Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

Data-parallel analysis supported by HDF5

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"Fermilab is America's particle physics and accelerator laboratory.

We bring the world together to solve the mysteries of matter, energy, space and time."

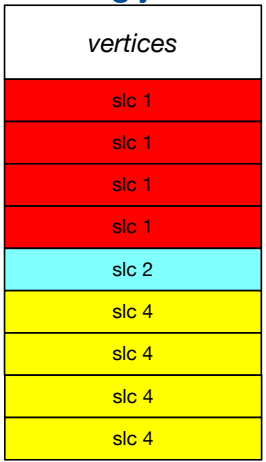
How we are currently using HDF5

- Most of HEP does not have a long history with HDF5.
  - The accelerator modeling community has been using more than 10 years (since v 1.6).
- We use it to store *tabular* data (HEP calls them *ntuples*)
  - for interactive analysis by scientists
  - for input to machine learning algorithms
- We are exploring its use for moderately large data sets
  - current analysis target is about 2 TB.
- HEP scientists program in (1) C++ and (2) Python
- One of our projects is concentrating on analysis using *pandas*, employing HDF5 to support easy-to-use parallel reading of datasets.

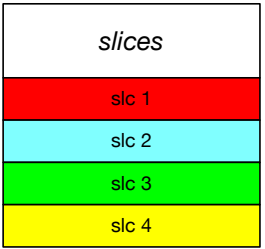
What are data storage looks like

- Tabular data
  - Use *group* to represent a table; read it into a *DataFrame*.
  - Use *dataset* to represent a column.
- Read table into a *pandas* DataFrame.
- Why not use support of HDF5 from *pandas*?
  - Our data sometimes contains multi-dimenional arrays, which don't seem well-supported by *pandas*.
  - Storing data using simple HDF5 concepts allow us to read the data with other tools as well.
- A complication: files have hundreds of tables, which do not all align. We need the equivalent of *joins* between tables — but joins are expensive.

Avoiding joins



Group verices by slice, to make first selection



Use vertex summary with slice information, for second level of selection.

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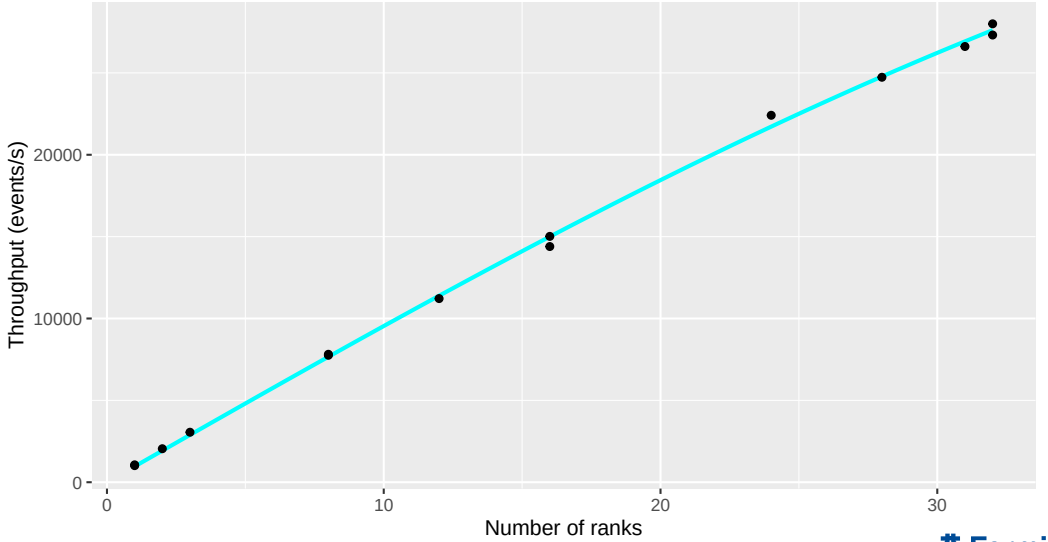
What analysis code looks like

- Analysis programs are MPI-based
- Physicists see *almost* no MPI code — they write as if for a serial process
  - Sometimes need a trivial reduction, adding results from the many ranks
- Framework core code handles data parallelism

```
def kNueCVNCut(tables): # input is a dict of DataFrames
    df = kCVNe(tables)  # apply a different named selection first
    dfRHC = df[kRHC(tables)==1] >= kNueCVNRHC # RHC-class data...
    dfFHC = df[kRHC(tables)!=1] >= kNueCVNFHC # FHC-class data...
    return pd.concat([dfRHC, dfFHC])          # Our result is the sum
```

Some performance measurements (32 core AMD K10 (Barcelona) server)



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What could make this easier

- We have to keep *index columns* (datasets) in each table (group) to let us align the data.
- We keep another index column to let us calculate spans of slices to be processed by each MPI rank.
- A clever indexing scheme would make this task easier. . .
- Efficient *sparse array* storage would make this trivial.