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Chapter 1

Computing in DUNE

This chapter briefly describes the DUNE computing model, which touches on all elements of the ND and FD and their physics programs. More detailed aspects of the model may be found in Appendix **??**. *DUNE will produce a complete technical design report for computing over the next two years.*

1.1 Overview

The Deep Underground Neutrino Experiment (DUNE) experiment will commission the first 10 kt fiducial mass far detector (FD) module between 2024 and 2026 with a long data-taking run, and the remaining three modules between 2026 and 2036. An active prototyping program is ongoing at the European Organization for Nuclear Research (CERN), where a short test beam run took place in 2018 with ProtoDUNE-SP, a 700 t, 15,360 channel prototype liquid argon time-projection chamber (LArTPC) with single-phase (SP) readout. Tests of a dual-phase (DP) detector of similar size began in mid-2019. The DUNE experiment has already benefited greatly from these initial tests. The collaboration has recently formed a formal computing and software consortium (CSC), with significant participation of European institutions and interest from groups in Asia, to develop common software and computing, and to formalize resource contributions.

The CSC resource model benefits from the existing Open Science Grid (OSG) and Worldwide LHC Computing Grid (WLCG) infrastructure developed for the LHC and broader HEP community. DUNE is already using global resources to simulate and analyze ProtoDUNE-SP data. Several European institutions are part of this resource pool, making significant contributions to the ProtoDUNE-SP and ProtoDUNE-DP programs. We expect this global computing consortium to grow and evolve as we begin gathering data from the full DUNE detector in the 2020s.

The long-term DUNE science program should produce volumes of raw data similar in scale to the data volumes that current LHC Run-2 experiments have already successfully handled. Baseline predictions for the DUNE data, depending on actual detector performance and noise levels, are

$\sim$30 PB of raw data per year. These data, with simulations and derived analysis samples, will need to be made available to all collaborating institutions. We anticipate that institutions around the world will both contribute and use storage and CPU resources for DUNE.

The DUNE computing strategy starts with considerable infrastructure in place for international computing collaboration, in part thanks to the LHC program. Additional large non-LHC experiments, such as Large Synoptic Survey Telescope (LSST), the Belle II B-factory experiment, and DUNE will begin operation over the next decade and must use and expand upon this model to encourage international cooperation. The broader HEP community is organizing common efforts through the HEP Software Foundation Collaboration (HSC) [1]. The HSC is an organization of interested parties using the extensive knowledge gained over the past two decades to anticipate the needs of experiments over the next two decades, and to develop a sustainable computing landscape for the HEP community. The HSC white papers and roadmaps emphasize common tools and infrastructure as the foundation of this landscape.

The DUNE computing strategy heavily leverages the HSC model of common tools and infrastructure, which encompass data movement and storage, job control and monitoring, accounting, and authentication. DUNE recognizes that other large-scale experiments have similar needs and will encounter complementary issues, thus driving worldwide cooperation on common tools as the most cost-effective way to fulfill the scientific missions of the experiments. DUNE pilot programs already use this model. Most recently in data management and storage, Fermi National Accelerator Laboratory (Fermilab), CERN, Rutherford Appleton Laboratory, and other research and academic institutions in the UK are collaborating on adapting and using the Rucio data management systems [2] to serve as the core data management system for DUNE.

This protoculture of international collaboration within DUNE was demonstrated during the 2018 test beam run of the ProtoDUNE-SP detector, which produced raw data at rates of up to 2 GB/s. These data were transferred and stored in the archive facilities at CERN and Fermilab, and replicated at sites in the UK and Czech Republic. In a more recent commissioning test for the ProtoDUNE-DP detector, similar data transmission rates were achieved to CERN, Fermilab, and the CCIN2P3 computer center in Lyon, France.

In total, 1.8 PB of raw data were produced during the ten-week test beam run, mimicking, within a factor of two, expected data rates and volumes from the initial running of the FD complex. The prototype run was used to examine and test the scalability of existing and proposed computing infrastructure and to establish operational experience within the institutions that have expressed interest in developing and constructing the DUNE computing environment. The planning for DUNE is primarily based on the measurements and information gained from the ProtoDUNE experience. These measurements are proofs-of-concept for many of the systems, and their behavior can be reliably extrapolated to the projected levels needed for the complete DUNE experiment.

The ProtoDUNE experience highlights the significant technical challenges that must be overcome by 2024 for DUNE. Among the most significant will be 1) the design of DUNE-specific systems able to integrate the large suite of ancillary data (e.g., configurations, calibrations, shower libraries) with the main time projection chamber (TPC) data stream; 2) the potentially extreme size of some physics interactions, notably supernova bursts, that could produce enough data to overwhelm conventional processors; and 3) the continuing need for evolution of computing architectures and

infrastructure over the next decade. These challenges are unique to DUNE where the limiting factor will be human effort.

In summary, the DUNE computing strategy must be global, working with partners worldwide, and collaborative because many of the computational challenges we face are also faced by other, similar experiments. We are extremely fortunate to have the ProtoDUNE experience and test data to exercise our computing infrastructure and develop algorithms for full DUNE operations, although we know significant and interesting challenges lie ahead.

1.2 Computing Consortium

1.2.1 Overview

The mission of the DUNE CSC is to acquire, process, and analyze both detector data and simulations for the collaboration. This mission must extend over all the primary physics drivers for the experiment and must do so both cost effectively and securely. The CSC provides the bridge between the online systems for data acquisition (DAQ) and monitoring and the physics groups who develop high-level algorithms and analysis techniques to perform measurements using the DUNE data and simulations. The CSC works with collaborating institutions to identify and provide computational and storage resources. It provides the software and computing infrastructure in the form of analysis frameworks, data catalogs, data transport systems, database infrastructure, code distribution mechanisms, production systems, and other support services essential for recording and analyzing the data and simulations.

The CSC works with national agencies and major laboratories to negotiate use and allocation of computing resources. This work includes support for near-term R&D efforts such as ProtoDUNE runs, and extends to designing, developing, and deploying the DUNE computing model and its requisite systems. This includes evaluating major software infrastructure systems to determine their usefulness in meeting the DUNE physics requirements. These evaluations should identify opportunities to adopt or adapt existing technologies, and to engage in collaborative ventures with HEP experiments outside of DUNE.

At first glance, the DUNE CPU and storage needs appear modest compared to the corresponding needs for the high-luminosity LHC experiments. However, the beam structure, event sizes, and analysis methodologies make DUNE very unlike collider experiments in event processing needs and projected computational budgets. In particular, the large DUNE event sizes (0.1-10 GB as opposed to 1-10 MB per detector readout) present a novel technical challenge when data processing and analysis are mapped onto current and planned computing facilities. The advent of high-performance computing systems optimized for parallel processing of large data arrays is a great advantage for DUNE. These architectures suit the uniform LArTPC raw data structure very well, in contrast to the more complex data structures and geometries present in conventional heterogeneous HEP data.

DUNE will require significant effort to adapt to emerging global computing resources that likely will be both more heterogeneous in computational capabilities (e.g., featuring CPU, GPU, and other advanced technologies) and more diverse in topological architectures and provisioning models. The DUNE CSC must be ready to fully exploit these global resources after 2026, allowing all collaborators to access the data and meet the scientific mission of the experiment.

1.2.2 Resources and Governance

The CSC was formed from an earlier ad hoc DUNE computing and software group. The governance structure for the CSC is described in Ref. [3]. The consortium coordinates work across the collaboration, but funding comes from collaborating institutions, laboratories, and national funding agencies.

The CSC has an elected consortium leader who is responsible for subsystem deliverables and represents the consortium in the overall DUNE collaboration. In addition, technical leads act as overall project managers for the CSC. The technical leads report to the overall consortium leader. CSC has both a host laboratory technical lead to coordinate between the DUNE project and Fermilab, the host laboratory, and an international technical lead to coordinate with other entities. At least one of the three leadership roles should be held by a scientist from outside the USA. CSC management currently appoints people to other roles, typically after a call for nominations. A more formal structure for institutional contributions and commitments is under consideration.

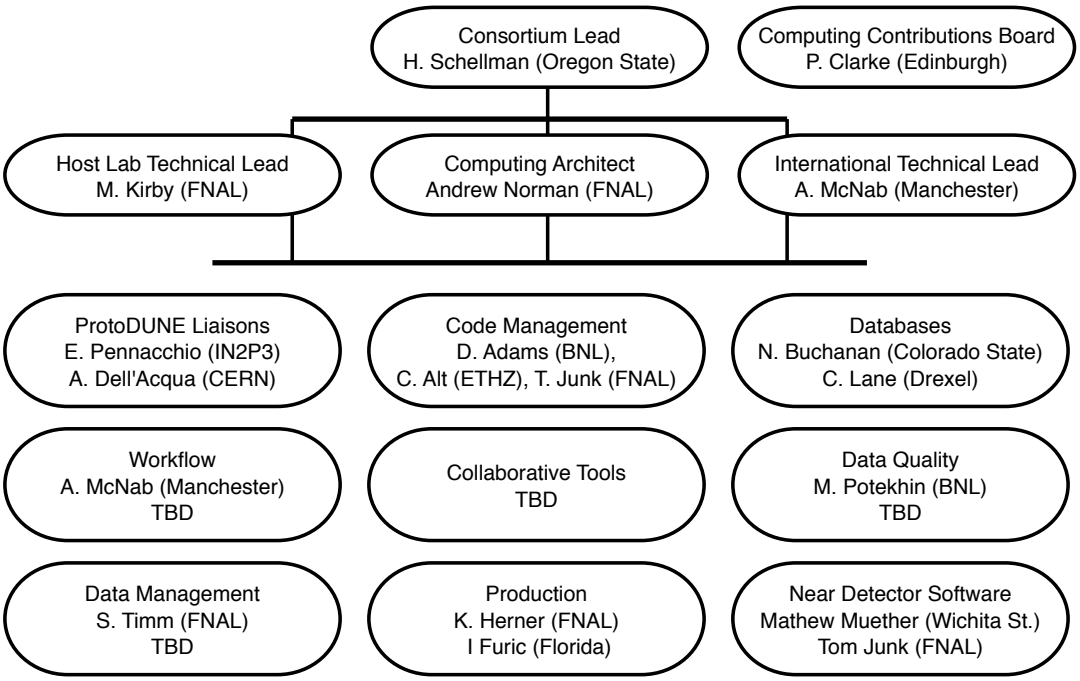


Figure 1.1: Organization chart for current CSC.

1.2.3 Scope of the Consortium

The CSC member institutions (Table 1.1) focus on the hardware and software infrastructure for offline computing. Responsibility for developing algorithms resides with the physics groups, and online systems at experimental sites are governed by the DAQ and cryogenic instrumentation and slow controls (CISC) consortia. The CSC defines interfaces, sets coding standards, and provides training. All groups coordinate closely to ensure that the full chain of data acquisition, processing, and analysis functions properly. Formal interfaces with the DAQ and controls groups are described in [4, 5].

The CSC operates at two levels: at the hardware level, where generic resources can be provided as in-kind contributions to the collaboration, and at the human level, where individuals and groups help develop common software infrastructure. The technology for hardware contributions (e.g., grid CPU and storage) exists and was successfully used during the ProtoDUNE-SP data run and its associated simulation and reconstruction. Highlights of that effort are discussed below and in Volume II, DUNE Physics, Chapter 4.

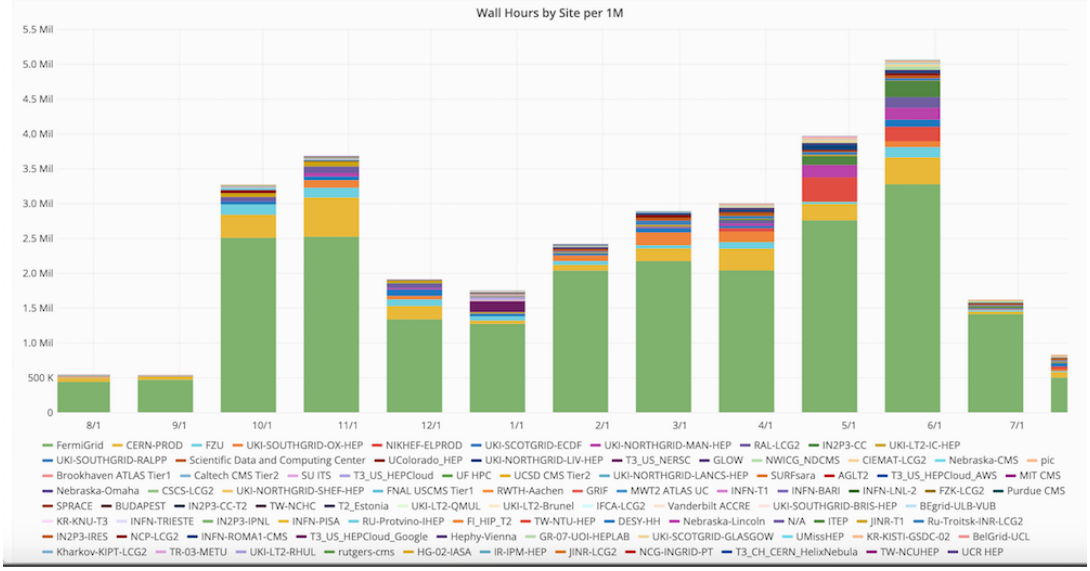


Figure 1.2: CPU wall-time from July 2018 to July 2019, the first peak shows ProtoDUNE-SP reconstruction while the second is dominated by data analysis and ProtoDUNE-DP simulation. A total of 31 million wall-hours were delivered with 24 M-hrs coming from Fermilab.

1.2.4 Hardware Resources

As illustrated in Figure 1.2, the DUNE collaboration has already used substantial global resources through the WLCG and OSG mechanisms. As the experiment evolves over the next five years, institutions and collaborating nations will be asked to formally pledge resources (both CPU and storage), and those resources will be accounted for and considered in-kind contributions to the collaboration. A computing resources board will be set up to administer this process and serve as liaison to national resource providers.

Several international partners are already contributing substantially to CPU resources, and we continue to integrate additional large national facilities. Most CPU resources are opportunistic, but Fermilab and CERN have committed several thousand processor cores and several PB of data storage. Additionally, DUNE is one of the first beneficiaries of the IRIS project (UK), which provides computing for astronomy and particle physics. We are working with OSG and WLCG to integrate reporting mechanisms for CPU use, so accurate monitoring of hardware contributions will be in place for a second planned ProtoDUNE run in 2021-2022 and the buildup to data taking in the mid 2020's.

1.2.5 Personnel

The advancement of a dedicated DUNE computing team responsible for operations and development of new tools specific to the DUNE experiment is ongoing. Figure 1.1 shows the current CSC organization, where only a few of the listed individuals are full-time on DUNE. Thus, we rely on common tools and techniques shared with other, smaller experiments at CERN and Fermilab. In particular, DUNE operates as one of several intensity frontier experiments at Fermilab where a substantial amount of shared resources can be accessed, but with few personnel assigned specifically to DUNE.

The full DUNE software and computing effort will be much larger than that for ProtoDUNE. The unique DUNE data footprint and anticipated evolution in processor technologies will require a major undertaking to construct and operate the necessary computing infrastructure. This infrastructure must be in place well before detector commissioning begins at Sanford Underground Research Facility (SURF).

Two basic design tenets are cooperation with the broader community and reuse of tools. Collaboration scientists will develop much of the high-level algorithms, but a dedicated group of experts with advanced programming and project management skills are needed to build and operate the core software infrastructure for the experiment. Personnel resources are similar to those required for LHCb and Belle II, which are collaborations of a similar size to DUNE. Based on a comparison to those experiments, approximately 20 full-time-equivalent (FTE) workers should be dedicated to ensure primary DUNE software and computing needs are met. This estimate of future personnel requirements follows from an assessment of the LHCb organization structure.

Appendix **??** describes computing personnel activities in detail. In summary, we will need approximately 20 FTE, with 10 FTE for a software development team that will create and maintain the primary software needed to run DUNE algorithms, and the distributed software infrastructure. Some of these efforts will be completed jointly with other collaborations and HSC/WLCG projects, but in return, DUNE must make substantive contributions to these common efforts. In addition to the software development effort, DUNE computing will require specific operational roles such as data manager, code librarian, and user support. Based on LHCb experience, we have identified ten such roles each requiring an FTE of 0.5 to 2.0. These roles can be filled by experienced DUNE collaborators or computing professionals, and their contributions to the experiment should be properly recognized as equivalent to efforts in construction or operation of the experiment.

Table 1.1: DUNE computing and software consortium members

Institution	Country
Centro Brasileiro de Pesquisas Físicas	Brazil
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York University	Canada
European Organization for Nuclear Research	CERN
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Laboratoire d'Annecy-le-Vieux de Physique des Particules	France
Tata Institute of Fundamental Research	India
Korean Institute for Science and Technology Information	Korea
Nikhef National Institute of Subatomic Physics	Netherlands
University of Bern	Switzerland
Centro de Investigaciones Energéticas, Medeioambientales y Technólogicas	Spain
University of Edinburgh	UK
The GridPP Collaboration	UK
University of Manchester	UK
Queen Mary University	UK
STFC Rutherford Appleton Laboratory	UK
Argonne National Laboratory	USA
University of California, Berkeley	USA
Brookhaven National Lab	USA
Colorado State University	USA
University of Colorado Boulder	USA
Fermi National Accelerator Laboratory	USA
University of Florida	USA
Lawrence Berkeley National Laboratory	USA
University of Minnesota	USA
Northern Illinois University	USA
University of Notre Dame	USA
Oregon State University	USA
SLAC National Accelerator Laboratory	USA
The University of Texas at Austin	USA
Valley City State University	USA

The CSC has instituted a series of workshops, which started with two on the topic of "Data Model and Infrastructure" in the summer and fall of 2019, to set the scope of the subprojects to prepare for a formal computing technical design report (TDR). Table 1.2 gives a draft timeline for the computing project.

1.2.6 Resource Contributions

The CSC resource board is developing a formal resource funding model. Currently, we would expect collaborating countries to contribute to computing physical resources and operational duties (e.g., shifts) distributed fairly and developed in consultation with the full DUNE collaboration. The core of the software development effort would mainly come from CSC members. Contributions will be a mix of CPU resources, storage, and personnel, with the mix tailored to the resources and capabilities of each country and institution. To date, these contributions have been voluntary and opportunistic, but will evolve to a more formal model similar to the pledges in the LHC experiments.

1.3 Data Types and Data Volumes

Offline computing for DUNE creates new and considerable challenges because of the experiment's large scale and diverse physics goals. In particular, the advent of LArTPCs with an exquisite resolution and sensitivity, combined with the enormous physical volume of the DUNE far detector and its large number of readout channels, presents challenges in acquiring, storing, reducing, and analyzing a prodigious amount of data — orders of magnitude more data than in previous neutrino experiments.

Neutrino experiments operate at low event rates, on the order of 1 Hz even for near detectors. Despite these low event rates, DUNE can generate enormous amounts of data from a single event. This leads to unique challenges in cataloguing, storing and reconstructing data, even though the total volume of data and CPU needs are significantly lower than in large collider experiments. At a collider, each of the billions of triggered beam crossings is reasonably small and effectively independent of the others. In contrast, a single DUNE trigger readout can be many GB in size and, in the case of a supernova candidate, many TB. Maintaining the coherence of such large correlated volumes of data in a distributed computing environment presents a significant challenge.

The rapidly changing computing landscape presents other challenges in this area, as the traditional HEP architecture of individual core processors running single-threaded applications is superseded by applications that efficiently use multiple processors and perhaps even require GPUs. At the same time, despite the rapid development of algorithms for LArTPC reconstruction, they are by no means mature. The ProtoDUNE-SP test at CERN in fall 2018 has contributed greatly to this development by providing a wealth of data that will inform the evolution of future DUNE computing models.

Table 1.2: Milestones for DUNE computing development. Data volumes assume 15 PB/year of compressed raw data starting in 2024.

Year	Activity	Integrated data, PB
2018		10
	ProtoDUNE-SP beam run	
2019		19
	ProtoDUNE-SP processing	
	ProtoDUNE-DP commissioning and data taking	
	Develop resource model	
	Develop high level task list	
2020		21
	Continue ProtoDUNE processing/operations Formalize international resource model	
	Build operations team	
	Evaluate data and computing models	
	Database design for hardware	
2021		25
	Produce Computing TDR	
	Framework modifications for HPC	
	Database design for conditions/configuration	
2022		39
	ProtoDUNE second beam run	
	Begin large scale purchases for FD commissioning	
2023		43
	Reconstruct/analyze ProtoDUNE results	
	Continue ProtoDUNE processing/operations	
	Support FD commissioning	
	Conditions and configuration data fully integrated	
	Acquire storage for first year of data from one module	
2024		66
	First real data from one FD module	
	Full operations team in place	
	Data analysis challenges	
2025		88
	Complete provisioning of hardware/storage for first beam run	
2026		111
	First beam run with two modules	

The CSC, SP DAQ, and host laboratory have agreed on a preliminary maximum data transfer rate from the FD to Fermilab of 100 Gbit/s, consistent with projected network bandwidths in the mid 2020s, and a limit of 30 PB/year raw data stored to tape. Calibration for the FD modules (10 PB/year/module to 15 PB/year/module) and beam and cosmic ray interactions in the near detector (ND) will dominate uncompressed data volumes. With a factor of four for lossless compression, we anticipate a total compressed data volume of 3 PB/year/module to 5 PB/year/module for the full FD; ND rates are not yet established but are likely smaller.

This section describes the make-up and rates of the data to be transfered.

1.3.1 Single-phase Technology Data Estimates

Each of the 150 SP module anode plane assemblies (APAs) (Section **??**) has 2,560 readout channels, each of which is sampled with 12 bit precision every 500 ns. For a TPC of this size, drift times in the liquid argon (LAr) are approximately 2.5 ms and the volume of raw data before compression is approximately 6 GB per 5.4 ms readout window. With no triggering and no zero suppression or compression, the volume of raw data for the four modules would be on the order of 145 exaB/year. Table 1.3 summarizes the relevant parameters for the SP technology. For our calculations of data volume, we assume lossless compression and partial, rather than full, readouts of regions of interest (ROIs) in the FD modules. We do not assume zero-suppression at the level of single channels.

Table 1.3: Useful quantities for computing estimates for SP readout.

Quantity	Value	Explanation
Far Detector Beam:		
Single APA readout	41.5 MB	Uncompressed 5.4 ms
APAs per module	150	
Full module readout	6.22 GB	Uncompressed 5.4 ms
Beam rep. rate	0.83 Hz	Untriggered
CPU time/APA	100 sec	from MC/ProtoDUNE
Memory footprint/APA	0.5-1GB	ProtoDUNE experience
Supernova:		
Single channel readout	300 MB	Uncompressed 100 s
Four module readout	450 TB	Uncompressed 100 s
Trigger rate	1 per month	(assumption)

1.3.2 Dual-phase Technology Data Estimates

A DP module will have 153,600 readout channels and a full drift time of 7.5 ms. Given 20,000 samples in an 8 ms readout, the uncompressed event size is 4.2 GB (for one drift window). Gas amplification leads to a high signal-to-noise (S/N) ratio, allowing lossless compression to be applied at the front end with a compression factor of ten; this brings the event size per module to 0.42 GB.

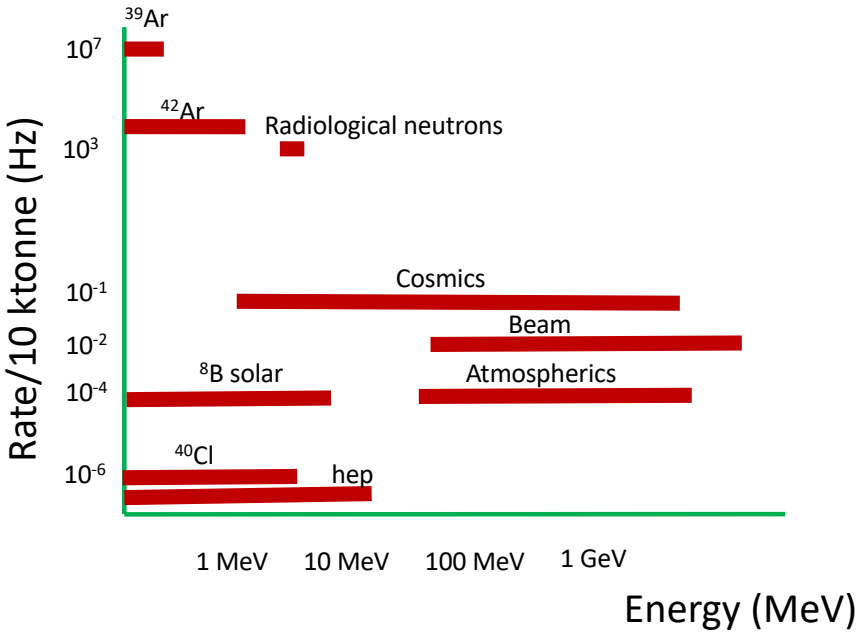


Figure 1.3: Expected physics-related activity rates in a single 10 kt SP module. Figure from Volume IV, The DUNE Far Detector Single-Phase Technology, Chapter 7.

Table 1.4: Summary of expected data rates for a single 10 kt SP module (from Volume IV, The DUNE Far Detector Single-Phase Technology). The rates assume no compression. ^{39}Ar decay candidates are temporarily stored for one to two months at a time. The same applies to fake supernova neutrino burst (SNB) data. Improved readout algorithms will be developed and evaluated with the initial data and are expected to reduce the data volume by about a factor of ten while retaining efficiency.

Source	Annual Data Volume	Assumptions
Beam interactions	27 TB	10 MeV threshold in coincidence with beam time, including cosmic coincidence; 5.4 ms readout
^{39}Ar, cosmics and atmospheric neutrinos	10 PB	5.4 ms readout
Radiological backgrounds	< 2 PB	< 1 per month fake rate for SNB trigger
Cold electronics calibration	200 TB	
Radioactive source calibration	100 TB	< 10 Hz source rate; single APA readout; 5.4 ms readout
Laser calibration	200 TB	10^6 total laser pulses; half the TPC channels illuminated per pulse; lossy compression (zero-suppression) on all channels
Random triggers	60 TB	45 per day

An FD DP module can be treated as twenty smaller detectors, each with a number of readout channels similar to ProtoDUNE-DP running in parallel, and each defining a sub-module ROI. For beam or cosmic events, it is possible to record only the interesting ROIs with the compressed size of a single ROI at 22 MB.

1.3.3 Data Rates

Figure 1.3 illustrates the raw rates and energy ranges for relevant physical processes in a single DUNE FD module.

1.3.3.1 Beam Coincident Rates

Requiring coincidence with the 10 µs LBNF beam spill would reduce the effective live time from $\sim$1.2 s to a 5.4 ms readout window (8 ms for DP), leading to an uncompressed event size of approximately 24 GB for four SP modules (somewhat less for DP) — still too much to record permanently at full rate. Only a few thousand true beam interactions in the FD modules are expected each year. Compression and conservative triggering based on photon detectors (PDs) and ionization should reduce the data rate from beam interactions by several orders of magnitude without sacrificing efficiency. Studies discussed in Volume IV, The DUNE Far Detector Single-Phase Technology, Chapter 7 indicate that high trigger efficiencies are achievable at an energy threshold of 10 MeV, leading to event rates for beam-initiated interactions of $\sim$6,400/year. Table 1.4, adapted from Volume IV Chapter 7, summarizes expected uncompressed rates from one SP module.

1.3.3.2 Near Detector

The ND configuration is not yet fully defined, but we do have substantial experience from T2K and MicroBooNE at lower energies, and MINERvA and NOvA at the DUNE beam energies on cosmic and beam interactions under similar conditions. We expect that the DUNE ND will have $\sim$1 beam interaction per m^3 per beam pulse, and non-negligible rates of cosmic rays. Initial estimates indicate that zero-suppressed data rates will be of order 10 MB/s with yearly data volumes less than a PB.

1.3.3.3 Processes not in Synchronization with the Beam Spill

Processes not associated with the beam spill include SNB physics, proton decay, neutron conversion, and atmospheric and solar neutrino interactions. These processes generally have less energy, making triggering more difficult, and they are asynchronous, thus requiring an internal or external trigger. In particular, SNB signals will consist of a large number of low-energy interactions spread throughout the FD volume over a period of 1-100 seconds. Buffering and storing 100 seconds of SNB data would require approximately 20,000 readout windows, or 460 TB for a four-module

readout. At a rate of one fake SNB event per month, this would generate 6 PB of uncompressed data per year. Reconstructing and analyzing these data will require substantial evolution in our software frameworks, which were developed to process small (1 MB to 100 MB) events on single processors. Updating the frameworks is a major upcoming task for the DUNE computing R&D.

1.3.3.4 Calibration

The FD modules will require continuous calibration and it is likely that these calibration samples will dominate the data volume. Cosmic-ray muons and atmospheric neutrino interactions will provide a substantial sample for energy and position calibrations. Dedicated runs with radioactive sources and laser calibration will also generate substantial and extremely valuable samples. Table 1.4 includes estimates for the SP module.

Electron lifetime in the detector volume can be monitored via ^{39}Ar decays at rates of $\sim$1/kg/sec. As discussed in the appendices for Volume II, DUNE Physics, a single 5 ms readout of the full detector would provide 50,000 decays for study. A small number of such readouts per day would provide a global monitor of conditions at the 1% level, but measurements sensitive on meter scales will require a factor of 10^4 more data, and can become a significant fraction of the calibration data stream. In summary, ^{39}Ar cosmic ray and atmospheric neutrino signals collected for calibration make up the bulk of the uncompressed SP data volume at $\sim$10 PB/year per module and will dominate the rates from the FD modules.

1.3.3.5 Zero Suppression

The data volumes discussed above are for non-zero-suppressed readout of the full FD. A combination of local triggering, zero suppression, and efficient lossless compression mechanisms can substantially reduce the final data volume. However, previous HEPexperience indicates that signal processing must be done carefully and is often done after data-taking, and when the data are well understood. As a result, early running often generates large data volumes while algorithms are being tuned. Experience from the Short-Baseline Neutrino (SBN) and ProtoDUNE experiments will help us develop these data movement and processing algorithms, but they may be applied later in the processing chain for SP. No zero-suppression is planned for DP.

1.3.4 Simulation

The bulk of data collected with the FD is likely to be background, with real beam interaction events in the FD numbering in the thousands per year, not millions. Thus, the size of beam event simulation samples may be smaller than the unprocessed raw data considered above. Simulation of lower-energy events should reflect the fact that they are very rare; they could be simulated in sub-volumes of the whole detector. While simulation will be important to the experiment, it is not expected to dominate the data volume as it does in many experiments.

Simulation inputs such as flux files, overlay samples, and shower libraries must be distributed to simulation jobs carefully. Proper simulation requires that these inputs be distributed in unbiased parcels, which from a technical standpoint can be difficult to do efficiently in a widely distributed environment. This will require thoughtful design.

1.3.5 Analysis

We anticipate that most analysis samples will be many times smaller than the raw data, however, since they are distinctive to particular analyses and even users, producing and cataloguing them will require carefully designed tools and substantial oversight. DUNE will need a mix of official samples, produced by physics groups and distributed through a common catalog and through common file transfer mechanisms, as well as small user samples on local disks.

Final oscillation parameter scans with a large number of parameters can be quite CPU-intensive. For example, the NOvA collaboration's recent physics results required tens of millions of high-performance computing (HPC) CPU hours at the NERSC facility at Lawrence Berkeley National Laboratory (LBNL). DUNE collaborators used simpler models but the same techniques to generate some of the results presented in Volume II, DUNE Physics. These large-scale analysis projects will require collaboration-wide coordination of resources and will benefit greatly from optimization for specific architectures.

1.3.6 Data Storage and Retention Policies

Some data samples, e.g., real neutrino and cosmic ray interactions in the FD, most of the ND data, and any real SNB events, will be extremely valuable and will require conservative and potentially redundant retention policies. Calibration samples, and possibly fake SNB triggers, may be stored temporarily and discarded after processing.

1.4 ProtoDUNE-SP Data

1.4.1 Introduction

ProtoDUNE-SP ran at CERN in the NP04 beamline from September to November of 2018. Before that run, several data challenges at high rate validated the data transfer mechanisms. The run itself has already served as a substantial test of the global computing model, and studies of cosmic rays continue.

This section describes the ProtoDUNE data design and the lessons learned from our experience.

1.4.2 Data Challenges

Starting in late 2017, a series of data challenges were performed with ProtoDUNE-SP. Simulated data were passed through the full chain from the event builder machines to tape storage at CERN and Fermilab at rates up to 2 GB/s. These studies allowed optimizing the network and storage elements well before the start of data taking in fall 2018. The full DUNE FD, in writing 30 PB/year, will produce data at rates similar to those in the 2018 data challenges. While accommodating the ProtoDUNE-SP data rates was not technically challenging, the integrated data volume from an experiment running 99% of the time over several decades will be.

1.4.3 Commissioning and Physics Operations

The first phase of operations involved commissioning the detector readout systems while the LAr reached full purity. During this period data were taken with cosmic rays and beam. Once high LAr purity was reached, ProtoDUNE-SP collected physics data with beam through October and half of November 2018. After the beam run, we continued to take cosmic ray data under varying detector conditions, such as modified high voltage and purity, and new readout schemes.

1.4.4 Data Volumes

ProtoDUNE-SP comprises a TPC consisting of six APAs, their associated PDs, and a cosmic ray tagger (CRT). In addition, the NP04 beamline is instrumented with hodoscopes and Cherenkov counters to generate beam triggers. Random triggers were generated at lower rates to collect unbiased cosmic ray information. During the test beam run, the TPC readout dominated the data volume. The nominal readout window during the beam run was 3 ms as a match to the drift time at full voltage (180 kV), which was maintained for most of the run. The TPC alone produced 138 MB/event without compression, not including headers. The uncompressed event size including all TPC information, CRT, and PD data was 170 MB to 180 MB. Data compression was implemented just before the October beam physics run, reducing this number to 75 MB. In all, 8.1 million beam events produced a total of 572 TB. An additional 2.2 PB of commissioning data and cosmic ray data was also recorded. Table 1.5 summarizes the data volumes recorded in ProtoDUNE-SP from October 2018 to October 2019.

Table 1.5: Data volumes recorded by ProtoDUNE-SP as of October 2019.

Type	Events	Size
Raw Beam	8.1 M	520 TB
Raw Cosmics	19.5 M	1,190 TB
Commissioning	3.86 M	388 TB
Pre-commissioning	13.89 M	641 TB

Events were written out in 8 GB raw data files, each containing approximately 100 events. The

beam was live for two 4.5 s spills every 32 s beam cycle, and data were taken at rates up to 50 Hz, exceeding the typical 25 Hz, leading to compressed DC rates of 400 MB/s to 800 MB/s from the detector.

1.4.5 Reconstruction of ProtoDUNE-SP Data

Thanks to substantial work by the 35 ton prototype, MicroBooNE, and the LArTPC community, high-quality algorithms were in place to reconstruct the TPC data. As a result, a first pass reconstruction of the ProtoDUNE-SP data with beam triggers was completed in December, 2018, less than a month after data taking ended. Results from that reconstruction are presented in Volume II, DUNE Physics, Chapter 4 with some highlights summarized here.

1.4.6 Data Preparation

Before pattern recognition begins, data from the ProtoDUNE detector is unpacked and copied to a standard format within the art framework based on ROOT objects. This reformatted raw data includes the waveform for each channel, consisting of 6,000-15,000 12-bit, 0.5 μsec samples. The first step in reconstruction is data preparation, which entails the conversion of each analog-to-digital converter (ADC) waveform into a calibrated charge waveform with signals proportional to charge. Once the data are prepared, hit-level ROIs are identified, and data outside these regions are discarded, significantly reducing data size. The data preparation process is described more fully in [6].

Figures 1.4 and 1.5 illustrate the transformation of TPC data during data preparation for one wire plane for 3 ms. A full 5.4 ms readout of a single 10 kt module would contain a factor of 750 times more information than this image.

1.4.7 Computational Characteristics of Data Preparation and Deconvolution

Decoding for ProtoDUNE-SP originally stored all six APAs in memory. Each 3 ms of APA readout consists of more than 15 M 16-bit values. Decompressing and converting this information to a floating point format causes substantial memory expansion. Data with a 7.5 ms window were also recorded. The input and output event sizes and reconstruction time scale were found to scale linearly with the readout window and with the number of APAs processed.

Processing each wire plane (three per APA) independently reduces the memory footprint because electrical signals correlate between channels within an APA wire plane but not between planes. However, although subdividing the detector into wire planes reduces the memory footprint for short (beam-related) readouts, this is not a viable solution for the long readouts expected for SNB events. We are still seeking the best strategy for these much larger ($\times 10,000$) time windows.

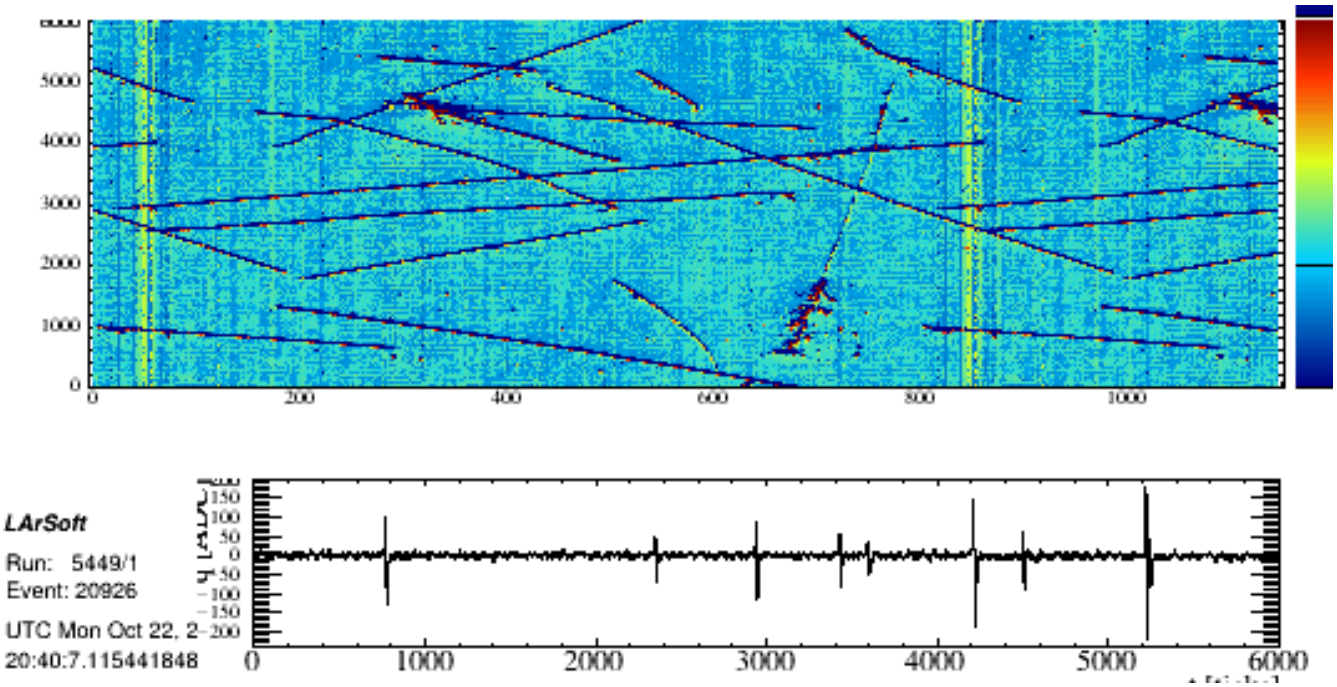


Figure 1.4: Example of pedestal-subtracted data for one ProtoDUNE-SP wire plane. The top pane shows the ADC values in a V (induction) plane (Section **??**) with the x axis as channel number and the y axis as time slice. The bottom pane shows the bipolar pulses induced on one channel.

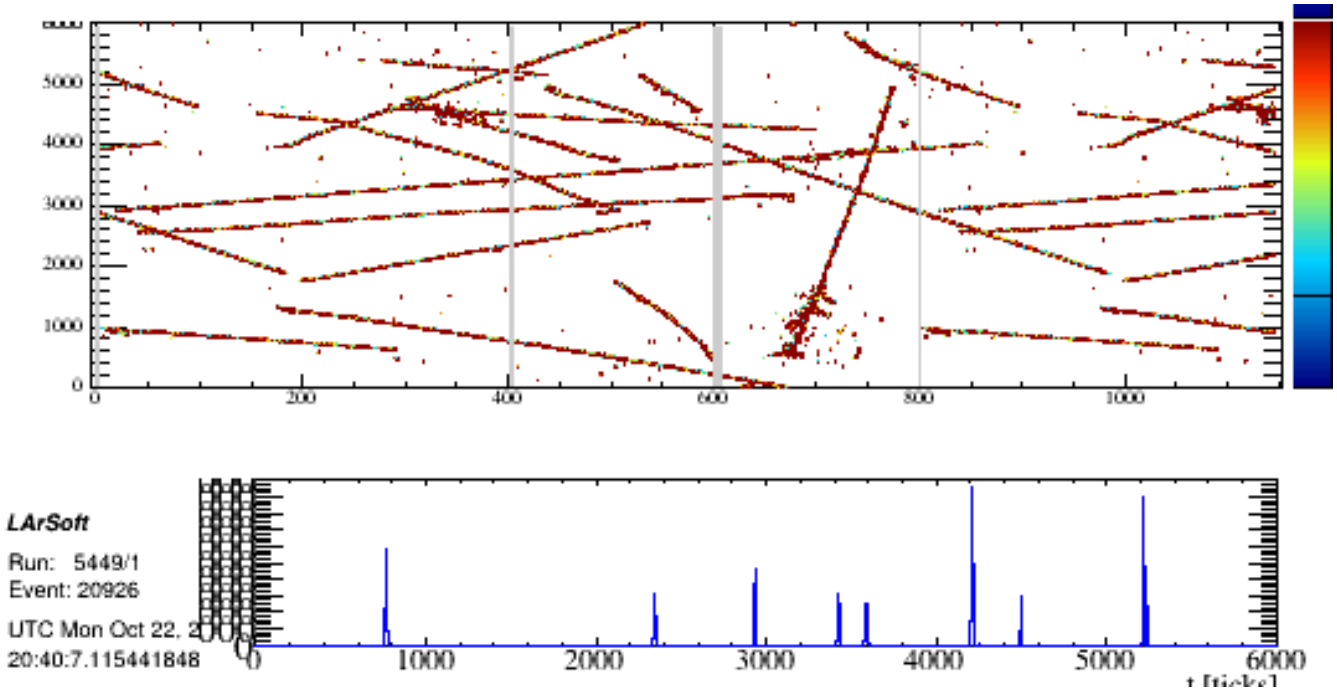


Figure 1.5: Pedestal-subtracted data for one ProtoDUNE-SP wire plane, as in Figure 1.4, after calibration, cleanup, deconvolution, and finding ROIs.

The DAQ consortium is exploring methods for segmenting large events (such as SNBs) into smaller ROIs in both time and space for efficient readout. As long as those regions are on the scale of single interactions, the resulting data should fit into a reasonable memory budget at the expense of tracking and collating many distributed interactions.

The operations performed in signal processing require few decisions but do include operations such as fast Fourier transforms and deconvolution. These operations are well suited for GPU and parallel processing. We are actively exploring multi-threaded processing for all data preparation algorithms.

1.4.8 Reconstruction Characteristics

Once ROIs have been identified, several 3D reconstruction packages are used. For the first reconstruction pass in November, the Pandora [7], Wire-Cell [8], and Projection Matching Algorithm (PMA) [9] frameworks were used. The results are described in Volume II, DUNE Physics. Figure 1.6, taken from that volume, illustrates the measured efficiency for the Pandora algorithm reconstructing a triggered beam particle as a function of momentum for the simulation and data for selected data taking runs. Figure 1.6 demonstrates that the efficiency is already high and reasonably well simulated.

Full reconstruction of these ProtoDUNE-SP interactions, with beam particles and approximately 60 cosmic rays per readout window, took approximately 600 s/event with 200 s each for the signal processing and hit finding stages; the remaining time was divided among three different pattern recognition algorithms. Output event records were substantially smaller (22 MB compressed) but were still dominated by information for TPC hits above threshold.

All these algorithms are run on conventional Linux CPUs using OSG/WLCG grid computing infrastructure. Deep learning techniques based on image pattern recognition algorithms are also being developed. Many of these algorithms can be adapted to run on HPC assets, although the optimal architecture for 3D reconstruction likely differs from that for hit finding.

1.4.9 Lessons Learned

The first ProtoDUNE-SP run has given us very valuable information for planning the full DUNE computing model.

- Data and simulation challenges led to a reasonably mature and robust model for acquiring, storing, and cataloging the main data stream at design rates.
- The experiment integrated several existing grid sites and used substantial opportunistic resources. This allowed initial processing of data within one month of the end of the run.
- Prototype infrastructure was in place for provisioning, authentication and authorization, data management, networking, file catalog, and workflow management.

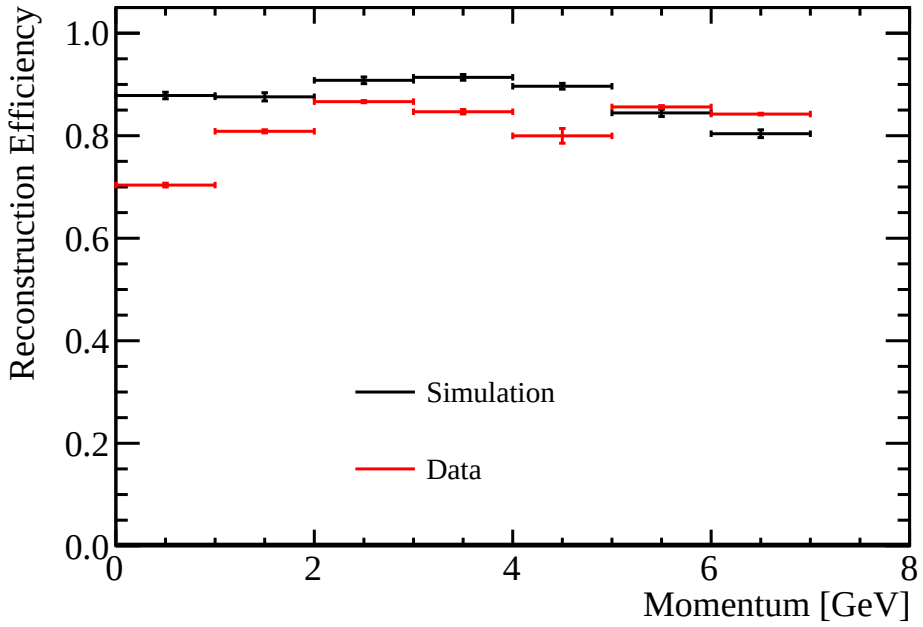


Figure 1.6: The efficiency of reconstruction for the triggered test beam particle as a function of particle momentum in data (red) and simulation (black). (Figure 4.30 from Volume II, DUNE Physics.)

- Reconstruction algorithms were available, permitting immediate studies of detector performance and calibration.
- Beam information was successfully integrated into processing through an IFbeam database.
- Auxiliary information from some systems, e.g., slow controls, was not fully integrated into processing. This led to a manual input of the running conditions by shift personnel, and offline incorporation of that information into the data catalog. This prompted a closer collaboration between the DAQ and CISC groups and the design of robust interfaces for configurations and conditions.

Overall, the ProtoDUNE-SP data taking and processing was a success, despite too much reliance on manual intervention because automated processes were not always in place. Considerable effort must go into integrating detector conditions, data migration, workflow systems, and HPCs with multi-threaded and vectorized software.

Glossary

35 ton prototype A prototype cryostat and single-phase (SP) detector built at Fermilab before the ProtoDUNE detectors. 17

analog-to-digital converter (ADC) A sampling of a voltage resulting in a discrete integer count corresponding in some way to the input. 17, 18

anode plane assembly (APA) A unit of the SP detector module containing the elements sensitive to ionization in the LAr. It contains two faces each of three planes of wires, and interfaces to the cold electronics and photon detection system. 11, 16, 17

art A software framework implementing an event-based execution paradigm. 17

Belle II B-factory experiment now running at KEK. 3, 7

European Organization for Nuclear Research (CERN) The leading particle physics laboratory in Europe and home to the ProtoDUNEs. (In French, the Organisation Européenne pour la Recherche Nucléaire, derived from Conseil Européen pour la Recherche Nucléaire. 2, 3, 7, 9, 15, 16

cryogenic instrumentation and slow controls (CISC) Includes equipment to monitor all detector components and liquid argon (LAr) quality and behavior, and provides a control system for many of the detector components. 6, 20

cosmic ray tagger (CRT) Detector external to the TPC designed to tag TPC-traversing cosmic ray particles. 16

computing and software consortium (CSC) DUNE computing and software consortium. 2, 4–7, 9, 11

data acquisition (DAQ) The data acquisition system accepts data from the detector front-end (FE) electronics, buffers the data, performs a trigger decision, builds events from the selected data and delivers the result to the offline secondary DAQ buffer. 4, 6, 11, 19, 20

DC direct coupling. 17

dual-phase (DP) Distinguishes one of the DUNE far detector technologies by the fact that it operates using argon in both gas and liquid phases. 2, 13, 14

DP module dual-phase DUNE far detector (FD) module. 11, 13

Deep Underground Neutrino Experiment (DUNE) A leading-edge, international experiment for neutrino science and proton decay studies. 2–7, 9, 10, 13–16, 19

far detector (FD) The 70 kt total (40 kt fiducial) mass liquid argon time-projection chamber (LArTPC) DUNE detector, composed of four 17.5 kt total (10 kt fiducial) mass modules, to be installed at the far site at SURF in Lead, SD, USA. 2, 3, 11, 13–16

Fermi National Accelerator Laboratory (Fermilab) U.S. national laboratory in Batavia, IL. It is the laboratory that hosts Deep Underground Neutrino Experiment (DUNE) and serves as its near site. 3, 5, 7, 11, 16

FTE full-time equivalent. A unit of labor for the project. One year of work from one person. 7

HEP high energy physics. 2–4, 9, 14

high-performance computing (HPC) high-performance computing facilities; generally computing facilities emphasizing parallel computing with aggregate power of more than a teraflop. 15, 19, 20

HEP Software Foundation Collaboration (HSC) A foundation that facilitates cooperation and common efforts in high energy physics software and computing internationally. 3, 7

IFbeam Database that stores beamline information indexed by timestamp. 20

liquid argon (LAr) Argon in its liquid phase; it is a cryogenic liquid with a boiling point of −90 °C (87 K) and density of 1.4 g/ml. 11, 16

liquid argon time-projection chamber (LArTPC) A time projection chamber (TPC) filled with liquid argon; the basis for the DUNE FD modules. 2, 4, 9, 17

Lawrence Berkeley National Laboratory (LBNL) US national laboratory in Berkeley, CA. 15

LHC Large Hadron Collider. 2–4, 9

LHCb LHC experiment dedicated to forward physics. 7

Large Synoptic Survey Telescope (LSST) 8.4 m telescope with 3.2G-pixel camera that will start taking data in 2023. 3

MicroBooNE The LArTPC-based MicroBooNE neutrino oscillation experiment at Fermi National Accelerator Laboratory (Fermilab). 13, 17

MINERvA The MINERvA neutrino cross sections experiment at Fermilab. 13

near detector (ND) Refers to the detector(s) installed close to the neutrino source at Fermilab. 11, 13, 15

NERSC National Energy Research Computing Facility at Lawrence Berkeley National Laboratory (LBNL). 15

NOvA The NOvA off-axis neutrino oscillation experiment at Fermilab. 13, 15

NP04 CERN North Area hadron beamline used for the SP test beam run. 15, 16

Open Science Grid (OSG) Open Science Grid. 2, 6, 7, 19

Pandora The Pandora multi-algorithm approach to pattern recognition. 19

photon detector (PD) The detector elements involved in measurement of the number and arrival times of optical photons produced in a detector module. 13, 16

Projection Matching Algorithm (PMA) A reconstruction algorithm that combines 2D reconstructed objects to form a 3D representation. 19

ProtoDUNE Either of the two DUNE prototype detectors constructed at European Organization for Nuclear Research (CERN). One prototype implements SP technology and the other dual-phase (DP). 3, 4, 7, 14, 15, 17

ProtoDUNE-DP The DP ProtoDUNE detector at CERN. 2, 3, 6, 13

ProtoDUNE-SP The SP ProtoDUNE detector at CERN. 2, 3, 6, 9, 15–20

ROI region of interest. 11, 13, 17–19

ROOT A modular scientific software toolkit. It provides all the functionalities needed to deal with big data processing, statistical analysis, visualisation and storage. It is mainly written in C++ but integrated with other languages such as Python and R. 17

Rucio Data management system originally developed by ATLAS but now open-source and shared across HEP. 3

signal-to-noise (S/N) signal-to-noise ratio. 11

Short-Baseline Neutrino (SBN) A Fermilab program consisting of three collaborations, MicroBooNE, SBND, and ICARUS, to perform sensitive searches for ν_e appearance and ν_μ disappearance in the Booster Neutrino Beam. 14

supernova neutrino burst (SNB) A prompt increase in the flux of low-energy neutrinos emitted in the first few seconds of a core-collapse supernova. It can also refer to a trigger command type that may be due to this phenomenon, or detector conditions that mimic its interaction signature. 12–15, 17, 19

single-phase (SP) Distinguishes one of the DUNE far detector technologies by the fact that it operates using argon in its liquid phase only. 2, 11, 14

SP module single-phase DUNE FD module. 11–14

Sanford Underground Research Facility (SURF) The laboratory in South Dakota where the Long-Baseline Neutrino Facility (LBNF) far site conventional facilities (FSCF) will be constructed and the DUNE FD will be installed and operated. 7

T2K T2K (Tokai to Kamioka) is a long-baseline neutrino experiment in Japan studying neutrino oscillations. 13

technical design report (TDR) A formal project document that describes the experiment at a technical level. 9

time projection chamber (TPC) A type of particle detector that uses an E field together with a sensitive volume of gas or liquid, e.g., LAr, to perform a 3D reconstruction of a particle trajectory or interaction. The activity is recorded by digitizing the waveforms of current induced on the anode as the distribution of ionization charge passes by or is collected on the electrode. 3, 11, 16, 17, 19

Wire-Cell A tomographic automated 3D neutrino event reconstruction method for LArTPCs. 19

Worldwide LHC Computing Grid (WLCG) Worldwide LHC Computing Grid. 2, 6, 7, 19

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