched filter true hits respectively. This allows a more  
1615 precise matching between the different groups of hits produced, as it will account for  
1616 any delays and distortions introduced by the FIR and the matched filters.

1617 In the case of the raw waveforms (with noise), I run the hit finder on them, with  
1618 different values of the threshold, after applying either the FIR or the matched filters. I  
1619 will name them simply standard hits and matched filter hits respectively. Then, I match  
1620 the generated hits to the true hits (the standard hits with the standard true hits and  
1621 the matched filter hits with the matched filter true hits). The matching is performed by  
1622 comparing the channel number and the timestamp of the hits. To count as a match,  
1623 I require that all hits with the same channel number and timestamp have overlapping  
1624 hit windows, i.e. the time windows between their hit end and hit start times need to

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**Figure 6.18:** 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.

overlap. If more than one hit in one of the groups have hit overlap with the same hit in the other group I only count the hit with closer hit peak time value.

The generation of the samples, the procedure to produce the standard hits (with the default FIR filter) and matched filter hits and the matching of these with the true hits is described in detail in App. ??.

To quantify the performance of the two hit finder approaches, I use a classical method from statistical classification known as confusion matrix [59]. This is basically a way of sorting the outputs of a binary classifier, considering the true values of the classification and the predicted values. It divides the outputs in four categories: true positive (TP, both true and predicted values are 1), false negative (FN, true value is 1 but predicted is 0), false positive (FP, true value is 0 but predicted is 1) and true negative (TN, both true and predicted values are 0)).

The contents of the confusion matrix allow us to compute other derived scores to judge the performance of our classifiers. In this study, I will make use of three of these

## 6.5. Using simulated samples

1639 metrics, namely the precision or positive predictive value:

$$\text{PPV} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \quad (6.22)$$

1640 the sensitivity or true positive rate:

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}, \quad (6.23)$$

1641 and the  $F_1$  score [60]:

$$F_1 = \frac{2\text{TP}}{2\text{TP} + \text{FP} + \text{FN}}, \quad (6.24)$$

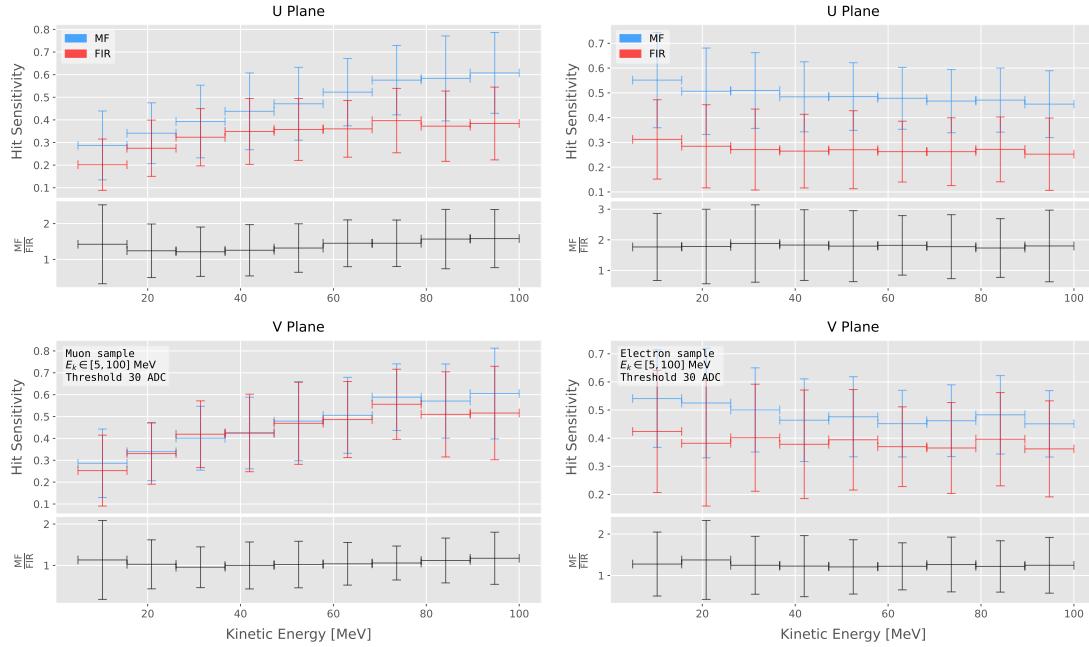
1642 which is the harmonic mean of the precision and the sensitivity.

1643 In our specific case I am not going to make use of the true negative value, as its  
1644 definition in this context can be ambiguous because one does not have clear instances in  
1645 the classification process. This way, I will only count the number of true positives as the  
1646 total amount of hits I can match between true and raw populations, the number of false  
1647 negatives will be the number of missing true hits and the false positive the number of  
1648 hits which do not match any true hit.

1649 In Fig. 6.18 I show the precision (blue), sensitivity (red) and  $F_1$  (green) scores I  
1650 obtained for different values of the threshold used in the hit finder for the case of the  
1651 muon sample. Because the matched filters are only applied to induction channels, I only  
1652 consider here hits coming from the U and V planes. The panel on the left corresponds  
1653 to the scores I got when I ran the hit finder on the FIR filtered waveforms, whereas the  
1654 right panel contains the scores for the matched filter case. The points are centered at  
1655 the threshold value used and represent the mean value obtained for each score using all  
1656 the generated events, while the error bars indicate one standard deviation around the  
1657 mean value.

1658 One can see that the precision for the matched filter case is lower when the thresholds  
1659 are very low, as the noise baseline is slightly amplified, but then rises to high values  
1660 quicker than for the FIR case. The other difference one can spot is that the sensitivity

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives

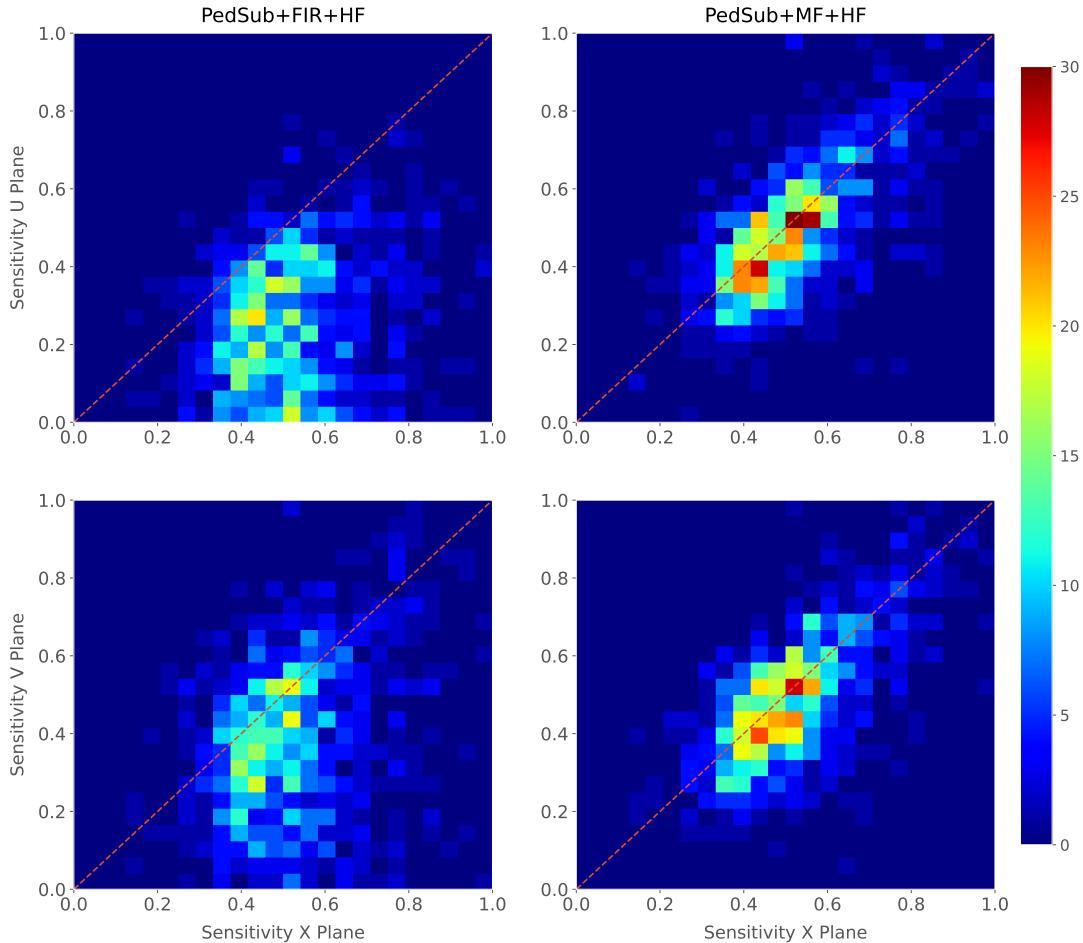


**Figure 6.19:** Dependence of the averaged hit sensitivity on the kinetic energy of the events for the matched filter (blue) and standard (red) hits, for the case of the muon (left panel) and electron (right panel) samples, separated between U (top plots) and V (bottom plots) induction wire planes. 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.

in the FIR case starts dropping faster at around the same threshold values where the precision stabilizes around 1, while in contrast for the matched filter this rapid decrease starts at higher threshold values. A similar scan for the same thresholds was performed for the electron sample in the same energy range, yielding similar results.

In Fig. 6.19 I show the averaged hit sensitivity versus the kinetic energy of the events, both for the matched filter hits (blue) and the standard hits (red). The left panel corresponds to the muon sample, whereas the one on the right corresponds to the electron sample, both with kinetic energies between 5 and 100 MeV. In each panel the top plot corresponds to hits in the U plane, while the bottom plot contains the same information for the V plane. Each plot contains two subplots, the one on the top shows 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.

## 6.5. Using simulated samples

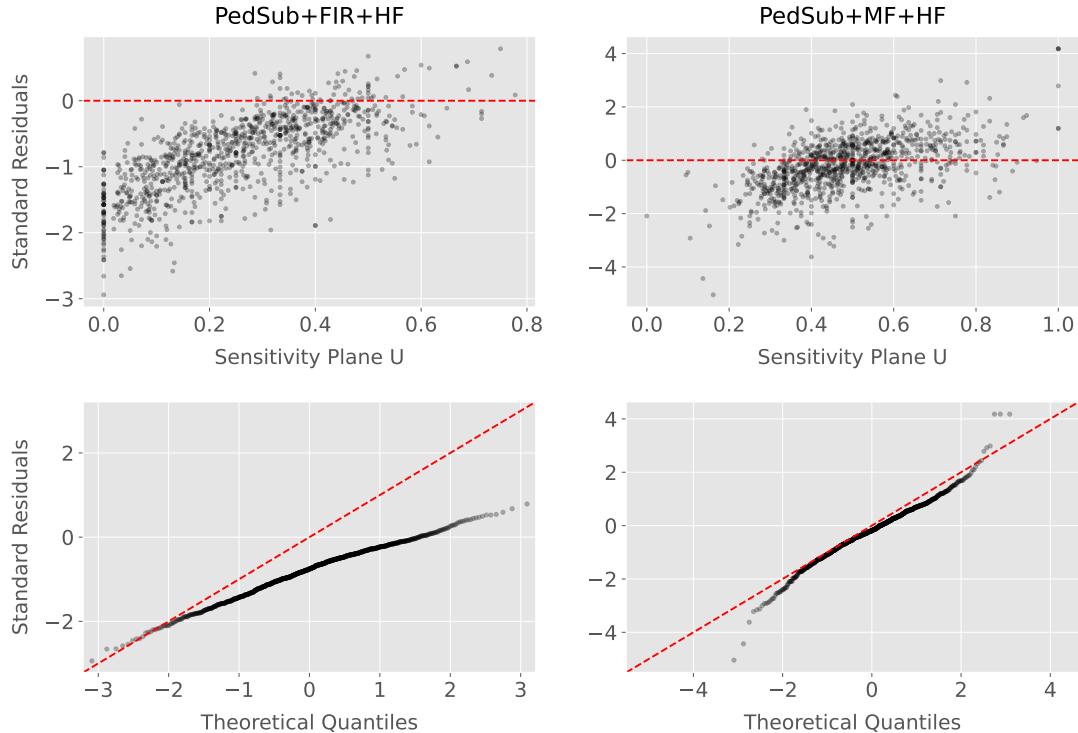


**Figure 6.20:** Distributions of the hit sensitivity in the U (top panels) and V (bottom panels) planes versus the hit sensitivity in the X plane, both for the standard hits (left panels) and the matched filter hits (right panels), in the case of the electron sample and a threshold of 30 ADC.

1673 The horizontal lines are placed at the mean value obtained in the fit and represent the  
 1674 width of the  $E_k$  bins used, while the vertical error bars indicate one standard deviation  
 1675 around that mean value. In both cases the threshold used was 30 ADC, as I required  
 1676 the precision to be higher than 0.99 for both matched filter and standard cases.

1677 One can see that, in general, the improvements are better for the U than for the V  
 1678 plane. While for the U channels I achieved a mean improvement of 50% and 80% for  
 1679 muons and electrons respectively, the improvement in the V plane is stalled at 10% and  
 1680 25%. Nevertheless, if I look at the sensitivities for the matched filter hits in both planes  
 1681 one can see these have similar mean values for each energy bin, while on the contrary

## Chapter 6. Matched Filter approach to induction wire Trigger Primitives



**Figure 6.21:** 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.

for the standard hits the sensitivity remains relatively high for the  $V$  plane. This way, it looks there was a less significant gain because the hit sensitivity was already high.

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

Furthermore, we can look at how the concurrence of hits between the different wire planes has changed. For any given event, I expect to have a similar number of hits in the three planes. As the ionisation electrons need to cross the  $U$  and  $V$  planes prior to reach the collection plane  $X$  they will induce current in those wire planes. A way to check the concurrence of hits across planes is looking at the relation between the hit sensitivities for each individual event. One cannot expect the sensitivities to be exactly equal across

## 6.5. Using simulated samples

1694 planes, but ideally they should be normally distributed around the diagonal.

1695 Fig. 6.20 shows the hit sensitivity in the U (top panels) and V (bottom panels)  
1696 planes versus the hit sensitivity in the X plane, for the case of the standard hits (left  
1697 panels) and the matched filter hits (right panels). All plots were generated for the  
1698 electron sample and a threshold of 30 ADC. From these one can see a clear trend,  
1699 when I use the standard hit finder chain the sensitivities in the induction planes are  
1700 systematically lower than the hit sensitivity in the X plane, i.e. most of the points sit  
1701 below the diagonal (red dashed line). In contrast, when the matched filters are applied,  
1702 the majority of the events are distributed around the diagonal. This points out that the  
1703 concurrence of hits across planes has improved.

1704 To exemplify the improvement I obtained, one can consider the residuals of the hit  
1705 sensitivities for the X and U planes. Assuming the diagonal hypothesis, i.e. given a  
1706 dataset of the form  $(x, y)$  for any  $x$  I take the predicted  $y$  value to be equal to the value  
1707 of  $x$ , I can compute the standard residuals for the hit sensitivities in U given the ones for  
1708 X. In Fig. 6.21 (top panels) I show these standard residuals against the corresponding  
1709 values of the hit sensitivity in the U plane, for our electron sample with kinetic energy  
1710 between 5 and 100 MeV. If I compare the scatter points in the case of the standard  
1711 hits (left panel) and the matched filter hits (right panel), I see that the residuals of the  
1712 standard hit finder case follow a certain pattern and their mean deviates from 0.

1713 To see clearly if the residuals are normally distributed, in Fig. 6.21 (bottom panels)  
1714 I plot the corresponding quantile-quantile plot for both the standard (left panel) and  
1715 matched filter (right panel) standard residuals. One can clearly see that the points for  
1716 the standard case follow a strongly non-linear pattern, suggesting that the residuals  
1717 do not follow a normal distribution. In contrast, for the matched filter hits the points  
1718 conform to a roughly linear path, implying that in this case the normality condition is  
1719 fulfilled.

1720 All these results hint at the fact that the concurrence of hits across the wire planes  
1721 can be strengthened by applying the matched filters.



1722 **Chapter 7**

1723 **DM searches with neutrinos from  
1724 the Sun**

1725 **7.1 Motivation**

1726 The idea of detecting neutrino signals coming from the Sun’s core to probe DM is not new.  
1727 The main focus of these searches has usually been high-energy neutrinos originated from  
1728 DM annihilations into heavy particles [61–64], although recent studies have proposed to  
1729 look at the low-energy neutrino flux arising from the decay of light mesons at rest in the  
1730 Sun [65–68] previously thought undetectable.

1731 In this chapter I try to demonstrate the capability of DUNE to constrain different  
1732 DM scenarios. I used the neutrino fluxes arising from DM annihilations in the core  
1733 of the Sun to compute the projected limits that DUNE would be able to set on the  
1734 annihilation rates in the Sun and the DM scattering cross sections.

1735 **7.2 Gravitational capture of DM by the Sun**

1736 The Sun and the centre of the Earth are possible sources of DM annihilations, specially  
1737 interesting because of their proximity. Their gravitational attraction ensured the capture  
1738 of DM from the local halo through repeated scatterings of DM particles crossing them.

## Chapter 7. DM searches with neutrinos from the Sun

1739 Only neutrinos produced from DM annihilations can escape the dense interior of these  
1740 objects. Therefore, neutrino telescopes are the most useful experimental layouts to  
1741 pursue DM searches from their cores.

1742 The neutrino flux from DM annihilations inside the Sun depends on the DM capture  
1743 rate, which is proportional to the DM scattering cross section, and the annihilation rate,  
1744 which is proportional to the velocity-averaged DM annihilation cross-section. The total  
1745 number of DM particles inside the Sun follows the Boltzmann equation [65]:

$$\frac{dN_{DM}}{dt} = C_{\odot} - A_{\odot} N_{DM}^2, \quad (7.1)$$

1746 where  $C_{\odot}$  and  $A_{\odot}$  are the total Sun DM capture and annihilation rates respectively.  
1747 In this expression I neglected the evaporation term, proportional to  $N_{DM}$ , which only  
1748 contribute for  $m_{DM} \lesssim 4$  GeV [69]. As the current threshold of neutrino telescopes is  
1749 a few GeV, this region falls below the probed range but can be important in future  
1750 low-energy projects.

1751 This equation has an equilibrium solution:

$$N_{DM}^{eq} = \sqrt{\frac{C_{\odot}}{A_{\odot}}}, \quad (7.2)$$

1752 which represents the amount of DM inside the Sun if the capture and annihilation have  
1753 reached equilibrium. As the Sun is approximately 4.6 Gyr old, it is usually assumed that  
1754 equilibrium has been achieved. Therefore, the anomalous neutrino flux from the Sun  
1755 would only depend on the DM scattering cross section, enabling us to set limits on this  
1756 quantity. If one does not assume equilibrium, some assumptions on the DM annihilation  
1757 cross section are necessary to extract predictions from neutrino signals.

1758 Here, I am going to consider three possible scenarios for the DM interactions: DM  
1759 scattering off electrons, spin-dependent (SD) and spin-independent interactions off nuclei.  
1760 For the case of these last two, the cross sections will be given in terms of the SD and  
1761 SI elastic scattering DM cross section off protons (assuming that DM interactions off

## 7.2. Gravitational capture of DM by the Sun

1762 protons and neutrons are identical),  $\sigma_p^{\text{SD}}$  and  $\sigma_p^{\text{SI}}$ , as [4, 65]:

$$\sigma_i^{\text{SD}} = \left( \frac{\tilde{\mu}_{A_i}}{\tilde{\mu}_p} \right)^2 \frac{4(J_i + 1)}{3J_i} |\langle S_{p,i} \rangle + \langle S_{n,i} \rangle|^2 \sigma_p^{\text{SD}}, \quad (7.3)$$

$$\sigma_i^{\text{SI}} = \left( \frac{\tilde{\mu}_{A_i}}{\tilde{\mu}_p} \right)^2 A_i^2 \sigma_p^{\text{SI}}, \quad (7.4)$$

1763 where  $\tilde{\mu}_{A_i}$  is the reduced mass of the DM-nucleus  $i$  system,  $\tilde{\mu}_p$  is the reduced mass of  
 1764 the DM-proton system,  $A_i$  and  $J_i$  the mass number and total angular momentum of  
 1765 nucleus  $i$  and  $\langle S_{p,i} \rangle$  and  $\langle S_{n,i} \rangle$  the expectation value of the spins of protons and neutrons  
 1766 averaged over all nucleons, respectively (see Ref. [70] for a review on spin expectation  
 1767 values).

1768 Since the Sun is mainly composed of Hydrogen, the capture of DM from the halo  
 1769 is expected to occur mainly through spin-dependent scattering. However, since the  
 1770 spin-independent cross section is proportional to the square of the atomic mass, heavy  
 1771 elements can contribute to the capture rate (even though they constitute less than 2%  
 1772 of the mass of the Sun). Heavy elements can also contribute to the spin-dependent cross  
 1773 section if the DM has also momentum-dependent interactions.

1774 DM particles can get captured by the Sun if after repeated scatterings off solar  
 1775 targets their final velocity is lower than the escape velocity of the Sun. In the limit of  
 1776 weak cross sections, this capture rate can be approximately written as [4]:

$$C_{\odot}^{\text{weak}} = \sum_i \int_0^{R_{\odot}} dr 4\pi r^2 \int_0^{\infty} du_{\chi} \frac{\rho_{\chi}}{m_{\chi}} \frac{f_{v_{\odot}}(u_{\chi})}{u_{\chi}} \omega(r) \int_0^{v_e(r)} dv R_i^-(\omega \rightarrow v) |F_i(q)|^2, \quad (7.5)$$

1777 where the summation extends over all possible nuclear targets. In this expression,  $R_{\odot}$   
 1778 is the radius of the Sun,  $\rho_{\chi}$  is the local DM density,  $m_{\chi}$  the mass of the DM particle,  
 1779  $f_{v_{\odot}}(u_{\chi})$  the DM velocity distribution seen from the Sun's reference frame,  $R_i^-(\omega \rightarrow v)$   
 1780 is the differential rate at which a DM particle with velocity  $v$  scatters a solar target of  
 1781 mass  $m_i$  to end up with a velocity  $\omega$  and  $|F_i(q)|$  is the nuclear form factor of target  $i$ .

1782 The differential scattering rate takes a rather simple form when considering velocity-

## Chapter 7. DM searches with neutrinos from the Sun

1783 independent and isotropic cross sections. In that case, this quantity is given by [4, 71]:

$$R_i^-(\omega \rightarrow v) = \frac{2}{\sqrt{\pi}} \frac{\mu_{i,+}^2}{\mu_i} \frac{v}{\omega} n_i(r) \sigma_i \left[ \chi(-\alpha_-, \alpha_+) + \chi(-\beta_-, \beta_+) e^{\mu_i(\omega^2 - v^2)/u_i^2(r)} \right], \quad (7.6)$$

1784 where  $\mu_i$  is the ratio between the DM mass and the mass of target  $i$ ,  $\mu_{i,\pm}$  is defined as:

$$\mu_{i,\pm} \equiv \frac{\mu_i \pm 1}{2}, \quad (7.7)$$

1785  $n_i(r)$  is the density profile of target  $i$  in the solar medium,  $u_i(r)$  is the most probable

1786 velocity of target  $i$  given by:

$$u_i(r) = \sqrt{\frac{2T_\odot(r)}{m_i}}, \quad (7.8)$$

1787 where  $T_\odot(r)$  is the temperature of the Sun, the quantities  $\alpha_\pm$  and  $\beta_\pm$  are defined as:

$$\alpha_\pm \equiv \frac{\mu_{i,+}v \pm \mu_{i,-}\omega}{u_i(r)}, \quad (7.9)$$

$$\beta_\pm \equiv \frac{\mu_{i,-}v \pm \mu_{i,+}\omega}{u_i(r)}, \quad (7.10)$$

1788 and the function  $\chi(a, b)$  is a Gaussian integral of the form:

$$\chi(a, b) \equiv \int_a^b dx e^{-x^2}. \quad (7.11)$$

1789 Finally, if one assumes the DM halo velocity distribution in the galactic rest frame

1790 to be a Maxwell-Boltzmann distribution, one can write the halo velocity distribution for

1791 an observer moving at the speed of the Sun with respect to the DM rest frame as:

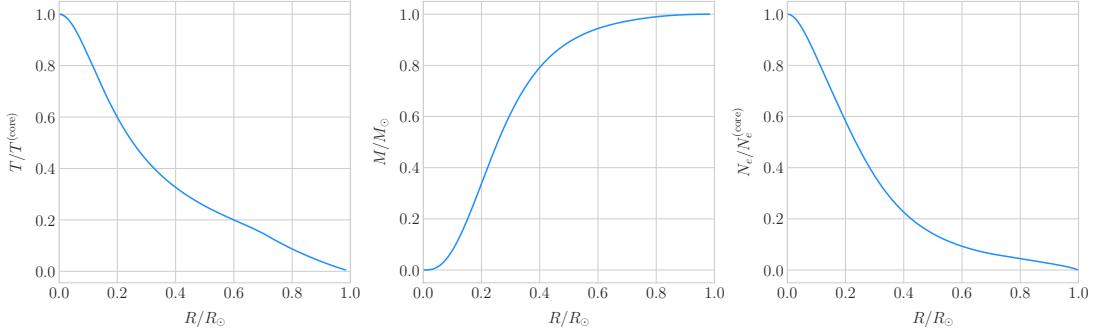
$$f_{v_\odot}(u_\chi) = \sqrt{\frac{3}{2\pi}} \frac{u_\chi}{v_\odot v_d} \left( e^{-\frac{3(u_\chi - v_\odot)^2}{2v_d^2}} - e^{-\frac{3(u_\chi + v_\odot)^2}{2v_d^2}} \right), \quad (7.12)$$

1792 where:

$$\omega^2 = u_\chi + v_e(r)^2, \quad (7.13)$$

1793 is the DM velocity squared,  $v_\odot$  the relative velocity of the Sun from the DM rest frame

## 7.2. Gravitational capture of DM by the Sun



**Figure 7.1:** Input solar parameters used in our capture rate computation as functions of the Sun's 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 [3].

1794 and  $v_d \simeq \sqrt{3/2}v_\odot$  the velocity dispersion.

1795 For the case of strong scattering cross section, Eq. (7.5) ceases to be valid, as it  
 1796 escalates indefinitely with the cross section. In that limit, the capture rate saturates to  
 1797 the case where the probability of interaction is equal to one, which can be written as:

$$C_\odot^{\text{geom}} = \pi R_\odot^2 \left( \frac{\rho_\chi}{m_\chi} \right) \langle v \rangle \left( 1 + \frac{3}{2} \frac{v_e^2(R_\odot)}{v_d^2} \right) \xi(v_\odot, v_d), \quad (7.14)$$

1798 where  $v_d = \sqrt{8/3\pi}v_d$  is the mean velocity in the DM rest frame and the factor  $\xi(v_\odot, v_d)$   
 1799 accounts for the suppression due to the motion of the Sun:

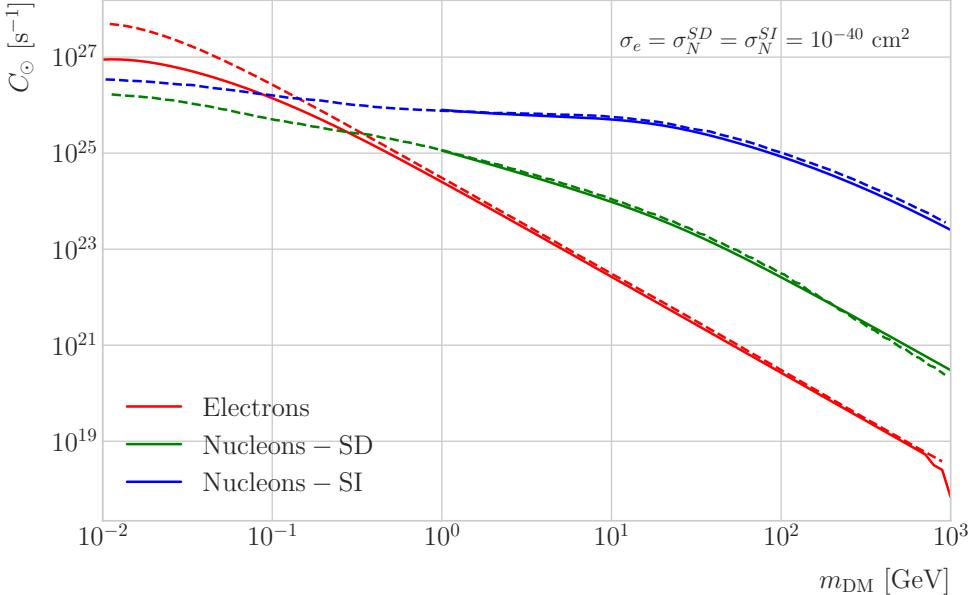
$$\xi(v_\odot, v_d) = \frac{v_d^2 e^{-\frac{3v_\odot^2}{2v_d^2}} + \sqrt{\frac{\pi}{6}} \frac{v_d}{v_\odot} (v_d^2 + 3v_e^2(R_\odot) + 3v_\odot^2) \text{Erf} \left( \sqrt{\frac{3}{2}} \frac{v_\odot}{v_d} \right)}{2v_d^2 + 3v_e^2(R_\odot)}. \quad (7.15)$$

1800 Having these into account, one can write the total capture rate as a combination of  
 1801 both contributions, allowing a smooth transition between the two, as:

$$C_\odot = C_\odot^{\text{weak}} \left( 1 - e^{C_\odot^{\text{geom}}/C_\odot^{\text{weak}}} \right). \quad (7.16)$$

1802 I computed the capture rate from Eq. (7.16) in the case of interactions with  
 1803 electrons. To do so, I used the standard solar model BS2005-OP [3]. Fig. 7.1 shows the

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.2:** 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. [4]. All the rates are shown for a choice of scattering cross section of  $\sigma_i = 10^{-40} \text{ cm}^2$ .

1804 three parameters from the solar model that are needed for the computation, the solar

1805 temperature (left panel), mass (central panel) and electron density (right panel) profiles.

1806 For the case of the interactions off nuclei, the computations are more convoluted

1807 as one needs to add up the contributions of the different most abundant nuclei in

1808 the Sun. Also, in contrast to the electron scenario where the form factor is trivially

1809  $|F_e(q)|^2 = 1$ , for any nucleus  $i$  one would need to consider some appropriate nuclear

1810 density distribution (either a Gaussian approximation, a Woods-Saxon distribution, etc)

1811 which would complicate the calculations even further.

1812 That is the reason why, at this stage of our study, I decided to take an alternative

1813 approach to the computation of the DM-nucleus capture rates. I used the **DarkSUSY**

1814 software, that allows us to compute these quantities performing a full numerical

1815 integration over the momentum transfer of the form factors. The default standard

1816 solar model used by **DarkSUSY** is BP2000<sup>1</sup> [72].

---

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

## 7.2. Gravitational capture of DM by the Sun

1817 In Fig. 7.2 I show the results I obtained for the capture rates, for the case of  
 1818 interactions off electrons (red solid line), SD (green solid line) and SI (blue solid line)  
 1819 interactions of nucleons. In all cases I used a value of the scattering cross sections of  
 1820  $\sigma_i = 10^{-40} \text{ cm}^2$ . Note here one of the limitations of the **DarkSUSY** approach, one can  
 1821 not extend the computation below  $m_{\text{DM}} = 1 \text{ GeV}$ . Nevertheless, this is not something  
 1822 to worry about in this case, as I will discuss next. As a comparison, I added also the  
 1823 values computed in Ref. [4] (same color scheme, dashed lines). One can see there is good  
 1824 agreement between these and the **DarkSUSY** computation of the SD and SI interactions  
 1825 for  $m_{\text{DM}} \geq 1 \text{ GeV}$ . In this regime their computations also matches quite well our  
 1826 result for the electron capture rate. However, these start to differ significantly below  
 1827  $m_{\text{DM}} = 1 \text{ GeV}$ , being their estimate up to a factor of 5 bigger than ours for low masses.  
 1828

1828 Let us comment briefly about the assumption I made before about not including  
 1829 an evaporation term in the Boltzmann equation. If I include this term in the equation  
 1830 (which will be proportional to the number of DM particles) the equilibrium solution  
 1831 takes the form:

$$N_{\text{DM}}^{eq} = \sqrt{\frac{C_{\odot}}{A_{\odot}}} \frac{1}{\kappa + \frac{1}{2} E_{\odot} \tau_{eq}}, \quad (7.17)$$

1832 where  $E_{\odot}$  is the total evaporation rate,  $\tau_{eq}$  is the equilibrium time in the absence of  
 1833 evaporation:

$$\tau_{eq} = \frac{1}{\sqrt{C_{\odot} A_{\odot}}}, \quad (7.18)$$

1834 and  $\kappa$  is defined as:

$$\kappa \equiv \sqrt{1 + \left( \frac{E_{\odot} \tau_{eq}}{2} \right)^2}. \quad (7.19)$$

1835 Now, it is easy to proof that in case evaporation dominates  $\kappa \gg 1$  and therefore:

$$N_{\text{DM}}^{eq} \simeq \frac{C_{\odot}}{E_{\odot}}. \quad (7.20)$$

1836 In contrast, if evaporation is irrelevant  $\kappa \simeq 1$  and one recovers Eq. (7.2).

---

model is relatively old and do not see why they are not using others like [3]. Maybe one can double-check in the code to make sure.

## Chapter 7. DM searches with neutrinos from the Sun

1837 In this way, one can define the evaporation mass as the mass for which the number  
1838 of DM particles in equilibrium approaches Eq. (7.20) at 10% level:

$$\left| N_{DM}^{eq}(m_{\text{evap}}) - \frac{C_{\odot}(m_{\text{evap}})}{E_{\odot}(m_{\text{evap}})} \right| = 0.1 N_{DM}^{eq}(m_{\text{evap}}). \quad (7.21)$$

1839 This can be regarded as the minimum testable mass one can reach using the annihilation  
1840 products of the DM in the Sun.

1841 It was reported in Ref. [4] that, in the case of both SD and SI DM interactions  
1842 off nuclei, this value ranges from 2 to 4 GeV depending on the specific scattering  
1843 cross section value, compatible with the usual assumptions in the literature. What is  
1844 interesting is the case of the electron capture. It was found that, when one applies a  
1845 cutoff in the velocity distribution of the DM trapped in the Sun slightly below the escape  
1846 velocity, the evaporation mass for the DM-electron interaction decreases remarkably. For  
1847 a moderate choice of  $v_c(r) = 0.9v_e(r)$  one gets an evaporation mass of around 200 to  
1848 600 MeV. This possibility opens a region of the parameter space that could be tested  
1849 with neutrino detectors.

### 1850 7.3 Neutrino flux from DM annihilations

1851 When WIMPs annihilate inside the Sun a flux of high-energy neutrinos is expected from  
1852 heavy quarks, gauge bosons and  $\tau^+\tau^-$  final states, which decay before losing energy  
1853 in the dense solar medium, as they will produce a continuum spectra up to  $E_{\nu} \sim m_{\chi}$   
1854 (in the case of direct annihilation to neutrinos one would have a line at  $E_{\nu} = m_{\chi}$ ) [66].  
1855 This kind of signal has been extensively studied in the literature, allowing to put strong  
1856 limits on the SD WIMP-proton cross section for large  $m_{\chi}$ . However, the number of  
1857 high-energy neutrinos per WIMP annihilation is small and the spectrum depends on the  
1858 unknown final state. Moreover, background rejection is easier for large  $m_{\chi}$  but neutrinos  
1859 with  $E_{\nu} \gtrsim 100$  GeV are significantly attenuated by interactions in the Sun.

1860 Nevertheless, most WIMP annihilation final states eventually produce a low-energy  
1861 neutrino spectrum. In this case one does not just consider the more massive final

## 7.4. Computing limits from solar neutrino fluxes

states but also annihilations into  $e^+e^-$ ,  $\mu^+\mu^-$  and light quarks [65]. 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  $\nu_\mu$  while in the case of pions one would have a  $E_\nu = 29.8$  MeV  $\nu_\mu$ . In practice only  $K^+$  and  $\pi^+$  contribute to these signals, as  $K^-$  and  $\pi^-$  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.

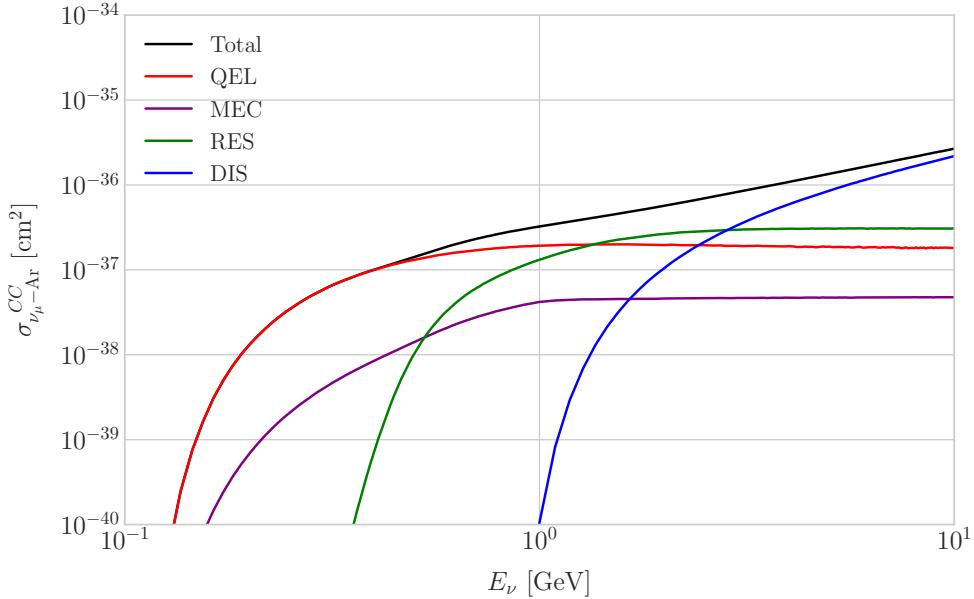
## 7.4 Computing limits from solar neutrino fluxes

In order 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:

$$N_B = \eta_B \int d\Omega \int_{E_{min}}^{E_{max}} dE_\nu \frac{d^2\Phi_{atm}^\mu}{dE_\nu d\Omega} \times \left( A_{eff}^{(\mu)}(E_\nu) T \right), \quad (7.22)$$

where  $\eta_B$  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 cross section and the number of nuclei in the fiducial volume of the detector. This way

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.3:** *NuWro* computed  $\nu_\mu - {}^{40}\text{Ar}$  charged-current scattering cross section as a function of the neutrino energy  $E_\mu$ . 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).

1888 for DUNE I can write:

$$A_{eff}^{(\mu)}(E_\nu) = (6.0 \times 10^{-10} \text{ m}^2) \left( \frac{\sigma_{\nu - \text{Ar}}^{(\mu)}(E_\nu)}{10^{-38} \text{ cm}^2} \right) \left( \frac{M_{target}}{40 \text{ kT}} \right), \quad (7.23)$$

1889 where  $\sigma_{\nu - \text{Ar}}^{(\mu)}$  is the  $\nu_\mu - {}^{40}\text{Ar}$  charged-current scattering cross section. In Fig. 7.3 I  
 1890 show the computed value of this cross section as a function of the neutrino energy  $E_\nu$ ,  
 1891 in the range of interest both for the atmospheric background and signal events. It was  
 1892 computed using the NuWro Monte Carlo neutrino event generator [73], including the  
 1893 charged-current contributions of the quasi-elastic scattering (red line), resonant pion  
 1894 exchange (green line), deep inelastic scattering (blue line) and meson exchange current  
 1895 (purple line).

1896 The background rejection will depend on the resolution of the detector and the  
 1897 selection one applies on the events. A geometry argument can be used to estimate  
 1898 the maximum background rejection one can achieve in this case, considering one can

## 7.4. Computing limits from solar neutrino fluxes

1899 efficiently discriminate all events coming from a direction different from that of the  
 1900 Sun. In that case, the optimal background efficiency will simply be the relative angular  
 1901 coverage of the Sun. Taking the angular diameter of the Sun as seen from the Earth to  
 1902 be  $0.5^\circ$ , I have:

$$\eta_B^{(opt)} \approx \frac{\pi \left(\frac{0.5}{2}\right)^2}{360 \times 180} \simeq 3.03 \times 10^{-6}. \quad (7.24)$$

1903 This value will give a very optimistic estimate of the number of background events.  
 1904 However, it can be regarded as an lower limit, as it represents the best case scenario.

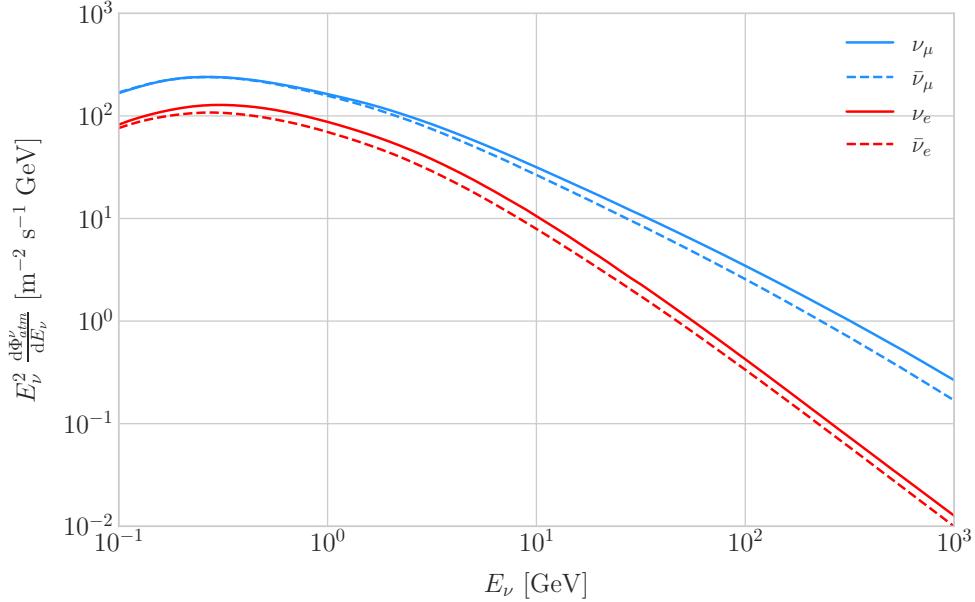
1905 In Fig. 7.4 I show the fluxes of atmospheric neutrinos at the Homestake mine during  
 1906 solar minimum, taken from Ref. [5]. The values are averaged over the two angular  
 1907 directions. In blue I have the flux of muon neutrinos while in red I indicate the flux  
 1908 of electron neutrinos. Additionally, the dashed lines correspond to both antineutrino  
 1909 species.

1910 Using these values for the muon neutrino and the corresponding total CC cross  
 1911 section, one can compute the number of expected background events by integrating over  
 1912 the given energy range (as in this case the angular integral is trivial). As for the energy  
 1913 range to integrate over, I choose the range for DUNE specified in [42],  $E_{min} = 10^{-1}$  GeV  
 1914 and  $E_{max} = 10$  GeV. Taking all these into account, I found the number of background  
 1915 events to be:

$$N_B \simeq \eta_B \times (3.827 \times 10^4) \times \left( \frac{\text{exposure}}{400 \text{ kT yr}} \right). \quad (7.25)$$

1916 In order to estimate the sensitivity of DUNE to this kind signal, one can consider a  
 1917 hypothetical data set where the number of observed neutrinos is taken to be the expected  
 1918 number of background events rounded to the nearest integer,  $N_{obs} = \text{round}(N_B)$  [74].  
 1919 Now, if I assume that the number of signal and background events seen by DUNE are  
 1920 given by Poisson distributions with means equal to the expected number of signal and  
 1921 background events,  $N_S$  and  $N_B$ , one can denote by  $N_S^{90}$  to the number of expected  
 1922 signal events such that the probability of having an experimental run with a number of  
 1923 events greater than  $N_{obs}$  is 90%. This number can be obtained as the numerical solution

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.4:** Expected atmospheric neutrino flux as a function of the neutrino energy  $E_\nu$  at Homestake at solar minimum, taken from Ref. [5]. The blue solid (dashed) line correspond to muon neutrinos (antineutrinos) and the red solid (dashed) line correspond to electron neutrinos (antineutrinos).

<sup>1924</sup> to the equation:

$$1 - \frac{\Gamma(N_{obs} + 1, N_S^{90} + N_B)}{N_{obs}!} = 0.9, \quad (7.26)$$

<sup>1925</sup> where  $\Gamma(x, y)$  is the upper incomplete gamma function.

<sup>1926</sup> The number of signal events is related to the neutrino flux from DM annihilations in  
<sup>1927</sup> a similar way as the background events to the atmospheric neutrino flux. In this case I  
<sup>1928</sup> have:

$$N_S = \eta_S \Gamma_A^{eq} \int_{z_{min}}^{z_{max}} dz \frac{dN_\nu}{dAdN_Adz} \times (A_{eff}^\mu(z)T), \quad (7.27)$$

<sup>1929</sup> where  $\eta_S$  is the signal efficiency,  $\Gamma_A^{eq}$  is the total annihilation rate of DM particles at  
<sup>1930</sup> equilibrium,  $\Gamma_A^{eq} = A_\odot (N_{DM}^{eq})^2$ ,  $z_{min}$  and  $z_{max}$  the minimum and maximum relative  
<sup>1931</sup> energies to integrate over (in such a way that  $z_{min,max} \leq E_{min,max}/m_{DM}$  for each  $m_{DM}$ )  
<sup>1932</sup> and  $dN_\nu/dAdN_Adz$  the muon neutrino flux per DM annihilation in the Sun.

<sup>1933</sup> Knowing  $N_S^{90}$  one can use the relation in Eq. (7.27) to obtain  $\Gamma_A^{eq,90}$  for different  
<sup>1934</sup> values of the DM mass. From there I can directly translate those values into the

## 7.5. Example: Kaluza-Klein Dark Matter

1935 upper limits for DUNE on the DM scattering cross sections, for a given exposure. The  
1936 relation between the annihilation rate and the DM-nucleon cross section comes from the  
1937 equilibrium condition through the solar DM capture rate. The details of the evolution  
1938 of the number of DM particles inside the Sun and the computation of the capture rates  
1939 are discussed in App. 7.2.

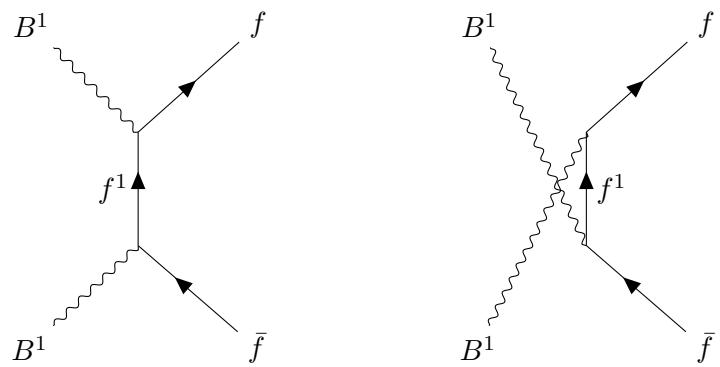
### 1940 7.5 Example: Kaluza-Klein Dark Matter

1941 Even though there are plenty of BSM theories which provide viable dark matter  
1942 candidates, Kaluza-Klein type of models [75, 76] within the universal extra dimensions  
1943 (UED) paradigm naturally predict the existence of a massive, stable particle that can  
1944 play the role of the dark matter. In the UED scenario all the SM fields can propagate  
1945 in one or more compact extra dimensions [77], as opposed to the idea of brane worlds  
1946 [78, 79], where just gravity can propagate in the bulk while SM particles live at fixed  
1947 points.

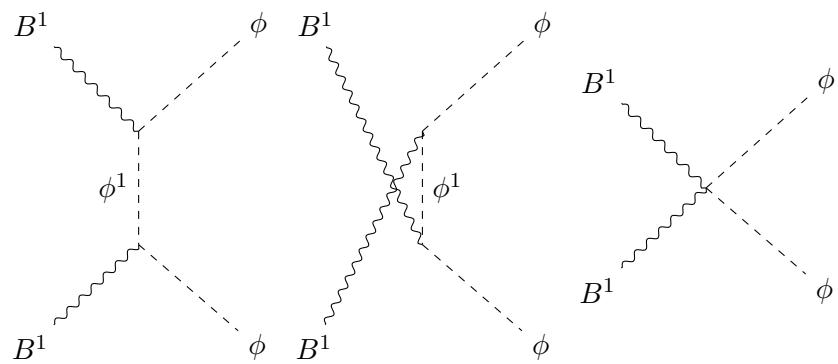
1948 Furthermore, in UED there is no violation of the translational invariance along the  
1949 extra dimensions, thus leading to degenerate KK modes masses and also the conservation  
1950 of the KK number in the effective four dimensional theory. At loop level, radiative  
1951 corrections and boundary terms shift the masses of the KK modes and break KK  
1952 number conservation into a KK parity. As a result, this theory only contains interactions  
1953 between an even number of odd KK modes and therefore the lightest among the first KK  
1954 excitations will be stable. This particle is usually denoted as the lightest Kaluza-Klein  
1955 particle (LKP) and its mass is proportional to  $1/R$ , being  $R$  the size of the extra  
1956 dimension.

1957 A viable DM candidate needs to be electrically neutral and non-baryonic, therefore  
1958 good candidates among the first Kaluza-Klein excitations would be the KK neutral  
1959 gauge bosons and the KK neutrinos [80]. Another possible candidate is the first KK  
1960 excitation of the graviton, which receives negligible radiate contributions and therefore  
1961 has a mass almost equal to  $1/R$ , but it has been shown that the lightest eigenstate from

## Chapter 7. DM searches with neutrinos from the Sun

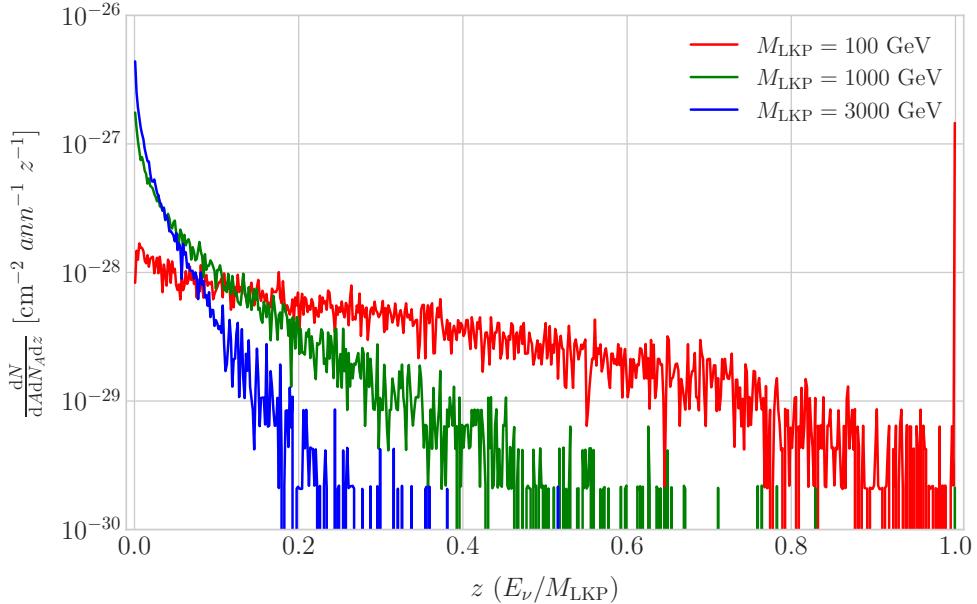


**Figure 7.5:** Feynman diagrams for  $B^1B^1$  annihilation into SM fermions.



**Figure 7.6:** Feynman diagrams for  $B^1B^1$  annihilation into a Higgs boson pair.

## 7.5. Example: Kaluza-Klein Dark Matter

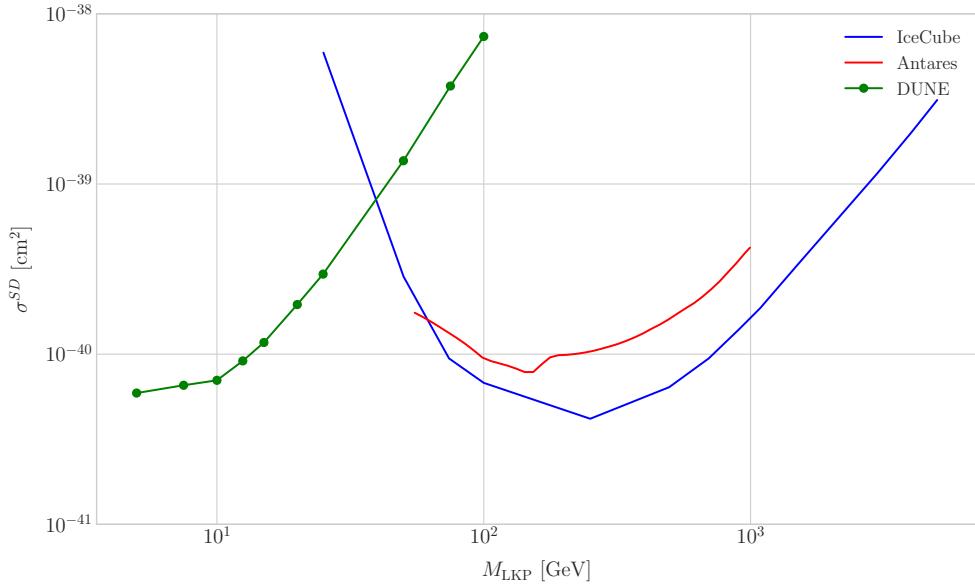


**Figure 7.7:** Computed spectra of muon neutrinos at the DUNE FD site from  $B^1$  annihilations in the Sun for three different values of  $M_{\text{LKP}}$ , plotted in relative energy units for legibility.

the mixing of the gauge mass states  $(B^1, W_3^1)$  would be lighter, as  $B^1$  and  $W_3^1$  receive negative radiative corrections [81]. It is also understood that, when these corrections become sizeable, the eigenstates become approximately pure  $B^1$  and  $W_3^1$  states as the Weinberg mixing angle grows small with the KK number [81]. In that case, the LKP can be well-approximated as being entirely  $B^1$ .

I need to compute the neutrino flux produced by the annihilations of the LKP in the core of the Sun, taking into account their propagation in the solar medium, as well as neutrino oscillations. To this end I used `WimpSim` [82, 83] to generate one million annihilation events in the Sun over a time span of four years and propagate them to the DUNE FD location ( $44^\circ 20' \text{ N}, 103^\circ 45' \text{ W}$ ), for different values of  $M_{\text{LKP}}$ . In Fig. 7.7 I show the obtained muon neutrino spectra arriving to the detector from LKP annihilations in the Sun, per unit area and per annihilation, plotted in relative energy units for different values of the mass. As one could expect the spectra get steeper the higher is the mass, due to the absorption of high-energy neutrinos in the solar medium. Also, one can see the peak at  $z = 1$  due to the direct annihilation into neutrinos  $\chi\chi \rightarrow \nu\bar{\nu}$ .

## Chapter 7. DM searches with neutrinos from the Sun

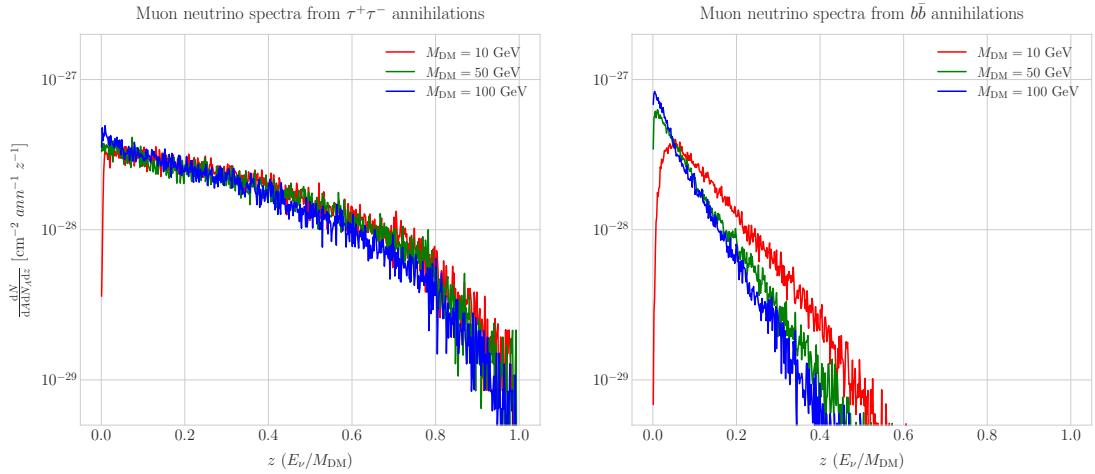


**Figure 7.8:** Projected 90% confidence level upper limit for DUNE (400 kT yr) on the spin-dependent  $B^1$ -proton scattering cross section as a function of  $M_{\text{LKP}}$  (green dots). I also show the previous limits from IceCube [6] (blue line) and Antares [7] (red line) on the LKP cross section. The shaded area represents the disfavoured region (at 95% confidence level) on the mass of the LKP from LHC data [8].

Now, one can estimate the sensitivity of DUNE to this particular model by using the methods I previously discussed. To begin with, I will use the optimistic estimation of the background efficiency in Eq. (7.24) to get our upper bound. Using it, one can directly compute the number of expected background events to be  $N_B = 0.1101$  for an exposure of 400 kT yr. Then, Eq. (7.26) give us a value of  $N_S^{90} = 2.20$  for the 90% exclusion number of expected signal events. By using the NuWro generated cross sections and the computed neutrino fluxes from  $B^1$  annihilations in the Sun I can estimate the limits on the SD and SI DM-nucleus cross section using the relation in Eq. (7.2) and the capture rates I computed with DarkSUSY.

In Fig. 7.8 I show the projected sensitive for DUNE on the spin-dependent  $B^1$ -proton scattering cross section versus the mass of the DM particle, for a exposure of 400 kT yr (green dots). I also include the previous results from IceCube [6] (blue line) and Antares [7] (red line). The shaded area represents the disfavoured region from combined searches for UED by ATLAS and CMS [8].

## 7.6. High energy DM neutrino signals



**Figure 7.9:** 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),  $50 \text{ GeV}$  (green line) and  $100 \text{ GeV}$  (blue line), plotted in relative energy units.

From the experimental point of view, this estimation lacked a detailed simulation of the detector response and thus this must be considered 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 [8] and other rare decay measurements [84, 85], it still constitutes an alternative indirect probe.

## 7.6 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

## Chapter 7. DM searches with neutrinos from the Sun

2007 those will produce usually a higher energy neutrino flux that will be out of reach for  
2008 DUNE (usually the maximum neutrino energy is taken to be  $E_{max} = 10$  GeV).

2009 In Fig. 7.9 I show the `WimpSim` [82, 83] generated muon neutrino spectra at the  
2010 DUNE FD location ( $44^\circ 20' N, 103^\circ 45' W$ ) from  $\tau^+\tau^-$  (left panel) and  $b\bar{b}$  (right panel)  
2011 annihilations in the core of the Sun, for different DM masses. Here, one can clearly see  
2012 the meaning of the previous distinction between hard and soft channels. For the same  
2013 DM mass value, the muon neutrino spectrum from the  $\tau^+\tau^-$  channel is more flat and  
2014 reaches higher energies than the one from the  $b\bar{b}$  channel, which drops faster.

2015 In this case, I prepared two sets of files, one for  $\tau^+\tau^-$  and the other for  $b\bar{b}$ , for DM  
2016 masses in the range from 5 to 100 GeV (actually for  $b\bar{b}$  the first mass point I took is  
2017 7.5 GeV, as a WIMP with  $m_{DM} = 5$  GeV can not kinematically self annihilate into  $b\bar{b}$ ).  
2018 Then, I prepared the `WimpSim` output fluxes in a specific way to use them as inputs to  
2019 `NuWro`, which simulates the neutrino interaction with the argon.

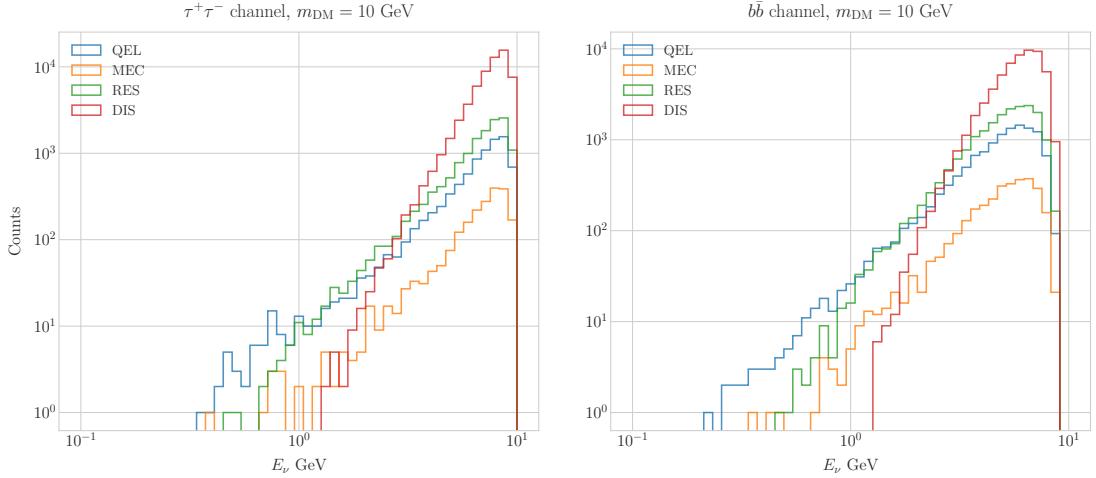
2020 Because `WimpSim` outputs an event list together with the fluxes, I can use the former  
2021 to generate the events. The direction of these is given in terms of the azimuth and  
2022 altitude angles viewed from the specified location, so first I need to convert these into the  
2023 DUNE FD coordinates. Once I have done it, each event can be processed with `NuWro`.  
2024 To increase the number of samples and optimise the computation time, I generate 100  
2025 interactions (i.e. `NuWro` events) for each `WimpSim` event<sup>2</sup>. I restrict the event generation  
2026 to charged current interactions, but I allow all the different contributions to the CC  
2027 cross section, i.e. quasielastic scattering (QEL), meson exchange current process (MEC),  
2028 resonant pion production (RES) and deep inelastic scattering (DIS). I just take into  
2029 account the CC contribution because I am only interested in final states with charged  
2030 leptons, as we have better chances of reconstructing the kinematics of CC events.

2031 For the atmospheric fluxes I follow a similar procedure, only that this time I do not  
2032 have a set of events but the fluxes binned in azimuth and altitude angles. This way, I  
2033 transform these to DUNE coordinates and process the fluxes for each bin separated with

---

<sup>2</sup>This 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.

## 7.6. High energy DM neutrino signals



**Figure 7.10:** Distribution of the muon neutrino energies from the  $\tau^+\tau^-$  (left panel) and  $b\bar{b}$  (right panel) annihilation channels, for  $m_{\text{DM}} = 10$  GeV, separated by CC interaction type: QEL (blue), MEC (orange), RES (green) and DIS (red).

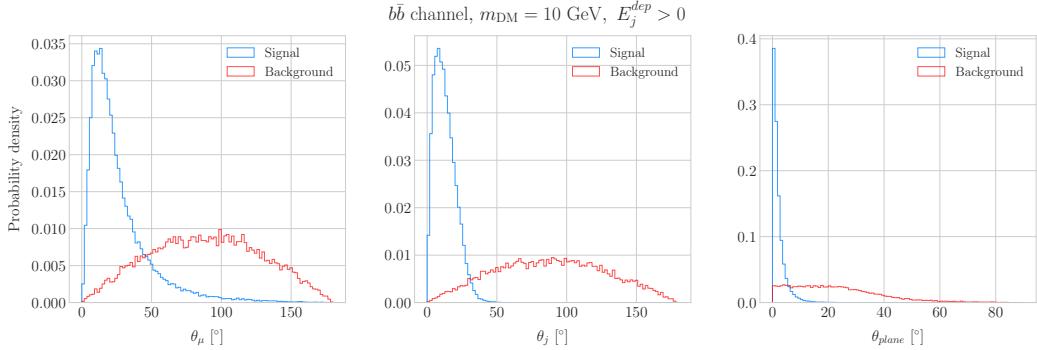
2034 NuWro.

2035 At this point, I have two sets of events with different energies and final states.  
 2036 In Fig. 7.10 one can see the distribution of the muon neutrino energies for the case  
 2037  $m_{\text{DM}} = 10$  GeV, both for the  $\tau^+\tau^-$  (left panel) and  $b\bar{b}$  (right panel) channels, separated  
 2038 by interaction. One can clearly see that there are different energy regimes where the  
 2039 primary interaction type is different. This leads to a plurality of event topologies,  
 2040 therefore making it difficult to implement a general approach to the selection of events  
 2041 in detriment of the background. As a way to proceed, I decided to split our samples,  
 2042 based on the different interaction modes and contents of the final state, into a CC DIS  
 2043 sample and a single proton CC QEL sample.

2044 **7.6.1 DIS events**

2045 To begin with, I consider the high energy part of the spectrum. In this region DIS events  
 2046 dominate, i.e. interactions of the form  $\nu_\mu + q_d(\bar{q}_u) \rightarrow \mu^- + q_u(\bar{q}_d)$ . Therefore, our final  
 2047 estates will contain a muon and a hadronic jet from the fragmentation of the outgoing  
 2048 quark. As all these events have  $E_\nu \gtrsim 1$  GeV the momentum transfer to the remnant  
 2049 nucleus is negligible, for this reason the neutrino energy can be effectively reconstructed

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.11:** Distributions of  $\theta_\mu$  (left panel),  $\theta_j$  (central panel) and  $\theta_{\text{plane}}$  (right panel) for the  $b\bar{b}$  sample with  $m_{\text{DM}} = 10$  GeV (blue) and the atmospheric background (red).

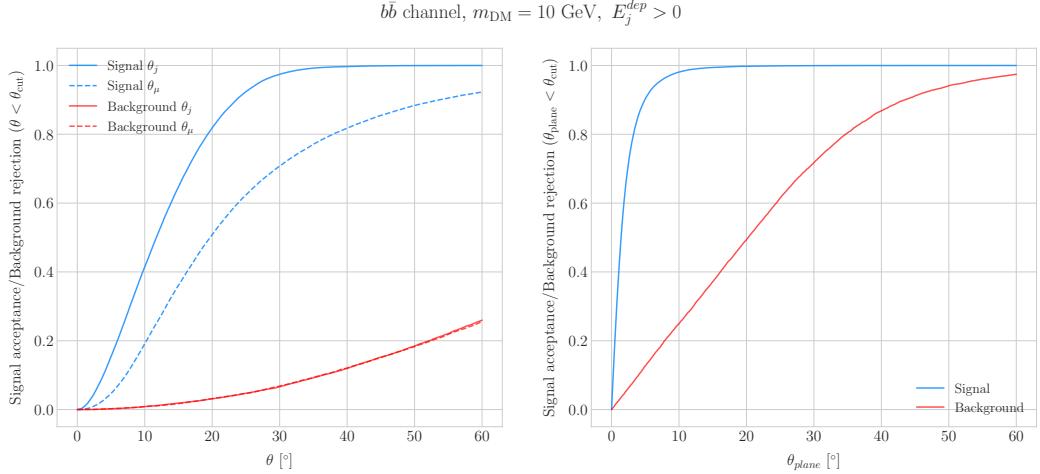
just taking into account the momenta of the muon and the jet. This technique was successfully used in Ref. [86] to select monoenergetic DM solar neutrino events from  $\nu\bar{\nu}$  annihilation channels.

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

To account for the limited angular resolution of the detector, I smeared the momenta of the muons and hadrons. In a liquid argon TPC muons are expected to be tracked with high precision, therefore I take the associated angular resolution to be  $1^\circ$ . In the case of jets, it is expected that for the hadrons dominating the cascade a detector like DUNE has an angular resolution between  $1^\circ$  to  $5^\circ$  [42], so I take the latter, more conservative, estimate.

As a first selection step, I will just take into account particles with kinetic energies above the detection threshold of DUNE. For muons and photons the specified threshold energy is 30 MeV, for charged pions 100 MeV and for other hadrons 50 MeV [42]. This way, if the outgoing muon in a certain event has an energy lower than the required

## 7.6. High energy DM neutrino signals



**Figure 7.12:** Left panel: signal efficiencies (blue lines) and background rejections (red lines) for events passing the cuts  $\theta < \theta_{\text{cut}}$  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  $\theta_{\text{plane}} < \theta_{\text{cut}}$  for the momentum conservation plane deviation.

threshold I will drop such event. For the case of hadrons and photons, I will only require to have at least one particle above the energy threshold, so then one can compute the jet momentum using the (smeared) momenta of the  $N$  particles above threshold as:

$$\vec{p}_j = \sum_{i=1}^N \vec{p}_i. \quad (7.28)$$

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

$$E_j^{\text{dep}} = m_{^{39}\text{Ar}} - m_{^{40}\text{Ar}} + \sum_{i=1}^N \sqrt{|\vec{p}_i|^2 + m_i^2}. \quad (7.29)$$

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

For the events I can compute the angles for the muon and jet with respect to the

## Chapter 7. DM searches with neutrinos from the Sun

2080 incoming neutrino as:

$$\cos \theta_\mu = \hat{p}_\nu \cdot \hat{p}_\mu, \quad (7.30)$$

$$\cos \theta_j = \hat{p}_\nu \cdot \hat{p}_j, \quad (7.31)$$

2081 and the deviation from the momentum conservation plane as:

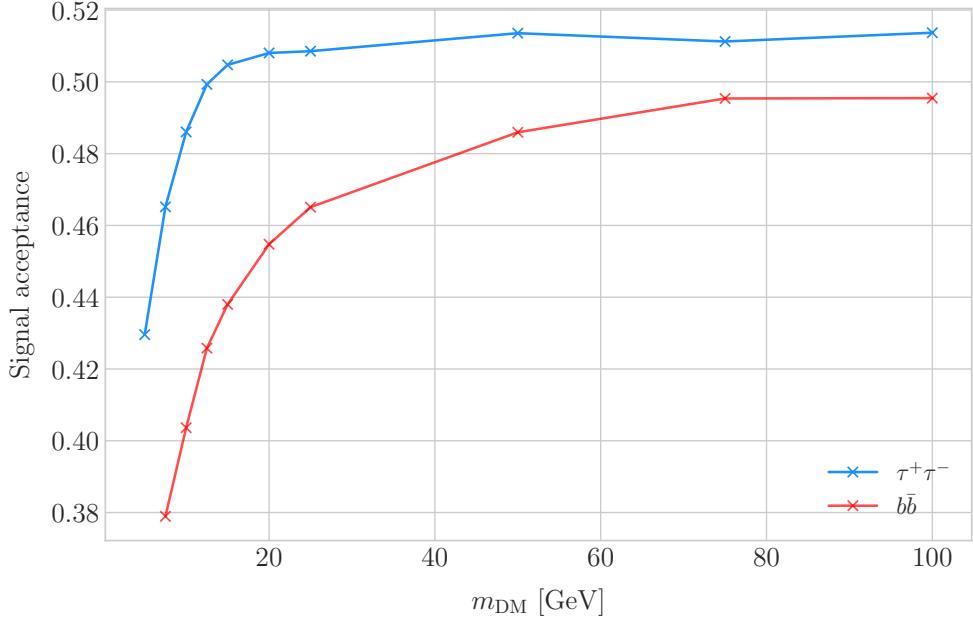
$$\sin \theta_{plane} = \left| \frac{\hat{p}_\mu \times \hat{p}_\nu}{|\hat{p}_\mu \times \hat{p}_\nu|} \cdot \hat{p}_j \right|. \quad (7.32)$$

2082 In Fig. 7.11 I show some distributions of these quantities for the case of the  $b\bar{b}$  sample  
 2083 with  $m_{DM} = 10$  GeV (blue histograms) and for the atmospheric backgrounds (red).  
 2084 In order to select the atmospheric events I followed the same criteria as for the signal  
 2085 events. However, because in the signal case I used the true direction of the neutrino  
 2086 as input, as it should be that of the Sun at that time and therefore known, in the  
 2087 atmospheric case I used a set of solar positions as our ansatz for the neutrino direction.  
 2088 From the distributions, one can see that the muon and the jet for the signal events are  
 2089 predominantly forward and also that the deviations from the momentum conservation  
 2090 plane are peaked at zero, as one should expect.

2091 Now, I can start applying cuts to maximise our signal selection efficiency while at  
 2092 the same time I try to minimise the amount of atmospheric background events passing  
 2093 the selection. To this end, I will need to find some lower and upper cuts for  $\theta_j$  and  
 2094  $\theta_\mu$  and an upper bound for  $\theta_{plane}$ . In Fig. 7.12 I show how upper bound cuts in the  
 2095 different angular variables affect the signal efficiency (blue lines) and the background  
 2096 rejection (red lines). Notice that the signal efficiency behaves in a quite different way  
 2097 when I apply cuts in the jet and the muon angles. On the contrary, the cuts on both  
 2098 variables have a similar effect on the background rejection.

2099 In order to obtain the optimal set of cuts, I perform a multidimensional scan. I  
 2100 do this separately for the  $\tau^+\tau^-$  and the  $b\bar{b}$  samples. For each case, I scan the possible  
 2101 cuts for each mass point and then I take the mean value of the signal efficiency for

## 7.6. High energy DM neutrino signals

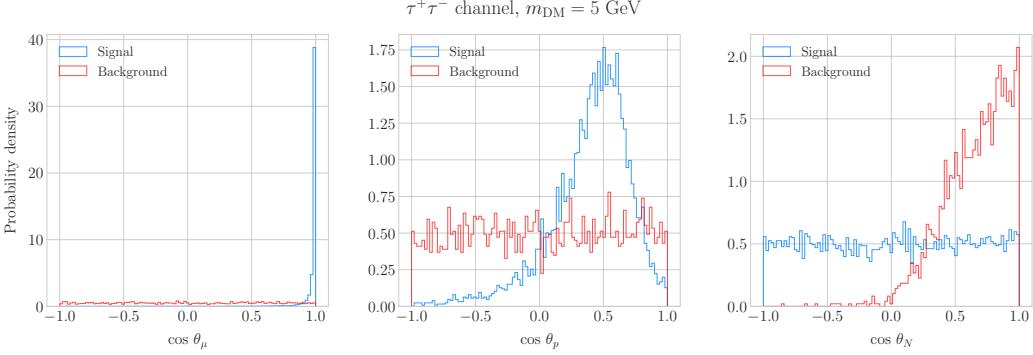


**Figure 7.13:** Signal efficiencies for the  $\tau^+\tau^-$  (blue line) and  $b\bar{b}$  (red line) DIS samples as functions of the DM mass,  $m_{\text{DM}}$ , obtained by applying the optimal angular cuts  $\theta_\mu < 27^\circ$ ,  $4^\circ < \theta_j < 26^\circ$  and  $\theta_{\text{plane}} < 3.5^\circ$ .

2102 each configuration, to get the mean efficiency for each set of cuts. I do a similar scan  
 2103 for the atmospheric sample independently. Then, I take the sets of cuts such that  
 2104 the background rejection achieved is greater than 99.8% and search for the one which  
 2105 maximises the  $\tau^+\tau^-$  and  $b\bar{b}$  sample mean efficiencies. I found that with the cuts  $\theta_\mu < 27^\circ$ ,  
 2106  $4^\circ < \theta_j < 26^\circ$  and  $\theta_{\text{plane}} < 3.5^\circ$  I get a background rejection of 99.80% while achieving  
 2107 a 49.40% and 44.92% mean signal efficiencies for the  $\tau^+\tau^-$  and  $b\bar{b}$  signals respectively.

2108 In Fig. 7.13 I show the signal efficiencies as a function of the DM mass for the  $\tau^+\tau^-$   
 2109 (blue line) and the  $b\bar{b}$  (red line) DIS events, after applying the cuts discussed above, as  
 2110 well as the energy threshold and hadronic visible energy selections. One can see that  
 2111 the efficiency grows with the mass, as annihilations of more massive DM particles will  
 2112 produce a neutrino spectrum centered at higher energies, where DIS events dominate.  
 2113 Notice also that the efficiency is higher for the  $\tau^+\tau^-$  case at every mass point, as in  
 2114 general this channel produces neutrinos at higher energies than the corresponding  $b\bar{b}$   
 2115 channel.

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.14:** Distributions of  $\cos \theta_\mu$  (left panel),  $\cos \theta_p$  (central panel) and  $\cos \theta_N$  (right panel) for the  $\tau^+\tau^-$  QEL sample with  $m_{\text{DM}} = 5 \text{ GeV}$  (blue) and the atmospheric background (red).

### 2116 7.6.2 Single proton QEL events

2117 Now, one can try to explore the low energy tail of the neutrino energy distributions. This  
 2118 regime is dominated by the QEL interactions, i.e. events of the type  $\nu_\mu + n \rightarrow \mu^- + p$ .  
 2119 In this case, as the typical energies are  $E_\nu \lesssim 1 \text{ GeV}$ , the momentum transfer to the  
 2120 remnant nucleus is sizeable. Therefore, I can not make the approximation I did before  
 2121 and assume that the momentum of the muon and the proton will give an adequate  
 2122 estimation of the reconstructed neutrino energy.

2123 In any case, as before, I can take the direction of the incoming neutrino as known.  
 2124 That way, one can estimate the energy of the neutrino as:

$$E_\nu^{reco} = E_\mu + E_p + m_{^{39}\text{Ar}} - m_{^{40}\text{Ar}}, \quad (7.33)$$

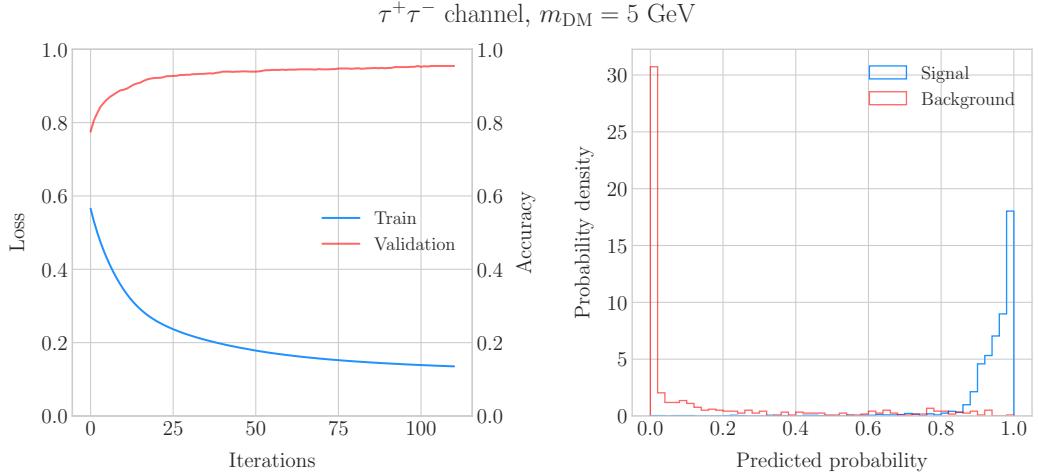
2125 and using momentum conservation I can write the momentum of the remnant nucleus  
 2126 as:

$$\vec{p}_N = \hat{p}_\nu (E_\mu + E_p + m_{^{39}\text{Ar}} - m_{^{40}\text{Ar}}) - \vec{p}_\mu - \vec{p}_p. \quad (7.34)$$

2127 As in the previous case, I need to drop the events where the muon or the proton fall  
 2128 below the kinetic energy detection threshold [42]. Also, I again apply a smearing to the  
 2129 momenta of the particles, a 1% for muons and 5% for protons.

2130 Having done that, one can compute the following angular variables for our selected

## 7.6. High energy DM neutrino signals



**Figure 7.15:** 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  $\tau^+\tau^-$  QEL signal with  $m_{\text{DM}} = 5 \text{ GeV}$  (blue) and the atmospheric background (red).

2131 events:

$$\cos \theta_\mu = \hat{p}_\nu \cdot \hat{p}_\mu, \quad (7.35)$$

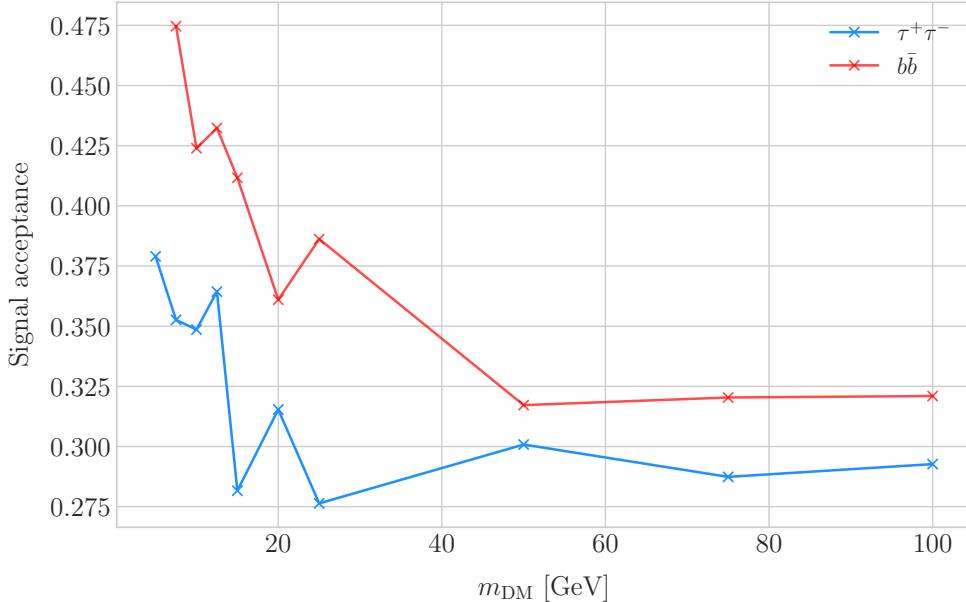
$$\cos \theta_p = \hat{p}_\nu \cdot \hat{p}_p, \quad (7.36)$$

$$\cos \theta_N = \hat{p}_\nu \cdot \hat{p}_N. \quad (7.37)$$

2132 Fig. 7.14 shows the distributions of these angular variables for the  $\tau^+\tau^-$  QEL  
 2133 sample with  $m_{\text{DM}} = 5 \text{ GeV}$  (blue) and the atmospheric background (red). Again, for  
 2134 the atmospheric events I used a random solar position as the ansatz for the incoming  
 2135 neutrino direction. Notice that now, opposed to the DIS case where the signal had very  
 2136 sharp distributions for the variables considered, the shapes of the angular distributions  
 2137 for signal and background are not that much different.

2138 This effectively means that the usual approach of applying simple angular cuts would  
 2139 not work as well as in the previous situation. Therefore, as a possible solution, I tried to  
 2140 use a multilayer perceptron (MLP) classifier to separate between signal and background  
 2141 events. Thus, the power of the hypothesis test will serve as an estimate of the signal

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.16:** Signal efficiencies for the  $\tau^+\tau^-$  (blue line) and  $b\bar{b}$  (red line) single proton QEL samples as functions of the DM mass,  $m_{\text{DM}}$ , 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%.

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 our events into training, validation and test samples. The input variables for the classifier were the reconstructed neutrino energy from Eq. (7.33) and the angular variables defined in Eqs. (7.35 - 7.37). I used the MLP classifier implemented in `scikit-learn` [87], 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  $\tau^+\tau^-$  QEL signal with  $m_{\text{DM}} = 5$  GeV is shown in Fig. 7.15. 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.

## 7.6. High energy DM neutrino signals

2156 The training stops either when the maximum number of iterations is reached (1000 in  
2157 this case) or when the accuracy for the validation sample reaches a certain tolerance  
2158 (I chose  $10^{-4}$  as our tolerance). On the right panel I have the distributions for the  
2159 predicted probability by the model, separated in true signal (blue) and background  
2160 (red) events, for the test sample. One can see that both populations are well separated,  
2161 obtaining a power of 44.97% and a size of 0.17% when I require a predicted probability  
2162 greater than 0.97.

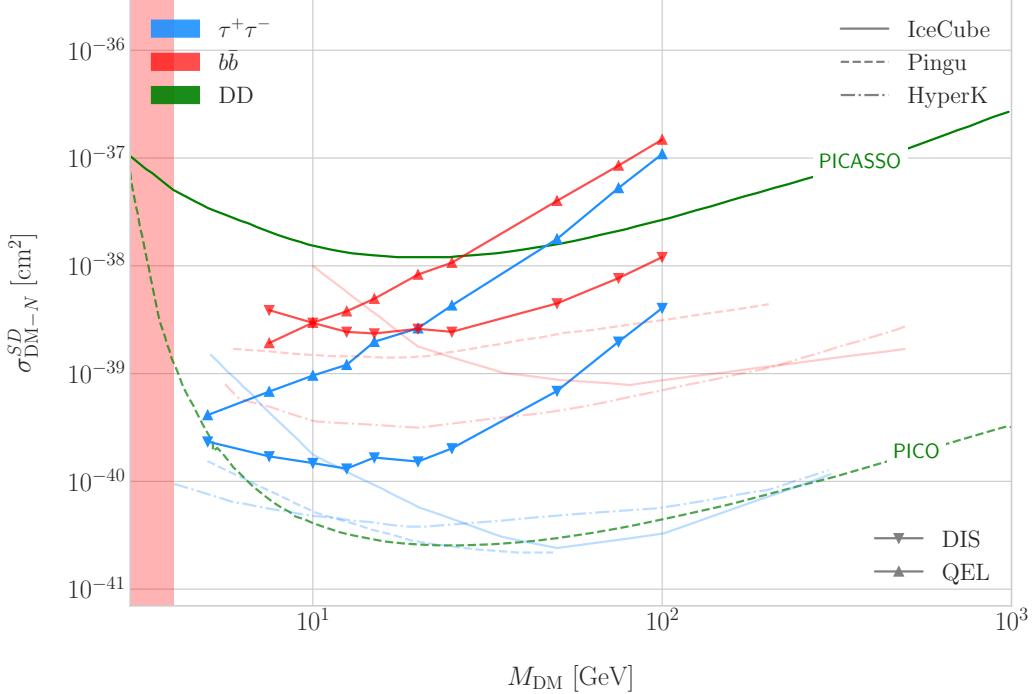
2163 Applying this criteria for each sample, I obtain the mean signal efficiencies shown in  
2164 Fig. 7.16. Notice that the efficiencies for the channel  $\tau^+\tau^-$  (blue line) are consistently  
2165 lower than the ones for the  $b\bar{b}$  channel (red line). This can be due to the fact that, for  
2166 each DM mass point, the neutrino spectrum coming from the  $b\bar{b}$  annihilation channel is  
2167 centered at lower energies when compared to the  $\tau^+\tau^-$  spectrum. This directly translates  
2168 into more low energy neutrinos undergoing QEL interactions, which give signals that  
2169 can be easily separated from the atmospheric background. This explanation also help us  
2170 understand why in both cases the signal acceptance drops when the DM mass increases.  
2171 In all cases, the background rejection took values between 99.8% to 99.9%. I will assume  
2172 a 99.8% background rejection value in all cases to keep our estimation conservative.

### 2173 7.6.3 Results

2174 In order to estimate the DM-nucleon cross section sensitivities in the present case I need  
2175 again to compute the expected number of background events. As I am now separating  
2176 events by interaction type Eq. (7.25) does not hold anymore, as in that case I integrated  
2177 over the total neutrino-argon cross section. In this instance, the expected background  
2178 events for DIS events is approximately given by:

$$N_B^{DIS} \simeq \eta_B^{DIS} \times (4.655 \times 10^3) \times \left( \frac{\text{exposure}}{400 \text{ kT yr}} \right), \quad (7.38)$$

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.17:** Projected 90% confidence level upper limit for DUNE (400 kT yr) on the spin-dependent DM-nucleon scattering cross section as a function of  $m_{\text{DM}}$ , for the annihilation channels  $\tau^+\tau^-$  (blue) and  $b\bar{b}$  (red) separated by interaction type (up triangles denote DIS interactions whereas down triangles represent QEL interactions). I also show the previous limits from IceCube [9] (solid lines) and the projected sensitivities for Pingu [10] (dashed lines) and Hyper-Kamiokande [11] (dash-dotted lines), as well as the direct detection limits from PICASSO [12] (solid green line) and PICO-60 C<sub>3</sub>F<sub>8</sub> [13] (dashed green line).

2179 whereas for QEL events we have:

$$N_B^{QEL} \simeq \eta_B^{QEL} \times (2.248 \times 10^4) \times \left( \frac{\text{exposure}}{400 \text{ kT yr}} \right). \quad (7.39)$$

2180 Now, using these together with Eqs. (7.26) and (7.27) one can obtain the 90% C.L.  
 2181 upper limit on the total annihilation rate at equilibrium for both kind of events. Then,  
 2182 applying the computed DM-nucleons capture rates I can translate these into limits on  
 2183 the DM-nucleon cross section by means of Eqs. (7.2), (7.5) and (7.6).

2184 Fig. 7.17 shows the obtained limits on the SD DM-nucleon cross section for DUNE,  
 2185 using the DIS (up triangles) and QEL (down triangles) events both for the  $\tau^+\tau^-$  (blue)  
 2186 and the  $b\bar{b}$  (red) samples, for an exposure of 400 kT yr. I also include the corresponding

## 7.7. Example: Leptophilic Dark Matter

2187 current limits from IceCube [9] (solid lines), as well as the projected sensitivities of Pingu  
2188 [10] (dashed lines) and Hyper-Kamiokande [11] (dash-dotted lines). For comparison, I  
2189 also show the reported direct detection limits from PICASSO [12] (solid green line) and  
2190 PICO-60 C<sub>3</sub>F<sub>8</sub> [13] (dashed green line).

2191 Notice that, for most of the mass range, the limits one can set by using the DIS  
2192 events are stronger than those of the QEL interactions, except for the low mass part  
2193 of both the  $\tau^+\tau^-$  and the  $b\bar{b}$  curves where the QEL events dominate. In general, the  
2194 expected sensitivity of DUNE for DM masses  $\lesssim 25$  GeV surpasses the stronger current  
2195 indirect limits. However, experiments like Hyper-Kamiokande are foreseen to have an  
2196 overall better sensitivity in this kind of searches, as they have a bigger active volume  
2197 and accept a broader energy range.

2198 A pending question is what happens when we add the RES and MEC charged-current  
2199 interaction contributions. In that case it would probably be more convenient to split  
2200 the samples by final state interaction topologies. Also, another necessary improvement  
2201 would be adding a full detector simulation and reconstructions. This will also require  
2202 considering the effect of poorly reconstructed events or final states containing neutral  
2203 particles such that they mimic the desired topology at the reconstruction level.

## 2204 7.7 Example: Leptophilic Dark Matter

2205 In general, the capture rate of DM particles by the Sun via interactions with electrons is  
2206 several orders of magnitude smaller than the capture via DM-nucleus scattering. Thus,  
2207 it would be sub-leading even when nucleon capture is loop suppressed. As I showed in  
2208 Fig. 7.2, the capture rate via scattering off electrons only surpasses the capture rates  
2209 via DM-nucleons interactions for DM masses  $\lesssim 100 - 500$  MeV.

2210 However, if one considers a model where DM-nucleon interactions are forbidden even  
2211 at loop level, then electron interactions will be the sole contributor to DM capture in  
2212 the Sun. One can describe such scenario where the DM particles couple to leptons but  
2213 not to the quark sector using effective operators.

## Chapter 7. DM searches with neutrinos from the Sun

2214 In general, assuming that the DM particle is a Dirac fermion, the dimension six  
2215 operators describing the interaction between two DM particles and two leptons can be  
2216 written as:

$$\mathcal{L}_{eff} = G \sum_i (\bar{\chi} \Gamma_\chi^i \chi) (\bar{\ell} \Gamma_\ell^i \ell), \quad (7.40)$$

2217 where  $G = 1/\Lambda^2$  is the effective coupling strength,  $\Lambda$  the cut-off of the effective field  
2218 theory and  $\ell$  denotes any lepton. In principle, one should consider all the possible  
2219 Lorentz structures  $\Gamma_f^i$  in order to have a complete set of effective operators.

2220 However, some combinations will induce interactions with nucleons at loop level. As  
2221 we are specifically interested in interactions which forbid any communication with the  
2222 quark sector, I will not consider those [88]. In addition, some of the effective operators  
2223 give rise to velocity-suppressed scattering cross sections between DM particles and  
2224 leptons. I will also neglect those, as the suppression goes with the square of the DM  
2225 halo velocity which in units of the speed of light is  $\sim 10^{-6}$ .

2226 This way, the only Lorentz tensor structure that do not induce interactions with  
2227 quarks at loop level and gives a contribution to the scattering cross section that is not  
2228 velocity suppress is the axial-axial interaction. The effective Lagrangian is then given  
2229 by:

$$\mathcal{L}_{eff} = \frac{c_A^\chi c_A^\ell}{\Lambda^2} (\bar{\chi} \gamma^\mu \gamma^5 \chi) (\bar{\ell} \gamma_\mu \gamma^5 \ell), \quad (7.41)$$

2230 where  $c_A^\chi$  and  $c_A^\ell$  are the couplings for the different species. As the DM coupling appears  
2231 as a common factor for any lepton choice, I will redefine the corresponding coupling  $c_A^\ell$   
2232 to absorb  $c_A^\chi$ . Also, for simplicity, I will assume that the couplings between the DM  
2233 particles and the leptons are flavour independent, i.e. I have just two couplings,  $c_A^e$  for  
2234 charged leptons and  $c_A^\nu$  for neutrinos.

2235 In the case of a scalar DM particle, the lowest order effective interaction with  
2236 leptons happens through a dimension five operator, generating scalar and pseudoscalar  
2237 interactions. However, the former induces interactions with quarks at two loop level  
2238 whereas the latter gives a velocity suppressed scattering cross section.

2239 From the effective Lagrangian in Eq. (7.41) it can be shown that the axial-axial

## 7.7. Example: Leptophilic Dark Matter

2240 contribution to the scattering cross section for the fermionic DM and a charged lepton  
2241 is given by:

$$\sigma_{\text{DM}-e}^{AA} = 3(c_A^e)^2 \frac{m_e^2}{\pi \Lambda^4}. \quad (7.42)$$

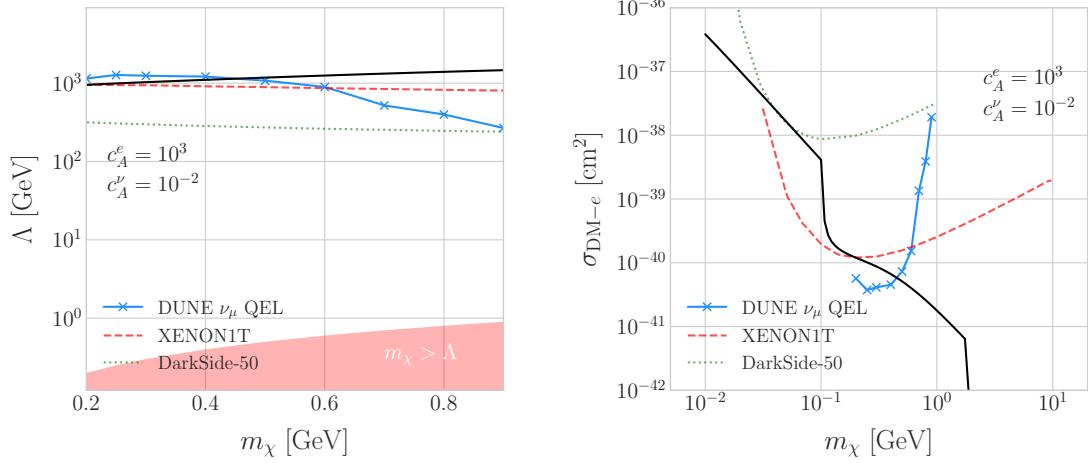
2242 If the DM interacts exclusively with fermions, then the only annihilation channels  
2243 that will give us a measurable neutrino flux coming out of the Sun are  $\tau^+\tau^-$  and  $\nu\bar{\nu}$ . The  
2244 former channel, already explored previously in the more mainstream scenario of the DM  
2245 capture via scattering off nucleons, is open only for  $m_{\text{DM}} > m_\tau \simeq 1776.86 \pm 0.12$  MeV  
2246 [89], a mass region where the solar DM capture by electrons is at least one order of  
2247 magnitude smaller than the capture via interactions with nucleons. On the contrary, the  
2248 latter allows us to explore a region where the capture rate via scattering off electrons  
2249 dominates over the rest.

2250 One downside of focusing in such low mass range is that it falls below the usual  
2251 limit of  $m_{\text{evap}} \sim 4$  GeV usually explored in the literature. The pretext to explore this  
2252 region is the result discussed previously reported in Ref. [4], where DM evaporation in  
2253 the Sun for the case of capture via electron scattering could be negligible for masses  
2254 as low as  $m_{\text{evap}} \sim 200$  MeV. This result is quite sensitive to the high velocity tail of  
2255 the DM velocity distribution in equilibrium inside the Sun, and therefore full numerical  
2256 simulations would be needed to assess the impact of this effect. However, this falls out of  
2257 the scope of our work.

2258 In this case, as I have a specific realisation of the interaction between the DM  
2259 and leptons, one can estimate the relic density of our DM for different values of the  
2260 couplings and the effective field theory scale  $\Lambda$ . The first step to do so is compute the  
2261 self-annihilation cross section. Because I consider cold relics, at the freeze-out time our  
2262 DM particles were non-relativistic and so one can expand the annihilation cross section  
2263 in terms of the relative velocity  $v$  between two annihilating DM particles as [90]:

$$\sigma_{\text{ann}}^{AA}|v| \approx \frac{1}{2\pi\Lambda^4} \sum_\ell \left(c_A^\ell\right)^2 m_\chi^2 \sqrt{1 - \frac{m_\ell^2}{m_\chi^2} \left[ \frac{m_\ell^2}{m_\chi^2} + \frac{1}{12} \left(2 - \frac{m_\ell^2}{m_\chi^2}\right) v^2 \right]}, \quad (7.43)$$

## Chapter 7. DM searches with neutrinos from the Sun



**Figure 7.18:** Left panel: Projected 90% confidence level sensitivity of DUNE (400 kT yr) to the scale  $\Lambda$  of an EFT containing only leptophilic DM axial-axial interactions (blue line). Right panel: In both cases the corresponding limits from DarkSide-50 [14] (dotted green line) and XENON1T [15] (dashed red line) are also shown, together with the configurations for which the correct relic density is achieved (black line), all for the coupling values  $c_A^e = 10^3$  and  $c_A^\nu = 10^{-2}$ .

where the sum includes all the possible lepton final states with mass  $m_\ell$ .  
 Solving the Boltzmann equation for the evolution of the DM density gives as a solution a relic density of:

$$\Omega_\chi h^2 \approx \frac{(1.04 \times 10^9) x_F}{M_{Pl} \sqrt{g_*} (a + 3b/x_F)}, \quad (7.44)$$

where  $x_F = m_\chi/T_F$  being  $T_F$  the freeze-out temperature,  $g_*$  the number of relativistic degrees of freedom at freeze-out and  $a$  and  $b$  the terms in the annihilation cross section expansion  $\sigma_{ann}|v| \approx a + bv^2 + \mathcal{O}(v^4)$ . Using the current best fit for the relic DM density  $\Omega_\chi h^2 = 0.1198 \pm 0.0012$  [91] one can use these relations to compute the required effective theory scale  $\Lambda$  at which the correct density is achieved for any combinations of  $m_\chi$  and  $c_A^\ell$ .

As discussed before, in the low DM mass region QEL interactions dominate. Moreover, if I focus on direct annihilation to neutrinos, the energy of the muon neutrino flux is known as it must be equal to the mass of the DM particle,  $E_\nu = m_\chi$ . That way, now I do not need to use Eq. (7.33) in order to estimate the momentum transfer to the

## 7.7. Example: Leptophilic Dark Matter

2277 remnant nucleus, I can simply take:

$$\vec{p}_N = \hat{p}_\nu m_\chi - \vec{p}_\mu - \vec{p}_p. \quad (7.45)$$

2278 To estimate the signal efficiency and background rejection for this case I used again  
2279 the MLP classifier from `scikit-learn`, using the same specifications as before. The  
2280 only difference now is that I add also the reconstructed neutrino energy as one of the  
2281 features to train the classifier with, because the characteristic monoenergetic flux for  
2282 each  $m_\chi$  value will help to distinguish between signal and background events.

2283 In this case, for masses below  $\sim 500$  MeV I obtain a signal efficiency close to unity  
2284 while keeping a background rejection of 99.9%. For bigger values of the mass, the signal  
2285 efficiency drops significantly if I require to keep the background acceptance under 0.01%.  
2286 However, because this kind of search is dominated by the background, sacrificing the  
2287 signal acceptance to keep the background rejection to a minimum enhances the reach  
2288 of the analysis. This way, for DM masses of the order of  $m_\chi \sim 1$  GeV I end up with  
2289 efficiencies as low as 1%.

2290 Now, estimating the number of background events using Eq. (7.39) one can go on  
2291 and apply Eqs. (7.26) and (7.27) together with Eq. (7.42) to derive the sensitivity of  
2292 DUNE to this kind of model. Fig. 7.18 (left panel) shows the potential reach of DUNE  
2293 to constrain the EFT scale  $\Lambda$  this model containing only leptophilic DM axial-axial  
2294 interactions (blue line), for a choice of couplings  $c_A^e = 10^3$  and  $c_A^\nu = 10^{-2}$ . I also included  
2295 the current limits on the DM-electron scattering cross section from DarkSide-50 [14]  
2296 (dotted green line) and XENON1T [15] (dashed red line), reworked with Eq. (7.42) to  
2297 show their implications for the EFT scale. The values of  $\Lambda$  for which the correct DM relic  
2298 density value is achieved for each mass are also shown (black line). This tells us that,  
2299 for that specific choice of couplings, DUNE would be sensitive to DM configurations  
2300 allowed by the relic density constraint up to a mass of  $m_\chi \sim 400$  MeV.

2301 In Fig. 7.18 (right panel) I show the same upper limits but for the DM-electron  
2302 scattering cross section. From this view one can see that DUNE would be able to

## Chapter 7. DM searches with neutrinos from the Sun

2303 offer complementary information to the low energy DM-electron interaction searches  
2304 performed by direct detection experiments, in a slightly higher mass range.

2305 With the present example, although it focuses on a very specific realisation of the DM  
2306 interactions, I show the potential of DUNE to constrain exotic DM scenarios. Thanks  
2307 to its low backgrounds and superb angular resolution DUNE will be able to help with  
2308 the systematic searches for dark sectors physics.

2309 Chapter 8

2310 Particle ID in GArSoft

2311 ND-GAr is a magnetised, high-pressure gaseous argon TPC (HPgTPC), surrounded by  
2312 an electromagnetic calorimeter (ECal) and a muon detector (commonly refer to as  $\mu$ ID).  
2313 A detailed discussion on the requirements, design, performance and physics of ND-GAr  
2314 can be found in the DUNE ND CDR [48] and the ND-GAr whitepaper (cite).

2315 In DUNE Phase II ND-GAr will fulfill the role of TMS, measuring the momentum  
2316 and sign of the charged particles exiting ND-LAr. Additionally, it will be able to measure  
2317 neutrino interactions inside the HPgTPC, achieving lower energy thresholds than those  
2318 of the ND and FD LArTPCs. By doing so ND-GAr will allow to constrain the relevant  
2319 systematic uncertainties for the LBL analysis even further.

2320 The goal of the present chapter is to review the requirements that the physics program  
2321 of DUNE impose on ND-GAr, present the current status of its design and describe the  
2322 GArSoft package, its simulation and reconstruction software.

2323 As decided during the DUNE Phase II workshop in June 2023 [reference], we want  
2324 to build ND-GAr physics case by showing:

- 2325 • That ND-GAr can constrain systematic uncertainties that ND-LAr might miss.
- 2326 • The impact on the neutrino oscillation results if such systematic uncertainties are  
2327 missed.
- 2328 • That ND-GAr is necessary to reach DUNE's main physics goals.

## Chapter 8. Particle ID in GArSoft

2329 This way, the design of ND-GAr will be physics driven.

2330 In order to study the effects of final state interactions (FSI) in CC interactions,  
2331 ND-GAr should be able to measure the spectrum of protons and charged pions at low  
2332 energies. ND-GAr also needs to be able to measure the pion multiplicity, specially for  
2333 energies above 100 MeV as at these energies the pions shower in the LAr, to inform the  
2334 pion mass correction in the ND and FD LArTPCs.

2335 In order to correctly identify electrons, muons, pions, kaons and protons ND-GAr  
2336 can use a combination of:  $dE/dx$  measurements in the HPgTPC,  $E_{ECAL}/p$  using the  
2337 ECAL total energy and the momentum obtained from magnetic spectroscopy in the  
2338 HPgTPC and penetration information through the ECAL and muon tagger.

### 2339 8.1 $dE/dx$ measurement in the TPC

2340 Among the parameters extracted from the track fitting, ionisation is particularly useful  
2341 for particle identification, as it is a function of the particle velocity. Although for the  
2342 case of relativistic particles this dependence is not very strong, measuring the track on  
2343 a large number of points may allow us to estimate the amount of ionisation accuratel.  
2344 This, paired with a measurement of the momentum, may allow us to identify the particle  
2345 type.

2346 The first calculation of the energy loss per unit length of relativistic particles using  
2347 a quantum-mechanical treatment is due to Bethe [?]. Using this approach, the mean  
2348 ionisation rate of a charged particle traveling through a material medium is (using  
2349 natural units  $G = \hbar = c = 1$ ):

$$\left\langle \frac{dE}{dx} \right\rangle = \frac{4\pi Ne^4}{m_e \beta^2} z^2 \left( \log \frac{2m_e \beta^2 \gamma^2}{I} - \beta^2 \right), \quad (8.1)$$

2350 where  $N$  is the number density of electrons in the medium,  $e$  the elementary charge,  $m_e$   
2351 is the electron mass,  $z$  the charge of the particle in units of  $e$ ,  $\beta$  is the velocity of the  
2352 particle,  $\gamma = (1 - \beta^2)^{-1}$  and  $I$  denotes the effective ionisation potential averaged over  
2353 all electrons. This relation is known as the Bethe-Bloch formula.

## 8.1. $dE/dx$ measurement in the TPC

From Eq. (8.1) one can see that the ionisation loss does not depend explicitly on the mass of the charged particle, that for non-relativistic velocities it falls as  $\beta^{-2}$ , then goes through a minimum and increases as the logarithm of  $\gamma$ . This behaviour at high velocities is commonly known as the relativistic rise. The physical origin of this effect is partly due to the fact that the transverse electromagnetic field of the particle is proportional to  $\gamma$ , therefore as it increases so does the cross section.

It was later understood that the relativistic rise could not grow indefinitely with  $\gamma$ . A way to add this feature in the Bethe-Bloch formula is by introducing the so-called density effect term. It accounts for the polarisation effect of the atoms in the medium, which effectively shield the electromagnetic field of the charged particle halting any further increase of the energy loss [?]. Denoting the correction as  $\delta(\beta)$ , one can rewrite Eq. (8.1) as:

$$\left\langle \frac{dE}{dx} \right\rangle = \frac{4\pi Ne^4}{m_e \beta^2} z^2 \left( \log \frac{2m_e \beta^2 \gamma^2}{I} - \beta^2 - \frac{\delta(\beta)}{2} \right). \quad (8.2)$$

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

Another standard method to compute the amount of ionisation a charged particle produces is the so-called photo-absorption ionisation (PAI) model proposed by Allison and Cobb [?]. Within their approach, the mean ionisation is evaluated using a semiclassical calculation in which one characterises the continuum material medium by means of a complex dielectric constant  $\epsilon(k, \omega)$ . However, in order to model the dielectric constant they rely on the quantum-mechanical picture of photon absorption and collision. Therefore, in the PAI model the computation of the ionisation loss involves a numerical integration of the measured photo-absorption cross-section for the relevant material.

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

## Chapter 8. Particle ID in GArSoft

2381 It happens that neither the Bethe-Bloch theory nor the PAI model from Allison and  
2382 Cobb offer a close mathematical form for the ionisation curve. This is the reason why a  
2383 full parametrisation of the ionisation curves can be useful. A parametrisation originally  
2384 proposed for the ALEPH TPC [?] and later used by the ALICE TPC [?] group that  
2385 manages to capture the features of the ionisation energy loss is:

$$f(\beta\gamma) = \frac{P_1}{\beta^{P_4}} \left( P_2 - \beta^{P_4} - \log \left[ P_3 + \frac{1}{(\beta\gamma)^{P_5}} \right] \right), \quad (8.3)$$

2386 where  $P_i$  are five free parameters. Hereafter, we will refer to Eq. (8.3) as the ALEPH  
2387  $dE/dx$  parametrisation.

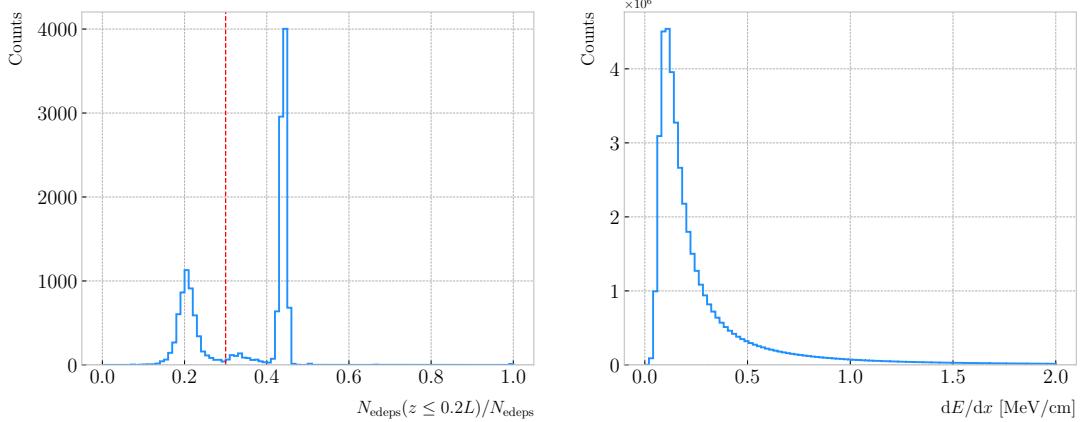
### 2388 8.1.1 Energy calibration

2389 In order to obtain the amount of energy loss by a charged particle due to ionisation  
2390 in our TPC we need to determine the conversion between the charge deposited in our  
2391 readout planes and the actual energy depositions. This procedure is known as energy  
2392 calibration.

2393 In a general, the first step of the calibration involves a non-uniformity correction,  
2394 to make sure that the detector response is uniform throughout the TPC. These are  
2395 typically divided into three categories, non-uniformities in the transverse  $YZ$  plane,  
2396 non-uniformities along the drift direction  $X$  and variations of the detector response  
2397 over time (would not apply to us as the detector is not built yet). These would correct  
2398 for effects such as electron diffusion and attenuation, space charge effects or channel  
2399 misconfiguration. However, because at the moment I am only interested in making sure  
2400 we recover a sensible result from our simulation, I will not apply uniformity corrections  
2401 to our charge deposits.

2402 Other effects, like electron-ion recombination or ADC saturation, lead to a non-linear  
2403 relation between the observed charge and the deposited energy in the detector, with the  
2404 observed readout charge saturating at high ionisation energies. In this case, because we  
2405 are dealing with gaseous argon and therefore recombination is not as important as in

## 8.1. $dE/dx$ measurement in the TPC



**Figure 8.1:** 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.

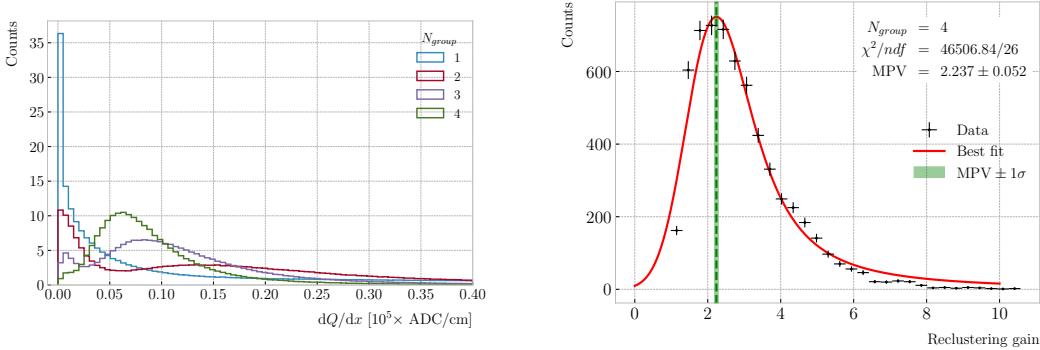
2406 liquid, we do not simulate recombination effects in the TPC. Even so, the simulation of  
 2407 the electronic response will still introduce charge saturation, and one needs to correct  
 2408 for it in order to obtain the exact amount of energy loss due to ionisation.

2409 By default, the track fitting algorithm in GArSoft provides a `TrackIonization`  
 2410 object associated to each reconstructed track. It contains two collections of charge  
 2411 deposits, one for each fitting direction, consisting on pairs of charge values ( $dQ$ , in ADC)  
 2412 and step sizes ( $dx$ , in cm).

2413 In order to estimate the ionisation loss in the ND-GAr TPC, I have used an MC  
 2414 sample consisting of single, isotropic protons propagating in the TPC. The starting points  
 2415 of the protons were sampled inside a  $50 \times 50 \times 25$  cm box centered at  $(100, -150, 1250)$ ,  
 2416 and their momenta are uniformly distributed in the range  $0.25 - 1.75$  GeV. I ran the  
 2417 simulated sample through GArSoft's default detector simulation and reconstruction, and  
 2418 then a custom analyser module that extracts the ionisation data together with other  
 2419 reconstructed track information from the Kalman fit.

2420 For studying the energy loss of the protons I select the reconstructed tracks that  
 2421 range out (i.e. slow down to rest) inside the TPC. A characteristic feature of the energy  
 2422 loss profile of any stopping ionising particle is the so-called Bragg peak, a pronounced

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**Figure 8.2:** 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.

peak that occurs immediately before the particle comes to rest. From Eq. (8.1) we can see that this behaviour is expected, as the energy loss for non-relativistic particles is inversely proportional to  $\beta^2$ . In data, a way of identifying the Bragg peak, and thus select the stopping particles, is checking the number of energy deposits towards the end of the track. In this case, I count the fraction of the Geant4 simulated energy deposits with a residual range value (the distance from a given energy deposit to the last deposit in the track trajectory) less than a 20% of the corresponding track length<sup>1</sup>. The distribution of this fraction of energy deposits for our proton sample is shown in Fig. 8.1 (left panel). We can clearly see two well separated peaks in this distribution, one centered at 0.2 and another, narrower, one centered at a higher value. The first one corresponds to non-stopping protons, as in that case the number of energy deposits towards the end of the track is uniformly distributed due to the absence of the Bragg peak. In that way, I apply a cut in this distribution, requiring that at least 30% of the simulated energy deposits sit in the last 20% of the tracks, to ensure that the Bragg peak is present.

Figure 8.1 (right panel) shows the distribution of the energy loss per unit length for the Geant4 simulated energy deposits of the selected stopping protons. We can see that

<sup>1</sup>As 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.

## 8.1. $dE/dx$ measurement in the TPC

it follows the expected shape of a Landau distribution, which describes the fluctuations of the ionisation energy losses [?]. 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 8.2 (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.

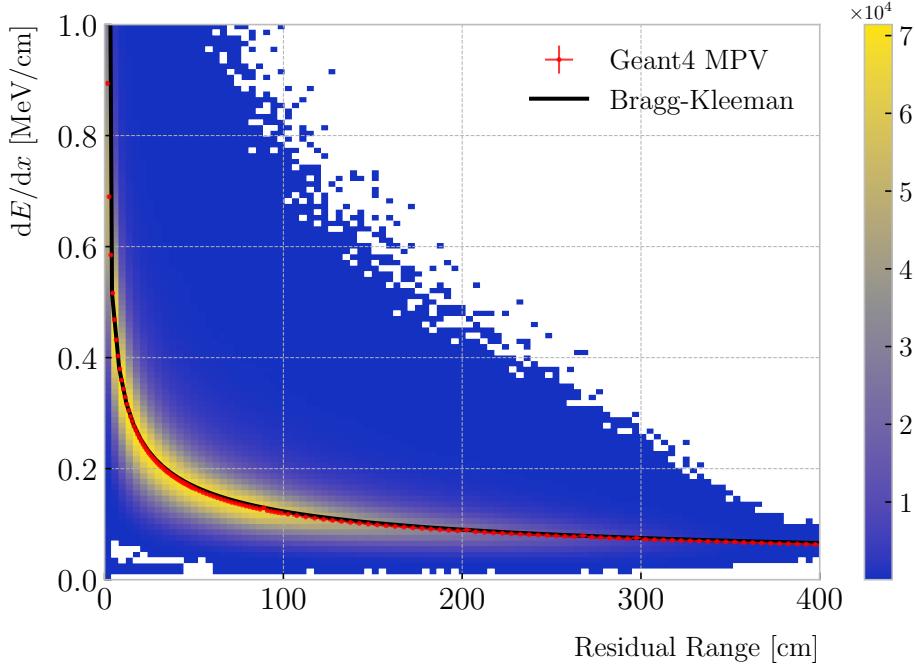
An extra factor I need to account for, when reclustering is applied, is how the overall  $dQ/dx$  per track changes. To do so, we can look at the ratio between the median  $dQ/dx$  after and before the reclustering. Figure 8.2 (right panel) shows the median enhancement in  $dQ/dx$  per track for the stopping proton sample in the case  $N_{group} = 4$ . Fitting a Landau distribution convolved with a Gaussian<sup>2</sup>, I estimate the most probable value of this ratio to be  $G_{group} = 2.24 \pm 0.05$ .

At this point, I am left with determining the conversion between the charge deposits per unit length  $dQ/dx$  and the energy deposits per unit length  $dE/dx$ . To this end, we need a way of comparing the two. I can use the residual range  $z$  to get a prediction of

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<sup>2</sup>In 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.

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**Figure 8.3:** 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. (8.4).

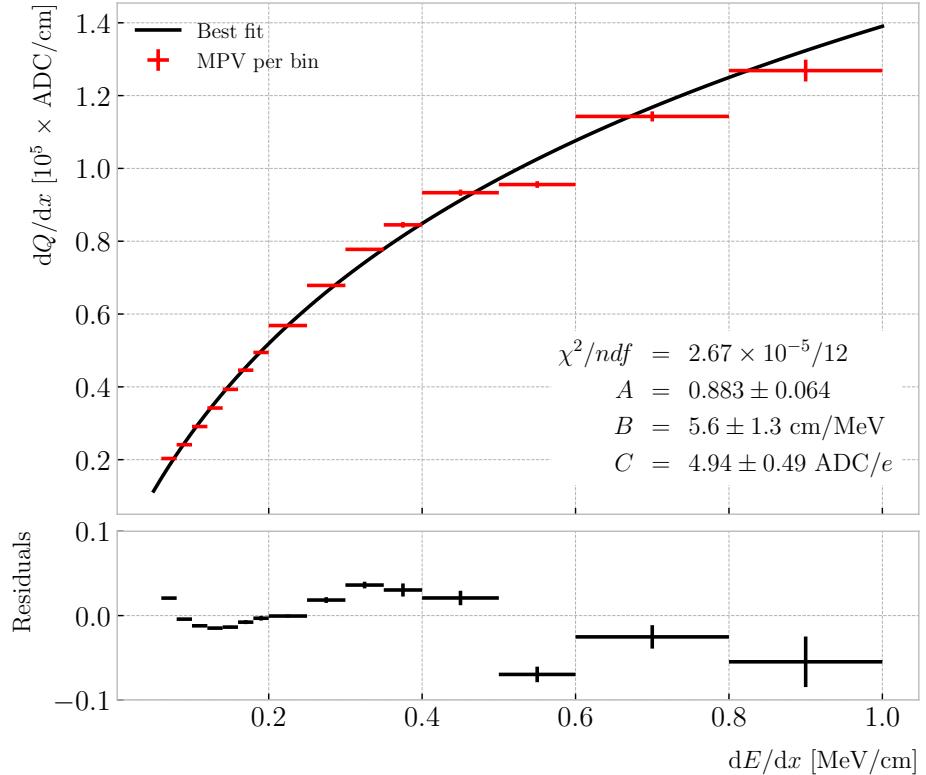
2467 the most probable  $dE/dx$  by using the following empirical parametrisation [?]:

$$\frac{dE}{dx}(z) = \frac{z^{\frac{1}{p}-1}}{p\Lambda^{\frac{1}{p}}}, \quad (8.4)$$

2468 which is quoted in the literature as the Bragg-Kleeman formula. In order to obtain the  
 2469  $p$  and  $\Lambda$  parameters I perform a fit using the energy losses and the residual ranges given  
 2470 by the Geant4 stage of our proton sample.

2471 Within our simulation, the residual range is sampled with a maximum size of  
 2472 5 mm. Therefore, to perform the fit to the Bragg-Kleeman formula, we can use a  
 2473 fine-grained residual range binning. For each of the residual range bins I extract the  
 2474  $dE/dx$  distribution and fit it to a LanGauss distribution, to obtain the value of the  
 2475 most probable  $dE/dx$  in the bin together with a statistical uncertainty. I then fit Eq.  
 2476 (8.4) to these most probable values and the centres of the residual range bins. This

## 8.1. $dE/dx$ measurement in the TPC



**Figure 8.4:** 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. (8.5).

procedure is depicted in Fig. 8.3, 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 Bragg-Kleeman relation to those values (black line). The best fit is obtained for the parameter values  $p = 1.8192 \pm 0.0005$  and  $\Lambda = 0.3497 \pm 0.0008 \text{ cm/MeV}^p$ <sup>3</sup>.

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

In order to parametrise the charge saturation, we can use the following logarithmic

<sup>3</sup>These strange units for  $\Lambda$  come from dimensional analysis, just to keep the Bragg-Kleeman formula (8.4) consistent.

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2486 function inspired by the modified box model for recombination:

$$\frac{dE}{dx} = \frac{e^{\frac{dQ}{dx}B\frac{W_{ion}}{G_{group}C}} - A}{B}, \quad (8.5)$$

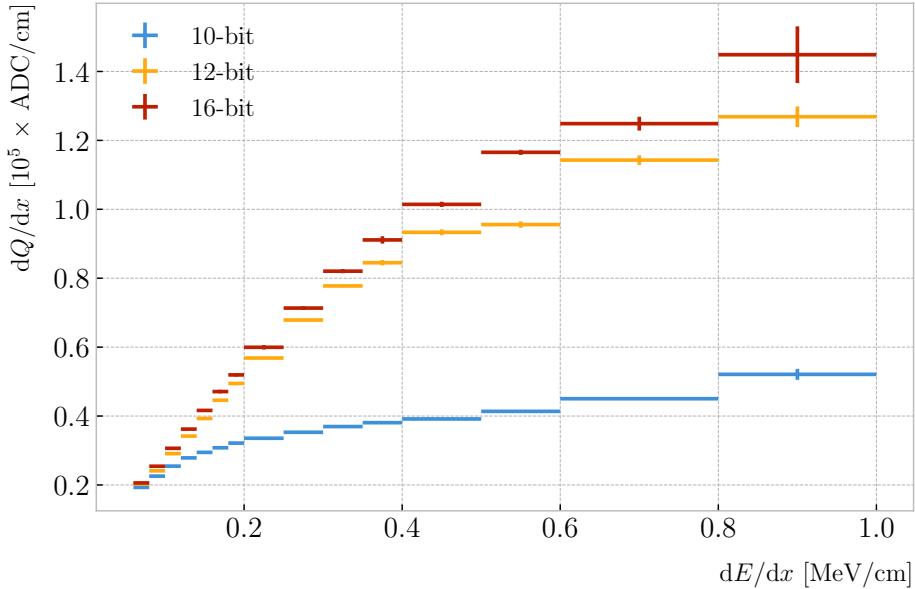
2487 where  $A$  and  $B$  are the calibration parameters we need to determine,  $W_{ion}$  is the average  
2488 energy to produce an electron-ion pair,  $G_{group}$  is the gain from the reclustering discussed  
2489 above and  $C$  is the calibration constant to convert number of electrons to ADC counts,  
2490 commonly refer to as gain (also to be obtained in the fit). In this case, I use a value for the  
2491 electron-ion production energy of  $W_{ion} = 26.4$  eV [?]. This value, used in our simulation  
2492 as well, was measured for gaseous argon in normal conditions, and therefore should  
2493 be checked in the future to describe correctly the high-pressure argon-CH<sub>4</sub> mixture of  
2494 ND-GAr.

2495 For the calibration fit I follow a procedure similar to the previous one for Eq. (8.4).  
2496 Binning the  $dE/dx$  range, I fit a LanGauss distribution to the corresponding  $dQ/dx$   
2497 distribution to obtain the most probable value. The resulting data points (red bars) are  
2498 shown in Fig. 8.4 (top panel), the horizontal error bars depict the width of the  $dE/dx$   
2499 bin whereas the vertical bars represent the error associated to the most probable value  
2500 estimation. A fit to the logarithmic function in Eq. (8.5) is also shown (black line).  
2501 For this I weighted the data points using the inverse of their relative error, obtaining  
2502 a reduced chi-square value of  $\chi^2/ndf = 2.22 \times 10^{-6}$ . The best fit parameters I found  
2503 from this fit are  $A = 0.883 \pm 0.064$ ,  $B = 5.6 \pm 1.3$  cm/MeV and  $C = 4.94 \pm 0.49$  ADC/e.  
2504 Figure 8.4 (bottom panel) shows the residuals between the data points and the fit.

2505 The value for the gain I obtained from the fit is in reasonable agreement with our  
2506 expectation. This value is set in GArSoft to 5 ADC/e by default.

2507 One interesting thing to check is what induces this non-linear relation between charge  
2508 and energy. The only effects that modify the amount of electrons reaching the readout  
2509 planes in the simulation are the transverse diffusion and the finite electron lifetime.  
2510 Once the electrons reach the readout chambers, the pad response functions are applied,  
2511 together with an electrons-to-ADC conversion and the ADC saturation limit.

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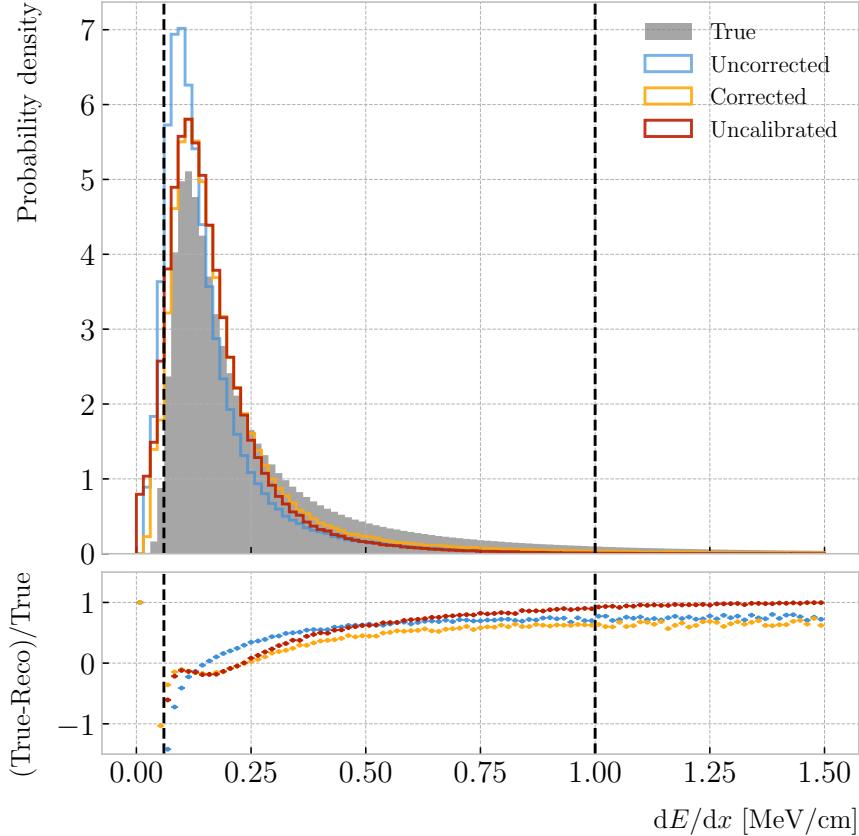
**Figure 8.5:** Fitted most probable  $dQ/dx$  values for each  $dE/dx$  bin for three different ADC bit limits, 10 (blue points), 12 (default, yellow points) and 16-bit (red points).

**Table 8.1:** Calibration parameters obtained from the fit of the ND-GAr simulated stopping proton sample to the calibration function from Eq. (8.5). The fits were performed for the 10, 12, and 16-bit ADC limits.

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

2512 By default, GArSot applies a 12-bit ADC limit, which can be changed in the  
 2513 simulation configuration. However, it can only be increased up to 16-bit, as we represent  
 2514 the ADC collection as a `std::vector<short>`. This way, I tried to change the saturation  
 2515 parameter to see how it affects the relation between reconstructed charge and energy.  
 2516 Figure 8.5 shows a comparison between the most probable  $dQ/dx$  for 10, 12 and 16-  
 2517 bit ADC limits. As expected, the lower the limit is the sooner the charge saturates.  
 2518 For higher ADC limits the relation between energy and charge remains linear up to  
 2519 higher  $dE/dx$  values, but even for the 16-bit limit the saturation is noticeable for values  
 2520  $\gtrsim 0.5$  MeV/cm.

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**Figure 8.6:** 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.

Table 8.1 shows the results of fitting the samples with 10 and 16-bits ADC limits to the calibration function from Eq. (8.5), using the weights based on their relative error 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 8.6 (top panel) shows the true (solid grey) and reconstructed (blue, labeled as uncorrected) distributions

## 8.1. $dE/dx$ measurement in the TPC

2530 together. The dashed vertical lines indicate the region of validity of the calibration fit, i.e.  
2531 the left and right edges of the first and last  $dE/dx$  bin respectively. Notice that these  
2532 histograms are area-normalised, as the total number of true energy deposits is much  
2533 higher than the number of reconstructed charge deposits. This is due to a combination  
2534 of effects, like the finite spatial resolution of the detector, the hit clustering used in the  
2535 track fitting and the reclustering we have applied here.

2536 The two distributions are significantly different. That can be seen clearly when  
2537 looking at the fractional residuals, shown in Fig. 8.6 (bottom panel). In particular,  
2538 the position of the peak is off, which could bias the mean energy loss predictions. It  
2539 seems like the difference between these may be due to an overall scaling factor. One  
2540 possibility is to scale the most probable value of the reconstructed distribution to  
2541 the most probable value predicted by Geant4. I do this by fitting both distributions  
2542 using a LanGauss function, obtaining  $dE/dx_{MPV, true} = 0.1145 \pm 0.0005$  MeV/cm and  
2543  $dE/dx_{MPV, reco} = 0.0928 \pm 0.0005$  MeV/cm for the true and reconstructed most probable  
2544 values respectively. These can be translated into an scaling factor  $S = 0.579 \pm 0.006$ .

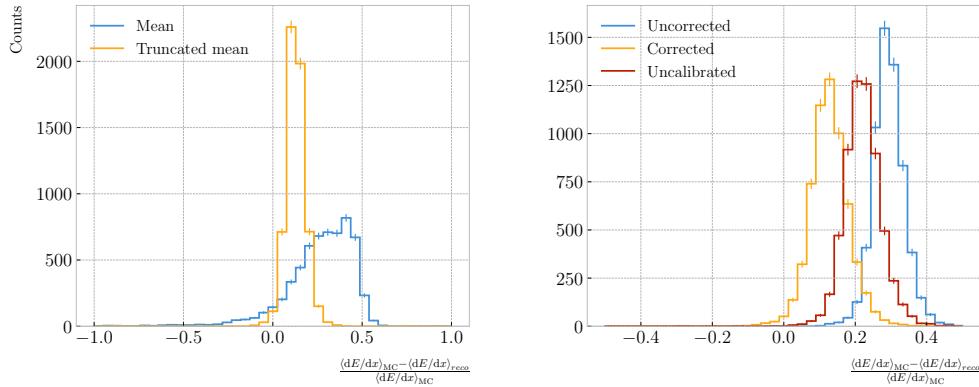
2545 The result of applying the scaling correction can be seen in Fig. 8.6 (top panel).  
2546 The corrected  $dE/dx$  distribution (yellow, labeled as corrected) peaks around the same  
2547 value the true distribution does, as expected. Moreover, the high energy region is also  
2548 slightly better described. For low ionisations, below the lower limit of the calibration  
2549 fit, the differences between true and reconstructed are still significant. This low energy  
2550 excess may be migration of some events from the peak region. The overall effect of the  
2551 correction can be seen in the fractional residual plot in Fig. 8.6 (bottom panel).

2552 One can also check what happens if instead of applying the logarithmic calibration we  
2553 simply scale the  $dQ/dx$  distribution (post reclustering) to have the same most probable  
2554 value as the true  $dE/dx$  distribution. In this case, following an analogous procedure to the  
2555 one described earlier, I found the scaling factor  $S_{uncalibrated} = 0.414 \pm 0.002$  MeV/ADC<sup>4</sup>.  
2556 The resulting distribution (red, labeled as uncalibrated) is also shown in in Fig. 8.6 (top  
2557 panel). The behaviour of the new distribution is similar to the corrected case at low

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<sup>4</sup>Notice that now the scaling factor is not dimensionless, as it acts more like a conversion factor here.

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**Figure 8.7:** Left panel: fractional residuals between the true and the corrected  $\text{d}E/\text{d}x$  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)  $\text{d}E/\text{d}x$  60% truncated means, for each event in the stopping proton sample.

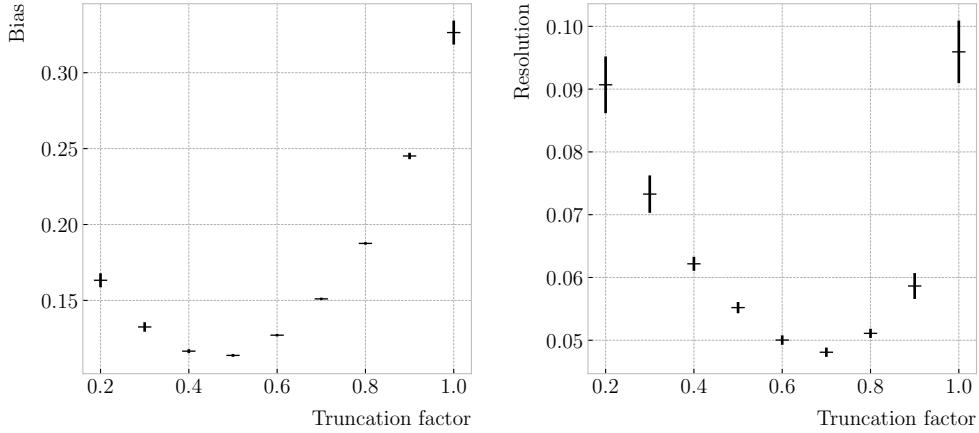
2558 energy losses, around the peak of the true distribution, but it is worse at describing the  
 2559 high energy tail. This is expected, it is in the high ionisation regime where saturation  
 2560 effects apply and therefore calibration is needed.

### 2561 8.1.2 Truncated $\text{d}E/\text{d}x$ mean

2562 Once we have a collection of  $\text{d}E/\text{d}x$  values for each reconstructed track, we can compute  
 2563 the corresponding most probable ionisation loss per unit length of the particle. This  
 2564 is the value predicted by the Bethe-Bloch or the PAI models, and together with a  
 2565 measurement of the momentum it allows for particle identification.

2566 However, estimating the most probable  $\text{d}E/\text{d}x$  value for each reconstructed track  
 2567 is not a trivial task. As mentioned before, the  $\text{d}E/\text{d}x$  distributions follow Landau-like  
 2568 distributions. Therefore, one should perform e.g. a LanGauss fit to correctly estimate  
 2569 the most probable values. Automating this kind of fits is often problematic, as they  
 2570 usually incur in convergence problems. Moreover, the reconstructed  $\text{d}E/\text{d}x$  distributions  
 2571 we obtain tend to have relatively small statistics, which may also produce poor fits. In  
 2572 practice, doing these unsupervised fits may degrade our performance, and a more robust  
 2573 method is preferred.

## 8.1. $dE/dx$ measurement in the TPC



**Figure 8.8:** 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.

2574 A possibility could be taking the mean of the reconstructed  $dE/dx$  distribution for  
 2575 each particle. The problem with this approach is that the high energy Landau tail,  
 2576 combined with our limited statistics, can induce large fluctuations in the computation  
 2577 of the mean. Imagine you have two protons with the same kinetic energy, but due to  
 2578 reconstruction problems in one case you did not get as many charge deposits reconstructed  
 2579 in its high ionisation loss region. If you do not remove the tails the computed  $dE/dx$   
 2580 means will be significantly different.

2581 In order to avoid those fluctuations, one can compute the mean of a truncated  $dE/dx$   
 2582 distribution instead. By keeping only a given fraction of the lowest energy deposits  
 2583 we obtain an estimate of the mean energy loss that is more resilient to reconstruction  
 2584 inefficiencies and statistical effects. Figure 8.7 (left panel) shows a comparison between  
 2585 the  $\langle dE/dx \rangle$  computed by taking the mean of the full distribution (blue line) and the  
 2586 60% lowest energy clusters (yellow line), for the stopping proton sample. The fractional  
 2587 residuals are computed for each proton, taking the corresponding means using their  
 2588 collections of true and reconstructed energy deposits. One can see that using the simple  
 2589 mean translates into a high bias and uncertainty in the  $\langle dE/dx \rangle$  estimation, whereas  
 2590 applying the truncation reduces both significantly.

2591 Additionally, I performed a comparison between the 60% truncated mean  $dE/dx$

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2592 obtained using the different calibration methods discussed earlier, namely the uncorrected  
2593 (blue), corrected (yellow) and uncalibrated (red) distributions. The results are shown  
2594 in Fig. 8.7 (right panel). While the widths of these distributions are similar, the bias  
2595 obtained for the corrected sample, i.e. calibration function and correction factor applied,  
2596 is a factor of  $\sim 2$  lower than in the uncalibrated case and almost three times smaller  
2597 than for the uncorrected sample.

2598 The next step is to optimise the level of truncation we are going to apply to our  
2599 data. To do so, I used different truncation factors, i.e. the percentage of energy-ordered  
2600 reconstructed energy deposits we keep to compute the mean, on the corrected  $dE/dx$   
2601 sample of the stopping protons. Then, following the same procedure of computing the  
2602 fractional residuals as before, I fitted the resulting histograms using a double Gaussian  
2603 function. This is simply the sum of two Gaussian functions of the type:

$$g(x; \mu, \sigma, A) = A e^{-\frac{(x-\mu)^2}{2\sigma^2}}. \quad (8.6)$$

2604 I do not add the classical normalisation factor of the Gaussian,  $1/\sqrt{2\pi}\sigma$ , therefore  
2605 the amplitude  $A$  simply represents the maximum of the function. One of the two  
2606 Gaussian functions describes the core part of the distribution, while the other captures  
2607 the behaviour of the tails.

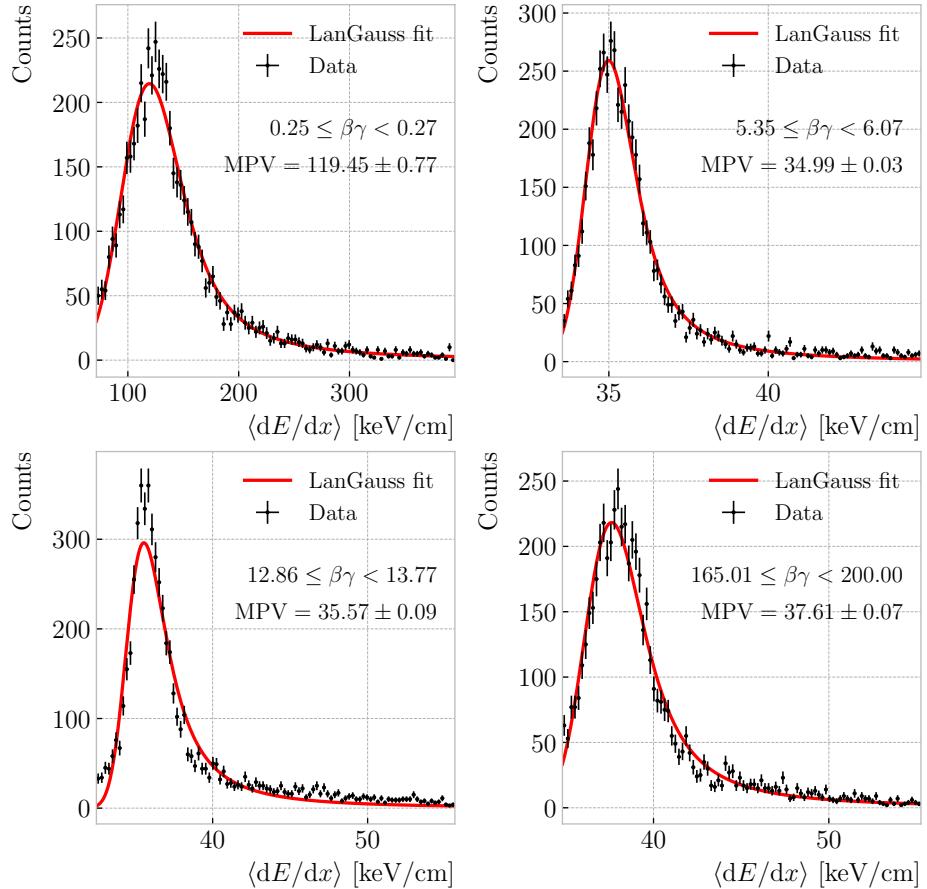
2608 For each truncation factor, I look at the bias and the resolution I obtain. I define  
2609 these as the weighted means of the corresponding parameters in the fits:

$$\bar{x} = \frac{A_{core} x_{core} + A_{tail} x_{tail}}{A_{core} + A_{tail}}, \quad (8.7)$$

2610 where  $A_{core}$  and  $A_{tail}$  are the amplitudes of the core and tail distributions respectively  
2611 and  $x$  is either the mean  $\mu$  or the width  $\sigma$  of said distributions.

2612 Figure 8.8 shows the bias (left panel) and the resolution (right panel) I obtained  
2613 for the stopping proton sample, using different values of the truncation. From these, it  
2614 can be seen that a truncation factor of 50% minimises the bias in the estimation, while

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**Figure 8.9:** Examples of the truncated mean  $dE/dx$  LanGauss fits for various  $\beta\gamma$  bins, from a simulated FHC neutrino sample.

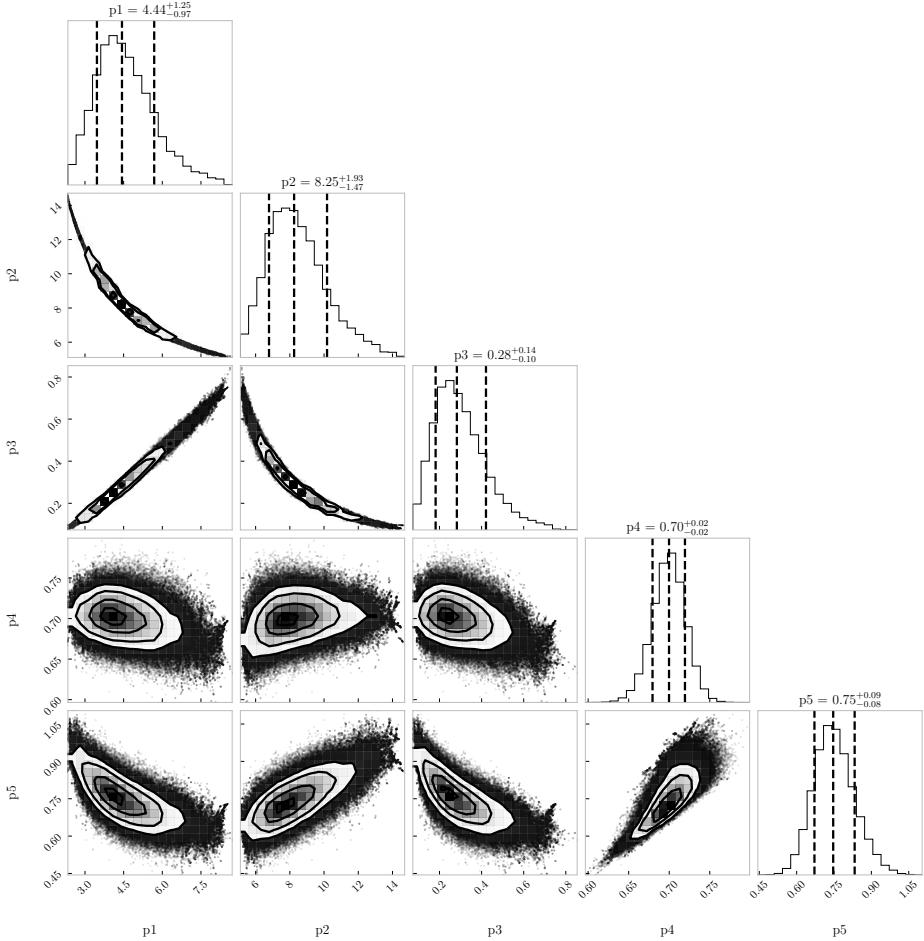
2615 70% gives the best resolution. That way, I settled on the intermediate value of 60%  
 2616 truncation, which yields a  $\langle dE/dx \rangle$  resolution of  $5.00 \pm 0.08$  % for stopping protons.

### 2617 8.1.3 Mean $dE/dx$ parametrisation

2618 Now that we have a way to estimate the mean energy loss of a particle in the HPgTPC,  
 2619 we can determine the value of the free parameters in the ALEPH formula, Eq. (8.3).  
 2620 For this, I used a sample of  $10^5$  reconstructed FHC neutrino events inside ND-GAr. In  
 2621 this case I cannot use the stopping proton sample, as we need to cover the full kinematic  
 2622 range of interest for the neutrino interactions in our detector.

2623 The original data does not contain an estimation of the velocity of the tracks, instead  
 2624 the tracks have a value for the reconstructed momentum and the associated PDG code

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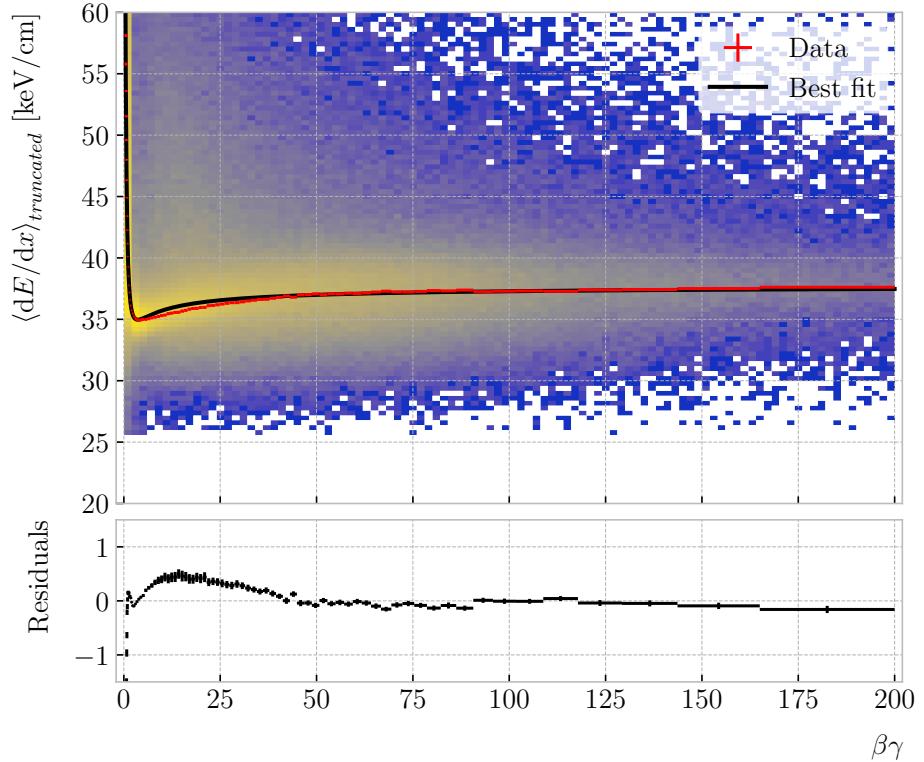
**Figure 8.10:** Resulting one and two dimensional projections of the posterior probability distributions of the ALEPH  $\langle dE/dx \rangle$  parameters obtained by fitting the 60% truncated mean  $dE/dx$  values from a FHC neutrino sample in ND-GAr. The vertical dashed lines in the 1D distributions represent the 16th, 50th and 84th percentiles.

of the Geant4-level particle that created the track. Therefore, one can select some of the particles in the data, in this case I selected electrons, muons, pions and protons, and compute  $\beta$  and  $\gamma$  using the reconstructed momentum and their mass. In terms of  $\beta\gamma$  the mean  $dE/dx$  does not depend on the particle species, so one can consider all the dataset as a whole. For this fit, I will express  $\beta$  in terms of the  $\beta\gamma$  product as:

$$\beta = \frac{\beta\gamma}{\sqrt{1 + (\beta\gamma)^2}}, \quad (8.8)$$

which can be easily proven from the definition of  $\gamma$ .

### 8.1. $dE/dx$ measurement in the TPC

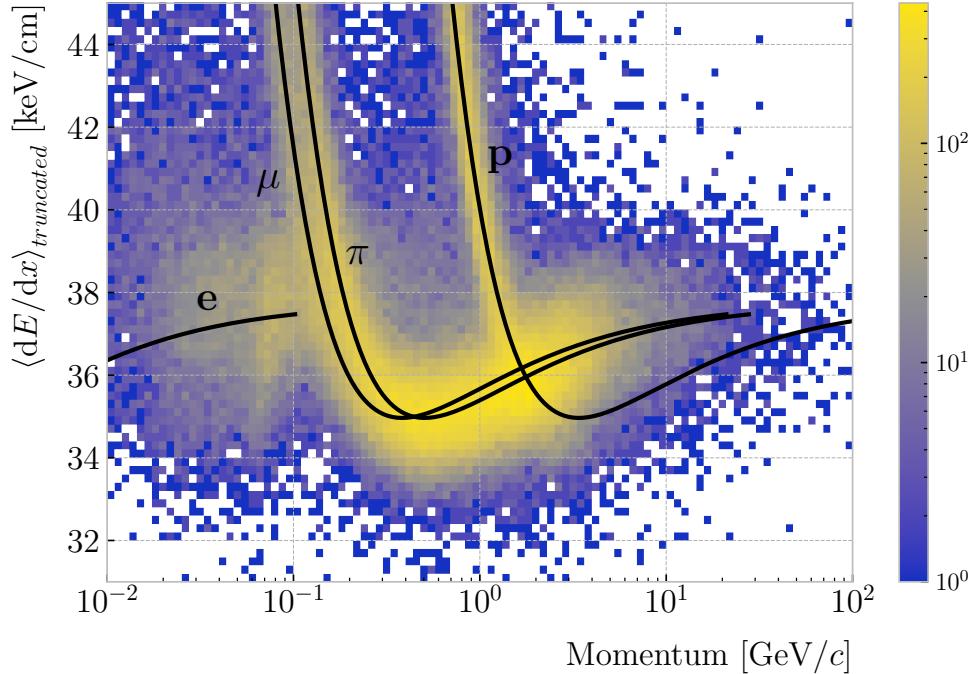


**Figure 8.11:** Truncated mean  $dE/dx$  obtained for the FHC neutrino sample as a function of the  $\beta\gamma$  product (upper panel). Also shown are the fitted most probable values for each  $\beta\gamma$  bin (red points) and the best fit obtained using the ALEPH parametrisation (black line). The residuals resulting from the fit are shown in the lower panel.

2631 Next, I bin the data in  $\beta\gamma$ . I chose a fine binning so as to capture the different  
 2632 features of the ionisation curve. Instead of fixing the bin width, I select them so each one  
 2633 has approximately the same statistics. Then, for each  $\beta\gamma$  slice, I compute the median  
 2634 and the interquartile range (IQR) of the  $\langle dE/dx \rangle$  distribution. Using these, I make a  
 2635 histogram in the range [median – IQR, median + 5 IQR], which I fit to a LanGauss  
 2636 function in order to extract the MPV. Using this range accounts for the asymmetric  
 2637 nature of the distributions, while also helps avoiding a second, lower maximum present  
 2638 at low  $\beta\gamma$ , probably a result of reconstruction failures.

2639 A few examples of these fits are shown in Fig. 8.9. The chosen values of  $\beta\gamma$  sit in  
 2640 very distinct points along the  $\langle dE/dx \rangle$  curve, going from the high ionisation region at  
 2641 low velocities (top left panel), to the minimum point (top right panel), the beginning of

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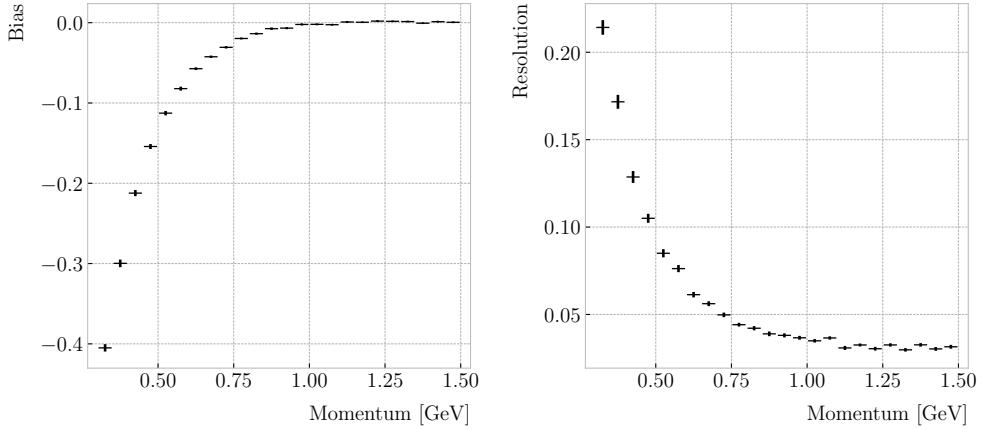
**Figure 8.12:** Distribution of the 60% truncated mean  $\langle dE/dx \rangle$  versus reconstructed momentum for the FHC neutrino sample. The black lines indicate the predictions of the ALEPH parametrisation for electrons, muons, charged pions and protons.

the relativistic rise (bottom left panel), and the plateau produced by the density effect (bottom right panel).

I used the resulting most probable  $\langle dE/dx \rangle$  values and the centres of the  $\beta\gamma$  bins as the points to fit to the ALEPH formula. For this particular fit I used the least-squares 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 8.10 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. 8.11 (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 underestimates for energy losses  $\gtrsim 50$  keV/cm, and the start of the relativistic raise,

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.13:** Estimated values of the mean  $dE/dx$  bias (left panel) and resolution (right panel) obtained for the true protons in a FHC neutrino sample.

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. 8.11 (bottom panel).

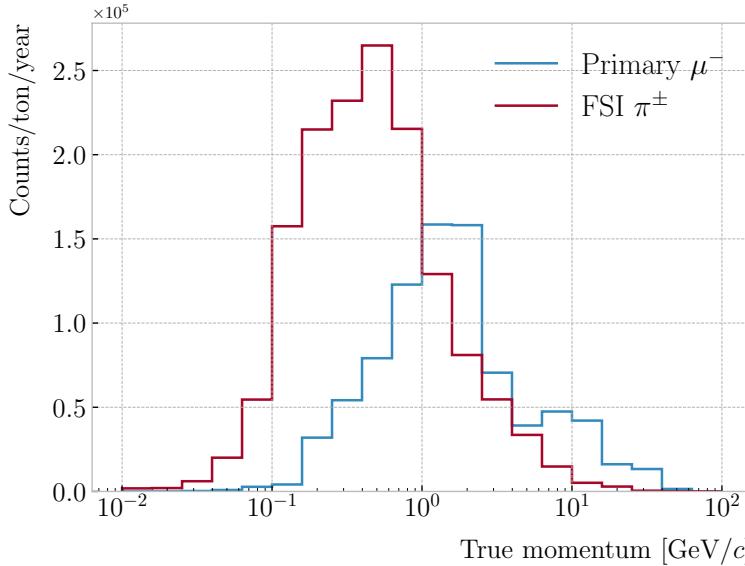
### 8.1.4 Particle identification

## 8.2 Muon and pion separation in the ECal and MuID

As it could be seen from Fig. 8.12, it is not possible to separate muons and charged pions in the HPgTPC using  $dE/dx$  for momenta  $\gtrsim 300 \text{ MeV}/c$ . In ND-GAr, approximately 70% of the interactions in FHC mode will be  $\nu_\mu$  CC (compared to the 47% of  $\bar{\nu}_\mu$  CC interactions when operating in RHC mode), while 24% are neutral currents. Out of these, around 53% and 47% of them will produce at least one charged pion in the final state, respectively. Figure 8.14 shows a comparison between the spectra of the primary muons and the charged pions for  $\nu_\mu$  CC interactions in ND-GAr producing one or more charged pions. From this, one can see that (i) the majority of muons and charged pions are not going to be distinguishable with a  $\langle dE/dx \rangle$  measurement, and that (ii) particle identification is necessary both to classify correctly the  $\nu_\mu$  CC events and identify the primary muon within them.

ND-GAr features two other subdetectors which can provide additional information

## Chapter 8. Particle ID in GArSoft



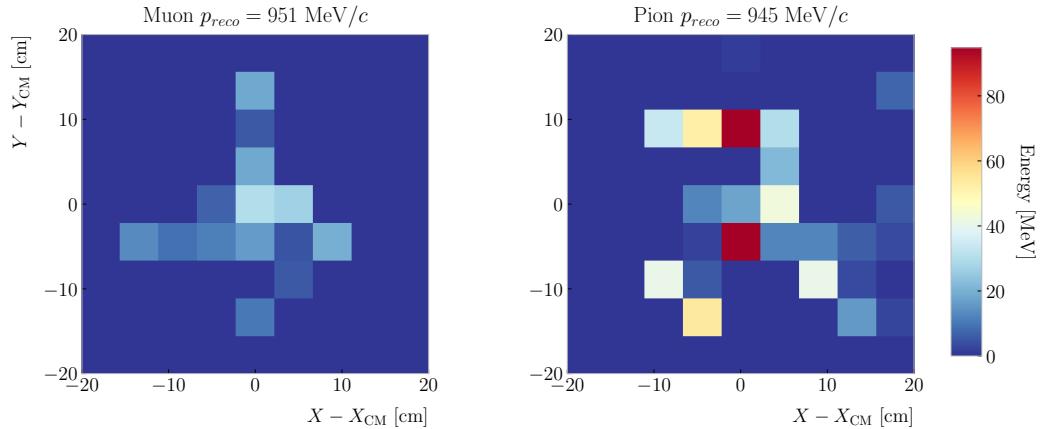
**Figure 8.14:** True momentum distribution for the primary muon in  $\nu_\mu$  CC  $N\pi^\pm$  interactions inside the fiducial volume of ND-GAr (blue line), compared to the post FSI charged pion spectrum (red line).

for this task, namely the ECal and MuID. The current ECal design, described in (ref section), consists of 42 layers, made of 5 mm of Pb, 7 mm of plastic scintillator and a 1 mm PCB board. The total thickness of this calorimeter is 1.66 nuclear interaction lengths or 1.39 pion interaction lengths. The MuID design is in a more conceptual stage, however it is envisioned to feature layers with 10 cm of Fe and 2 cm of plastic scintillator<sup>5</sup>. With its three layers, it will have a thickness of 1.87 or 1.53 nuclear or pion interaction lengths, respectively.

Because pion showers are dominated by inelastic nuclear interactions, the signatures of these particles in the calorimeter will look significantly different from those of muons. Although our ECal is not thick enough to fully contain the hadronic showers of the charged pions at their typical energies in FHC neutrino interactions, they can still be used to understand whether the original particle was more hadron-like or MIP-like. In Fig. 8.15 I show two examples of energy distributions created by a muon (left panel) and a charged pion (right panel) of similar momenta interacting in the ECal. These

<sup>5</sup>It 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.

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.15:** 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.

2687 figures represent the transverse development of the interactions. For each of them, I  
 2688 computed the principal component and centre of mass of the interaction, projecting  
 2689 the position of the hits onto the plane perpendicular to that direction, and taking the  
 2690 distances relative to the centre. It can be seen that the muon follows an almost MIP-like  
 2691 behaviour, being the central bin in the histogram the one with the highest deposited  
 2692 energy. On the other hand, the pion not only deposits more energy overall, but also this  
 2693 energy is more spread-out among the different hits. It is this kind of information that  
 2694 would allow us to tell apart muons from pions.

2695 This way, I identify three main action points that need to be addressed if one wants  
 2696 to use these detectors to distinguish between muons and charged pions. These are:

- 2697 1. the way we make the associations between tracks in the HPgTPC to the activities  
 2698 (what in GArSoft we call clusters) in the ECal and the MuID,
- 2699 2. what variables or features one can extract from the calorimeters that encapsulate  
 2700 the information we are interested about,
- 2701 3. and how to carry out the classification problem.

## Chapter 8. Particle ID in GArSoft

### 2702 8.2.1 Track-ECal matching

2703 One of the main players in the muon and pion separation is the way we associate clusters  
2704 in the ECal to reconstructed tracks in the TPC. Missing some associations or making  
2705 wrong ones can bias the ECal quantities that we can use for classifying particles. The  
2706 current algorithm in GArSoft provides precise associations, i.e. most of the associations  
2707 that it produces are correct, but it appears to miss an important number of associations  
2708 (at least when using the default configuration).

2709 The current TPC track-ECal cluster association algorithm is divided in four parts.  
2710 It first checks whether the track end point fulfils certain conditions to be extrapolated.  
2711 There are two cut values in this step, one for the drift direction and other radial.

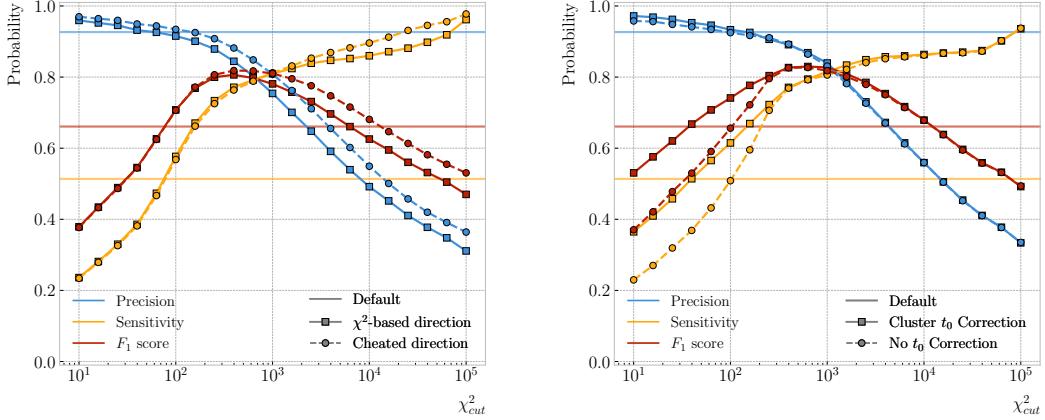
2712 If the point can be extrapolated, the code computes the coordinates of the centre  
2713 of curvature using the Kalman fit estimates at the track end ( $y, z, 1/R, \phi, \tan\lambda$ ). It  
2714 then compares the distance between this and the cluster in the  $(z, y)$  plane with  $R$ . This  
2715 introduces another cut in the perpendicular direction.

2716 The next step is different for clusters in the barrel or in one of the end caps. If it  
2717 is a barrel cluster the algorithm extrapolates the track up to the radial distance of the  
2718 cluster. There are three possible outcomes, the extrapolated helix can cut the cylinder  
2719 of radius  $r_{clus}$  two, one or zero times. I get the cut point that is closer to the cluster and  
2720 check that it is either in the barrel or the end caps. Computing the difference between  
2721 the  $x$  coordinates of the cluster and the extrapolated point, the module checks that this  
2722 is not greater than a certain cut. If the cluster is in an end cap, I propagate the track  
2723 up to the  $x$  position of the cluster. Then, the algorithm computes the angle in the  $(z, y)$   
2724 plane between the centre of curvature and the cluster,  $\alpha$ , and the centre of curvature  
2725 and the propagated point,  $\alpha'$ . A cut is applied to the quantity  $(\alpha - \alpha')R$ .

2726 If the cluster contains more than a certain number  $N$  of hits, I apply an extra cut to  
2727 the dot product of the direction of the track at the propagated  $x$  value and the cluster  
2728 direction.

2729 The code makes sure to only associate one end of the track (if any) to a cluster.

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.16:** 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  $\chi^2$ -based direction estimator (squares) and cheating the directions (circles), for different values of the  $\chi^2$  cut. Right panel: comparison of the performance of the new algorithm when applying the cluster  $t_0$  correction (squares) and when (circles).

2730 However, it can associate more than one track to the same cluster. This makes sense,  
2731 as different particles can contribute to the same cluster in the ECal, but it makes it  
2732 difficult to quantify the relative contributions of the tracks to a certain cluster.

2733 As a way of comparing the performance of this algorithm, a new, simpler association  
2734 module was written. The goal was to have a simple and robust algorithm, which depends  
2735 on as few parameters as possible and that can produce a one-to-one matching between  
2736 tracks and ECal clusters.

2737 For each reconstructed track, the new algorithms applies the same procedure to the  
2738 forward and the backward fits irrespective of their end point positions. It first gets the  
2739 Kalman fit parameters at the corresponding end point together with the  $X$  position,  $x_0$ ,  
2740 ( $y_0$ ,  $z_0$ ,  $1/R$ ,  $\phi_0$ ,  $\tan\lambda$ ).

2741 For each ECal cluster, I compute the radial distance to the centre of the TPC and  
2742 find the  $\phi$  value in the range  $[\phi_0, \phi_0 + \text{sign}(R)\phi_{max}]$  that makes the propagated helix  
2743 intersect with the circle defined with such radius. The  $(x, y, z)$  position of the helix for  
2744 the  $\phi$  value found (if any) is then computed. In case there are two intersections, I keep  
2745 the one that minimises the distance between  $(y, z)$  and  $(y_c, z_c)$ .

2746 I then calculate  $\chi^2$  value based on the Euclidean distance between the propagated

## Chapter 8. Particle ID in GArSoft

2747 point and the cluster:

$$\chi^2/ndf = \frac{\sum_{n=0}^2 (x^{(n)} - x_c^{(n)})^2}{3}. \quad (8.9)$$

2748 If there was no intersection I store a  $-1$  instead. In the end, for each reconstructed track  
2749 in the event one ends up with two collections of  $\chi^2$  values, one for each ECal cluster  
2750 and fit directions.

2751 The current code only supports having ECal clusters associated to one end of each  
2752 track. We have two options to decide what track end to keep. The first one tries to  
2753 cheat the selection, looking at the distance between the two track ends and the true  
2754 start position of the associated MC particle. The second one keeps the track end with  
2755 more  $\chi^2$  entries below the cut.

2756 This feature of only considering one track end limits the algorithm, making it not  
2757 suitable for reconstructing events with particles originating outside the TPC. However,  
2758 as for the moment the main concern of the group is the study of neutrino interactions  
2759 off the gaseous argon, this is an acceptable assumption.

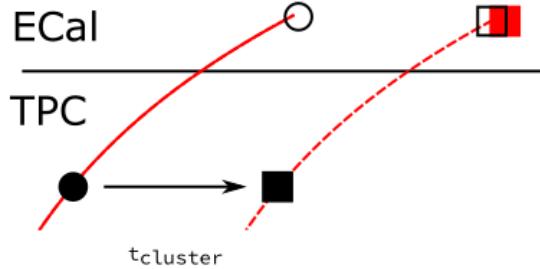
2760 In order to associate a cluster to a track, I take all clusters with a  $\chi^2$  value in the  
2761 range  $[0, \chi_{cut}^2]$ . If a cluster has been assigned to more than one track we leave it with  
2762 the one with the lowest  $\chi^2$ .

2763 This default behaviour of the algorithm can be modified to associate more than one  
2764 track to each cluster. Not only that, but the  $\chi^2$  values can be used to assign relative  
2765 weights to the different contributions.

2766 To evaluate the performance of the association method, I use a binary classification  
2767 approach. In this case, I check the leading MC Track IDs associated to the reconstructed  
2768 tracks and ECal clusters. I count an association as true positive (TP) if both Track  
2769 IDs coincide. An association is considered false positive (FP) when the Track IDs are  
2770 different. If a cluster has not been associated to any track but it shares the Track ID  
2771 with a reconstructed track it is counted as a false negative (FN).

2772 For the testing, I used a sample of 10000 FHC neutrino events inside the HPgTPC.  
2773 Figure 8.16 (left panel) shows the precision (blue line), sensitivity (yellow line), and  $F_1$

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.17:** 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,  $t_{cluster}$ .

2774 score (red line) I obtained for different values of  $\chi^2_{cut}$ . For comparison, the same metrics  
 2775 computed for the default algorithm with the current configuration are also shown (dashed  
 2776 lines). In the case of the new algorithm, I used both the  $\chi^2$ -based method to estimate  
 2777 the track direction described earlier (square markers) and the cheated direction from the  
 2778 Geant-level information (circle markers). For either of these we achieve similar values of  
 2779 the precision compared to the old code, while having a considerably higher sensitivity.  
 2780 It can be seen that cheating the direction of the tracks only makes a difference at high  
 2781  $\chi^2_{cut}$ , past the optimal value of the cut around the  $F_1$  score maximum. Therefore, I set  
 2782 the  $\chi^2$  method as the default.

2783 One of the possible weak points of this approach is that it relies on the position along  
 2784 the drift direction to make the decisions. Within the current ND-GAr design implemented  
 2785 in GArSoft, the timing information is provided by the ECal. That effectively means  
 2786 that prior to make the track-ECal associations the reconstructed  $x$  positions of the track  
 2787 trajectories differ from the simulated ones by an amount:

$$x_{reco}^{(n)} - x_{sim}^{(n)} = v_{drift} t_0, \quad (8.10)$$

2788 where  $v_{drift}$  is the mean drift velocity in our medium and the initial time is in the range  
 2789  $t_0 \in [0, t_{spill}]$  where  $t_{spill}$  is the spill length. For a 10  $\mu\text{s}$  spill this translates into a  
 2790 maximum 30 cm uncertainty on the drift direction position.

2791 The current default in GArSoft sets  $t_0 = 0$ , but the functionality to randomly sample

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2792 this within the spill time is in place. Therefore, we need to understand what is the impact  
2793 of a non-zero  $t_0$  on the associations algorithm and foresee possible ways of minimising a  
2794 loss in performance.

2795 Figure 8.17 represents a possible option to tackle the association problem when  
2796 having events with a non-zero initial time  $t_0$ . The black and white circles represent the  
2797 original points, whereas the squares indicate the corrected positions. The end points of  
2798 the track and the propagated points up to the cluster radius are indicated using filled  
2799 and unfilled markers respectively. The red square represents the position of the cluster.

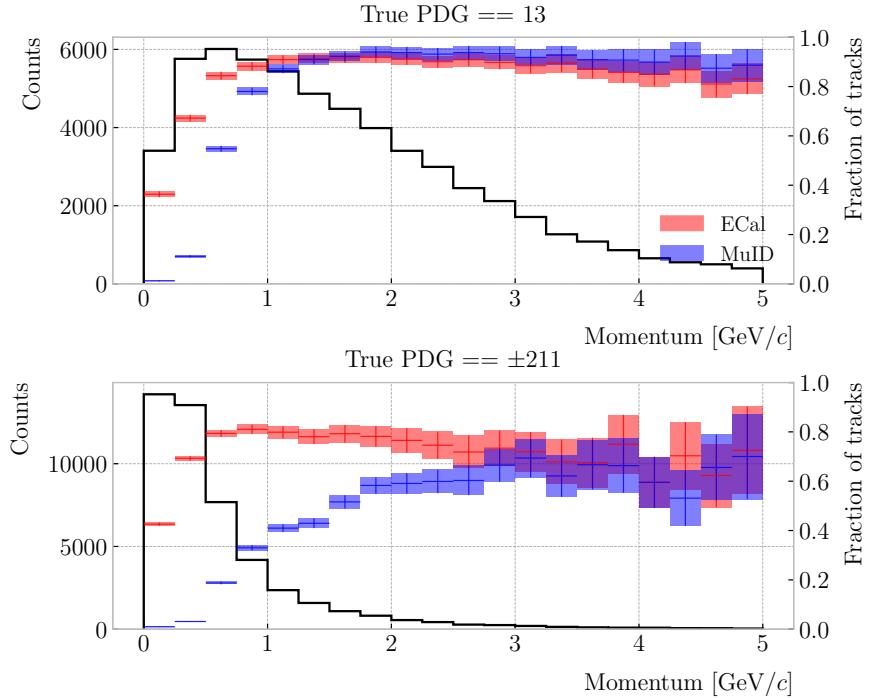
2800 Here I try to correct for the drift coordinate position using the time associated to the  
2801 cluster. Assuming that the drift time is much larger than the propagation time,  $t_{cluster}$   
2802 could be used as a good estimation of the  $t_0$ . An alternative can be using the earliest  
2803 time associated to a hit in said cluster. Doing this for each cluster before computing  
2804 the  $\chi^2$  value could be used as an alternative to knowing the specific value of the  $t_0$ , as  
2805 when the association is correct this will provide the right correction but its impact is  
2806 small enough to not change the position significantly in the case the cluster does not  
2807 correspond to a given track.

2808 I tested the effect of this correction again using a sample of 10000 FHC neutrino  
2809 events. Figure 8.16 (right panel) shows the precision (blue line), sensitivity (yellow line),  
2810 and  $F_1$  score (red line) for the case the cluster  $t_0$  correction is applied (square markers)  
2811 and for the no correction case (circle markers), as a function of  $\chi^2_{cut}$ . In this case, the  
2812 differences are particularly notorious at low values of the cut. It makes sense, as the  $t_0$   
2813 effect becomes subdominant when the distance we consider grows large. Overall, the  
2814 correction increases the sensitivity while keeping the precision almost unchanged. As a  
2815 result, I apply the  $t_0$  correction to the generated samples as the default.

### 2816 8.2.2 Classification strategy

2817 The problem of the muon and charged pion separation has to be viewed in the broader  
2818 context of the particle identification in our detector. Focusing on the beam neutrino  
2819 interactions, it is clear that we are going to have muons and pions spanning a broad

## 8.2. Muon and pion separation in the ECal and MuID

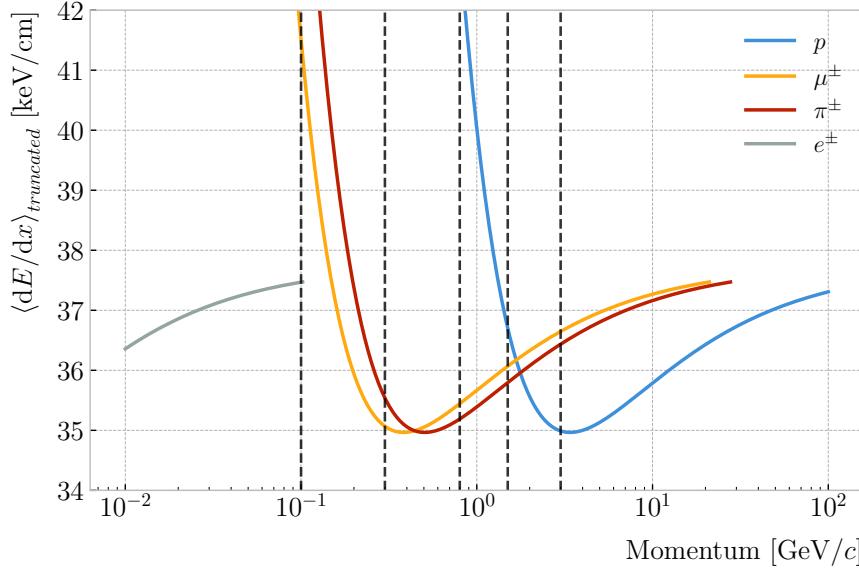


**Figure 8.18:** Momentum distribution for the reconstructed muons (top panel) and charged pions (bottom panel) in a FHC neutrino sample, together with the fraction of them reaching the ECal (red) and MuID (blue). Each entry corresponds to a reconstructed track, backtracked to a true muon or pion which has not produced any other reconstructed track.

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 protons as possible.

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**Figure 8.19:** 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.

2832     Figure 8.18 shows the momentum distribution of the reconstructed muons (top) and  
 2833     pions (bottom) in a FHC sample. It also contains the fraction of particles reaching the  
 2834     ECal (red) and MuID (blue), for the different momentum bins. In Fig. 8.19 I show the  
 2835     mean  $dE/dx$  of different particles as a function of the momentum, computed using the  
 2836     ALEPH parametrisation with the best fit parameters found in Subsec. 8.1.2.

2837     Using these two figures as references, I decided to approach the classification by  
 2838     dividing the problem into six different momentum regions. A summary of these can be  
 2839     found in Tab. 8.2. The basic idea is to exploit all the information that is available in  
 2840     each region and . For the problem at hand, I prepared separated samples of isotropic  
 2841     single muons and pions, with momenta uniformly distributed along the corresponding  
 2842     momentum range. Each sample contains 50000 events of the corresponding particle  
 2843     species. I did not generate samples for the first region, as it is assumed that the separation  
 2844     can be achieved using  $dE/dx$  only. For the last region, I generated particles up to a  
 2845     momentum of 10  $\text{GeV}/c$ , as that is well above the typical energies of muons and pions  
 2846     from FHC neutrino interactions in ND-GAr.

## 8.2. Muon and pion separation in the ECal and MuID

**Table 8.2:** 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             |
| $\geq 3.0$ GeV/c | Use ECal and MuID for muons and pions, $dE/dx$ and ToF for protons |

2847        Additionally, I prepared another sample of 100000 FHC neutrino events. For each  
 2848      interaction, I select the reconstructed particles which were backtracked to true muons or  
 2849      charged pions. I use this dataset to perform validation checks, to see how the models  
 2850      trained with the single particle data generalise to a more realistic scenario.

2851        To tackle this classification problem, I make use of Boosted Decision Trees (BDT). A  
 2852      decision tree uses a flowchart-like structure to make decisions based on some input data.  
 2853      It starts from a root node, which represents the complete dataset, and then it splits  
 2854      this based on the variable or feature which gives the best separation between classes,  
 2855      creating two new nodes. The process repeats for each node until it reaches a certain  
 2856      limit, like a maximum number of splits or some tolerance criteria. The last set of nodes  
 2857      are often called leave nodes, and represent the final prediction of the classifier.

2858        Boosting refers to a family of methods to combine the predictions from multiple  
 2859      classifiers, following a sequential approach where each new model learns from the errors  
 2860      of the previous one. The process starts with a simple decision tree, which is used to  
 2861      make predictions on the training data. Then, the data points misclassified by the first  
 2862      model are assigned higher weights, and another decision tree is trained on the data with  
 2863      adjusted weights. The predictions of the two trees are then combined, and the cycle  
 2864      repeats for a predefined number of iterations. Gradient boosting uses the direction of  
 2865      the steepest error descent to guide the learning process and improve the accuracy with  
 2866      each iteration.

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### 2867 8.2.3 Feature selection and importance

2868 Using the reconstructed tracks as a starting point, I compute a number of ECal and  
2869 MuID variables for each of them. As there can be more than one cluster associated to a  
2870 track, what I do is collect all associated clusters and compute these variables from the  
2871 complete collection of associated hits. For the MuID, because it only features three layers  
2872 and typically there will be less hits, I also allow single hits to be associated with tracks<sup>6</sup>.  
2873 I can roughly divide the variables in three types: energy-related, geometry-related and  
2874 statistical. In the following, I briefly describe the variables related exclusively to the  
2875 ECal:

2876 • Energy-related ECal

- 2877 – ECal total energy (ClusterTotalEnergy): sum of the energy of all the ECal  
2878 hits.
- 2879 – Mean ECal hit energy (HitMeanEnergy): mean of the hit energy distribution.
- 2880 – Standard deviation ECal hit energy (HitStdEnergy): standard deviation of  
2881 the hit energy distribution.
- 2882 – Maximum ECal hit energy (HitMaxEnergy): maximum of the hit energy  
2883 distribution.

2884 • Geometry-related ECal

- 2885 – Mean distance hit-to-cluster (DistHitClusterMean): mean of the distance  
2886 distribution between the hits and the corresponding cluster's main axis.
- 2887 – RMS distance hit-to-cluster (DistHitClusterRMS): root mean square of the  
2888 distance distribution between the hits and the corresponding cluster's main  
2889 axis.
- 2890 – Maximum distance hit-to-centre (DistHitCenterMax): maximum of the  
2891 distance distribution between the hits and the centre of the TPC.

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<sup>6</sup>At 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.

## 8.2. Muon and pion separation in the ECal and MuID

- 2892 – Time-of-Flight velocity (TOFVelocity): slope obtained when fitting a straight  
2893 line to the hit time versus hit distance to the centre (i.e.  $d = v \times t$ ).

2894 • **Energy and geometry ECal**

- 2895 – Radius 90% energy (Radius90E): distance in the hit-to-cluster distribution  
2896 for which 90% of the total energy is contained in the hits that are closer to  
2897 the axis (i.e. radius that contains 90% of the energy).

2898 • **Statistical ECal**

- 2899 – Number of hits (NHits): total number of hits associated to the track.  
2900 – Number of layers with hits (NLayers): not really a count of all layers with  
2901 hits but the difference between the last and the first layer with hits.

2902 Figure 8.20 shows the distributions of three different ECal variables, separating true  
2903 muons (blue) and charged pions (red), for the five momentum ranges considered. I chose  
2904 to show one feature from each category, namely the mean energy per hit (left column),  
2905 the mean distance between the hits and the centre of the cluster (middle column), and  
2906 the number of ECal layers with hits (right column). These give an idea of the separating  
2907 power of the different features, and how it changes considerably with the energy. In  
2908 the number of layers with hits distributions, the peak at 6 is due to the fact that the  
2909 first six ECal layers sit inside the pressure vessel<sup>7</sup>. Therefore, some of the particles get  
2910 stopped crossing it, never making it to the seventh layer.

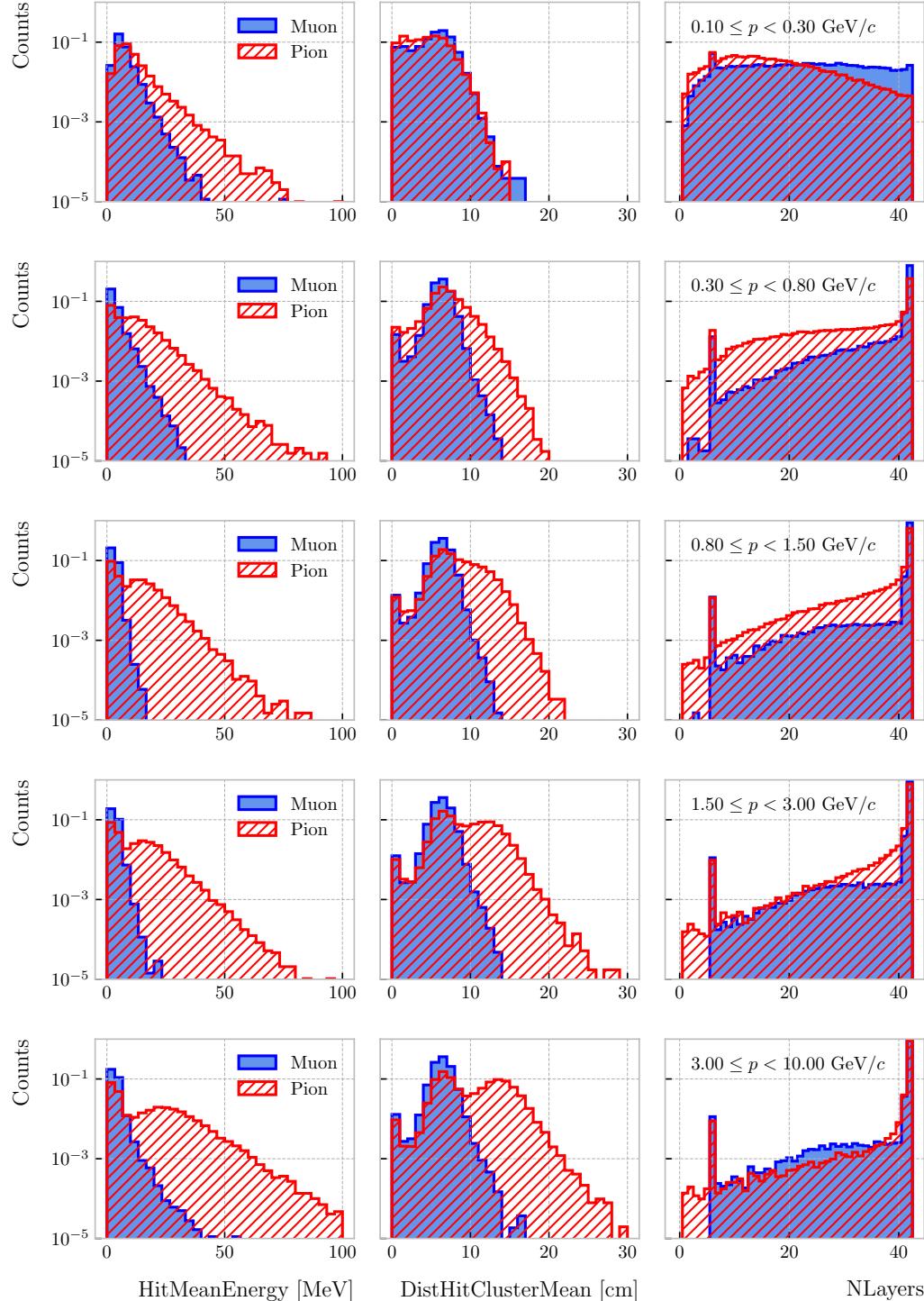
2911 In the case of the MuID, because at low momenta a significant fraction of the particles  
2912 do not make it past the ECal, I only consider the information coming from this detector  
2913 for momenta  $\geq 0.8$  GeV/ $c$ , i.e. for the last three momentum regions. The variables I  
2914 extract from it are the following:

2915 • **Energy-related MuID**

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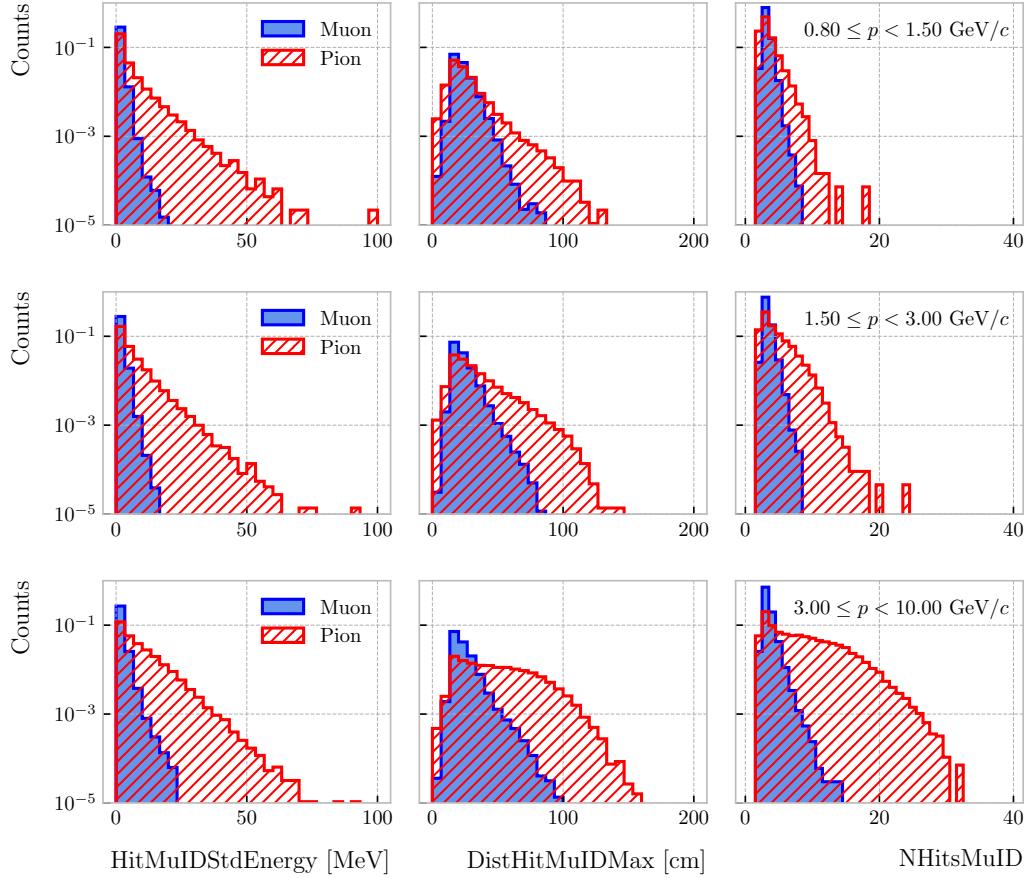
<sup>7</sup>Note to self: check this. I thought the ECal barrel had 8 layers of tiles, and that all of them were inside the pressure vessel.

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**Figure 8.20:** 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.

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.21:** 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.

- 2916           – MuID total energy (ClusterMuIDTotalEnergy): sum of the energy of all the
- 2917            MuID hits.
- 2918           – Mean MuID hit energy (HitMuIDMeanEnergy): mean of the MuID hit energy
- 2919            distribution.
- 2920           – Standard deviation MuID hit energy (HitMuIDStdEnergy): standard deviation
- 2921            of the MuID hit energy distribution.
- 2922           – Maximum MuID hit energy (HitMuIDMaxEnergy): maximum of the MuID
- 2923            hit energy distribution.

- 2924           • **Geometry-related MuID**

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- 2925        – Maximum distance MuID hit-to-hit (DistHitMuIDMax): maximum distance
- 2926              between pairs of MuID hits (not sure this is a good variable, distribution
- 2927              looks nuts).
- 2928        – Maximum distance MuID hit-to-centre (DistHitCenterMuIDMax): maximum
- 2929              of the distance distribution between the MuID hits and the centre of the
- 2930              TPC.

### 2931        • Statistical MuID

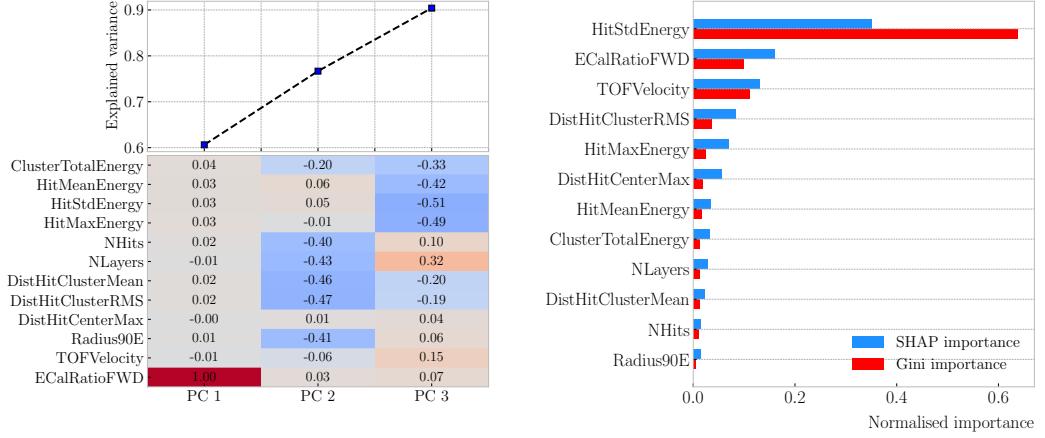
- 2932        – Number of hits (NHitsMuID): total number of MuID hits associated to the
- 2933              track.
- 2934        – Number of layers with hits (NLayersMuID): not really a count of all layers
- 2935              with MuID hits but the difference between the last and the first layer with
- 2936              MuIDhits.

2937        Figure 8.21 shows the distributions of three different MuID variables, separating true  
2938        muons (blue) and charged pions (red), for the three momentum ranges which use the  
2939        muon tagger information. In this case I decided to standard deviation of the MuID hit  
2940        energy distribution (left column), the maximum distance between the MuID hit pairs  
2941        (middle column), and the number of MuID hits (right column). These variables are used  
2942        together with the ECal features at high momenta, providing additional disambiguation  
2943        power.

2944        Once our features have been defined, one can do some exploratory analysis to  
2945        understand how well the variables describe the target class, and avoid the black-box  
2946        approach by what features are most relevant for the learning process. This way, I  
2947        performed a feature analysis for each of the momentum ranges I divided this classification  
2948        problem into. It follows three steps: first a principal component analysis (PCA), followed  
2949        by a feature importance study using Gini and Shapley values, and finally a feature  
2950        permutation importance analysis.

2951        The PCA is useful to understand the variance of the feature space. It is an  
2952        unsupervised machine learning technique that allows the user to perform a dimensionality

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.22:** 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  $0.3 \leq p < 0.8$  GeV/c.

reduction. It uses a singular value decomposition of the input features to project them into a lower dimensional space. The idea is to find the matrix  $\mathbf{C}_m$ , whose columns are the first  $m$  orthonormal eigenvectors of the input covariance matrix. Consider the  $n \times p$  real matrix of input data  $\mathbf{X}$ , where  $n$  is the number of samples and  $p$  the number of features. If  $\mathbf{X}$  is centred, i.e. the means of its columns are equal to zero, we can write the covariance matrix of  $\mathbf{X}$  as  $\mathbf{C} = \mathbf{X}^\top \mathbf{X} / (n - 1)$ . This matrix can be diagonalised, yielding:

$$\mathbf{C} = \mathbf{V} \mathbf{L} \mathbf{V}^\top, \quad (8.11)$$

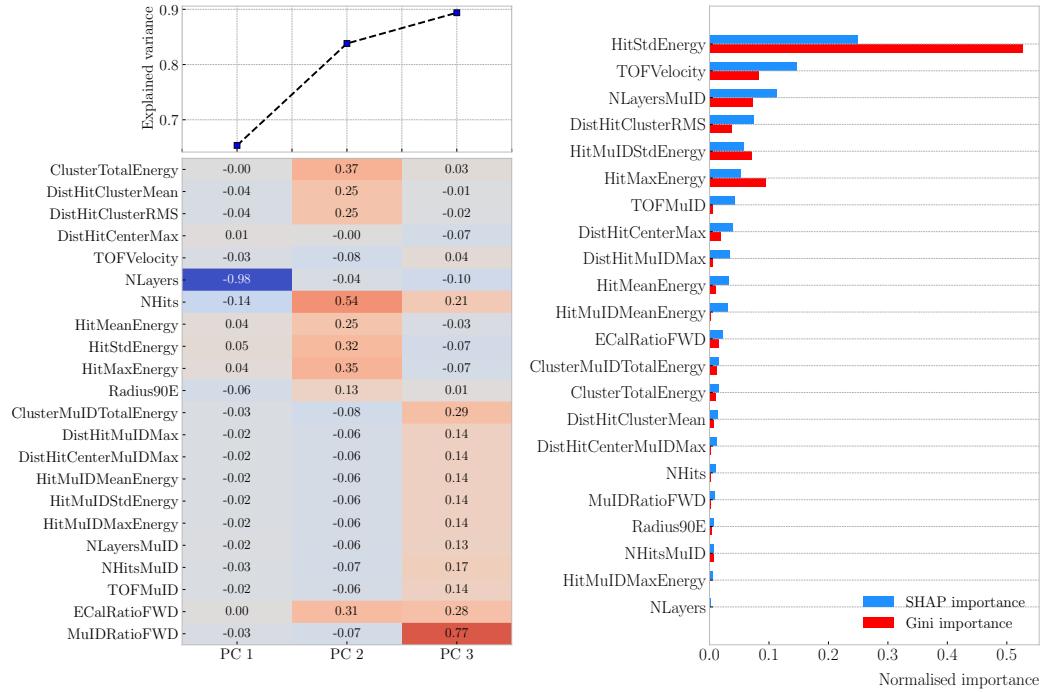
where  $\mathbf{V}$  is a matrix of eigenvectors and  $\mathbf{L}$  a diagonal matrix with eigenvalues  $\lambda_i$ . Then, performing SVD on  $\mathbf{X}$  gives us:

$$\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{W}^\top, \quad (8.12)$$

where  $\mathbf{U}$  is a unitary matrix, whose columns are called left singular vectors,  $\mathbf{S}$  is a diagonal matrix of single values  $s_i$ , and  $\mathbf{W}$  is another unitary matrix, its columns known as right singular vectors. This way, we can write:

$$\mathbf{C} = \mathbf{W} \mathbf{S} \mathbf{U}^\top \mathbf{U} \mathbf{S} \mathbf{W}^\top / (n - 1) = \mathbf{W} \frac{\mathbf{S}^2}{n - 1} \mathbf{W}^\top. \quad (8.13)$$

## Chapter 8. Particle ID in GArSoft



**Figure 8.23:** 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  $0.8 \leq p < 1.5 \text{ GeV}/c$ .

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:

$$Y = \mathbf{C}_m^\top X. \quad (8.14)$$

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.

Centring is necessary when using SVD to obtain the eigenvectors of the covariance matrix, as only in that case we can do the identification with the right singular vectors from the input data. Scaling is needed when variables are on different scales, as some can then dominate the PCA procedure.

## 8.2. Muon and pion separation in the ECal and MuID

2975 I used the PCA module of `scikit-learn`, together with the `RobustScaler`, which  
 2976 centres the data and scales it based on the interquartile range. In Fig. 8.22 (left panel)  
 2977 and Fig. 8.23 (left panel) I show the results I obtained from the PCA for the momentum  
 2978 ranges  $0.3 \leq p < 0.8 \text{ GeV}/c$  and  $0.8 \leq p < 1.5 \text{ GeV}/c$ , respectively. Notice that in  
 2979 the second case the number of features increases considerably, as this is the first region  
 2980 which uses the MuID variables. I found that, in all the cases, adding a fourth PC does  
 2981 not add additional information. As it can be seen in the top panels of the figures, the  
 2982 cumulative explained variance is already over 80% with three PCs.

2983 The bottom panels show the contribution of the variables to the principal axes. For  
 2984 the two first momentum regions, I observe a tendency of the energy-related and the  
 2985 geometry-related ECal variables to be clustered together. For the other ranges, when  
 2986 I include the MuID variables, there seems to be a division between ECal and MuID  
 2987 variables. For these, it seems like the number of ECal layers with hits also plays an  
 2988 important role.

2989 The next step in the analysis is to quantify the importance of the features based on  
 2990 two additional metrics, namely the Gini and the Shapley values. The Gini importance,  
 2991 often called mean decrease impurity, is based on how much a feature contributes to the  
 2992 purity improvement at the splits in each decision tree. The purity is measured in terms  
 2993 of the Gini impurity index, defined as:

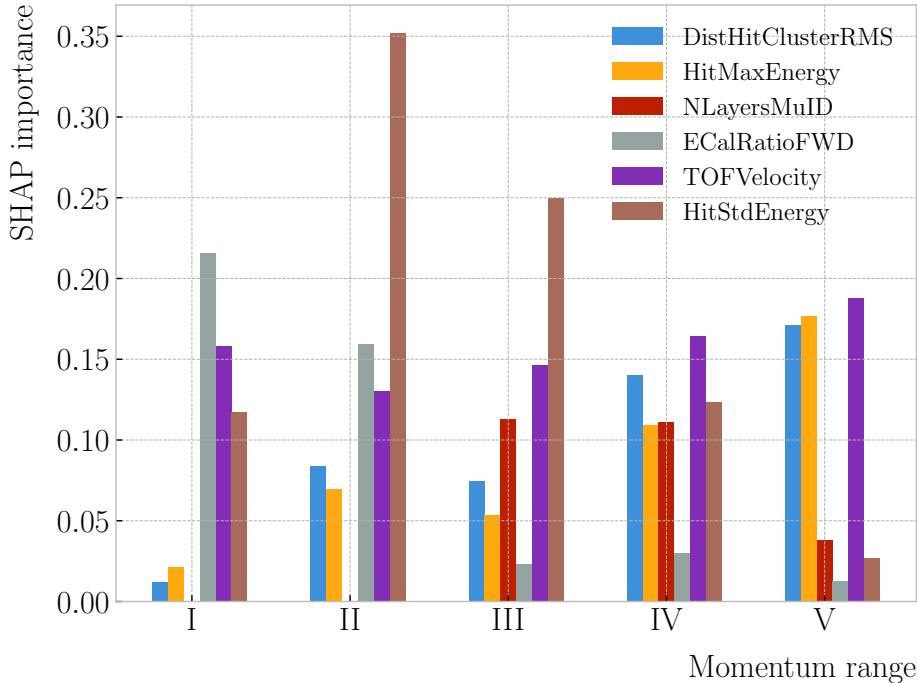
$$I_G = 1 - \sum_i f_i, \quad (8.15)$$

2994 where  $f_i$  is the fractional abundance of the  $i$ -th class. Then, for each split one can  
 2995 compute the weighted decrease in impurity as:

$$\Delta_G = \frac{N_t}{N} \left( I_G - \frac{N_t^R}{N_t} I_G^R - \frac{N_t^L}{N_t} I_G^L \right), \quad (8.16)$$

2996 where  $N$  represents the total number of samples,  $N_t$  the number of samples at the current  
 2997 node,  $N_t^R$  and  $N_t^L$  the number of samples in the right and left children respectively,

## Chapter 8. Particle ID in GArSoft



**Figure 8.24:** Evolution of the SHAP importance for the top six most important features across all five momentum ranges.

2998  $I_G$  is the Gini impurity at the current node, and  $I_G^R$  and  $I_G^L$  the Gini impurities of the  
 2999 resulting right and left children.

3000 For each decision tree, one will have a normalised vector with the accumulated  
 3001 decrease in Gini impurity for each feature. In the case of a BDT, the feature importances  
 3002 are simply the mean for all the estimators in the ensemble<sup>8</sup>.

3003 The concept of Shapley values originated in the context of game theory, and it  
 3004 measures the marginal contribution of a feature in enhancing the accuracy of a classifier.  
 3005 Take  $F$  to be the set of all features in a problem, and  $S \subseteq F$  the subset of features. To  
 3006 compute the Shapley value of the  $i$ -th feature, one has to train a model with that feature  
 3007 present,  $f_{S \cup \{i\}}$ , and another model trained without it,  $f_S$ . This has to be repeated for  
 3008 all possible combinations of subsets  $S \subset F \setminus \{i\}$ , and evaluating the models predictions

---

<sup>8</sup>Note 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.

## 8.2. Muon and pion separation in the ECal and MuID

3009 on the appropriate sets of data  $x_S$ . This way, the Shapley value results:

$$\varphi_i = \sum_{S \subset F \setminus \{i\}} \frac{|S|! (|F| - |S| - 1)!}{|F|!} [f_{S \cup \{i\}}(x_{S \cup \{i\}}) - f_S(x_S)]. \quad (8.17)$$

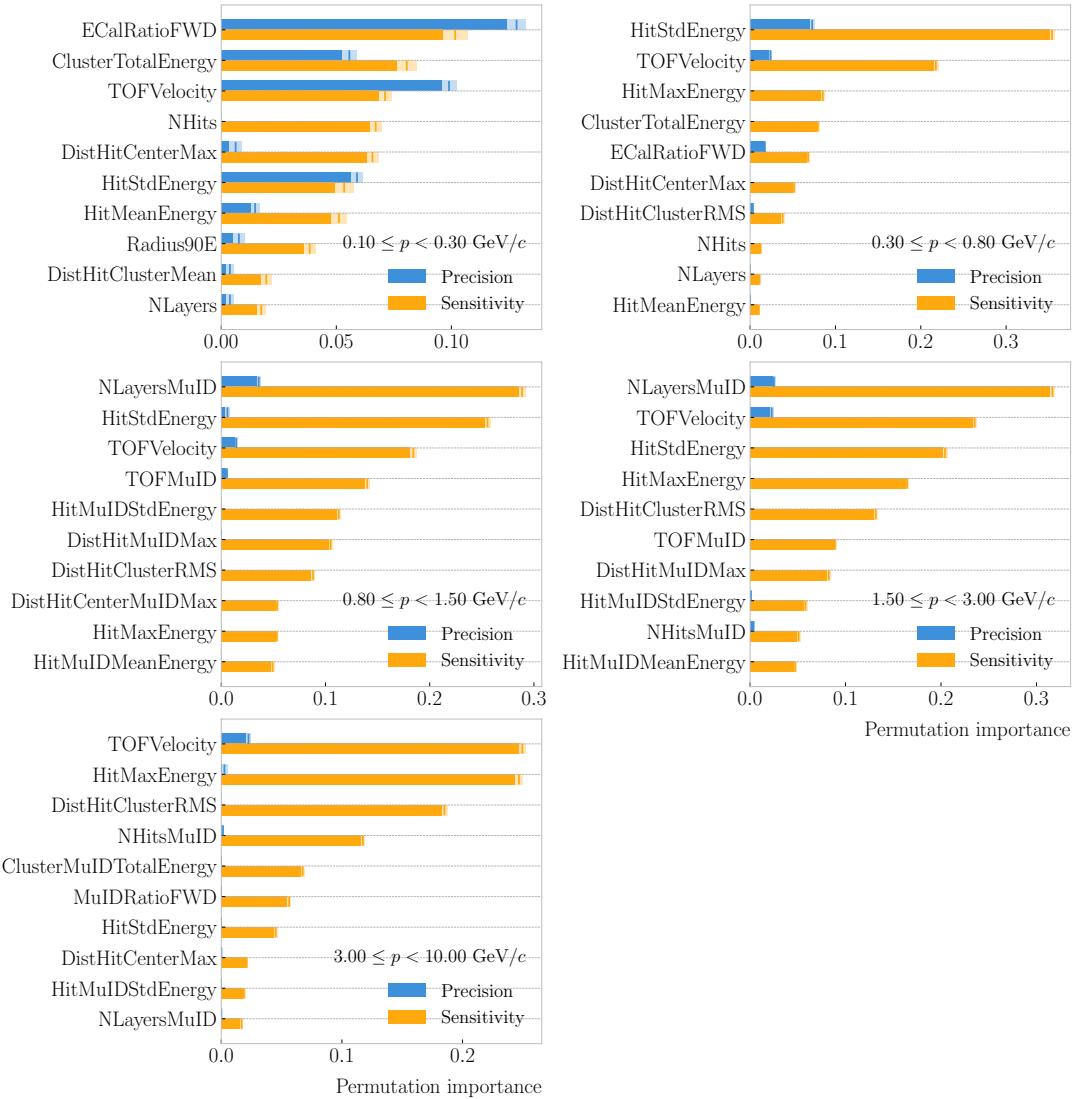
3010 I trained the `GradientBoostingClassifier` from `scikit-learn` with the default  
 3011 configuration in order to evaluate both the Gini and Shapley importances. The Gini  
 3012 scores are automatically computed by `scikit-learn`, using the training data. For the  
 3013 Shapley importance, I used the implementation from the `SHAP` package, computing  
 3014 it using the test sample. The results can be seen in Fig. 8.22 (right panel) and  
 3015 Fig. 8.23 (right panel), again for the momentum ranges  $0.3 \leq p < 0.8 \text{ GeV}/c$  and  
 3016  $0.8 \leq p < 1.5 \text{ GeV}/c$ . The length of the bars denote either the SHAP (blue) or the Gini  
 3017 (red) importance of the feature. One interesting thing to notice is that, when looking at  
 3018 the Gini importance, there is always one feature that dominates over the rest. This is  
 3019 not the case for the SHAP importance, where importances tend to be more balanced.

3020 Across all momentum ranges, I observe that the most important features are. For  
 3021 the five momentum ranges considered, only six variables sit in the top five at least once.  
 3022 Figure 8.24 shows the evolution of the SHAP importance of these six features. It is  
 3023 interesting to see that the time-of-flight variable keeps its importance almost unchanged  
 3024 for all momenta. Also, it looks like the ECal energy ratio gets less relevant the higher the  
 3025 momentum is, but the RMS of the hit-to-cluster distance distribution and the maximum  
 3026 ECal hit energy become more important in the last momentum ranges.

3027 The last step in the feature selection analysis is the feature permutation. This  
 3028 technique measures the contribution of each feature to the performance of a model by  
 3029 randomly shuffling its values and checking how some scores degrade. For the present  
 3030 case, I am interested in the precision or purity, and the sensitivity or efficiency, as these  
 3031 two are the most relevant metrics from a physics point of view. The `scikit-learn`  
 3032 module provides the user with a method to perform the permutation scans.

3033 The results of these are shown in Fig. 8.25. For the different momentum ranges  
 3034 I show the permutation importances for the ten most important features. For each

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**Figure 8.25:** 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.

## 8.2. Muon and pion separation in the ECal and MuID

3035 of the variables I report the effect the permutations have on the precision (blue) and  
3036 sensitivity (yellow) of the models. The bars indicate the importance value, with the  
3037 lighter part representing one standard deviation around the mean (hinted as an additional  
3038 vertical line). Something to notice is that, in the first momentum region, the feature  
3039 permutations have an effect on both the precision and the sensitivity. However, for the  
3040 rest the precision is almost unaffected, while the sensitivity changes are considerably  
3041 larger.

3042 It is also interesting to see that most of the variables identified as important here  
3043 are the same I found when looking at the Shapley values. The behaviour of these across  
3044 the momentum ranges is also similar, with the same patterns of some features being  
3045 important at low momenta and then dropping in importance for the high momentum  
3046 ranges.

3047 Wit this, I conclude the study of the features. I have prepared the training and  
3048 testing datasets and understood what features are likely to have the largest impact on  
3049 the performance of the classifiers.

### 3050 8.2.4 Hyperparameter optimisation

3051 Any BDT requires the user to specify a number of parameters that will dictate its  
3052 behaviour. They can be divided into two categories: (i) tree-specific parameters, which  
3053 affect each individual tree in the model, and (ii) boosting parameters, which control the  
3054 boosting operation in the model. The value of these so-called hyperparameters affect the  
3055 performance and predictive power of the models. Therefore, one needs to carefully select  
3056 their optimal values in order to extract as much information as possible from the data.

3057 From all the parameters used to define a tree in the `scikit-learn` implementation  
3058 of the BDT classifier, I only consider a subset of them. This is due to the fact that some  
3059 are mutually exclusive, but also because I noticed that others have little effect on the  
3060 problem at hand. Therefore, the parameters I investigate are the following:

- 3061 • `min_samples_split`: defines the minimum number of samples required in a node  
3062 to be considered for splitting. Higher values prevent a model from learning relations

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3063        which might be highly specific to the particular sample, but may lead to under-fitting  
3064        if the value is too low.

3065        • `min_samples_leaf`: defines the minimum samples required in a leaf node. For  
3066        imbalanced problems it should take a low value, as there will not be many cases  
3067        where the minority class dominates.

3068        • `max_depth`: maximum depth of a tree. Useful to prevent over-fitting, as higher  
3069        depth will allow a model to learn relations specific to the training sample.

3070        In the case of the boosting parameters, the ones I look at are:

3071        • `learning_rate`: determines the impact of each tree on the final outcome. Low  
3072        values make the model robust to the specific characteristics of a tree, and thus  
3073        allow it to generalise well. However, that usually requires a large number of trees  
3074        to model the data properly.

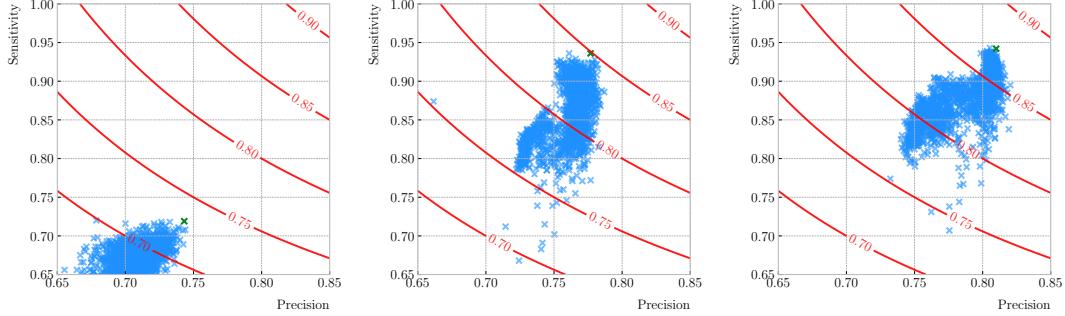
3075        • `n_estimators`: number of sequential trees to be trained. In general, BDTs are  
3076        fairly robust at higher number of trees but it can still overfit at a point.

3077        • `subsample`: fraction of observations to be selected for each tree. Values slightly  
3078        less than 1 make the model robust by reducing the variance.

3079        In general, hyperparameters depend on each other. Thus, it is not possible to  
3080        optimise them independently. In the literature, we find two main strategies to explore  
3081        the hyperparameter space. We could use a grid search, in which one discretises a  
3082        portion of the space of hyperparameters and evaluates the model at each point. Another  
3083        approach is the randomised search, where a certain number of random configurations of  
3084        hyperparameters are explored.

3085        In this case, I used the random search to scan the hyperparameter space. Also,  
3086        because it is not guaranteed that a set of hyperparameters can be efficiently applied  
3087        across different datasets, I perform the optimisation for each of the momentum ranges  
3088        considered. Table 8.3 shows the list of hyperparameters considered, and the range within

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.26:** 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.

3089 which I let them vary. I decided to fix the number of estimators to 400 in all cases, as  
3090 its value is correlated with that of the learning rate.

3091 I evaluate 10000 different hyperparameter configurations for each momentum range.  
3092 For the hyperparameter tuning, I used subsamples containing 10% of the full datasets,  
3093 keeping the original proportions between classes, in order to reduce the computational  
3094 load. The performance of the models was assessed using a stratified 3-fold cross-validation  
3095 with replacement. Cross-validation involves dividing the data in a number of subsets,  
3096 training the model using some of them, and testing it with the rest. In our case, I  
3097 divide the data in 3 equal-sized subsets, maintaining the class proportions of the original  
3098 dataset. Then, for 3 consecutive iterations, I train the models using 2 of the subsets  
3099 while I compute the precision and sensitivity scores with the other. This approach  
3100 provides a more robust estimate of the performance on unseen data.

3101 Figure 8.26 shows the results in the precision versus sensitivity plane, for the  
3102 momentum regions I, III and V (from left to right). The contours represent the curves  
3103 of equal  $F_1$ -score, i.e. the harmonic mean of the precision and the sensitivity. In order  
3104 to select the optimal configurations (indicated in the plots with a green cross), I chose  
3105 the point with the highest  $F_1$ -score.

3106 The results for the different momentum ranges are summarised in Tab. 8.3. One  
3107 can see some consistency in hyperparameter choices, with models generally preferring

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**Table 8.3:** 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 |

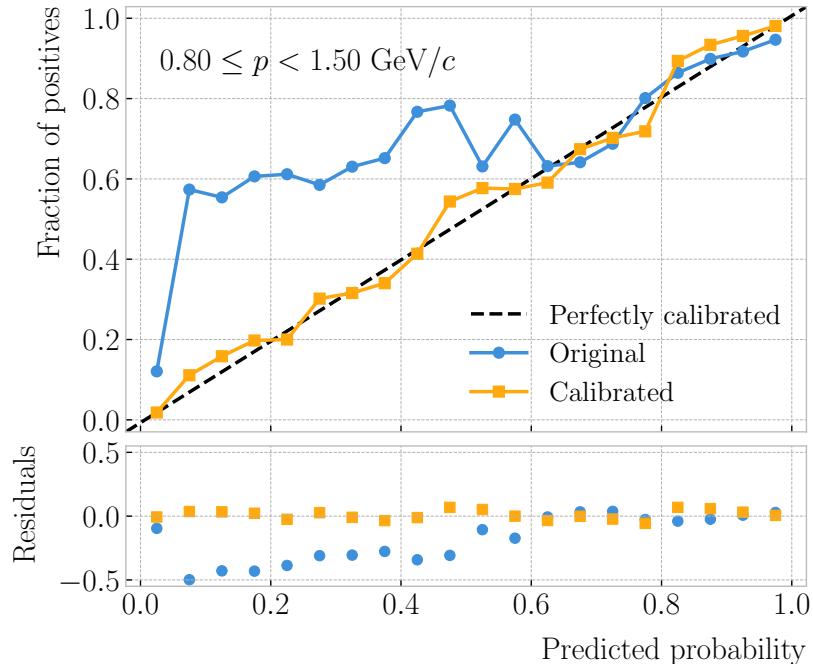
**Table 8.4:** Performance metrics of the BDTs with optimal hyperparameters, for the different momentum ranges.

| Metric       | Value $\pm 1\sigma$ |                   |                   |                   |                   |
|--------------|---------------------|-------------------|-------------------|-------------------|-------------------|
|              | I                   | II                | III               | IV                | V                 |
| Accuracy     | $0.779 \pm 0.003$   | $0.812 \pm 0.003$ | $0.846 \pm 0.002$ | $0.861 \pm 0.003$ | $0.874 \pm 0.002$ |
| Precision    | $0.769 \pm 0.003$   | $0.752 \pm 0.005$ | $0.788 \pm 0.002$ | $0.805 \pm 0.003$ | $0.815 \pm 0.003$ |
| Sensitivity  | $0.745 \pm 0.009$   | $0.921 \pm 0.006$ | $0.965 \pm 0.002$ | $0.967 \pm 0.002$ | $0.976 \pm 0.001$ |
| $F_1$ -score | $0.757 \pm 0.004$   | $0.828 \pm 0.003$ | $0.867 \pm 0.002$ | $0.879 \pm 0.002$ | $0.889 \pm 0.002$ |
| ROC AUC      | $0.868 \pm 0.003$   | $0.865 \pm 0.003$ | $0.899 \pm 0.002$ | $0.902 \pm 0.002$ | $0.911 \pm 0.001$ |

3108 small values for the tree-specific parameters, small learning rate, and relatively large  
 3109 subsample sizes.

3110 Now that I have obtained the optimal values of the hyperparameters, I can train  
 3111 the different BDTs. In this case I use the complete datasets, keeping 20% of the data  
 3112 for testing. Table 8.4 shows the values of the different performance metrics obtained  
 3113 using the selected hyperparameters and 5-fold cross-validation. The last row indicates  
 3114 the value of the area under the receiver operating characteristic (ROC) curve. This  
 3115 represents the sensitivity of a model as a function of the false positive rate. I have  
 3116 included it here as it is a classic model metric used in the machine learning community.  
 3117 Overall, there is a clear trend of models performing better at higher momentum.

## 8.2. Muon and pion separation in the ECal and MuID



**Figure 8.27:** Reliability diagrams for the BDT classifier used in the momentum range  $0.3 \leq p < 0.8$  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).

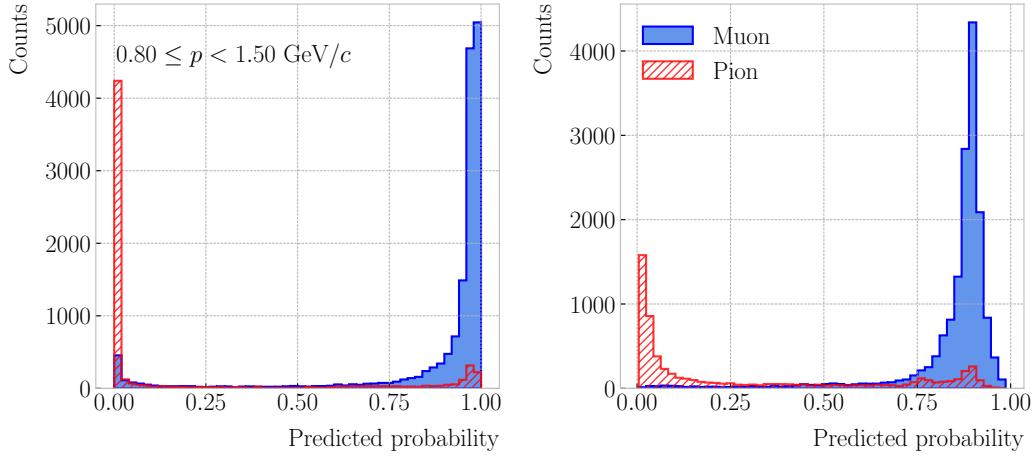
### 3118 8.2.5 Probability calibration

3119 So far, the trained BDTs are able to provide predictions of the class labels. Ideally,  
 3120 one would like the output of a classifier to give a confidence level about the prediction.  
 3121 However, it is not straightforward to interpret the outputs of our BDTs in terms of  
 3122 probabilities.

3123 A way to visualise how well the predictions of a classifier are calibrated is using  
 3124 reliability diagrams [92]. They represent the probability of the positive label versus the  
 3125 probability predicted by the classifier. These can be obtained by binning the predicted  
 3126 probabilities, and then compute the conditional probability  $P(y_{true} = 1 | y_i \leq y_{pred} <$   
 3127  $y_{i+1})$  by checking the fraction of true positive instances in each bin. The reliability  
 3128 diagram of a perfectly calibrated classifier would be a diagonal line.

3129 In this case, I try to correct the raw response of the classifiers by applying a sigmoid

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**Figure 8.28:** 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  $0.3 \leq p < 0.8 \text{ GeV}/c$ .

3130 function:

$$\sigma(x; A, B) = \frac{1}{1 + e^{Ax+B}}, \quad (8.18)$$

3131 where the parameters  $A$  and  $B$  are real numbers determined using the method of least  
3132 squares.

3133 For each classifier, I perform a grid search to obtain the optimal values of  $A$  and  $B$ .  
3134 For any pair, I compute the predicted probabilities as  $y_{pred} = \sigma(y_{raw}; A, B)$ , where  $y_{raw}$   
3135 are the raw predictions of the classifier<sup>9</sup>. Then, I calculate the corresponding reliability  
3136 curve, and take the sum of the squared residuals between it and the response of the  
3137 perfectly calibrated classifier.

3138 Figure 8.27 shows the reliability diagrams for the original (blue) and calibrated  
3139 (yellow) probability predictions of the classifier for the III momentum range,  $0.3 \leq p <$   
3140  $0.8 \text{ GeV}/c$ . The original response of the classifier is given by  $y_{pred} = \sigma(y_{raw}; -2, 0)$ ,  
3141 which is the transformation applied by `scikit-learn` to produce the probability estimate.  
3142 Notice how the calibrated prediction matches the ideal response much better than the  
3143 original, across all the probability range.

3144 One can also compare the responses of the uncalibrated and calibrated classifiers

---

<sup>9</sup>In `scikit-learn` these correspond to the outputs of the `decision_function` method.

### 8.3. ECal time-of-flight

3145 broken down by true particle type, as shown in Fig. 8.28. It can be seen that the  
3146 distributions for both muons (blue) and charged pions (red) smoothen after calibration,  
3147 but still the separating power of the classifier remains unchanged.

3148 At this point, having the trained classifiers and the probability calibration parameters,  
3149 I am able to assess the performance of the classification strategy in a physics-relevant  
3150 case.

#### 3151 8.2.6 Performance

### 3152 8.3 ECal time-of-flight

#### 3153 8.3.1 Arrival time estimations

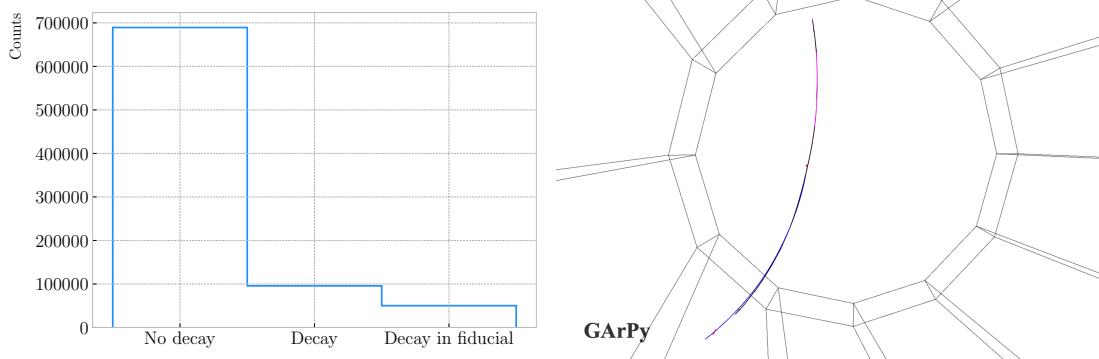
#### 3154 8.3.2 Proton and pion separation

### 3155 8.4 Charged pion decay in flight

3156 As discussed previously, in GArSoft the TPC tracks are formed after a pattern recognition  
3157 algorithm and a Kalman filter are applied to the TPC clusters. These two steps can  
3158 find discontinuities in the track candidates (e.g. due to a particle decay) when these  
3159 so-called breakpoints are large enough. However, for some, more subtle, cases they may  
3160 miss them and form a single reconstructed track. It has been noted in the literature  
3161 that Kalman filters offer, as a by-product, additional information to form test statistics  
3162 to identify these breakpoints [?, ?].

3163 Considering the mean life of the charged pion,  $\tau = (2.6033 \pm 0.0005) \times 10^{-8}$  s, one  
3164 can estimate that about 12% of the pions with momentum  $p \sim \mathcal{O}(500 \text{ MeV})$  (roughly  
3165 the peak of the pion momentum distribution in  $\nu_\mu$  CC interactions off argon) decay  
3166 inside the TPC. Figure 8.29 (left panel) shows the amount of charged pions decaying  
3167 in the full TPC and fiducial volumes from an isotropic, monoenergetic sample of  $10^5$   
3168 negatively charged pions with  $p = 500 \text{ MeV}$ . We see that about 10% of those decayed,  
3169 with more than half of them decaying inside the TPC fiducial volume.

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**Figure 8.29:** Left panel: number of non-decaying, decaying and decaying in the fiducial volume pions for a MC sample of  $10^5$ ,  $p = 500$  MeV 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.

3170     Figure 8.29 (right panel) shows an example event display of a charged pion (magenta  
 3171   line) decays in flight inside the TPC, but because the angle of the muon (blue line) is  
 3172   small both were reconstructed as one single track (black line). In this case, the composite  
 3173   track reaches the ECal, where it undergoes a muon-like interaction, thus being classified  
 3174   as a muon.

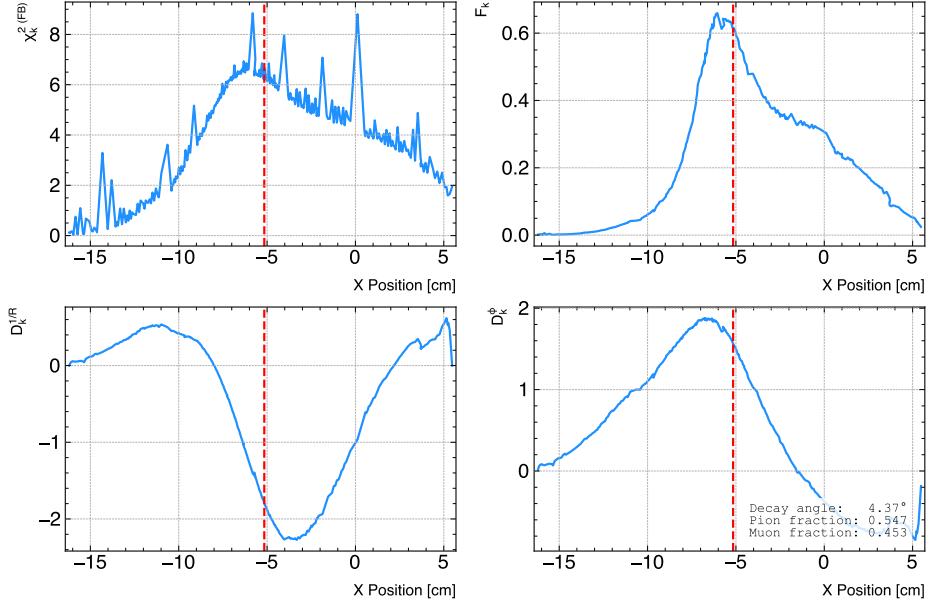
3175     A way to understand what decaying pion tracks were totally or partially reconstructed  
 3176   together with the daughter muon is looking at the relative energy contributions to the  
 3177   reconstructed track. In order to select a sample of such events, I require that a minimum  
 3178   50% of the total energy comes from the pion and at least 20% from the muon.

3179     To identify potential decays we can use the information we obtain from the Kalman  
 3180   filter at each step of the fitted track. The simplest test we can think about is computing  
 3181   the  $\chi^2$  of the mismatch between all the parameters in the forward and the backward fits:

$$\chi_k^{2(FB)} = (\hat{x}_k^B - \hat{x}_k^F)^T [V^{(\hat{x}_k, B)} + V^{(\hat{x}_k, F)}]^{-1} (\hat{x}_k^B - \hat{x}_k^F), \quad (8.19)$$

3182   where  $\hat{x}_k^F$ ,  $\hat{x}_k^B$  are the Kalman filter state vector estimates at step  $k$  in the forward and  
 3183   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.  
 3184   Using the values of the  $\chi^2$  at measurement  $k$  for the forward and backward fits we can

## 8.4. Charged pion decay in flight



**Figure 8.30:** Values of  $\chi_k^2(FB)$  (top left panel),  $F_k$  (top right panel),  $D_k^{1/R}$  (bottom left panel) and  $D_k^\phi$  (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.

3185 compute another  $\chi^2$  value that characterises the overall track fit:

$$\chi_{track}^2 = \chi_k^2(F) + \chi_k^2(B) + \chi_k^2(FB), \quad (8.20)$$

3186 which remains approximately constant for all  $k$ .

3187 An alternative approach proposed in the context of the NOMAD experiment was  
 3188 using a fit with a more elaborate breakpoint hypothesis, so we can perform a comparison  
 3189 of the  $\chi^2$  with and without breakpoints. This can be achieved by using some alternative  
 3190 parametrisation with extra parameters, which allows some of the track parameters to  
 3191 be discontinuous at certain points. A decay changes the momentum magnitude and  
 3192 direction, so we can use the new state vector:

$$\alpha = \left( y, z, 1/R_F, 1/R_B, \phi_F, \phi_B, \tan\lambda_F, \tan\lambda_B \right)^T. \quad (8.21)$$

3193 As we already have the estimates from the standard Kalman filter and their

## Chapter 8. Particle ID in GArSoft

3194 covariance matrices at each point, we do not need to repeat the Kalman fit for the new  
3195 parametrisation. Instead, I can compute the values of  $\alpha$  at each point  $k$  that minimise  
3196 the  $\chi^2$  resulting from comparing them to  $\{\hat{x}_k^B, \hat{x}_k^F\}$ . Introducing the two  $5 \times 8$  matrices:

$$H^F = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad H^B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (8.22)$$

3197 we can write this as:

$$\begin{aligned} \chi_k^{2(FB)}(\alpha) &= (\hat{x}_k^F - H^F \alpha)^T [V^{(\hat{x}_k, F)}]^{-1} (\hat{x}_k^F - H^F \alpha) \\ &\quad + (\hat{x}_k^B - H^B \alpha)^T [V^{(\hat{x}_k, B)}]^{-1} (\hat{x}_k^B - H^B \alpha). \end{aligned} \quad (8.23)$$

3198 The minimum of  $\chi_k^{2(FB)}(\alpha)$  is found when the measured new state vector takes the  
3199 value:

$$\hat{\alpha}_k = V^{(\hat{\alpha}_k)} H^T (V^{(\hat{x}_k)})^{-1} \hat{X}, \quad (8.24)$$

3200 where  $\hat{X} = \{\hat{x}_k^B, \hat{x}_k^F\}$ ,  $V^{(\hat{x}_k)}$  is the block diagonal matrix formed by  $V^{(\hat{x}_k, F)}$  and  $V^{(\hat{x}_k, B)}$   
3201 and  $V^{(\hat{\alpha}_k)}$  is the covariance matrix of  $\hat{\alpha}_k$ , given by:

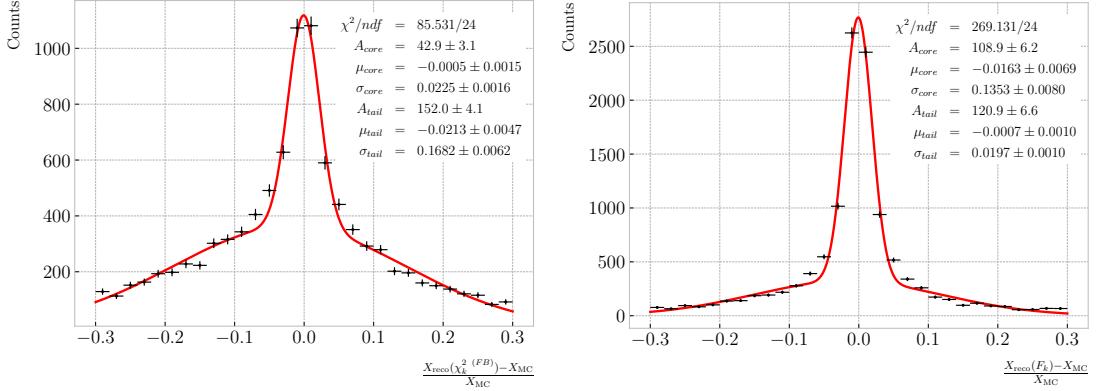
$$V^{(\hat{\alpha}_k)} = (H^T (V^{(\hat{x}_k)})^{-1} H)^{-1}. \quad (8.25)$$

3202 From these new fit estimates we can compute the  $F$  statistic, which tells us whether  
3203 the model with breakpoint provides a statistically significant better fit:

$$F_k = \left( \frac{\chi_{track,k}^2 - \chi_{full,k}^2}{8 - 5} \right) / \left( \frac{\chi_{full,k}^2}{N - 8} \right). \quad (8.26)$$

3204 One can also compute the signed difference of the duplicated variables divided by  
3205 their standard deviation at each point. These represent how significant the discontinuity

## 8.4. Charged pion decay in flight



**Figure 8.31:** 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).

3206 in each variable is. For any variable  $\eta$  we can write it as:

$$D_k^\eta = \frac{\hat{\eta}_k^B - \hat{\eta}_k^F}{\sqrt{\text{Var}[\hat{\eta}_k^F] + \text{Var}[\hat{\eta}_k^B] - 2\text{Cov}[\hat{\eta}_k^F, \hat{\eta}_k^B]}}. \quad (8.27)$$

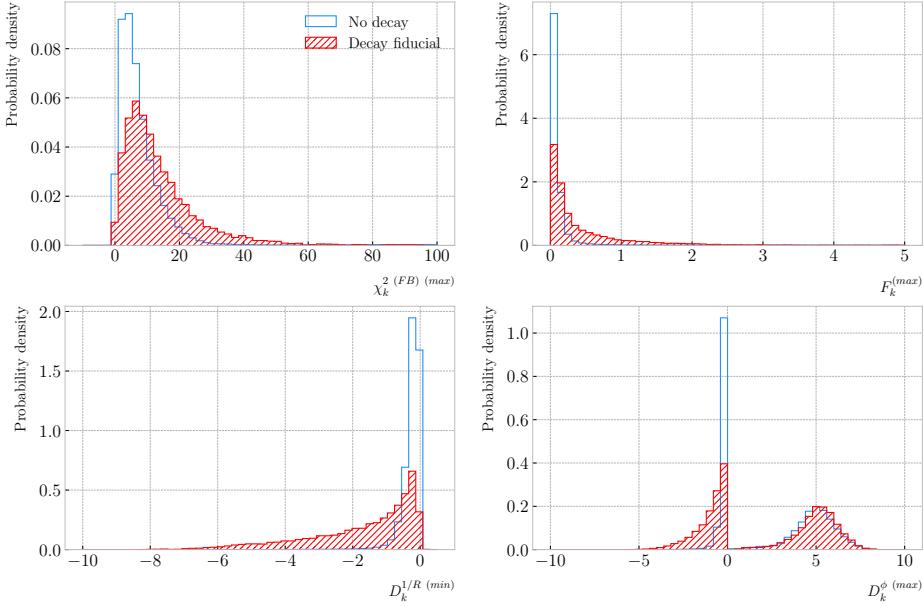
3207 In our case, the relevant ones to look at are  $D_k^{1/R}$  and  $D_k^\phi$ .

3208 Figure 8.30 shows the values of  $\chi_k^2(FB)$ ,  $F_k$ ,  $D_k^{1/R}$  and  $D_k^\phi$  as functions of the position  
3209 along the drift direction, for an example reconstructed track with 55.5% of the energy  
3210 coming from the charged pion and 45.5% from the daughter muon. The true position of  
3211 the decay is indicated (dashed red lines). Notice how  $\chi_k^2(FB)$  and  $F_k$ ,  $D_k^{1/R}$  reach their  
3212 maxima near the decay point. In the former case this indicates a large forward-backward  
3213 difference in the track fit. In the later it represents that the extended state vector  
3214 improves the fit particularly around that point.

3215 I can estimate the decay position finding resolution by computing the difference  
3216 between the  $X$  position of the maxima of  $\chi_k^2(FB)$  and  $F_k$  and the  $X$  position of the  
3217 true decay. Figure 8.31 represent the the fractional residual distributions for both cases,  
3218 from the sample of tracks containing pion decays. Fitting a double Gaussian to the  
3219 distributions (red lines) I find a resolution of 13.62% and 7.45% respectively.

3220 In principle, the  $F$ -statistic should follow a Fisher distribution with (8 – 5) and

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**Figure 8.32:** 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  $D_k^\phi$  (bottom right panel) for non-decaying reconstructed pion tracks (blue) and tracks which include the decay inside the fiducial volume (red).

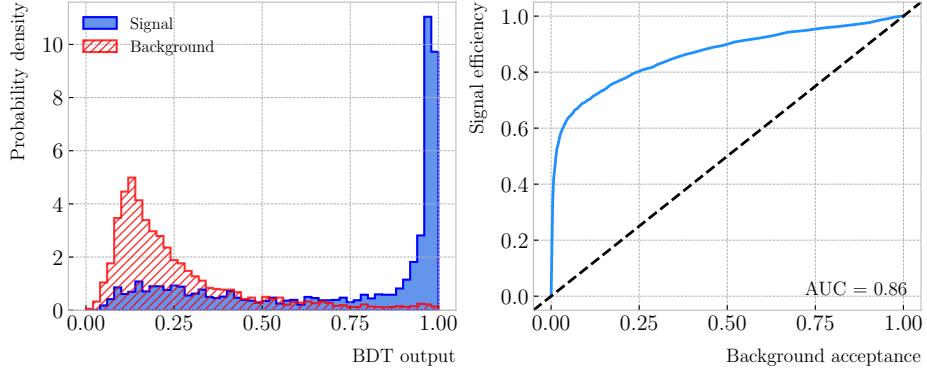
3221 ( $N = 8$ ) degrees of freedom under the null hypothesis. In most of our cases  $N \sim \mathcal{O}(100)$ ,  
 3222 so the probability density functions will look very similar. In this case, it is safe to take  
 3223 the limit  $N \rightarrow \infty$  in the Fisher PDF:

$$\begin{aligned}\tilde{f}(x; a - b) &= \lim_{N \rightarrow \infty} f(x; a - b, N - a) \\ &= \frac{2^{-\frac{a-b}{2}}}{\Gamma(\frac{a-b}{2})} (a - b)^{\frac{a-b}{2}} x^{\frac{a-b}{2}-1} e^{-\frac{a-b}{2}x}.\end{aligned}\tag{8.28}$$

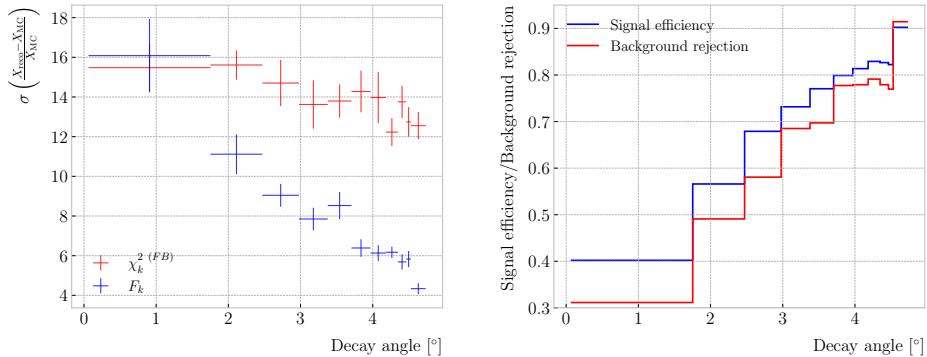
3224 In our case  $a - b = 8 - 5 = 3$ , so we would obtain a p-value of 0.05 at  $x = 2.60$ .

3225 Figure 8.32 contains the distributions of the maxima of  $\chi_k^{2(FB)}$ ,  $F_k$  and  $D_k^\phi$  and the  
 3226 minima of  $D_k^{1/R}$  for a sample of non-decaying pion tracks (blue) and another sample of  
 3227 reconstructed tracks containing part of the pion and the daughter muon from a decay  
 3228 inside the fiducial volume (red). Notice that, even though the values of  $F_k^{(max)}$  for the  
 3229 decay sample are typically larger than for the non-decaying one, just a small fraction of  
 3230 the events go beyond the aforementioned value of  $F = 2.60$ . Therefore, from a practical

## 8.4. Charged pion decay in flight



**Figure 8.33:** 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 8.34:** 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.

3231 point of view, it is not the most efficient variable to use for selecting the decay events.

3232 However, looking at the  $D_k^{1/R \text{ (min)}}$  distribution we can see there is a big difference  
 3233 between non-decaying and decaying events in this variable. One can use a combination  
 3234 of these four variables to distinguish between the pion decay events (signal) and the  
 3235 non-decaying pions (background).

3236 An approach to this classification could be using a boosted decision tree (BDT). One  
 3237 of the advantages of BDTs is that they are easy to interpret and identify the relative  
 3238 importance of the different input variables. Training a BDT with 400 estimators and a  
 3239 maximum depth of 4 I can obtain an efficient classification without overtraining. Figure

## Chapter 8. Particle ID in GArSoft

3240 8.33 (left panel) shows the distribution of probabilities predicted by the BDT for a test  
3241 sample. The signal efficiency as a function of background acceptance, the so-called ROC  
3242 curve, is shown in Fig. 8.33 (right panel). With a relative importance of 0.83, the most  
3243 important variable turned out to be  $D_k^{1/R \text{ (min)}}$ .

3244 One thing we can check is how the resolution to the decay and the signal efficiency in  
3245 the classification changes with the true decay angle. Using an equal-frequency binning  
3246 for the decay angles, we can repeat the previous steps for each bin.

3247 Figure 8.34 (left panel) shows the dependence on the decay angle of the decay finding  
3248 resolution. We can see that for the  $\chi_k^2 \text{ (FB)}$  maximum location method the resolution  
3249 consistently lies between 12 to 16%. However, the  $F_k^{(max)}$  approach gives a significantly  
3250 better resolution for high angle values, reaching the 4 – 6% range for decay angles  $\geq 4^\circ$ .

3251 For the classification dependence on the angle, I use the same classifier I trained  
3252 before but evaluating the test sample for each individual angular bin. I compute the  
3253 signal efficiency in each bin for a fixed value of the background rejection, in this case  
3254 90%. Similarly, for the background rejection estimation I use a fixed signal efficiency  
3255 value of 90%. Figure 8.34 (right panel) represents the change in signal efficiency (blue)  
3256 and background rejection (red) with the value of the true decay angles.

### 3257 8.4.1 Track breakpoints

## 3258 8.5 Neutral particle identification

### 3259 8.5.1 ECal clustering

3260 Another important reconstruction item is the clustering algorithm of ECal hits in  
3261 GArSoft. The default module features a NN algorithm that treats all hits in the same  
3262 way, independently of the layer each hit comes from. However, the current ECal design  
3263 of ND-GAr has two very different types of scintillator layers. The inner layers are made  
3264 out of tiles, which provide excellent angular and timing resolutions. On the other hand,  
3265 the outer layers are cross scintillator strips. That way, an algorithm that treats hits  
3266 from both kinds of layers differently may be able to improve the current performance.

## 8.5. Neutral particle identification

3267     Inspired by the reconstruction of T2K’s ND280 downstream ECal [?], the idea was  
3268    to put together a clustering module that first builds clusters for the different ECal views  
3269    (tiles, strips segmented in the  $X$  direction and strips segmented in  $Y$  direction), and  
3270    then tries to match them together to form the final clusters.

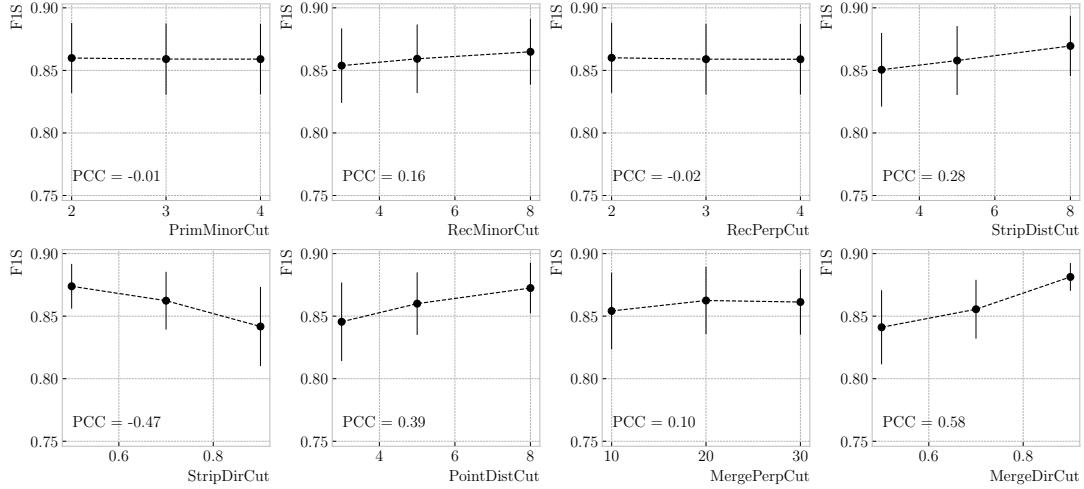
3271     Working on a module-by-module basis, the algorithm first separates the hits depending  
3272    on the layer type they come from. Then, it performs a NN clustering for the 3 sets of  
3273    hits separately. For the tile hits it clusters together all the hits which are in nearest-  
3274    neighbouring tiles and nearest-neighbouring layers, for strip hits it looks at nearest-  
3275    neighbouring strips and next-to-nearest-neighbouring layers (as the layers with strips  
3276    along the two directions are alternated). For strip clusters an additional cut in the  
3277    direction along the strip length is needed.

3278     After this first clustering I then apply a recursive re-clustering for each collection  
3279    of strip clusters based on a PCA method. In each case, we loop over the clusters with  
3280     $N_{hits} \geq 2$ , computing the centre of mass and three principal components. Propagating  
3281    these axes up to the layers of the rest of the clusters, we check if the propagated point  
3282    and the centre of mass of the second cluster are within next-to-nearest-neighbouring  
3283    strips. An additional cut in the direction along the strip length is also needed. Moreover,  
3284    I require that the two closest hits across the two clusters are at most in next-to-nearest-  
3285    neighbouring strips. I merge the clusters if these three conditions are satisfied. The  
3286    re-clustering is repeated until no more cluster pairs pass the cuts.

3287     The clusters in each strip view are combined if their centres of mass are close enough  
3288    and they point in the same direction. An alternative approach for the strip cluster  
3289    merging could be to compute the overlap between the ellipsoids defined by the principal  
3290    axes of the clusters, and then merge the pair if the overlap exceeds some threshold.  
3291    Further study is needed to understand if this change would have an impact in the overall  
3292    clustering performance.

3293     To merge the tile clusters to the combined strip clusters I propagate the principal  
3294    axis of the strip cluster towards the inner layers, up to the centre of mass layer of the  
3295    tile cluster. I merge the clusters if the distance between the propagated point and the

## Chapter 8. Particle ID in GArSoft



**Figure 8.35:** 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  $\nu_\mu$  CC interaction events.

3296 centre of mass is bellow a certain cut.

3297 The last step is to check if clusters in neighbouring modules should be merged  
 3298 together, both across two barrel modules, across end cap modules and between barrel  
 3299 end cap modules. I check the distance between the two closest hits in the pair of clusters  
 3300 and merge them if it passes this and an additional direction cut.

3301 Figure ?? presents an example of the clustering steps relevant for strip layer hits, from  
 3302 the input hits (top left panel) to the NN clustering (top right panel) and re-clustering  
 3303 (bottom left panel) for each strip view and the final merging strip clusters (bottom  
 3304 right panel). It shows the hits from a single ECal barrel module in a  $\nu_\mu$  CC interaction  
 3305 event with a neutral pion and a proton in the final state. The two clusters on the left  
 3306 correspond to the photon pair from the  $\pi^0$  decay and the one on the upper right corner  
 3307 is associated to the proton.

3308 This algorithm has a total number of eight free parameters that need to be optimised.  
 3309 I used a sample of 1000  $\nu_\mu$  CC interactions in order to obtain the optimal configuration of  
 3310 clustering parameters. This sample was generated up to the default ECal hit clustering  
 3311 level, so then I could run the new clustering algorithm each time with a different

## 8.5. Neutral particle identification

**Table 8.5:** Summary of parameters and sampled values used in the optimisation of the clustering algorithm.

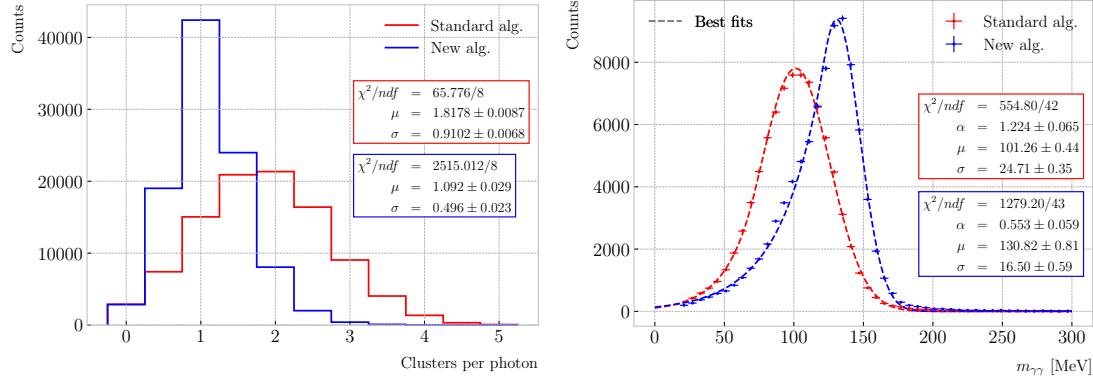
| Name         | Units  | Sampled values | Description                                                                  |
|--------------|--------|----------------|------------------------------------------------------------------------------|
| PrimMinorCut | strips | 2, 3, 4        | Distance along 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                                    |

3312 configuration of parameters. As the number of parameters is relatively large, I only  
 3313 performed a coarse-grained scan of the parameter space. Sampling each of the eight  
 3314 parameters at three different points each I obtain 6561 different configurations. These  
 3315 parameters, together with the used values, are summarised in Tab. 8.5.

3316 In order to measure the performance of the clustering, I use a binary classification  
 3317 approach. For each formed cluster, I identify the Geant4 Track ID of the matching MC  
 3318 particle and the energy fraction of each hit. Then, I assign to each cluster the Track ID  
 3319 with the highest total energy fraction. For each of the different Track IDs associated to  
 3320 the clusters, I select the cluster with the highest energy (only from the hits with the  
 3321 same Track ID). I identify such a cluster as the main cluster for that Track ID. I count  
 3322 as true positives (TPs) the hits with the correct Track ID in each main cluster. False  
 3323 positives (FPs) are the hits with the incorrect Track ID for the cluster they are in, not  
 3324 only main clusters. The false negatives (FNs) are the hits with the correct Track ID in  
 3325 clusters other than the main.

3326 Figure 8.35 shows the computed  $F_1$ -score values for the different cuts. In each case,  
 3327 the central value represents the mean of the  $F_1$ -score distribution for the specified value  
 3328 of the corresponding variable and the vertical error bar represents one standard deviation

## Chapter 8. Particle ID in GArSoft



**Figure 8.36:** Left panel: distributions of the number of ECal clusters per photon from  $\pi^0$  decays for the standard (red) and new (blue) clustering algorithms. Right panel: reconstructed invariant mass distributions for photon pairs from single  $\pi^0$  events using the standard (red) and new (blue) ECal clustering algorithms.

3329 around the mean. Also shown are the Pearson correlation coefficients of these central  
 3330 values. We can see that five of the variables have a sizeable effect on the  $F_1$ -score, with  
 3331 an absolute difference between the last and first values as big as 4%.

3332 The working configuration is obtained as follows. I first select all configurations  
 3333 with purity  $\geq 90\%$ . Among those, I choose the combinations that yield the maximum  
 3334  $F_1$ -score. If more than one configuration remains I select the one with the highest  
 3335 sensitivity. Doing so, I end up with a parameter configuration with an efficiency of 88%  
 3336 and a 90% purity. Compared with the default algorithm, which gives an efficiency of  
 3337 76% and a purity of 91% for the same sample, I have managed to improve the efficiency  
 3338 by a factor of 1.16.

### 3339 8.5.2 $\pi^0$ reconstruction

3340 One of the potential applications of the new ECal hit clustering is the reconstruction of  
 3341 neutral particles, in particular pions. Neutral pions decay promptly after being produced,  
 3342 through the  $\pi^0 \rightarrow \gamma\gamma$  channel  $(98.823 \pm 0.034)\%$  of the time. The photon pair does  
 3343 not leave any traces in the HPgTPC (unless one or both of them converts into an  
 3344 electron-positron pair), but each of them will produce an electromagnetic shower in  
 3345 the ECal.

## 8.5. Neutral particle identification

3346 To test the potential impact of the new algorithm in  $\pi^0$  reconstruction, I generated  
3347 a MC sample of single, isotropic neutral pions inside the HPgTPC. All pions were  
3348 generated with a momentum  $p = 500$  MeV and their initial positions were uniformly  
3349 sampled inside a  $2 \times 2 \times 2$  m box aligned with the centre of the TPC. I ran both the  
3350 default and the new clustering algorithms, using for the latter the optimised configuration  
3351 discussed above.

3352 The first thing to notice is that the number of clusters produced per photon has  
3353 decreased. Figure 8.36 (left panel) shows these distributions for the default (red) and  
3354 new (blue) algorithms. Using a simple Gaussian fit, we see that the mean number of  
3355 ECal clusters per photon went from  $1.82 \pm 0.01$  to  $1.09 \pm 0.03$ . This effectively means that  
3356 with the new algorithm the ECal activity of one true particle is typically reconstructed  
3357 as a single object. From the reconstruction point of view this can be an advantage. As  
3358 now most of the photon energy ends up in a single ECal cluster, I can simply use cluster  
3359 pairs to identify the  $\pi^0$  decay.

3360 In general, one calculates the invariant mass of the photon pair as:

$$m_{\gamma\gamma} = \sqrt{2E_1E_2(1 - \cos \theta)}, \quad (8.29)$$

3361 where  $E_i$  are the energies of the photons and  $\theta$  the opening angle between them. In this  
3362 case I can use the energies deposited in the ECal and their incident directions. This  
3363 quantity is computed for all possible pairs of clusters, using their position together with  
3364 the true decay point. In a more realistic scenario, e.g.  $\nu_\mu$  CC interaction, one could use  
3365 the position of the reconstructed primary vertex instead. I also tried to use the principal  
3366 direction of the clusters, but that approach gave considerably worse results. For each  
3367 event I only keep the pair with an invariant mass closer to the true  $\pi^0$  mass value.

3368 Figure 8.36 (right panel) shows the invariant mass distributions for the photon pairs  
3369 we get using the default (red) and the new (blue) ECal clustering algorithms. For the fit  
3370 I used a modified version of the Crystal Ball function [?], obtained by taking the limit

## Chapter 8. Particle ID in GArSoft

3371 where the parameter controlling the power-law tail goes to infinity:

$$f(x; N, \mu, \sigma, \alpha) = N \cdot \begin{cases} e^{\frac{\alpha(2x-2\mu+\alpha\sigma)}{2\sigma}}; & x \leq \mu - \alpha\sigma, \\ e^{-\frac{(x-\mu)^2}{2\sigma^2}}; & x > \mu - \alpha\sigma. \end{cases} \quad (8.30)$$

3372 Comparing the fitted mean and standard deviation values for the Gaussian cores, we  
3373 see that the distribution for the new algorithm is a 67% narrower and also peaks much  
3374 closer to the true  $m_{\pi^0}$  value, going from  $101.3 \pm 0.4$  MeV to  $130.8 \pm 0.6$  MeV.

<sup>3375</sup> Chapter 9

<sup>3376</sup> Event selection in ND-GAr

<sup>3377</sup> 9.1 CAFs and CAFAna

<sup>3378</sup> 9.2 Event selection

<sup>3379</sup> 9.2.1  $\nu_\mu$  CC selection

<sup>3380</sup> 9.2.2 Charged pion multiplicity



<sup>3381</sup> Chapter 10

<sup>3382</sup> Conclusions



<sup>3383</sup> Appendix A

<sup>3384</sup> An appendix



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