Large Scale Monte Carlo Simulation of Neutrino Interactions Using the Open Science Grid and Commercial Clouds

A. Norman, J. Boyd, G. Davies, E. Flumerfelt, K. Herner, N. Mayer, P. Mhashilhar, M. Tamsett, S. Timm

1Fermi National Accelerator Laboratory, Batavia IL, USA
2Indiana University, Bloomington IN, USA
3Tufts University, Boston MA, USA
4University of Sussex, Brighton, UK
E-mail: anorman@fnal.gov

Abstract. Modern long baseline neutrino experiments like the NOνA experiment at Fermilab, require large scale, compute intensive simulations of their neutrino beam fluxes and backgrounds induced by cosmic rays. The amount of simulation required to keep the systematic uncertainties in the simulation from dominating the final physics results is often 10x to 100x that of the actual detector exposure. For the first physics results from NOνA this has meant the simulation of more than 2 billion cosmic ray events in the far detector and more than 200 million NuMI beam spill simulations. Performing these high statistics levels of simulation have been made possible for NOνA through the use of the Open Science Grid and through large scale runs on commercial clouds like Amazon EC2. We details the challenges in performing large scale simulation in these environments and how the computing infrastructure for the NOνA experiment has been adapted to seamlessly support the running of different simulation and data processing tasks on these resources.

1. Overview
The NOνA experiment is a long baseline neutrino experiment designed to measure the oscillation probabilities for $\nu_\mu \rightarrow \nu_e$ ($\nu_e$ appearance) and $\nu_\mu \rightarrow \nu_\mu$ ($\nu_\mu$ disappearance. The experiment can do this for both neutrino and anti-neutrino beam running conditions resulting in for four independent oscillation measurements. These measurements are then used both alone and in combination with each other to place constraints on the mixing parameters that are described by the PMNS 3-flavor mixing model.

The NOνA experiment, as shown in Fig. 1, features a fine grain 14 kton, far detector based on 344,064 15 m long detections cells using a mineral oil based liquid scintillator and wavelength shifting fiber optic readout[1] which is located 810 km from the beam source at an angle of 14 mrad from the primary beam axis. The far detector is located on the Earth’s surface at the Ash River Laboratory in Minnesota. The surface location of the detector results in the detector being subject to more than 180 kHz of cosmic ray induced activity. The experiment also features a near detector located at Fermilab at a depth of 100 m which is designed to measure the NuMI1

1 Neutrinos at the Main Injector
Figure 1. The 14 kton NOνA far detector is located at the Ash River site in northern Minnesota, 810 km and 14 mrad off of the primary beam axis from the NuMI neutrino beam’s origin at Fermilab. A similar 200 ton near detector is located 100 m underground at Fermilab.

beam composition and flux prior to neutrino oscillations.

NOνA is particularly sensitive to being able to resolve the neutrino mass hierarchy problem, by determining the sign of the neutrino mass splitting $\Delta m^2_{31}$. This sensitivity is due to the experiment’s long baseline between target and far detector and ability to detect the $\nu_e$ appearance signature. This sign indicates whether the state $\nu_3$ is the heaviest or lightest of the neutrino mass eigenstates. These two possibilities determine whether the neutrino sector follows a “normal” mass/flavor structure similar to the charged leptons, where the electron is the lightest lepton an the $\tau$ the heaviest, or whether the neutrino sector follows an “inverted” hierarchy where the state that couples the least to the $\nu_e$ flavor state is the lightest. These measurements are extremely sensitive to the $\nu_e$ appearance probability and as a result require high statistics modeling of both signal and background channels to be able to make precision estimates of the mixing parameters.

2. Simulation Needs

The precision nature of the measurements that the NOνA experiment can make rely not only on the high quality of the data that is produced by the far and near detectors, but on the ability of the Monte Carlo based simulation code to model the neutrino beams, cosmic ray fluxes and the interaction and response characteristics of particles within the detectors. Critical to NOνA s science goals are detailed understandings of the beam related and cosmic ray induced backgrounds which mimic the oscillation signatures for both the $\nu_e$ charged current topology or the $\nu_\mu$ charged current topology, or distort the reconstructed energy distributions of either of these signatures which are directly linked to the determination of the mixing parameters.

The primary physics channel that contributes to these backgrounds are neutral current interactions with a $\pi^0$ in the final state. These interactions results in an electromagnetic shower which mimics the same shower topology as a $\nu_e$ charged current event. The other primary backgrounds are mis-reconstructed $\nu_\mu$ charged current interactions, and cosmic ray induced backgrounds. The simulated and observed backgrounds from each of these channels along with their propagation through the NOνA selection chain are shown in Table 1.

The NOνA far detector is located on the surface with only a 3 m earth equivalent over burden. This results in a tremendous flux of cosmic ray muons and other cosmic ray induced particles
Simulation Data

| Cut               | $\nu_e$ Signal | NC Beam $\nu_e$ | $\nu_\mu$ CC | Cosmic Ray | All Background |
|-------------------|----------------|-----------------|--------------|------------|----------------|
| All Events        | 36.7           | 380             | 28.1         | 557        | 19M            | 19M            |
| Pre-selection     | 24.7           | 83.5            | 2.9          | 30.0       | 56k            | 56k            |
| Vertex Gap        | 24.6           | 81.8            | 2.9          | 29.6       | 55k            | 55k            |
| $P_T/P$           | 22.0           | 59.6            | 2.6          | 24.3       | 1248           | 1334           |
| Maximum Y         | 21.2           | 57.4            | 2.5          | 23.0       | 834            | 917            |
| Neutral Net       | **13.9**       | 3.9             | **1.5**      | 0.7        | 0.5            | **6.5**        |
| Library Template  | **14.0**       | 3.5             | 1.5          | 1.1        | 0.9            | **7.0**        |

Table 1. NOνA background rates for the $\nu_e$ determined from the 2014/2015 simulation campaigns and comparisons of Monte Carlo to real far detector cosmic ray data. Rates are broken out by the selection chain criteria that are applied during the analysis process.

Impinging on the detector. These particles have the ability to penetrate deep enough, through in active regions of the detector, and interact in such a manner that they can appear to again mimic the $\nu_e$ or $\nu_\mu$ interaction topologies.

Understanding these backgrounds would require massive simulation campaigns to generate cosmic ray and beam fluxes, and detailed reconstruction and analysis work compare the simulated fluxes to the observed spectra in the detectors.

For the first set of detector data that NOνA experiment analyzed, it was necessary to simulate a cosmic ray exposure with high enough statistics that all portions of the NOνA detector’s phase space were sampled sufficiently to provide certainty in the backgrounds estimates. For this procedure the nominal detector exposure for the first data set, corresponding to the approximately 120 s of live detector readout, needed to be simulated at 100× the nominal exposure to provide sufficient certainty in the background estimates. This resulted in the projection that almost 3.3 hours of cosmic ray exposure, or nearly 1.8 billion cosmic ray interactions would have to be generated and propagated through the NOνA detector. [2]

In addition, neutrino beam simulation also needed to be generated and propagated through the NOνA near and far detectors to understand the neutral current backgrounds, reconstruction efficiencies and intrinsic $\nu_e$ content of the beam. This modeling of the beam related backgrounds required a sample the was nearly 10× the nominal exposure of $6 \times 10^{20}$ protons on target (PoT) of the first analysis set, or over 197 million NuMI beam events. The energy distributions of these samples are shown in Fig. 2.

This level of simulation work required that computing resources outside of the Fermilab campus computing clusters be leveraged and that the NOνA simulation code and infrastructure be adapted to modern grid and cloud computing environments.

3. Adaptation of Simulation Code

The adaptation of the NOνA simulation and analysis code stack to run at arbitrary sites around the globe required significant modifications to four major aspects of the computing model. The NOνA code would need to allow for code relocation, would need to provide compatibility across a variety of different operating system flavors, would have to allow for application distribution to foreign computing elements and clusters and would have to structure data movement to permit both copy in and copy out facilities to arbitrary locations.

3.1. Code Relocation

The first step in modifying the NOνA code base was to perform a detailed audit of the more than 459,000 lines of NOνA collaboration written analysis code. This audit was designed to
Figure 2. Simulation of neutrino interaction energy spectra broken out by interaction type for the NuMI neutrino beam. Statistical errors corresponding to one year of nominal beam exposure ($6 \times 10^{20}$ POT) shown. This simulation required the full simulation of over 197 million NuMI beam events.

Figure 3. Simulation of the $\nu_\mu$ quasi-elastic energy spectra with and without oscillations for a total exposure of $18 \times 10^{20}$ POT at full 14 kton detector mass. This simulation required extensive beam and full detector modeling.

Figure 4. Comparison of the output of the neural net corresponding $\nu_\mu$ CC identification for cosmic ray background Monte Carlo simulations and actual cosmic ray data data taken with the NOvA far detector. The more than 1.8 billion cosmic ray Monte Carlo events have been scaled down to match the detector data.

detect all instances where developers had either relied on locations including absolute paths based off of the structure of the software distribution as it was installed on the Fermilab central NAS systems, or had failed to use run-time reconfigurable paths to locate any type of input file source. The audit also reveal dependencies within the NOvA code base where developers had referenced files that were located outside of the official code distribution trees, often times in their own home directories or development areas. All of these path dependencies were remove so that code trees could be arbitrarily relocated to a different machine or storage system with only the need to modify run time environment settings.
The code was also audited so that it was compatible with being homed on an immutable, read-only volume. This required that I/O calls within the code be audited to ensure that configuration information, auxiliary data files, temporary files and other types of caches either be explicitly accessed through read-only methods or not exist within the code’s distribution trees. This resulted in the detection of numerous direct I/O calls which were improperly opening files in the base code’s release trees, or inadvertently placing temporary information within the tree. These access methods were modified and temporary information was relocated to use standard temporary file locations and access patterns.

Third party products and external packages or libraries that the NO\textnu A software depends on were packaged as relocatable UPS\textsuperscript{2} products\textsuperscript{3} and organized in independent product tree areas corresponding to the software distribution they support (e.g. NovaNearline\textsubscript{externals} supports the NovaNearline distribution).

The full software stack was then reorganized to be organized under a simple “base prefix”, as shown in Fig. 5 so that the code distribution could be re-homed at run time through the setting of simple environment paths and the use of UPS setup functions to configure specific dependency chains.

3.2. Operating System Compatibility
The NO\textnu A code stack was designed to compatible with both Scientific Linux Fermi 5 and 6. However the heterogeneous nature of the open science grid and other campus grids, can cause library version conflicts between the NO\textnu A code and the libraries that maybe installed on a local compute node. NO\textnu A ensures compatibility with the host operating system where the jobs run two separate ways.

First all the third party packages and external dependancies that code base relies on are packaged as relocatable UPS products with strong architecture, operating system flavor and product specific version information. The NO\textnu A software sets up a dependency tree at run time with the corresponding package versions, system flavors and architectures that are detected from the host system where the software is running. It then fully configures the code to run on this architecture or if an incompatibility is detected, the code aborts execution appropriately. This method is used to provide the full compiler suite and associated libraries that the software was built against as well as many domain specific packages that the software requires.

The second way in which the NO\textnu A code distribution ensures compatibility with the host operating system, is through a specific set of “compatibility” libraries. This library collection

\textsuperscript{2} Unix Product Support

\textsuperscript{3} UniversitextPath Support

**Figure 5.** Top level of the fully relocatable NO\textnu A software tree after reorganization under a common base path structure. Each major code tree has a parallel structure which contains all of the external dependencies that are needed for build and release as well as the run time dependencies.
was assembled to provide a fully “matched” set of libraries which are typically provided by the host platform, but which are known to be fully compatible with the NOνA software. By providing a full set of matched libraries that can override those provided by the host OS, NOνA can ensure that any differences between the states of different grid clusters are removed from the operational environment that the software sees. In the same manner that external dependencies are packaged as UPS products, the NOνA compatibility libraries are likewise packaged as a fully flavored and versioned UPS product so the that run time environment can choose the proper version to use.

3.3. Code Distribution

The packaging of the NOνA software stack as a fully relocatable, re-homable, read-only volume allows for the experiment to distribute full binary releases for multiple platforms and architectures via the CVMFS platform[4]. Using the CVMFS system, NOνA distributes the full 2 TB simulation and analysis code distribution for all official code releases that have been made in the last two years along with all of their supporting dependencies.

The base CVMFS repository is replicated out to the Open Science Grid through the official OSG stratum 1 servers, and through this mechanism become available at all sites that are participating in the OSG. Initially NOνA used a repository hosted directly by the OSG in the form of the shared Oasis CVMFS service. The NOνA code base, due to its size and use patterns was determined to be a candidate for its own dedicated CVMFS repository and in March of 2015 the NOνA code base was ported to a dedicated repository hosted by Fermilab and replicated out to the OSG by the stratum 1 servers. This repository was made available on the OSG as nova.opensciencegrid.org and has been used by the NOνA collaboration to run their code at sites that are direct collaborator in the NOνA, as well as sites that accept the Fermilab and NOνA VO.

3.4. Data Movement

The last step in making the NOνA software fully compatible with the Open Science Grid and commercial cloud providers, providing a path for both input and output data to reach the simulation and analysis jobs. To do this the NOνA code was fully integrated with the SAM data handling system which has been modernized to use standard HTTP communications channels[5]. The SAM system employs a data handling model in which the data is brought to the individual jobs at run time and for which no pre-placement of large datasets are necessary.

NOνA’s integration with SAM takes advantage of the full metadata catalog and replica catalog that the system provides, to intelligently schedule data movement to jobs that run both local to the Fermilab site, as well as those that run at remote sites. For NOνA, specific sites known or dedicated storage elements (or in the case of Amazon, the S3 storage resource) are used by the SAM system to stage data into the site or to buffer data for egress from the site. NOνA also leveraged the use of the Fermi File Transfer Service (F-FTS) to simplify the registration, cataloging and archiving of the output data that was generated by remote sites.

4. Simulation Campaigns on Grid and Cloud Resources

The project to adapt the NOνA code based to the requirements described in section 3 resulted in the ability to run the NOνA simulation and analysis suite at remote computing sites that had access to the Open Science Grid provided Oasis CVMFS service. During 2014 and 2015, NOνA used this capability to run over 2 million hours of simulations on distributed resources. These campaigns focussed primarily on the simulation of cosmic ray samples and NuMI beam described in section 2. The campaigns leveraged resources of more than 20 sites around the world as shown in Fig. 6. These sites included commercial cloud resource that were instantiated through Amazon Web Services (AWS), as well as sites who are members of the NOνA collaboration and...
other general OSG sites where were accessed in a purely "opportunistically" manner. Under this opportunistic model, large grid sites made idle resources available to OSG community and those resources were then consumed on a first-come first-server basis by participating OSG VOs. NO\(\nu\)A was one of the first communities, in the Intensity Frontier program at Fermilab, to demonstrate the viability of using opportunistic resources through the OSG for completing large scale simulation and data analysis tasks.

Submission of jobs to remote resources was managed through the glideinWMS system [6]. The system provides a uniform user interface which aggregates together local, grid and cloud resources. In turn, GlideinWMS uses the HTCondor system [7] to provision the remote resources. In the case of Grid sites, the glideinWMS system submits a pilot job to the site act as a "placeholder" for the actual user job. In the case of Cloud resources, the system makes a request to or invokes the provisioning system that is used to instantiate a specific virtual machine image, associated with a predefined count, on the cloud provider’s resources. When the remote resources are successfully reserved or become available, the requirements of individual jobs in the submission queue are matched against the capabilities being provided by the different pilot mechanisms and the actual user jobs are dispatched to the sites accordingly.

As part of a pilot program investigating the large scale use of cloud computing for scientific analysis, NO\(\nu\)A engaged in the generation of far detector cosmic ray Monte Carlo events using Cloud resources provided at Fermilab and through Amazon Web Services [8]. In the largest trial of this pilot program, NO\(\nu\)A ran 1,000 concurrent simulations on both FermiCloud\(^3\) and AWS.

For large scale Monte Carlo production, NO\(\nu\)A ran on the AWS platform, scheduling 3,300 simulations using 525 separate dual core virtual machines. This burst processing configuration of resources was able to produce 3.3 Million Far Detector Cosmic Ray events in the span of approximately 6 hours from the time of initial submission. The campaign produced 467 GB of output data that was directly transferred back to the storage systems at Fermilab through the standard data management and data handling systems described in Section 3.4. The total cost of the burst simulation campaign was $449, with a cost of $398 for the computation and $51 for data egress. This campaign demonstrated the ability of using cloud bursting for the generation of critical datasets that are time sensitive and require extremely a fast turn around between submission and availability for analysis. As was done in the pilot programs with the

\(^3\) Fermilab’s Cloud platform using OpenNebula
OSG, NOνA fully demonstrated their compatibility with cloud environments and the viability of running large scale scientific workflows on commercial clouds. This demonstration has opened up these avenues of analysis to other experiments in the intensity frontier program at Fermilab who are able to leverage the NOνA infrastructure and parts of the NOνA code stack to run similar simulations on AWS and else where.

5. Conclusions
The NOνA experiment has made significations changes in an effort to adapt their code base and computing model to permit their simulation and analysis code to run effectively on the Open Science Grid and on commercial cloud resources like Amazon’s AWS platform. These resources were used in 2014 and 2015 to make substantial contributions to the generation of over 1.8 billion cosmic ray interactions in the NOνA far detector and the simulation of over 197 million neutrino beam spills.

These simulation campaigns have demonstrated the ability of commercial cloud resources to provide large amounts of “burst” computational resources for the quick turn around of critical datasets, and have been used in this mode to generate cosmic ray background samples for the first NOνA analysis results.

The use of grid and cloud computing will be expanded in the coming year, as NOνA will use funds awarded through a grant by AWS Educate program to analyze the 2014/2015 neutrino dataset. These efforts will allow for over 2.1 million CPU hours, nearly 20% of the projected computational needs of the dataset, to be run on cloud resources. When these resources are combined with the resources provided by the Open Science Grid and other distributed computing facilities, NOνA may be able to nearly double in 2015/2016 the total analysis and simulation work that would have otherwise been possible using only dedicated Fermilab computing resources.

Acknowledgements
The author acknowledges support for this research was carried out by the Fermilab scientific and technical staff. Fermilab is Operated by Fermi Research Alliance, LLC under Contract No. De-AC02-07CH11359 with the United States Department of Energy

References
[1] Ayres D et al. 2007 The NOνA technical design report Tech. rep. FERMILAB-DESIGN-2007-01
[2] Norman A 2014 The NOνA experiment, the first 12 months of commissioning, operations and physics data XXVI International Conference on Neutrino Physics and Astrophysics
[3] Votava M, et al. 1991 Ups unix product support 7th real time conference
[4] Buncic P et al. 2010 Journal of Physics: Conference Series 219 042003
[5] Illingworth R A 2014 Journal of Physics: Conference Series 513 032045
[6] Sfiligoi I et al. 2009 The pilot way to grid resources using glideinwms Computer Science and Information Engineering, 2009 WRI World Congress on vol 2 pp 428–432
[7] Team Condor http://research.cs.wisc.edu/htcondor/htc.html
[8] Timm S et al. 2015 Cloud services for the fermilab scientific stakeholders 21st International Conference on Computing in High Energy and Nuclear Physics