DUNE Software Framework Requirements Taskforce Report

Executive Summary

This taskforce report was commissioned by the DUNE computing consortium. The scope of the report was to provide an enumeration of the needs of the DUNE experiment, as driven by its physics mission, in regards to a software framework for data processing and analysis.

The taskforce was composed of representatives from the different physics missions of DUNE, scientists with extensive experience with large scale data processing and analysis from outside of DUNE[1] and technical experts in software framework design, including the current conveners of the HSF[2] frameworks working group.

Task force members

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General framework requirements

For ease of reference, this executive summary lists the enumerated framework requirements defined by the Software Framework Requirements Task Force, more info on the task force can be found here:
https://wiki.dunescience.org/wiki/Software_Framework_Requirements_Task_Force

Brave readers are encouraged to read the full document to understand the context and nuances of each of the requirements, the wording here is the same as the full text. While there may be overlap, the complete set of requirements as derived from various considerations is presented and no attempt at reducing this list is made here, rather that is left to framework designers when drawing up specifications. Considerations on “Utilities” and “Desired Features” are also presented at the end of the document to capture useful discussions and provide additional context.

We list in the following the formal requirements determined by the taskforce.

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[1] Included scientists from ATLAS, CMS, Belle II, NOvA, MicroBooNE, CDF and D0
[2] High Energy Physics Software Foundation

(1) The framework must separate data and algorithms.

(2) The framework must separate the persistent data representation from the in-memory representation seen by algorithms.

Configuration requirements

(3) The framework should provide a Turing complete configuration language as a foundational component so that it can ensure coherence of its configuration.

(4) The framework should provide a suitable API so that algorithm writers can ensure their required parameters are self-describing and validatable.

(5) The framework configuration system needs to have a robust persistency and versioning system that makes it easy to document and reproduce previous results. It must be possible to create, tag, check-sum, store and compare configurations. This configuration management system should be external to the framework or data files so that configurations can reliably be reused and audited.

(6) The resulting state of the configured framework and its components should be deterministic and precisely reproducible given a set of environmental conditions which include the available hardware, operating system, input data, etc.

(7) The ensemble of the framework+environmental conditions must give reproducible results.

(8) It is desirable that it should be possible to only configure those framework components required for a particular data processing use case.

(9) It must be possible to derive the input data requirements for any algorithm, in order to define the sequence of all algorithms needed for a particular use case.

Concurrency and Multithreading

(10) It is (therefore) desirable that the framework should help facilitate the use of multi-threaded data processing and facilitate access to co-processors in an efficient manner.

(11) It is highly desirable that it be possible to write algorithmic code independently of the framework.

(12) ***It is highly desirable that the framework be sufficiently modular in design to allow re-use of framework services and functionality both within and outside of the framework context, as far as that is possible.***

(13) The framework must be able to schedule thread-safe and non-thread-safe work appropriately.

Reproducibility and provenance

(14) The framework must provide a full provenance chain for any and all data products which must include enough information to reproduce identically every persistent data product. By definition, the chain will also need to include sufficient information to reproduce the transient data passed between algorithm modules, even though the product is not persisted in the final output.

(15) The framework must provide full provenance information and all of the metadata required to ensure reproducibility.

Random numbers, machine learning and conditions

(16) It is highly desirable that the framework broker access to random number generators and seeds in order to guarantee reproducibility.

(17) The framework should give special attention to machine learning inference in the design, both to allow simple exchanges of inference backends and to record the provenance of those backends and all necessary versioning information.

(18) The framework must provide a conditions service that is a single point of access to conditions data.

(19) The configuration of the framework conditions service should ideally be via one configuration parameter (a global tag).

(20) It must be possible to override a subset of global tag configured conditions for testing purposes.

Data and I/O layer

(21) The framework must support reading and writing different persistent data formats.

(22) The framework I/O functionality must be backward compatible across versions.

(23) A mechanism for user-defined schema evolution of data products needs to be provided.

(24) The framework must provide a mechanism to register/associate and to run/apply custom serialization/deserialization and compression/decompression algorithms to data on write/read of that data from a persistable form.

(25) The framework should support compression on output data in a manner that is transparent to users and is configurable. It must be possible to disable the automatic compression of output data or provide compression transforms that are effectively identity transforms.

(26) The framework should allow a configurable maximum output file size and provide appropriate file-handling functionality.

Memory management

(27) The framework must be able to operate on subsets of a Trigger Record. Specifically, it must be possible to break Trigger Records down into smaller chunks (e.g. one APA) and be able to stitch those chunks back together. For supernovae, it must also be possible to reuse a fraction (nominally 100 us) of the previous chunk (nominally 5ms) of data to allow stitching in time.

(28) Data products should not occupy memory beyond their useful lifetimes.

(29) The framework must manage memory of data products in the Data Store.

(30) The framework needs to support skimming/slimming/thinning for data reduction.

(31) The framework needs to be able to read and write several parallel data streams (including friend trees). Labelling of data objects across streams should be intuitive and not error prone. Provenance information should support correlating related data objects across streams.

(32) The framework needs to allow experiment code to mix simulation and (overlay) data.

Physics analysis

(33) It must be possible to define arbitrary units of execution that are independent of Trigger Records. It must be possible to correlate these units to Trigger Records for exposure accounting, and experiment conditions.

(34) The framework should make minimal assumptions about the data model, i.e. it should not assume an event-by-event paradigm.

(35) Analysis must be able to use particle-candidate-based control flow, without any constraints arising from the event-by-event paradigm.

(36) The framework must support partial reading of the persistent data and must not require reading an entire Trigger Record unless required (i.e. it must not force the entire Trigger Record to be read).

(37) Calibration, reconstruction, and selection algorithms must be framework-agnostic, i.e. able to run transparently in any official DUNE framework where equivalent requisite data products exist.

(38) The framework should be easily portable and capable of running on local resources.

(39) The same code developed and tested on local resources must scale to large resources. This should include HPC resources as far as possible.

(40) Analysis files must record their parent framework files, but no Trigger Record provenance is required. The full provenance information need not be retained in analysis files as this could easily become larger than the data itself.

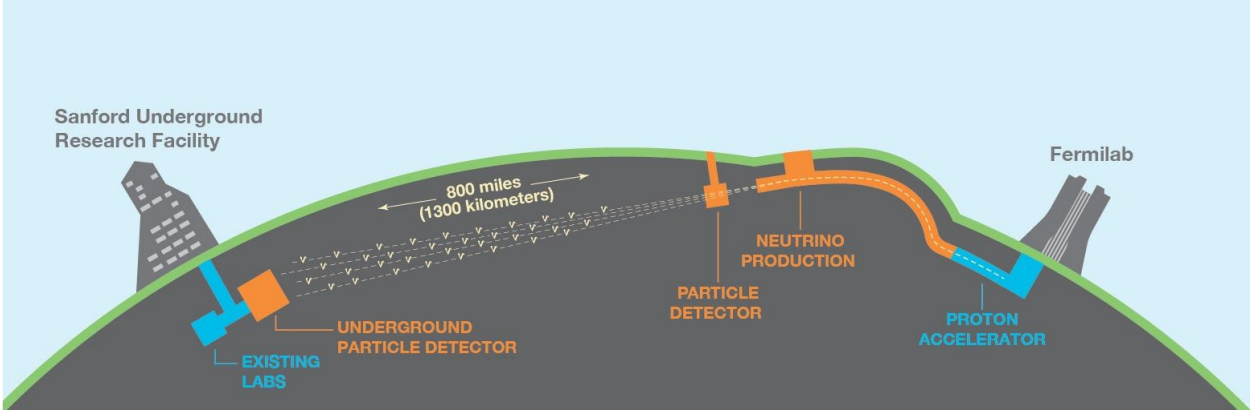
(41) The framework must have native support for exposure accounting (POT and live-time), so as to make errors of this sort difficult.

(42) The framework should provide some means of cross-referencing (labelling) multiple input streams to correlate them in order to facilitate evaluation of systematic uncertainties.

(43) The framework should be able to work with both ND and FD data on an equal footing, and within the same job.

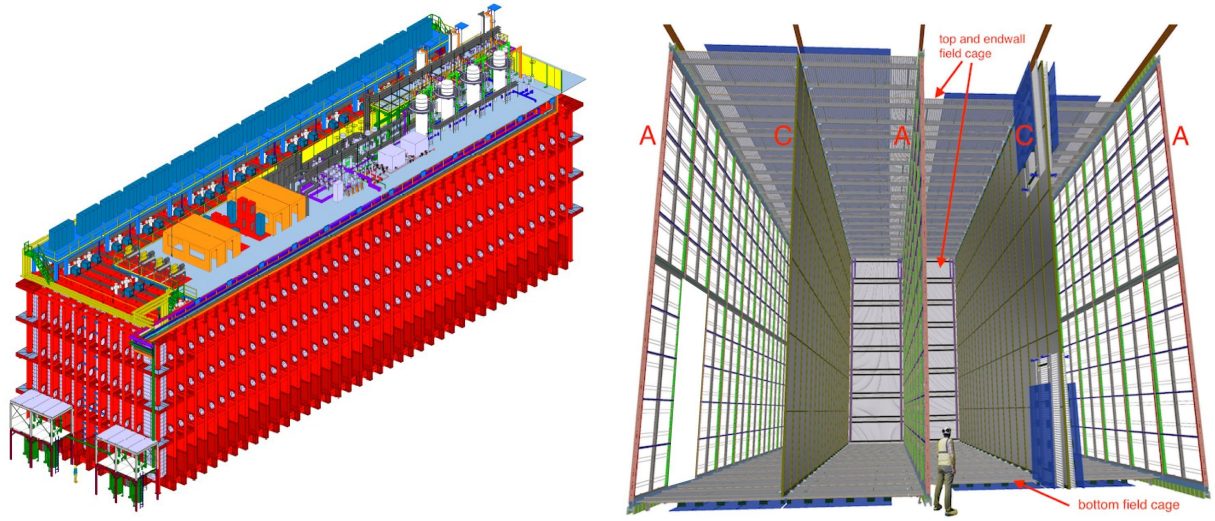
A very brief introduction to DUNE and DUNE Data Structure for Non-experts

The nature of the DUNE detector and its readout structure necessitate the definition of a number of conceptual terms that are used throughout this report for describing the requirements that are placed on the framework. We define and describe these core terminologies here, together with a very brief introduction to the DUNE detector itself, more information can be found at www.dunescience.org.



Schematic of the DUNE experiment concept, showing Fermilab (right) producing a high intensity neutrino beam that passes through two particle detectors, one close to the beam source and the other 800 miles away at the Sanford Underground Research Facility.

The DUNE experiment concept is to produce a high intensity neutrino beam at Fermilab. The neutrino beam passes first through a Near Detector (labelled “Particle Detector”) and then a Far Detector (“Underground Particle Detector”) 800 miles away at the Sanford Underground Research Facility. The Near Detector could be compared to modern collider experiment detectors, albeit with features unique to DUNE. The Far Detector, however, is truly enormous and produces data volumes which drive many of the most challenging requirements of the DUNE software framework. Hence the reader should be familiar with some basic DUNE Far Detector concepts in order to make sense of the discussions in this document. A glossary of essential terms for both the DUNE detector and software framework concepts is also given below.



(Left) Schematic of a Far Detector cryostat that houses one 10kTonne Far Detector module at the Sanford Underground Research Facility and (Right) A Far Detector module with Anode (A) and Cathode (C) planes shown. The blank rectangle on the left-most Anode plane illustrates the size of one Anode Plane Assembly (APA), where the adjacent drift volume is readout. A Far Detector module consists of 150 APAs, the final DUNE Far Detector will comprise four Far Detector modules.

Detector Glossary

Readout ([Detector] Drift): The unit of detector readout corresponding to the time it takes for ionization to fully traverse the active volume of the detector, from the furthest point in the volume to the readout plane. This serves as the minimum unit of detector readout.

Trigger Window: A temporal region extending from a start time t0 to an end time t0+Δt, for which the trigger system has detector activity, or for which it is desirable to readout the detector's data acquisition system.

Trigger Record: The set of one or more Readout Drifts that occur in overlap with a Trigger Window. This is the unit of data which is collated and recorded by the DAQ system and which forms the initial unit of data for the DUNE computing model.

APA Readout: The subset of a trigger record which corresponds to the data from a single anode plane assembly (APA). This is a spatially distinct region of the detector.

Region of Interest (ROI): A time/space region of the readout waveform data that rises above a detection threshold when transformed by a Fourier transform algorithm into a uni-polar representation.

Hit: A collection or clustering of samples in the waveform representation which are identified by an ROI as being above a suppression threshold (or suppression algorithm). These form the basis for spatial analysis of the data and the formation of tracks.

Interaction [Candidate]: Subset of an APA Readout which corresponds to activity which may constitute the interaction or passage of particles through the detector. A single Trigger Window may have multiple Interactions which are topologically distinct from each other or may overlap.

Software Framework Glossary

Data Atom: A discrete unit of information (detector data or simulation) which can be natively processed (looped over) by a framework.

Event: For collider experiments, events represent the natural data atom at least in the early stages of reconstruction that tend to dominate the requirements of software frameworks. For DUNE, the Trigger Record more accurately assumes that role and “event” is not used in this document to avoid confusion. Readers from collider experiment backgrounds may often find it useful to substitute the word “event” when you read “Trigger Record”.

Event-by-event paradigm: As the concept of an “event” is common in collider experiments, the software frameworks developed by those experiments often employ an event-by-event data processing paradigm, with the event being the data atom for the framework. We refer to that data processing paradigm in this document where relevant.

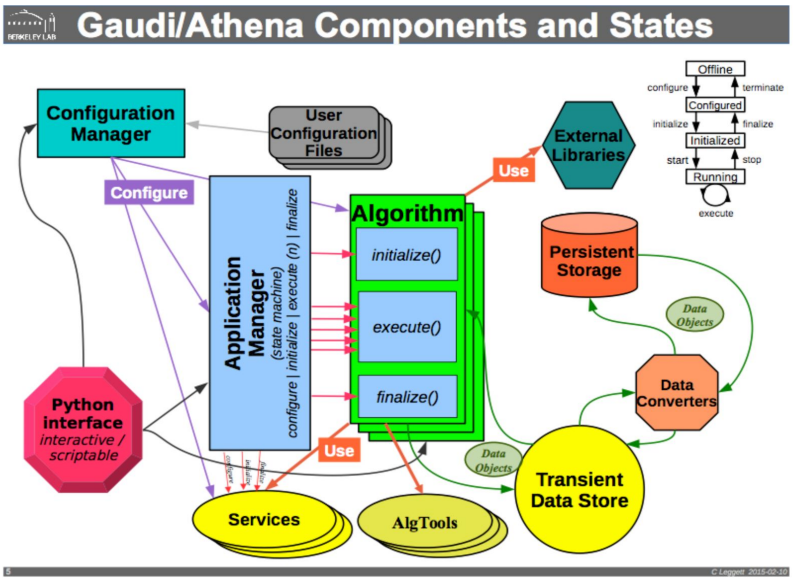
DUNE Software Framework Requirements Taskforce Report

Full Report

Document Scope

Many experiments use data processing frameworks to process their data in a reliable way and to provide a structure for many authors to contribute algorithmic code. The main aim of this document is ***to define the physics-based requirements of the software framework*** that DUNE will use to process data, herein referred to as "the framework". Requirements are highlighted in ***bold italic*** for the executive reader and are enumerated in parentheses. The primary use cases considered relate to simulation and reconstruction of DUNE data in production runs using DUNE's distributed computing resources. Substantial and unique algorithmic functionality exists in established code and providing support for their continued exploitation is critical.

In the classic implementation, the *framework* is an executable program that loops over units of data and executes physics code that resides in *modules* (called *algorithms* in Gaudi) that are scheduled by that framework. The code in these modules is provided the means to read and write data and has access to other information (e.g. conditions data) via *services*. Services, tools and modules are all configurable and dynamically loaded. In the model envisioned here, most of the framework code resides in supporting services and the term "framework" refers to those services and the supporting libraries as well as the framework executable(s).



Schematic of the Gaudi/Athena framework components and states. Physics code resides in modules in (proto)DUNE, which are called Algorithms in Gaudi/Athena.

Late-stage processing, referred to here as “analysis”, could in principle use the same framework and that may be very advantageous, or even necessary, in certain use cases. Unlike production runs, analysis is characterised by rapid R&D cycles and an expectation of fast turnaround, often using ad hoc data and metadata. Therefore general framework design is an important topic considered here as it can easily, although unintentionally, effectively exclude the analysis use case by making rapid R&D very difficult. These design considerations are discussed with the aim of providing guidance for the final design, while the final design choices must be taken by the framework design team. The design of the framework will impose constraints on developers and these will need to be accepted by the developer community and documented with the framework. To the extent that is possible, it is highly desirable that the same services and tools can be configured and accessed inside and outside the framework executable. This has the implication that much of the functionality traditionally provided by the framework executable (scheduling, reading and writing of data) be accessible outside of the framework context.

Heterogeneous computing and concurrency in general already plays an important role in scientific computing, promising greater speed and efficiency so long as we can utilise the disparate resources well. Again, general design considerations are presented here to provide guidance for the framework design. Technical design choices of e.g. whether developers should have direct access to concurrency tools like TBB, or whether they should be brokered by the framework is left to the framework design team.

An important use case not considered in this document is the use of the data processing framework in the online environment, particularly for a high-level trigger (HLT) which will present its own unique requirements (e.g. early termination of a trigger chain, forced accept, etc.). The most striking feature of the HLT usage pattern is the need to process a subset of data, usually corresponding to some region of interest. This pattern arises naturally in the use cases considered here.

General framework requirements

Frameworks typically use state transitions similar to those used in data acquisition and run control, including configuration, initialization, execution (where algorithmic code is typically run) and finalization. These state transitions are used by the framework to guarantee that all framework components have their work scheduled coherently. The components of a framework depend on the particular design but key requirements are

(1) the framework must separate data and algorithms

(2) the framework must separate the persistent data representation from the in-memory representation seen by algorithms.

For ease of reference, the "Data Store" is defined as the framework's repository for storing data in memory beyond the lifetime of particular algorithms. More detail on these broad requirements follow in later sections.

The framework needs to perform many different data processing steps with potentially very many different variations. As the code base will be rather large, targeted (re)compilation for particular purposes is not desirable, especially if e.g. only a handful of parameters for one algorithm need to be changed. Instead, the components of the framework are configured to perform a particular task in a particular way, e.g. performing signal processing on raw input data.

Configuration requirements

Configuration is distinct from initialization of the framework objects; configuration happens first. Given that RAII is an important concept for multi-threaded design, it is best to have a fully configured framework instance in the initialization phase. Given the abundance of variations that make up HEP workflows a robust and easily programmable configuration system is a foundational component of all modern frameworks. Some use a strictly declarative language and some use a Turing complete language. The former must be augmented with scripts that write the declarations in a Turing complete language (usually it is part of the workflow management system, WMS) because it turns out that control flow is a requirement. Given this, there is a requirement that:

(3) the framework should provide a Turing complete configuration language as a foundational component so that it can ensure coherence of its configuration.

The WMS needs to be able to supply framework configuration parameters such as input file(s) or random number seeds to each framework application instance, which it should do using the framework's configuration language. To minimise errors, these parameters should be self-describing and validatable, and so:

(4) the framework should provide a suitable API so that algorithm writers can ensure their required parameters are self-describing and validatable.

The framework should provide the concept of parameter sets that are nestable. The set of all parameter sets that define a framework application instance should be identifiable, referred to here as a FrameworkConfigID. Tracking that identity is one of the ingredients necessary to ensure scientific reproducibility. However some parameters do not (and should not) change the algorithmic results, such as a debug print flag. Independent of the state of such a flag it should be possible to define equivalence between FrameworkConfigIDs.

(5) The framework configuration system needs to have a robust persistency and versioning system that makes it easy to document and reproduce previous results. It must be possible to create, tag, check-sum, store and compare configurations. This configuration management system should be external to the framework or data files so that configurations can reliably be reused and audited.

Further fundamental requirements related to the framework configuration to guarantee reproducibility are:

(6) The resulting state of the configured framework and its components should be deterministic and precisely reproducible given a set of environmental conditions which include the available hardware, operating system, input data, etc.

(7) the ensemble of the framework+environmental conditions must give reproducible results.

Following on from the discussion of supporting fast analysis R&D:

***(8) it is desirable that it should be possible to only configure those framework components required for a particular data processing use case*.**

This generates a further requirement that

(9) it must be possible to derive the input data requirements for any algorithm, in order to define the sequence of all algorithms needed for a particular use case.

Concurrency and Multithreading

The arrival of concurrency and heterogeneous architectures has added a further level of complication for framework designers and developers alike. Much of the existing

code-base still relies heavily on serial programming for CPU architectures, meanwhile the co-processor market is evolving rapidly resulting in a diverse hardware landscape. Both multi-threading and co-processors present challenges for both frameworks and developers.

(10) It is therefore desirable that the framework should help facilitate the use of multi-threaded data processing and facilitate access to co-processors in an efficient manner.

For developers, highly modular code must be encouraged, allowing evolution or replacement of sub-algorithms that lend themselves to particular approaches. It is assumed that algorithmic code will be organized in "algorithm modules" and this term is used in this document. The codebase will therefore likely contain several alternatives for (sub)algorithms, the choice of which would depend on the available hardware. The framework will need to run in heterogeneous and potentially dynamic environments where the availability and type of co-processors may be known late. While the design of this technically challenging aspect is left to framework developers, it is worth pointing out the added challenge of developing algorithms for diverse hardware if the framework does not easily allow it. Therefore:

(11) it is highly desirable that it be possible to write algorithmic code independently of the framework.

This also helps keep the gap between analysis and production code as low as possible. Furthermore,

(12) ***it is highly desirable that the framework be sufficiently modular in design to allow re-use of framework services and functionality both within and outside of the framework context, as far as that is possible.***

Multi-threading presents additional, well-documented challenges, particularly given that many important libraries are not thread-safe. Summarising briefly: algorithmic code, including sub-algorithms, should be thread-safe and must declare their compatibility to the framework.

(13) The framework must be able to schedule thread-safe and non-thread-safe work appropriately.

Thread-safety implicitly includes a general requirement on developers that algorithms and their sub-algorithms do not store state information in a thread-unsafe manner. Further, data exchange should be done in controlled ways to ensure thread-safety, e.g. via some service which manages transient data - again the implementation of this challenging aspect is left to the framework designers.

Reproducibility and provenance

The reproducibility of physics results and the knowledge of how physics results were obtained is essential to DUNE and to the neutrino community as a whole. It must be possible both to replicate physics results using identical input data, or to repeat an analysis using a different set of input data with an identical sequence of identically configured algorithms. Therefore,

(14) the framework must provide a full provenance chain for any and all data products which must include enough information to reproduce identically every persistent data product. By definition, the chain will also need to include sufficient information to reproduce the transient data passed between algorithm modules, even though the product is not persisted in the final output.

The need for transient data products is driven by the large Trigger Record sizes that can be encountered in the DUNE data, and whose transformation may be required, but for storage considerations are not written out.

The use of highly parallel and heterogeneous computing environments leads to additional provenance requirements regarding the execution ordering and computing architectures on which the algorithms were executed. The need for this information arises because of the possibility of different computing architectures producing different results, and of accelerators and other computing offload mechanisms producing different results than serially executed or non-accelerated codes (i.e. GPU accelerated code producing different results than the same code executed on the host processor). Therefore

(15) the framework must provide full provenance information and all of the metadata required to ensure reproducibility.

This will include the computing architecture, including any specialized hardware used, on which the application is run as well as the runtime environment, execution model and concurrency level that the application used. It is likely that a full picture of the

necessary metadata will also require information only known to the workflow management system. In such a complex environment, it is highly desirable that the framework provide support to allow the effect of configuration changes and computing environments to be easily understood.

Random numbers, machine learning and conditions

DUNE will use several libraries outside of the framework software stack, and it will also be necessary to record the precise versions of all of these libraries to guarantee reproducibility of the physics results. It is noted that containers (docker et al) could potentially make provenance tracking easier in this respect. Random number generation is an important aspect of code and given the additional complications of multi-threading and co-processors:

(16) it is highly desirable that the framework broker access to random number generators and seeds in order to guarantee reproducibility.

One important source of external libraries relates to machine learning, and machine learning inference is expected to play a significant role in all stages of data processing including analysis.

(17) The framework should give special attention to machine learning inference in the design, both to allow simple exchanges of inference backends and to record the provenance of those backends and all necessary versioning information.

In addition to the Trigger Record data, data processing requires access to other data from various sources, for example slow controls, detector status, beam component status. Such data is referred to generically as “conditions data” and also includes e.g. detector calibrations and any data external to the Trigger Record. The time granularity or “interval of validity” of this data varies by source and is typically of much coarser granularity than individual Trigger Records, e.g. calibrations may be valid for months of data taking. Meanwhile there are often several versions of conditions data and correlations between conditions data is not uncommon, making the coherent management of conditions data a challenge in itself. For this reason, conditions data management should be external to the framework.

Access to the external conditions data should preferably proceed via REST interfaces that support loose coupling of the framework and the external conditions management system. As conditions data may need to be transformed from its persistent format into a

format required by an algorithm, and as multi-threading makes the cache validity of conditions data complicated:

(18) the framework must provide a conditions service that is a single point of access to conditions data.

(19) The configuration of the framework conditions service should ideally be via one configuration parameter (a global tag).

Developers must not hard-code conditions data in their algorithms, although

(20) it must be possible to override a subset of global tag configured conditions for testing purposes.

Developers usually find it convenient if such alternative conditions payloads can be provided outside of the main managed conditions system, e.g. via a local file.

Data and I/O layer

The main aim of this document is to describe the data processing steps for simulation and reconstruction of DUNE data. The first stage of processing in offline jobs, after job configuration and initialization, is reading in detector data. Offline jobs must read in data produced directly by the data acquisition system and also data produced by Monte Carlo simulation. Input data files may be retrieved from a persistent storage system, delivered over a network, or reside on local storage.

(21) The framework must support reading and writing different persistent data formats.

Every version of the framework must be able to read data files written by that version of the framework and all previous versions, with no loss in functionality or change in meaning of the data elements.

(22) The framework I/O functionality must be backward compatible across versions.

We do not require forward compatibility, in which data written with newer versions of the framework are also readable by older versions. Cases in which forward compatibility is

broken need to be documented as far as possible, however, as these are breaking changes.

Experimenters may change their minds about the contents of data products. For example, data members may be added because they were initially not included in the design but later found to be necessary, and rather than create a new data product, an expansion of an old one is more convenient. Framework programs reading old and new data files need to behave seamlessly if the data product has changed definition.

(23) A mechanism for user-defined schema evolution of data products needs to be provided.

The DUNE data model allows for Trigger Record data to be stored in persistable representations which are generated by customized hardware or which are optimized for specific acceleration hardware or computing systems. As a result, the data model expects that data will have custom “packed” representations that do not conform to 32-bit or 64-bit little-endian words. Furthermore, compression of the raw waveform data will be performed in the DAQ, though some data may arrive uncompressed. Some highly compressible data products may benefit from dedicated compression algorithms scheduled to run before output. Therefore,

(24) the framework must provide a mechanism to register/associate and to run/apply custom serialization/deserialization and compression/decompression algorithms to data on write/read of that data from a persistable form.

Data products that do not have dedicated compression algorithms associated with them can still benefit from automatic compression that is enabled by default.

(25) The framework should support compression on output data in a manner that is transparent to users and is configurable. It must be possible to disable the automatic compression of output data or provide compression transforms that are effectively identity transforms.

Experience shows that it is highly desirable to be able to configure a maximum file size such that output files are the correct size for efficient storage and for units of data processing; currently a file size of several GBs is considered optimal. As this requires the closure of an existing output file and creation and opening of a new file (with sensible filename) then this needs to be addressed at the framework level.

(26) The framework should allow a configurable maximum output file size and provide appropriate file-handling functionality.

Memory management

An issue that arises during data read-in and decompression and unpacking is the memory footprint used. The DUNE Far Detector is big. Supernova-burst (SNB) processing in the DUNE Far Detector presents unique challenges due to the large volume of data that are produced in each Trigger Record. An uncompressed SNB Readout for 100 seconds will take about 120TB of storage for one single-phase far detector module for just the TPC wire data, and DUNE will have four detector modules. These data will be divided into smaller chunks both in time and by detector component. For single-phase detector modules, these components are likely to be the anode plane assemblies (APA) due to the granularity of the data preparation processing.

In the first stage of offline processing, waveforms from the channels are de-noised and deconvolved, and pulses that are approximately Gaussian appear in the processed waveforms. Because the 100s of SNB Readout from each channel must be artificially broken into small chunks in time, there is the potential to introduce edge effects at the chunk boundaries. In order to avoid this, about 100 microseconds of data spanning the boundary on both sides must be used in processing the chunks.

A common ratio of RAM to CPU cores on existing grids is 2 GB/core. Memory usage beyond this results in poor performance and can lead to job eviction depending on the resource configuration. An uncompressed DUNE Far Detector module Trigger Record will be larger than this, about 6 GB. A supernova Trigger Record of 100s will be more than five orders of magnitude bigger again. Clearly the framework will need to be able to act on subsets of Trigger Records, while respecting the overlap criteria noted above in order to avoid creating artefacts.

(27) The framework must be able to operate on subsets of a Trigger Record. Specifically, it must be possible to break Trigger Records down into smaller chunks (e.g. one APA) and be able to stitch those chunks back together. For supernovae, it must also be possible to reuse a fraction (nominally 100 us) of the previous chunk (nominally 5ms) of data to allow stitching in time.

Data unpacking and initial processing can be arranged to operate on these subsets. In order to realize the benefit from operating in this way, however, intermediate data products that are no longer needed must no longer occupy space in memory. Data

products that have been written out and are no longer needed in memory are also good examples of those that can be evicted from memory, but there are also cases of intermediate products which must be flushed instead of written out.

(28) Data products should not occupy memory beyond their useful lifetimes.

As noted in “General Considerations”, the framework must be aware of which algorithms need which data products, while the algorithmic code, by nature of its modularity and re-use/reconfigurability, is expected to be unaware of what other components may be run in the same job. Therefore, the framework must be responsible for garbage collection, capable of freeing up memory at the earliest possible time. Furthermore, the framework will need to respect the memory constraints imposed by the processing environment which will entail supporting partial reading of data objects into memory and potentially purging any data objects or partial data objects not immediately required.

(29) The framework must manage memory of data products in the Data Store.

Frameworks need to provide configurable, flexible I/O access so that experiments can control the output of their jobs in fine-grained detail. This is needed to save on storage and also experimenter time, as smaller datasets take less time to analyze than larger ones.

(30) The framework needs to support skimming/slimming/thinning for data reduction.

Similarly, processing and analysis is made much more convenient (or even possible) if the skimmed/slimmed/thinned output streams can be associated with information in other streams that may be stored separately. Some analyzers may need the auxiliary data streams while others may not, and so a framework job that produces outputs for collaboration use would need to read all of the necessary streams. This also allows efficient use of storage, as data does not need to be co-located in the same file to be available for processing. In the case of writing, I/O cost can be very efficiently amortized if several output streams can be written based on one input file.

(31) The framework needs to be able to read and write several parallel data streams (including friend trees). Labelling of data objects across streams should be intuitive and not error prone. Provenance information should support correlating related data objects across streams.

A common offline job need that goes beyond the 1->1 input to output data model is mixing real Trigger Record data with Monte Carlo simulation. Monte Carlo simulation is often not sufficiently realistic, perhaps it fails to capture the time dependence of detector conditions or the generator or detector simulation simply lacks sufficient accuracy for the physics use case. In this case, Monte Carlo simulation can be augmented by adding actual detector data, e.g. to embed single tracks or entire Trigger Records into simulated data and reconstruct them as if they were actual Trigger Records. This can lead to a 2->many input output situation with asynchrony in both input and output.

(32) The framework needs to allow experiment code to mix simulation and (overlay) data.

Physics analysis

A SNB Trigger Record may have thousands of interesting physics interactions in it. They will be small tracks ("stubs"), of order of tens of wires hit in each plane, distributed through the detector and in time during the long Trigger Record. A convenient analysis workflow will save regions of interest to smaller files containing only data needed to analyze the small tracks and not the large amounts of waveform data containing only electronics noise and radiologicals. Most other Trigger Records, initiated by cosmic rays, beam neutrino interactions and atmospheric neutrino interactions, will have only one interaction in a Far Detector module. Some cosmic rays arrive in bundles with other cosmic rays, even at the 4850' level, and these are interesting to read out.

The near detector, on the other hand, will have many neutrino interactions per LBNF spill. The Gaseous Argon Near Detector Component (ND-GAr) expects 60 overlaid interactions per spill, mostly originating in its calorimeter, which has fast timing capabilities and thus can be used to separate particles belonging to different Trigger Windows. The liquid-argon TPC near detector will have order of 20 interactions per spill. Some downstream analyses will benefit from and expect upstream analyses to divide a Trigger Record's data into subsets based on classification algorithms that are intended to separate one interaction from another. These physics regions of interest, usually called "slices", are then what physicists expect to use as a unit of execution, i.e. they loop over slices in their analysis code.

(33) It must be possible to define arbitrary units of execution that are independent of Trigger Records. It must be possible to correlate these units to Trigger Records for exposure accounting, and experiment conditions.

Here, experiment conditions refers to data collected outside of the Trigger Record data stream. It consists of monitoring data from slow controls, detector status, and beam component status.

Data analysis presents its own challenges, and requires different tradeoffs to the preceding simulation/reconstruction/particle identification stages. Analysis includes the extraction of oscillation parameters, but is not limited to that, encompassing, as a minimum, comparisons between data and Monte Carlo, extraction of calibration and detector performance parameters, cross-section measurements, measurements of atmospheric, solar, and supernova neutrinos, and searches for non-standard phenomena.

The event-by-event paradigm is not a good match here. Spectra are filled by looping over neutrino candidates, or any other particle candidate, but then may undergo substantial processing in their own right. For example, the main work of an oscillation fit is the evaluation of many different combinations of oscillation and nuisance parameters. While slices provide sub Trigger Record control flow, particle candidate control flow ignores the Trigger Record structure entirely.

Efficient data access for typical analysis workflows is also very different to data processing using the event-by-event paradigm. It is very common to require access to only a small subset of the Trigger Record information (the variables required to make a cut, or reconstruct a quantity), and for the amount of information to vary across Trigger Records (e.g. in the case of early rejection in a physics analysis selection). For example ROOT TTrees use a “column-wise” data layout to make this access pattern efficient, but any serialization using the event-by-event paradigm will produce “row-wise” data. This may have implications on the persistent and transient Data Models and corresponding I/O layer implementations. Taking the above into consideration, the requirements for the framework are:

(34) The framework should make minimal assumptions about the data model, i.e. it should not assume an event-by-event paradigm.

(35) Analysis must be able to use particle-candidate-based control flow, without any constraints arising from the event-by-event paradigm.

(36) The framework must support partial reading of the persistent data and must not require reading an entire Trigger Record unless required (i.e. it must not force the entire Trigger Record to be read).

If these requirements cannot be reasonably satisfied then it is highly likely analysis would need to use a different framework to that used for data processing, but it is noted that e.g. Belle II has a similar dichotomy satisfied by one framework.

In the case where the data-processing and analyses frameworks are separated, it is desirable for a level of compatibility to be maintained between the frameworks. In previous experiments, there is a common pattern where, as the analysis framework matures, graduate students cease to be able to develop in the data-processing framework. To avoid this, compatibility layers may be required to allow algorithms (such as calibration, reconstruction, and selection methods) to transparently plug into either framework, to the extent it is possible.

(37) Calibration, reconstruction, and selection algorithms must be framework-agnostic, i.e. able to run transparently in any official DUNE framework where equivalent requisite data products exist.

Analysis work will be undertaken by a large number of collaborators, with varying levels of experience. In many cases, rapid feedback and iteration will be required to make progress. Meaningful analysis work must be possible with resources available locally to collaborators (single CPU, few gigabytes of memory, <100GB of disk). It must be possible to produce relevant histograms on interactive timescales (ie minutes). This re-emphasises the earlier requirements in General Considerations and in addition:

(38) The framework should be easily portable and capable of running on local resources.

Experience shows that oscillation fits accounting for large numbers of systematic uncertainties are resource intensive, while analysts will likely only have access to modest local resources for prototyping and development. Therefore the framework should make scaling and concurrency transparent both to the analyst and the developer as far as possible. The use of declarative analysis techniques should be strongly encouraged to support this even when co-processors (and low-level implementation) changes.

(39) The same code developed and tested on local resources must scale to large resources. This should include HPC resources as far as possible.

Analysis files, of course, are derived from the data-processing framework files, and it must be possible to reconstruct this history. Due to the very large number of Trigger Records expected to be summarized in a single analysis file, the size requirements, and the fact that per Trigger Record information remains available in the parent files, we require:

(40) Analysis files must record their parent framework files, but no Trigger Record provenance is required. The full provenance information need not be retained in analysis files as this could easily become larger than the data itself.

One common and insidious class of mistakes is errors in exposure accounting and normalization. This is also a problem that is entirely solvable at the technical level. Each individual Trigger Record (beam spill or other trigger) has exposure associated with it, whether POT or livetime or both. When filling a summary histogram from processing Trigger Records, the exposure should be calculated and stored as an integral part of the histogram, and operations between histograms should take correct notice of the exposure, e.g. ratio of one large exposure sample to a smaller exposure sample should produce a dimensionless ratio that has allowed for the differing exposures.

(41) The framework must have native support for exposure accounting (POT and livetime), so as to make errors of this sort difficult.

All but the simplest analyses require a treatment of systematic uncertainties. There are three main technical means by which these systematics can be introduced. The most common, and most convenient, is reweighting. For example, the effect of various cross-section and flux uncertainties may be encapsulated by applying weights to Trigger Records of certain categories, to increase or decrease their representation in the final spectra. Secondly, Trigger Record data may be shifted. For example, an energy scale uncertainty may be most conveniently represented by rewriting of Trigger Records to increase or decrease reconstructed energies by a certain amount. Finally, the least convenient method is alternate simulation samples. The profusion of files requiring processing and bookkeeping makes this a heavyweight option, but in the case of uncertainties early in the analysis chain with complex effects, it may be the only way to handle them accurately. The treatment of systematics is cross-cutting across all

analyses, it is important it is handled correctly, and the framework is able to offer substantive technical assistance.

In addition to being able to handle multiple input data streams:

(42) The framework should provide some means of cross-referencing (labelling) multiple input streams to correlate them in order to facilitate evaluation of systematic uncertainties.

For oscillation analysis, it will be important to work with both Near and Far detector data. Whether in an explicit joint fit, or where extracting constraints from the ND to apply to the FD analysis, there must be a uniformity in the treatment of various systematics. In general, experience gained with the Near Detector (where the majority of analysis work is likely to happen) should be transferable to the Far Detector. This re-emphasises the importance of the framework making minimal assumptions about the Data Model.

(43) The framework should be able to work with both ND and FD data on an equal footing, and within the same job.

While most of the focus at this stage of the experiment is on other tasks, in the long run analysis work will dominate. The outsized influence of decisions about data formats and analysis infrastructure mean that they should be afforded specially-careful consideration. This is also a very dynamic area, with rapid timescales and the possibility of important new ideas, so we must also remain flexible.

Appendix

Utilities

It should be possible to read/write framework-format data outside of the framework.

Utilities must be supplied that list data product names, sizes, and compressed sizes in files written by the framework.

Desired features

Care must be taken by the experiments to label mixtures of real data and simulated data as simulations. Experiment code may expect MC truth labels on all objects when in fact only some may be available, or possibly all are absent by choice. A method or a flag that returns a binary “isRealData” value may be too coarse-grained. Issues that need to be addressed are the handling of bookkeeping: Trigger Record numbering, handling of MC truth information in what otherwise is a data Trigger Record, and any code that performs different actions on MC and data. Analyzing mixed data will almost certainly require access to values from run conditions and calibration databases, and these have to be understood that they are the ones the user desires.

Another goal to think about without formally requiring it is to allow and encourage the overlapping of computation and I/O operations. I/O operations often take significant wall-clock time that can be used for computation if possible. The framework should support concurrent execution of both I/O and algorithm components and in a manner that allows for multiple units of data, not limited to just Trigger Records, to be processed concurrently (data pipelining).

Production processing usually involves one or more subsequent reprocessing passes, either after calibration constants have been calculated from the data or from external sources, or to accommodate new algorithms. Sometimes these reconstruction passes start with raw data as input, and sometimes they can take advantage of previous passes initial data processing stages (such as signal processing) and work on higher-level objects, such as hits. The framework needs to allow for this sort of workflow to be configured and run by the experiments. Sometimes the results of an

earlier processing pass need to be compared with those of a later pass, and the option to keep both sets of results in the output for comparison is useful.

It should be possible to reprocess data produced by the framework, both in re-running some or all previously run processing steps, and to add new processing steps. The output must be properly labeled and configurable so that the output of the earlier processing steps may be distinguished, dropped or retained.

The fully processed data and Monte Carlo from the experiment are likely to run to multiple terabytes. In order for analysis, which must necessarily consume the entire dataset, a hugely reduced data representation is required. It would be technologically feasible to do this by aggressive summarizing and slimming of the framework files from previous stages, and this does have some benefits, but due to the radically different demands of analysis and the benefits of alternate structurings of the data we explicitly do not make this a requirement or even a recommendation.

Experience has shown the importance of compatibility between disparate analysis efforts. This allows work on improving the data formats and analysis framework to be shared, allows experience and expertise from one area to carry over to another without retraining, reduces the opportunity for bugs, and saves huge amounts of time spent attempting to compare between or reconcile analyses.

There should be a common analysis data format, shared by virtually all analysis efforts.

Of course, this does not mean all analyses must use precisely the same files. Different aspects of data analysis will require radically different physics selections, and use non-overlapping properties of the data. We refer only to technical compatibility. This skimming work is expected to be common, and analysis is expected to iterate substantially more rapidly than data processing, including the inevitable respins for mistakes.

It should be possible to create a new iteration of the analysis files from the data-processing framework files on a reduced timescale (weeks) and to create skim files rapidly (days).