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Chapter 1

Computing Roles and Collaborative Projects

1.1 Roles

This appendix lists computing roles for DUNE derived from a comparison with existing similar roles on the LHCb experiment at CERN. LHCb is similar in size and data volumes to Deep Underground Neutrino Experiment (DUNE).

Distributed Computing Development and Maintenance - 5.0 FTE

> This role includes oversight of all software engineering and development activities for packages needed to operate on distributed computing resources. The role requires a good understanding of the distributed computing infrastructure used by DUNE as well as the DUNE computing model.

Software and Computing Infrastructure Development and Maintenance - 6.0 FTE

> This role includes software engineering, development, and maintenance for central services operated by DUNE to support software and computing activities of the project.

Database Design and Maintenance - 0.5 FTE

> This role includes designing, maintaining, and scaling databases for tasks within DUNE.

Data Preservation Development - 0.5 FTE

> This role includes activities related to reproducibility of analysis as well as data preservation, which requires expert knowledge of analysis and the computing model.

Application Managers and Librarians - 2.0 FTE

Application managers handle software applications for data processing, simulation, and analysis, and also coordinate activites in the areas of development, release preparation, and deployment of software package releases needed by DUNE. Librarians organize the overall setup of software packages needed for releases.

Central Services Manager and Operators - 1.5 FTE

The site manager and operators are responsible for the central infrastructure and services of the DUNE distributed computing infrastructure. This includes coordination with the host laboratory for services provided to DUNE.

Distributed Production Manager - 0.5 FTE

Distributed production managers are responsible for the setup, launch, monitoring, and completion of processing campaigns executed on distributed computing resources for the experiment. These include data processing, Monte Carlo (MC) simulation, and working group productions.

Distributed Data Manager - 0.5 FTE

The distributed data manager is responsible for operational interactions with distributed computing disk and tape resources. The role includes but is not limited to helping to establish new storage areas and data replication, deletion, and movement.

Distributed Workload Manager - 0.5 FTE

The distributed workload manager is responsible for operational interactions with distributed computing resources. The role includes activities such as helping to establish grid and cloud sites.

Computing Shift Leaders - 1.4 FTE

The shift leader is responsible for the experiment's distributed computing operations for a week-long period starting on a Monday to the following Sunday. Shift leaders chair regular operations meetings during their week and attend general DUNE operations meetings as appropriate.

Distributed Computing Resource Contacts - 0.5 FTE

Distributed computing resource contacts are the primary contacts for the DUNE distributed computing operations team and for the operators of large (Tier-1) sites and regional federations. They interact directly with the computing shift leaders at operations meetings.

User Support - 1.0 FTE

User support (software infrastructure, applications, and distributed computing) underpins all user activities of the DUNE computing project. User support personnel respond to

questions from users on mailing lists, Slack-style chat systems, and/or ticketing systems, and are responsible for documenting solutions in knowledge bases and wikis.

Resource Board Chair - 0.1 FTE

This role is responsible for chairing quarterly meetings of the Computing Resource Board, which includes representatives from the various national funding agencies that support DUNE, to discuss funding for and delivery of the computing resources required for successful processing and exploitation of DUNE data.

Computing Coordination - 2.0 FTE

Coordinators oversee management of the computing project.

1.2 Specific Collaborative Computing Projects

The HEP computing community has come together to form a HEP Software Foundation Collaboration (HSC)[1] that, through working groups, workshops, and white papers, guides the next generation of shared HEP software. The DUNE experiment's time scale, particularly the planning and evaluation phase, is almost ideal for allowing the HSC to develop effective contributions. Our overall strategy for computing infrastructure is to carefully evaluate existing and proposed field-wide solutions, to participate in useful designs, and to build our own solutions only where common solutions do not fit and additional joint development is not feasible. This section describes some of these common activities.

1.2.1 LArSoft for Event Reconstruction

Several neutrino experiments using the liquid argon time-projection chamber (LArTPC) technology share the Liquid Argon Software (LArSoft)[2] reconstruction package. MicroBooNE, SBND, DUNE, and others share in developing a common core software framework that can be customized for each experiment. This software suite and earlier efforts in other experiments made the rapid reconstruction of the ProtoDUNE-SP data possible. DUNE will contribute heavily to the future evolution of this package, in particular, by introducing full multi-threading to allow parallel reconstruction of parts of large events, thus anticipating the very large events expected from the full detector.

1.2.2 WLCG/OSG and the HEP Software Foundation

The Worldwide LHC Computing Grid (WLCG) organization [3], which combines the resource and infrastructure missions of the LHC experiments, has proposed a governance structure called Scien-

tific Computing Infrastructure (SCI) that splits out dedicated resources for LHC experiments from the general middleware infrastructure used to access those resources. In a white paper submitted to the European Strategy Group in December 2018 [4], a formal SCI organization is proposed. Many other experiments worldwide are already using this structure. As part of the formal transition to SCI, the DUNE collaboration was provisionally invited to join the WLCG management board as observers and to participate in the Grid Deployment Board and task forces. Our participation allows us to contribute to the technical decisions on global computing infrastructure while also contributing to that infrastructure. Many of these contributions involve the broader HEP Software Foundation efforts.

Areas of collaboration are described in the following sections.

1.2.2.1 Rucio Development and Extension

Rucio[5] is a data management system originally developed by the ATLAS collaboration and is now an open-source project. DUNE has chosen to use Rucio for large-scale data movement. Over the short term, it is combined with the sequential access via metadata (SAM) data catalog used by Fermi National Accelerator Laboratory (Fermilab) experiments. DUNE collaborators at Fermilab and in the UK are actively collaborating on the Rucio project, adding value for both DUNE and the wider community.

Besides DUNE, the global Rucio team now includes Fermilab and Brookhaven National Laboratory (BNL) staff, CMS collaborators, and the core developers on ATLAS who initially wrote Rucio. DUNE computing and software consortium (CSC) members have begun collaborating on several projects: (1) making object stores (such as Amazon S3 and compatible utilities) work with Rucio (a large object store in the UK exists for which DUNE has a sizable allocation); (2) monitoring and administering the Rucio system, and leveraging the landscape system at Fermilab; and (3) designing a data description engine that can be used to replace the SAM system we now use.

Rucio has already proved to be a powerful and useful tool for moving defined datasets from point A to point B. Rucio appears to offer a good solution for file localization but it lacks the detailed tools for data description and granular dataset definition available in the SAM system. The rapidly varying conditions in the test beam have shown that we need a sophisticated data description database interfaced to Rucio's location functions.

Efficient integration of caching into the Rucio model will be an important component for DUNE unless we can afford to have most data on disk to avoid staging. The dCache model, a caching front end for a tape store, is used in most Fermilab experiments. In contrast, LHC experiments such as ATLAS and CMS work with disk storage and tape storage that are independent of each other.

1.2.2.2 Testing New Storage Technologies and Interfaces

The larger HEP community[6] currently has a data organization, management, and access (DOMA) task force in which several DUNE collaborators participate. It includes groups working on authorization, caching, third party copy, hierarchical storage, and quality of service. All are of interest to DUNE because they will determine the long-term standards for common computing infrastructure in the field. Authorization is of particular interest; they are covered in Section 1.2.2.4.

1.2.2.3 Data Management and Retention Policy Development

A data life cycle is built into the DUNE data model. Obsolete samples (old simulations and histograms and old commissioning data) need not be maintained indefinitely. We are organizing the structure of lower storage to store the various retention types separately for easy deletion when necessary.

1.2.2.4 Authentication and Authorization Security and Interoperability

Within the next few years, we expect the global HEP community to change significantly the methods of authentication and authorization of computing and storage. Over that period, DUNE must collaborate with the USA and European HEP computing communities on improved authentication methods that will allow secure but transparent access to storage and other resources such as logbooks and code repositories. The current model requires individuals to be authenticated through different mechanisms for access to USA and European resources. Current efforts to expand the trust realm between European Organization for Nuclear Research (CERN) and Fermilab should allow a single sign-on for access to the two laboratories.

1.2.3 Evaluations of Other Important Infrastructure

The DUNE CSC is still evaluating some major infrastructure components, notably databases, and workflow management systems.

The Fermilab *conditions* database is being used for the first run of ProtoDUNE, but the Belle II [7] system supported by BNL is being considered for subsequent runs [8].

We are evaluating DIRAC [9] as a workflow management tool and plan to investigate PANDA [10], as well, to compare against the current GlideInWMS, HT Condor, and POMS solution that was successfully used for the 2018 ProtoDUNE campaigns. Both DIRAC and PANDA are being integrated with Rucio and several LHC and non-LHC experiments use them.

Glossary

ATLAS One of two general-purpose detectors at the LHC. It investigates a wide range of physics, from the search for the Higgs boson to extra dimensions and particles that could make up dark matter (DM). 5

Brookhaven National Laboratory (BNL) US national laboratory in Upton, NY. 5, 6

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. 6

CMS Compact Muon Solenoid experiment at CERN. 5

computing and software consortium (CSC) DUNE computing and software consortium. 5, 6

DIRAC Computing workflow management designed for LHCb and now used by many HEP experiments. 6

data organization, management, and access (DOMA) data organization, management, and access efforts through the HEP Software Foundation. 6

Deep Underground Neutrino Experiment (DUNE) A leading-edge, international experiment for neutrino science and proton decay studies. 2–6

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. 5, 6

HEP high energy physics. 4–6

HEP Software Foundation Collaboration (HSC) A foundation that facilitates cooperation and common efforts in high energy physics software and computing internationally. 4

Liquid Argon Software (LArSoft) A shared base of physics software across LArTPC experiments. 4

liquid argon time-projection chamber (LArTPC) A time projection chamber (TPC) filled with liquid argon; the basis for the DUNE far detector (FD) modules. 4

LHC Large Hadron Collider. 4–6

LHCb LHC experiment dedicated to forward physics. 2

Monte Carlo (MC) Refers to a method of numerical integration that entails the statistical sampling of the integrand function. Forms the basis for some types of detector and physics simulations. 3

MicroBooNE The LArTPC-based MicroBooNE neutrino oscillation experiment at Fermi National Accelerator Laboratory (Fermilab). 4

ProtoDUNE Either of the two DUNE prototype detectors constructed at European Organization for Nuclear Research (CERN). One prototype implements single-phase (SP) technology and the other dual-phase (DP). 6

ProtoDUNE-SP The SP ProtoDUNE detector at CERN. 4

Rucio Data management system originally developed by ATLAS but now open-source and shared across HEP. 5, 6

sequential access via metadata (SAM) A data-handling system to store and retrieve files and associated metadata, including a complete record of the processing that has used the files. 5

SBND The Short-Baseline Near Detector experiment at Fermilab. 4

Scientific Computing Infrastructure (SCI) Proposed extension of the infrastructure component of Worldwide LHC Computing Grid (WLCG) to other experiments. 4, 5

Worldwide LHC Computing Grid (WLCG) Worldwide LHC Computing Grid. 4, 5

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