Introduction to HDF5

https://github.com/ResearchComputing/Final_Tutorials

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Overview

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Data Model

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What is HDF5

Hierarchical **D**ata **F**ormat version 5 (HDF5).

- Designed for scientific, high volume data.
- Is a file format to manage data.
  - multidimensional arrays
  - tables
  - compounded structures
  - images
- Software library and tools that provide access to manage data in these files.
- Gives the developer access to manipulate groups and datasets rather than binary streams.

Why Use HDF5

Have you ever asked yourself

- How to handle petabytes of data?
- How to access your data?
  - across a cluster
  - remotely
  - on different platforms
- Majority of granting agencies require:
  - data management plan
  - quality assurance plan
  - open access to the data

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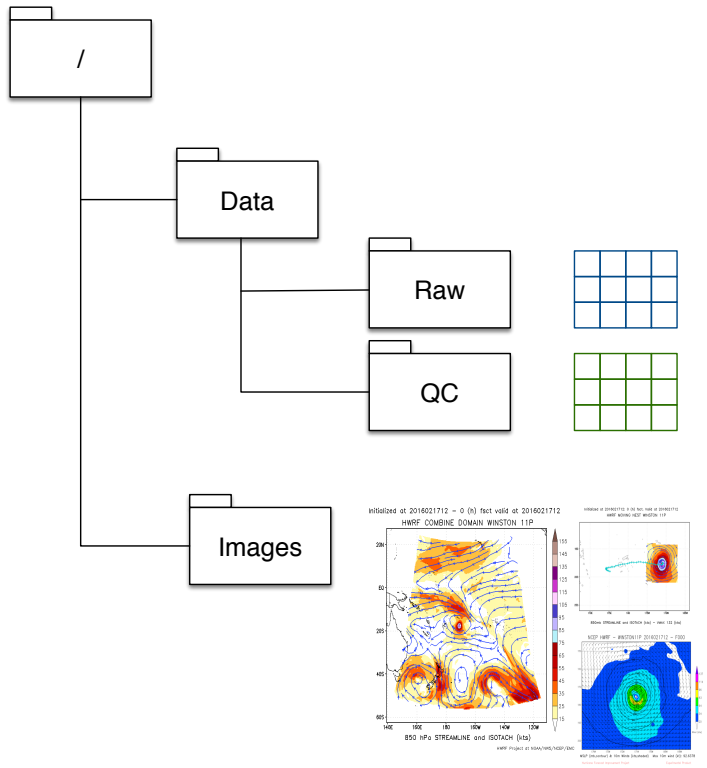
HDF5 Data Model

A HDF5 file is a container that can have groups, links and datasets.

- File - a contiguous string of bytes in a computer store (memory, disk, etc.), and the bytes represent zero or more objects of the model.
- Group - a collection of objects (including groups).
- Link - the way objects are connected.
- Dataset - a multi-dimensional array of data elements with attributes.
- Image - a dataset that are intended to be interpreted as an image.



- Table - a compounded data type to represent a table.
- Dataspace - a description of the dimensions of the dataset.
- Datatype - a description of a specific class of data element including its storage layout.
- Attribute - a named data value associated with a group, dataset, or named datatype.
- Property List - a collection of parameters (some permanent and some transient) controlling options in the library.

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HDF5 Datasets

HDF5 Datasets organize and contain your data. They consist of:

Metadata

- datatype (real, integer, …)
- layout (rank, rows, columns)
- properties (units)

Data

```
HDF5 "MIELLAJOKKA.h5" {
GROUP "/" {
   GROUP "010708-MIELLANJOKKA-1-3D" {
      DATASET "Emission" {
         DATATYPE  H5T_IEEE_F64LE
         DATASPACE  SIMPLE { ( 636 ) / ( 636 ) }
         DATA {
         (0): 240, 240.5, 241, 241.5, 242, 242.5, 243, 243.5,
         ...
         (630): 555, 555.5, 556, 556.5, 557, 557.5
         }
         ATTRIBUTE "Units" {
            DATATYPE  H5T_STRING {
               STRSIZE 2;
               STRPAD H5T_STR_NULLTERM;
               CSET H5T_CSET_ASCII;
               CTYPE H5T_C_S1;
            }
            DATASPACE  SCALAR
            DATA {
            (0): "nm"
            }
         }
      }
```

Attributes

Attributes are something you attach to a dataset that provides extra information.

- Describes the intended use of the dataset or group.
- User defined.
- Optional.

For example the location of a reading or the temperature when the reading occurred.

Virtual File Layers

HDF5 provides a virtual file layer which you can extend.

- POSIX
- STDIO
- MPI-IO

You do not need to be an MPI expert to use the parallel IO layer in HDF5.

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HDF5 on Janus

On Janus since the modules are hierarchical, we need to load the prerequisites.

- Serial

```
login04 ~$ ml intel
login04 ~$ ml hdf5
```

- Parallel (MPI-IO)

```
login04 ~$ ml intel
login04 ~$ ml impi
login04 ~$ ml hdf5
```

HDF5 Tools I

Which provides the following programs

Command	Description
`h5cc`	Simplifies compiling C programs (`h5pcc`)
`h5fc`	Simplifies compiling Fortran programs (`h5pfc`)
`h5debug`	Debugs an existing HDF5 file at a low level
`h52gif`	Converts a HDF5 image to a GIF
`gif2h`	Converts a GIF file to a HDF5 file
`h5diff`	Compares two HDF5 files
`h5dump`	Dumps a HDF5 file to ascii
`h5import`	Import ascii or binary data to a HDF5 file

HDF5 Tools II

Command	Description
`h5ls`	List information about a HDF5 file
`h5repack`	Repacks a file w/o compression/chunking
`h5repart`	Repartitions a file or family of files
`h5copy`	Copies objects to a new HDF5 file
`h5mkgrp`	Makes a group in a HDF5 file
`h5stat`	Display object and metadata information

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HDF5 IO Sequence

Very similar to normal IO sequence, only a few additional items need to be specified.

- open/create a file
- specify the dataspace
- create the dataset
- write the data
- close the file

HDF5 Fortran API

The fortran API is the same as the C API, however subroutines have a `_f` suffix and the last parameter is the return status.

C	Fortran
ierr = H5open(void)	H5open_f(ierr)

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Write a 20×20 matrix to a file.

The code is provided on Janus in
`/projects/tibr1099/meetup/Intro_HDF5`

`Makefile`	Build definitions
`kinds.f90`	Precision definitions
`hdf_swrite.f90`	Serial example
`hdf_pwrite.f90`	Parallel example

Questions?

Online Survey

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