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Some HEP experience with HDF5

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How we are currently using HDF5

- Most of our use is recent; HEP does not have a long history with HDF5.
- 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 large data sets
- HEP scientists program in (1) C++ and (2) Python
- We have provided some C++ library code to make creation of ntuple files simpler.
- Uptake in our community is encouraging:
  - The NOvA experiment is using this in large-scale data processing.
  - The multi-lab and multi-university SciDAC project “HEP Data Analytics on HEP” is making use of it in research.

In a Nutshell

- C++ template-based library for writing tabular data to HDF5.
  - Table -> HDF5 Group.
  - Column -> HDF5 Dataset.
  - Row element -> scalar or fixed size array of basic type (including variable and fixed-length strings).
- Requires C++11 and recent compiler (*e.g.* GCC newer than 6.4 verified); C++14 preferred for more intuitive syntax.
- Produces standard HDF5 files readable with *e.g.* `h5py` or C API.

Detail

- Table structure (column types and ranks) determined at compile-time; column names, extents at runtime.
- Row-based data entry: each column is an extensible dataset of row elements.
- Built on a “thick-thin” wrapper providing:
  - Exception-safe, resource-managed classes for HDF5 entities such as files, property lists, groups, datasets, and dataspaces.
  - Error handling via exceptions and an all-purpose call wrapper for HDF5 functions returning a possible error condition.
- Convenience functions `make_ntuple()`, `make_column()` and `make_scalar_column()` allow easy specification of column metadata such as filters.

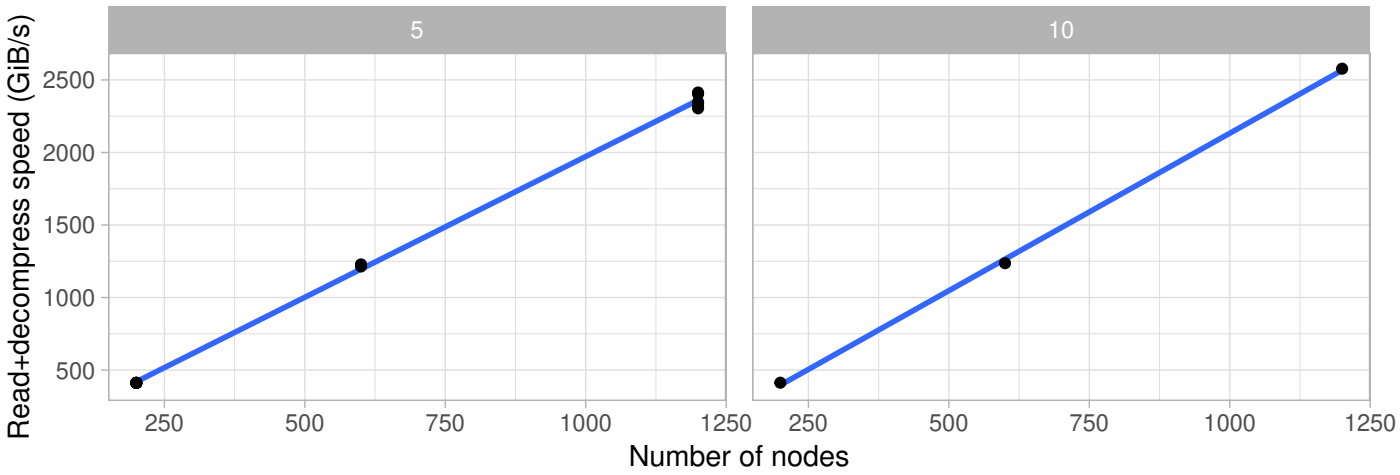
Simple things are very simple

```
// Define the ntuple
Ntuple<int, double> nt("simple.hdf5", // File.
                       "data",        // Table name (group).
                       {"A", "B"}     // Column names.
                      );

// Data to store
std::array<int, 3> idata { 1, 2, 3 };
std::array<double, 3> ddata { 4.5, 5.5, 6.5 };

// Insert the data
for (auto i = 0; i < 3; ++i) {
 nt.insert(idata[i], ddata[i]);
}
```

Complicated things are fairly simple

```
auto data =
  make_ntuple({"less-simple.hdf5", "g1"},
              make_column<int, 2>("A", {2, 3}),
              make_scalar_column<double>("B",
               {PropertyList{H5P_DATASET_CREATE}
                 (&H5Pset_shuffle)
                 (&H5Pset_deflate, 7u)}));
int i1data[] = {  1,  2,  3,  4,  5,  6,
                  7,  8,  9, 10, 11, 12,
                 13, 14, 15, 16, 17, 18 };
double d1data[] = { 1.01, 2.02, 3.03 };
for (auto i = 0; i < 3; ++i) {
  // Array -> address, value -> scalar or address.
  data.insert(&i1data[i*2], d1data[i]);
}
```

We are pleased with the read performance



These results are running on Cori at NERSC, using 200/600/1200 KNL nodes, 64 MPI ranks per node, in a Python program, reading 42 TiB of LArIAT experiment raw data, compressed into a single 4.2 TiB file. Panels show performance with 5 and 10 TiB Burst Buffer allocations.

The addition we would like the most

- We store (redundantly) index information in our tables (e.g. run number, subrun number, event number to identify a row in a table).
- We would prefer to store the relevant data at a location defined by *run*, *subrun*, and *event* “coordinates” in a 3-d space (and we need 4-, 5-, .. n-D spaces).
- But only a few “cells” of such a structure would be filled.
- We really need *efficient sparse multi-dimensional arrays*.

What we are finding hard

- Concatenation of files is hard to make efficient (i.e, to scale well)
  - concatenation means combining the rows of tables in similarly-structured input files into a single outpt file.
- Parallel writing in Python with filters (e.g. compression) is not currently possible.
  - ... but that is `h5py`, not really HDF5