**Project Goals**

- Extend physics reach of LHC and neutrino experiments
  - Event generator tuning
  - Neutrino oscillation and cross-section measurements
  - Detector simulation tuning

- Transform how these physics tasks are carried out through ASCR math and data analytics
  - High-dimensional parameter fitting,
  - Workflows supporting automated optimization
  - Distributed dataset management storage and access (*in situ*) for experiment data
  - Introduction of data-parallel programming within analysis procedures

- Accelerate HEP analysis on HPC platforms
**Collaboration**

- Collaboration between DOE Office of High Energy Physics and Advanced Scientific Computing Research (ASCR supports the major US supercomputing facilities)
  - LHC and neutrino physics: N. Buchanan (CSU, NOvA/DUNE), P. Calafiura (LBNL, LHC-ATLAS), Z. Marshall (LBNL, LHC-ATLAS), S. Mrenna (FNAL, LHC-CMS), A. Norman (FNAL, NOvA/DUNE), A. Sousa (UC, NOvA/DUNE)
  - Optimization: S. Leyffer (ANL), J. Mueller (LBNL)
  - Workflow, Data Modeling: M. Paterno (FNAL), T. Peterka (ANL), R. Ross (ANL), S. Sehrish (FNAL)
- J. Kowalkowski – PI (FNAL)

Accomplishments

- First NOvA neutrino oscillation analysis using NERSC
  - Time-to-result improved by 50x; first round completed within 16 hours
  - Used ~30M hours on Cori (and part of Edison) across two runs
- Prototype event store (**HEPnOS**) built for serving data to HEP analysis codes
- Data-parallel NOvA pre-analysis event selection procedure
  - NOvA accepted ownership of HDF conversion software for their data
- Improved understanding of ATLAS and CMS data through generator tuning with Pythia, Rivet, and Professor
  - Evolution of generator tuning algorithms, optimization of data selection, and development of DIY workflow
  - Generator tuning on unexploited LHC jet data and detector simulation tuning
- Community interactions:
  - CHEP: Event selection, Rational polynomial approximations in Professor, NOvA analysis

**HEPnOS**: [https://xgitlab.cels.anl.gov/sds/HEPnOS/wikis/home](https://xgitlab.cels.anl.gov/sds/HEPnOS/wikis/home)
NOvA Neutrino Oscillation Measurements

- Compare data with neutrino oscillation hypothesis
  - Extract best-fit oscillation parameters and associated confidence intervals
  - Compute rejection significance for non-optimal parameter values
- Cannot assume gaussian errors for oscillation measurements
  - (1) Low statistics and (2) parameters probed near physical boundaries
  - Require computationally-intensive calculation for confidence intervals

\[ P(\nu_\mu \rightarrow \nu_\mu) \simeq 1 - \sin^2(2\theta_{23}) \sin^2 \left( 1.267 \Delta m^2_{32} \frac{L}{E} \right) \]
NOvA Neutrino + Antineutrino Analysis

- NOvA uses some of the most complicated fitting procedures in neutrino physics
  - Simultaneous multi-dimensional fits for neutrino and anti-neutrino data
  - Complexity of high dimensional parameter space requires billions of functional fits
  - Multi-Universe techniques utilized for proper statistical corrections

- Large-scale analysis campaigns carried out at NERSC Cori for the first time
  - First run occurred May 7th, over 1.1 million running jobs
  - Second round of calculations occurred May 24th (both Cori and Edison)
  - Consumed 37M CPU-hours in 42 hours over both runs
  - New facilities and procedures enthusiastically received by NOvA collaboration – desire accelerating transfer of other key analyses

- NOvA revealed first set of electron antineutrino appearance results on June 4th at the Neutrino 2018 conference

NOvA Analysis run: Project support

- Required coordinated effort from SciDAC-4, Fermilab, the NOvA collaboration, and NERSC staff.
  - Analysis and technical effort directed by SciDAC/NOVA laboratory and university Postdocs and students
  - Provided excellent training ground for utilizing HPC centers and tools
- HEPCloud enabled large-scale resource provisioning, workload management, and monitoring at NERSC
- Broke several records
  - Accuracy: 8x higher resolution than any prior result
  - Turnaround: 50x faster - results reviewed in <24 hours
  - Scale: ~1M active cores – biggest Condor pool ever
- This work completes a first year major milestone:
  - Forms baseline for analysis calculations with current data, providing major scientific results
  - Reproduced 2017 results for validation
  - Future HPC refactoring will be compared with this result.
Neutrino analysis workflow

• Advancements using HPC leadership facilities
  – Analysis using full dataset across all layers, managed using tools and techniques developed by RAPIDS institute
  – Utilize multi-dimensional fitting procedures from FastMATH institute

• Initial tasks
  – Basic data models for NOvA and LArSoft and datasets mapped into HPC NVRAM-based hierarchical storage systems using ASCR services and tools through the Mochi project
  – Demonstration of fast event selection using DIY
  – Full automation of Feldman-Cousins analysis prescription with Decaf
HEP data management

- Make high-volume reconstructed physics object data available to analysis workflows
  - Leverage existing modular frameworks and extensible data models
  - Starting point: Use actual LArSoft Tracks, Hits, Associations from ProtoDUNE simulation
- Allow facility services to distribute data at any scale, using existing abstractions
  - Runtime ROOT replacement using RAPIDS for I/O
  - Include all levels (or layers) of data aggregation with metadata
  - Data distribution and data parallelism implicit to user
- Application access
  - Exploit event independence
HEPnOS: Fast Event-Store for HEP

Goals:
• Manage physics event data from simulation and experiment through multiple phases of analysis
• Accelerate access by retaining data in the system throughout analysis process
• Reuses components from Mochi ASCR R&D project

Properties:
• Write-once, read-many
• Hierarchical namespace (datasets, runs, subruns)
• C++ API (serialization of C++ objects)

Components:
• Mercury, Argobots, Margo, SDSKV, BAKE, SSG
• New code: C++ event interface
  Map data model into stores
Parallel event pre-selection

• Motivation
  – Fast assessment of event selection used for final analyses
  – Measure effects of event filtering

• Current situation
  – NOvA slice data held in 17K ROOT files across
  – ~27 million events are reduced to tens using ROOT macros applying physics “cuts”

• New method
  – Data prepared for analysis using workflow shown below
  – End state: >50 groups (tables), each with many attributes

• First selection procedure uses Python/MPI/HDF/Pandas on HPCs
  – Global index allow data alignment across tables within one rank
  – Simple composition of cut expressions with Pandas
  – Data parallelism implicit

![Workflow diagram]
Event generators

- Event generators are numerical models used in HEP for describing particle collisions
- 100s of tunable parameters reflecting years of modeling wisdom, made to reproduce experimental measurements
- Professor: a system for tuning a set of parameters to a set of observations; widely used in HEP
  - Relies on hand-picked parameters and observations
  - Only limited sets of parameters can be simultaneously tuned because of computing costs
  - Only simple event generators can be integrated because of computing costs
- Goals: automate, optimize, expand tools, and tune more parameters, exploit neglected data
**Optimizations**

- **Optimization effort:** develop new methods to efficiently identify and optimize only the most relevant tuning parameters in event generator application
- **FASTmath connection:** develop methods for efficient high-dimensional computationally expensive simulation optimization that are general enough to be applicable to a wide range of science problems
- **Our approach:** Formulation as “outer loop” optimization problem
  - Pragmatic approach for balancing deficiencies in physics modeling across a large variety of data
- **Early results:** Optimization performs better than manual data selection
Tuning with data from search analyses

- Generator tuning normally performed with “unfolded” data
  - Specialized measurements (e.g. underlying event, jet properties)
  - Wide variety of data available not previously used for tuning

- Use fast simulation to model detector effects, and tune directly to search data
  - First results compare well to tune with measurement

- Expands data that can be used and kinematic range
  - Tune event generators in phase space regions most interesting to LHC searches
The same mechanism used for tuning event generators can be applied to detector simulation – Here: proof of principle with fast simulation, using the same tools and workflow as before

Parameters normally taken from papers published by the experiments – Labor-intensive process; not always applicable to search regions, where these fast simulations are most used

Can be extended to provide an LHC search-data based fast simulation tune

Tune of jet resolution based on ATLAS dijet search data
Coming soon (end of summer) …

- Parallel NOvA analysis event pre-selection run on HPC facilities
  - HDF with Python, then with C++/DIY application
- First version of Feldman-Cousins correction with DIY
- HEPnOS and large-scale LArSoft dataset load and access
  - ProtoDUNE simulation: use of track/hit objects
  - LArIAT waveform – test using DSP app using DIY
- Generator tuning run

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Engagements

• RAPIDS
  – DIY: now within generating tuning and neutrino analysis applications, soon will be used within event selection and physics object access applications
  – Mochi: used within HEPnOS
  – Decaf: will first be doing an evaluation for overall tuning workflow

• Stefan Hoeche’s SciDAC project
  – Helping define HDF event format and workflows for parallel data access

• FASTMath
  – Combinatorics, binary constraint satisfaction problems: path and schedule optimizations

• HEP community
  – Pythia, Professor, Rivet, art framework, gallery, ROOT, other generators
Potential synergies

• RAPIDS
  – Northwestern University: parallel data access with netCDF
  – HDF Group: improved C++ (14, 17, and beyond), data modeling tools and schema aids
  – Performance tuning: will need help with parallel FS access tuning and vectorization of analysis codes

• FASTMath
  – Sparse grids and MCMC alternatives, high dimensional integration of expensive function

• HEP experiments: Neutrino community and GENIE tuning