Rethinking I/O: Using HPC resources within HEP

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Scalable I/O Workshop
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What we have been challenged with

- Greatly increase usage of HPC resources for HEP workloads
  - After all, many more compute cycles will be available in HPC than anywhere else.
- Can we …
  - Provide for large-scale HEP calculations
  - Demonstrate good resource utilization
  - Use tools available on HPC systems (we believe this is a practical decision)
- Scalable I/O has been one of the major concerns

Efforts have been underway to tackle challenges

- Big Data explorations (SCD)
  - New (to HEP) methods for performing analysis on large datasets
  - Began with Spark, moved to python/numpy/pandas/MPI
- HDF for experimental HEP (Fermilab LDRD 2016-010)
  - Organizing data for efficient access on HPC systems (HDF)
  - Organizing programs for efficient analysis of data with Python/numpy/MPI
- HEP Data Analytics on HPC (SciDAC grant)
  - Collaboration between DOE Office of High Energy Physics and Advanced Scientific Computing Research (ASCR supports the major US supercomputing facilities)
  - Physics analysis on HPC linked to experiments (NOvA, DUNE, ATLAS, CMS)

Questions to be addressed

- How ought data be organized and accessed?
  - Assuming usual HPC facility with a global parallel file system
  - A deeper memory hierarchy than we are used to
- How should the applications be organized?
  - Is our current programming model appropriate?
  - How do we achieve necessary parallelism?
  - What libraries should we be using?
- How will the operating systems and run-time environment affect our computing operations and software?
  - Are the software build and deployment tools we have in place adequate?
  - What if we could analyze an entire dataset all at once?
  - Can we benefit from tighter integration of workflow and application?

Plan of attack

- Choose representative problems to solve
  - NOvA analysis workflows, LArTPC processing, generator tuning
- Choose toolkits and libraries that could help
  - HDF5
  - ASCR data services geared towards HPC
  - Python with numpy, MPI, and Pandas
  - Container technology
  - DIY as a solution for data parallelism
- Facilities to be used initially:
  - NERSC Cori (KNL and Haswell)
  - ALCF Theta

Guiding principles, requirements, and constraints

- We aim to greatly reduce the time it takes to process HEP data.
- We need to redesign our workflows and code to take full advantage of HPC systems.
  - to use well-established parallel programming tools and techniques
  - to make sure these tools and techniques are sufficiently easy to use
  - We need programs that are adaptable to different “sizes” of jobs (numbers of nodes used) without changing the code.
  - We want data designed for partitioning across large machines.
- We want to partition data (and processing) by things that are meaningful in the *problem domain* (events, interactions, tracks, wires, . . .), not according to *computing model artifacts* (e.g. Linux filesystem files).
  - parallelism *implicit*

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Experimental contexts for our work

- LArTPC wire storage, access, and processing
- Event selection for neutrino analysis
- Object store for physics data
- Physics generator data access

LArTPC wire storage, access, and processing

Noise removal from LArIAT waveforms

- LArIAT is a LArTPC (Liquid Argon Time Projection Chamber) test beam experiment
- Converted all LArIAT raw data sample to one HDF5 file
  - Started with 200K art/ROOT data files
  - ~42 TB of digitized waveforms (4.2 TB compressed)
  - 15,684,689 events.
  - Waveform data from u and v wireplanes (240 wires per plane, 3072 samples per wire)
- Reorganized the data using HDF to be more amenable for parallel processing
- Processing the entire LArIAT raw data sample
  - First step of reconstruction is noise reduction using FFTs

Example MPI code: processing many events at one time

```
# first and last are calculated by library code, to tell
# this function call what part of the data set it is to
# work on.
adc_data = adcdataset[first:last] # read block of array
adc_floats = adc_data.astype(float)
# view data as an array of wires, rather than as events
adc_floats.shape = (nevts*WIRES_PER_PLANE, SAMPLES_PER_WIRE)
waveforms = transform_wires(adc_floats) # real work done here
# view the data as events again
waveforms.shape(nevts, WIRES_PER_PLANE, SAMPLES_PER_WIRE)
```

Parallelism is *entirely implicit*, and entirely data parallel.

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Example code: processing many wires

- All the real work is done in the numpy library, implemented in C.
  - The library ***can*** use multithreading, or *vectorization*, to get the most performance from the hardware.
- The script that launches the application specifies how many processes to use:
  - mpirun -np 76800 python process_lariat.py **<**filename**>**
  - This starts 76800 communicating parallel instances of our program — equivalent to running 76800 jobs all at once.

```
def transform_wires(wires):
    ftrans = numpy.fft.rfft(wires, axis=1)
    filtered = THRESHOLDS * ftrans
    return numpy.fft.irfft(filtered, axis=1)
```


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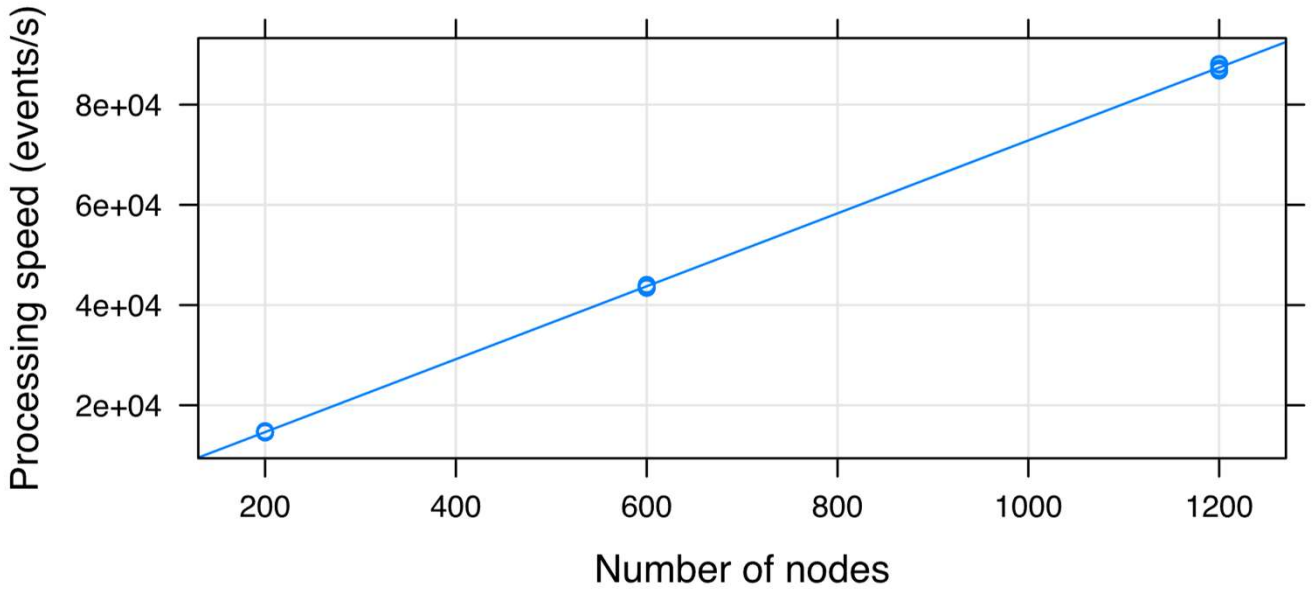
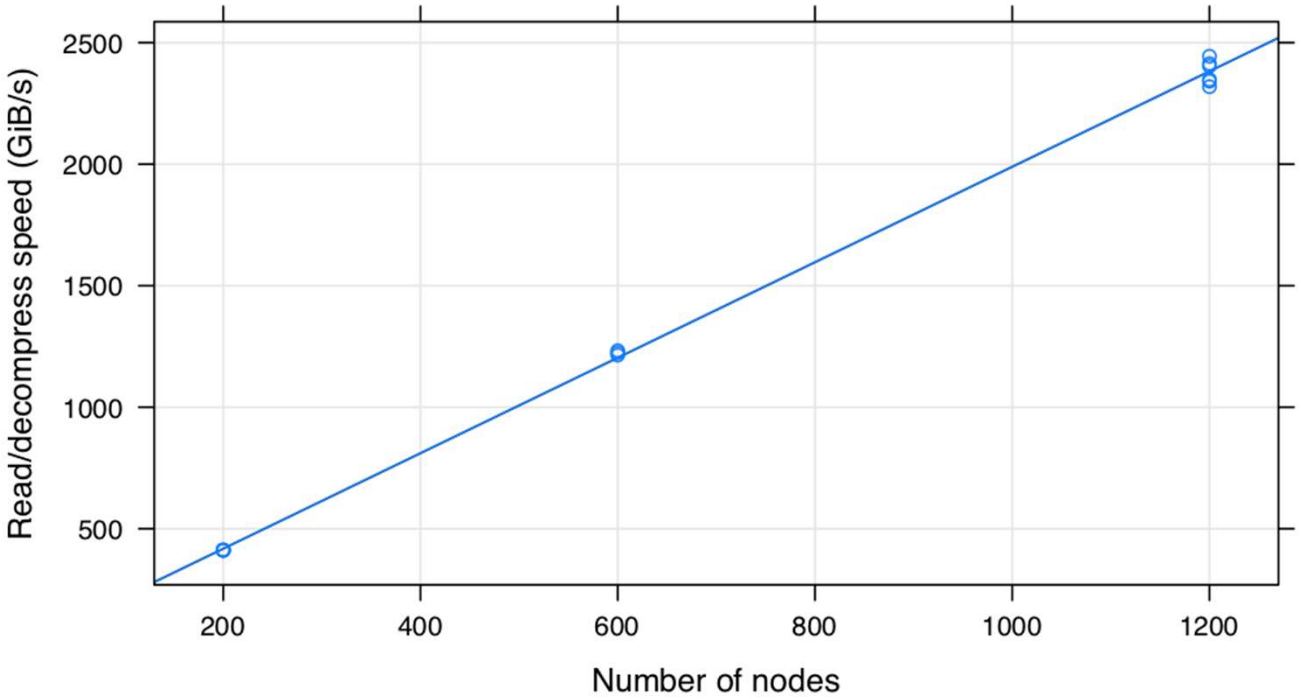
Processing speed for full analysis being done



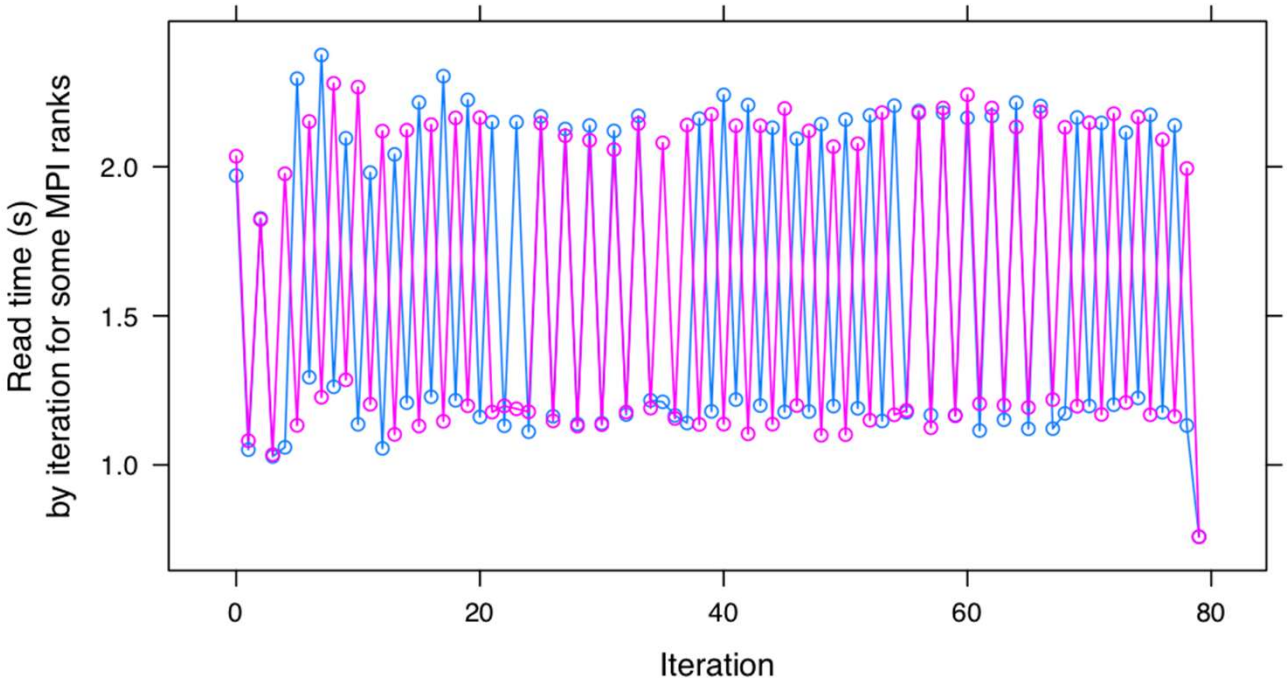
- Entire LArIAT dataset processed in three minutes (at 1200 nodes)
- Shows perfect scaling

Read speed – how does the I/O scale?



- Read + decompression speed for the whole application
- Nearly perfect strong scaling

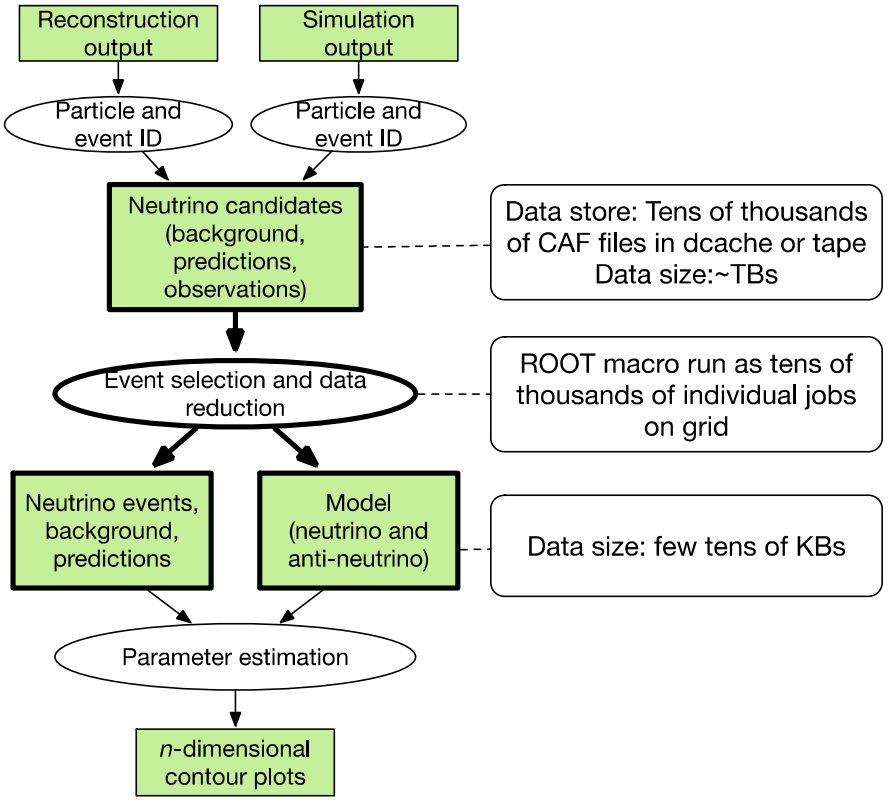
We should be able to do better …



- Different colors correspond to different ranks in the application
- Slower iterations within the application are twice as slow as faster ones (81 iterations in whole run)

Event selection for neutrino analysis

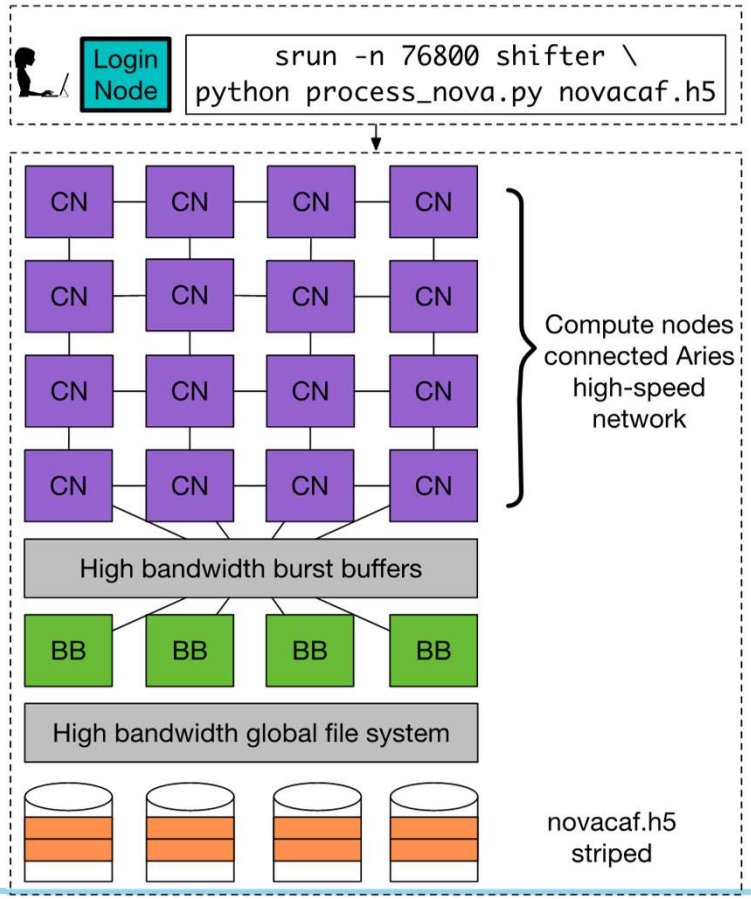
Traditional solution for oscillation parameter measurement



High-level organization of processing

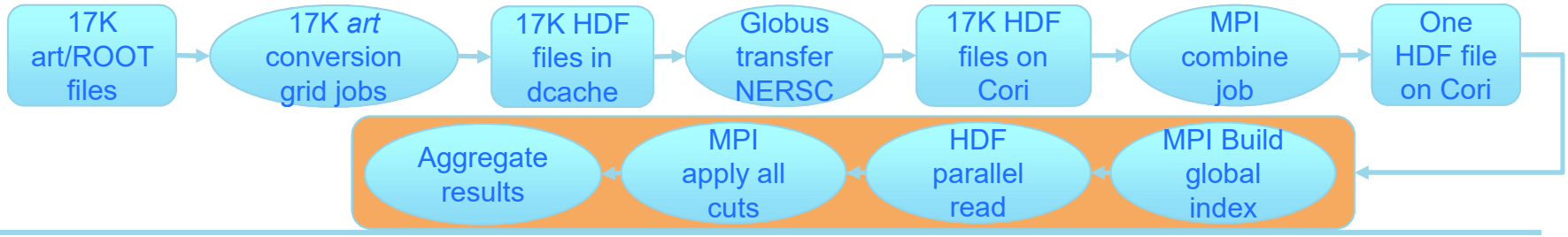
- We want to minimize …
  - *Reading*
  - *Communication* and *synchronization* between ranks
- We organize the data into a single HDF5 file, containing many different tables
  - some tables have one entry per slice
  - some have a variable number of entries per slice
- We want to process all data for a given *slice* in a single rank.
  - the *slice* is NOvA's "atomic" unit of processing, like a collider *event*.
  - for data that represent per-slice information, this is trivial
  - for other data, we need to do some work to ensure each rank has the correct data.

HPC solution



Parallel event pre-selection

- 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



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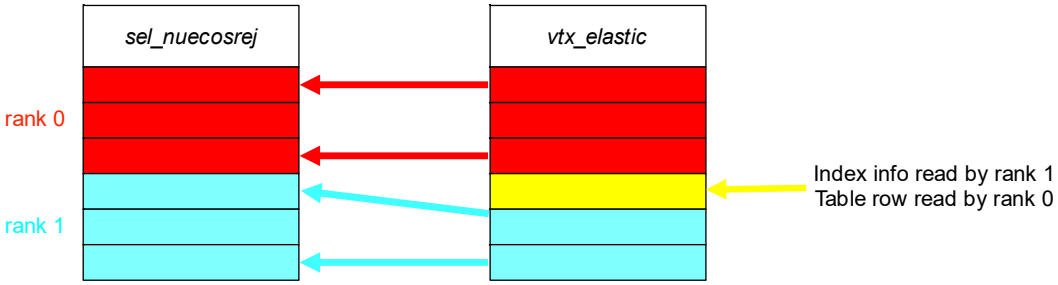
Distributing and reading information

- Each rank reads its “fair share” of index info from each table.
  - identifies which rank should handle which event, for most even balance
  - identifies range of rows in table that correspond to each event (all slices)



- Event “ownership” information distributed to all ranks
  - this assures no further communication between ranks is needed while evaluating the selection criteria on a slice-by-slice basis.
  - perfect data parallelism in running all selection code
- Each rank reads *only* relevant rows of relevant columns from relevant tables
  - all relevant data read by some rank
  - no rank reads the same data as another

Example selection code

```
def kNueSecondAnaContainment(tables):
    df = tables['sel_nuecosrej']
    return (df.distallpngtop > 63.0) & \
           (df.distallpngbottom > 12.0) & \
           (df.distallpngeast > 12.0) & \
           (df.distallpngwest > 12.0) & \
           (df.distallpngfront > 18.0) & \
           (df.distallpngback > 18.0)
```

- Selection can be done on multiple columns of a table.
- Logical operations are connected by & operator.
- Data parallelism is totally *implicit.*
- Returns an array with one logical value per *slice*.

```
def vtxelasticzCut(tables):
    df = tables['vtx_elastic']
    df['good'] =
        (df.vtxid == 0) & (df.npng3d > 0)
    KL = ['run', 'subRun', 'event', 'slice']
    return df.groupby(KL)['good'].agg(np.any)
```

- *vtx_elastic* table has one entry per *vertex;* may be more than 1 per slice.
- *groupby* combines results for all vertices in one slice.
- Returns an array with one logical value per *slice*.

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Current status

- NOvA has taken ownership of our HDF “ntuple” production code
  - They will use this in their own future production.
  - Especially interested in using for machine learning; many tools work with HDF5 files.
- We will be comparing performance with C++-MPI implementation.
- Integration with larger workflow that is also part of the SciDAC project
  - use of changes in event selection criteria to evaluation systematic uncertainties in the mixing parameter measurements
  - one integrated MPI program, to take best advantage of HPC platform.

Object store for physics data

HEPnOS: Fast Event-Store for HEP (on HPC)

Goals:

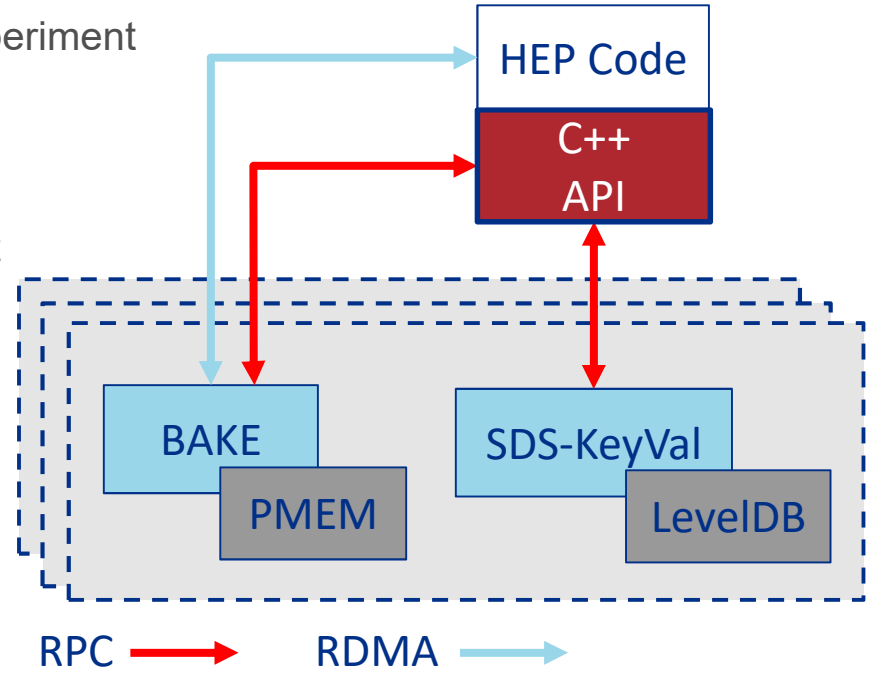
- Manage physics event data from simulation and experiment through multiple phases of analysis
- Accelerate access by retaining data in the system throughout analysis process
- Reuses components from Mochi ASCR R&D project

Properties:

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

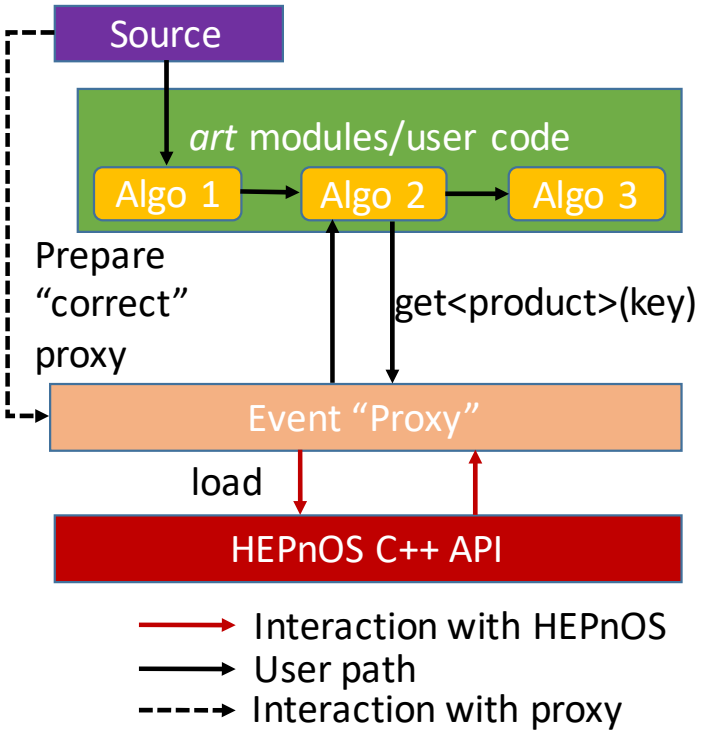
Components:

- Mercury, Argobots, Margo, SDSKV, BAKE, SSG
- **New code: C++ event interface**
  Map data model into stores



Our first use of HEPnOS

- Make high-volume reconstructed physics object data available to analysis workflows
  - Use existing *art* framework and gallery library
  - Starting point: Use actual LArSoft *Tracks*, *Hits*,and *Associations* from ProtoDUNE simulation
- Allow HPC facility services to distribute data at any scale, using existing HEP abstractions
  - Runtime ROOT File I/O replacement using HEPnOS
  - Include all levels (or layers) of data aggregation with metadata
- Data distribution and data parallelism implicit to user



Event currently interacts with *art*/ROOT File

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Current status and future direction

- Prototype test programs are running:
  - one to read from existing art/ROOT data files, and to write to the new data store
  - one to read from the new data store, and verify the integrity of the data
- We are using Docker containers for easy portability of development environment
  - Some of us develop on macOS laptops, others on a variety of Linux installations
  - We will deploy to NERSC (through Shifter) and ALCF (through Singularity)

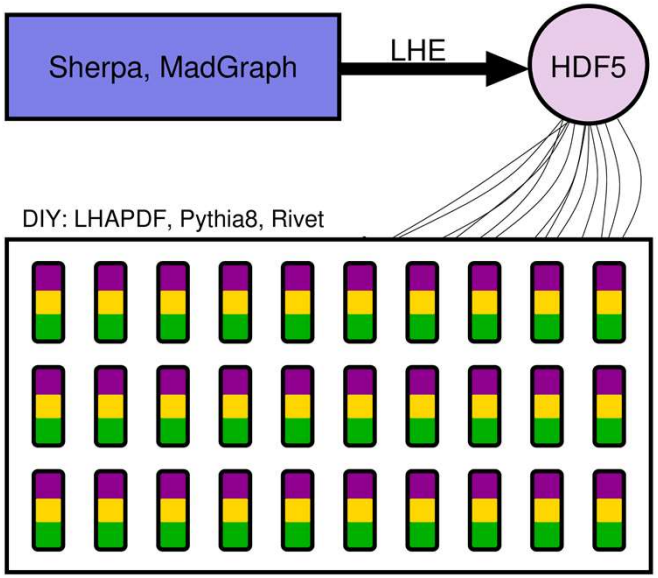
- The dataset (description and name) is included in the namespace
  - Interesting to have direct access to any part from any process on any node
  - Opens up new workflow possibilities
  - Can readily represent and access things below the event, such as NOvA slices

Physics generator data access

Matrix element (ME) calculations and physics generators

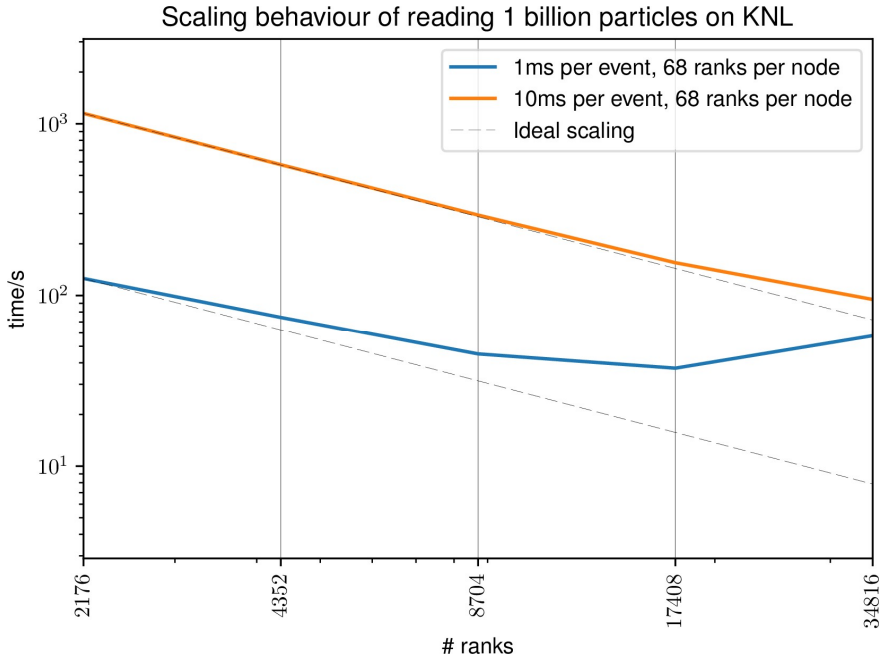
- Adequate predictions of many observables require input from matrix element generators
  - e.g. Getting angular distribution of jets correct
- ME generators (Sherpa, MadGraph) are used to generate high-multiplicity parton-level events
  - LHE description is the typical representation
  - Used as input to Pythia8 to get fully simulated events
- XML-based LHE data format is unsuitable for HPC
- Task is to write LHE data in HDF5 instead
  - We can accumulated all the XML data into one HDF5 file
  - Also working on writing HDF5 directly from Sherpa
- Will work seamlessly with our new DIY-based generator applications that tie together Pythia8, LHAPDF, and Rivet

Generator data available for any size study



- Organization of running Pythia8 on HPC facilities

- I/O will not be an issue



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Summary

- This work may be useful to inform other projects that are ongoing or starting
- NOvA has embraced the work we are doing here
  - Took ownership of the HDF writer module
- Converting full HEP experiment datasets has been very difficult
  - Heavily influenced by ROOT tree structure (NOvA tuple organization)
  - Complexity of data structures (LArSoft RawDigits class and others)
  - Some data structures have been reorganized (vectorization becomes straightforward)
- Python was excellent for prototyping; further work is needed to determine if we are getting the best performance possible.
  - Pandas provides a powerful set of abstractions for analysis tasks
  - Comparisons of C++ and python/pandas forthcoming

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Future directions

- Performance studies and tuning will continue
- Upcoming C++ codes will be using DIY, and possibly additional HPC-centric workflow tools such as Decaf
- Will be working with HEPCloud on integrating dataset handling.
- Looking into
  - Adding Summit as a platform
  - Making sure that analysis involving heterogeneous computing is handled
- As we move towards working within the *art* framework, similar techniques will be applied:
  - read the right information into memory,
  - use vectorized libraries for high-level operations on the data,
  - use the network to round up results that are distributed around the system

Acknowledgements

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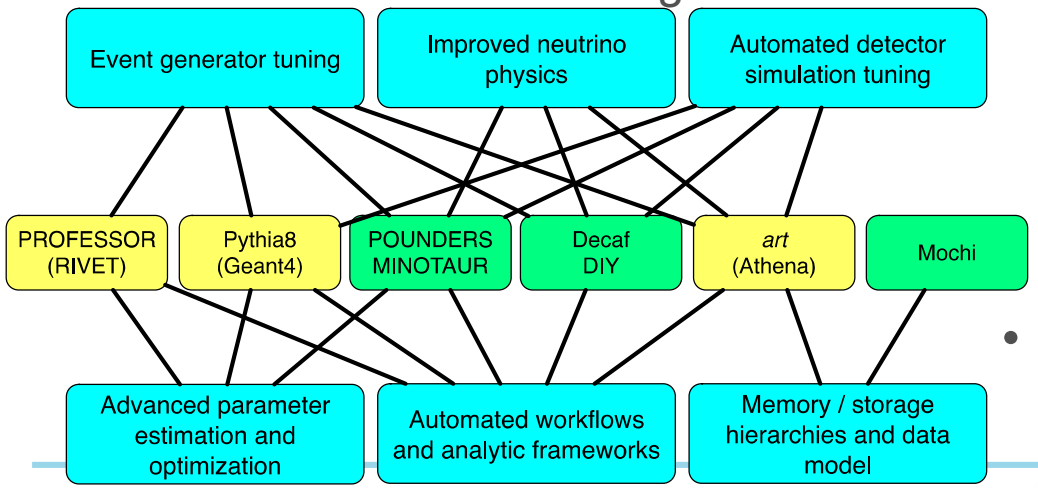
HEP Data Analytics on HEP: Goals

- 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

http://computing.fnal.gov/hep-on-hpc/