Introduction to HDF5

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Why HDF5?

- Have you ever asked yourself:
  - How will I deal with one-file-per-processor in the petascale era?
  - Do I need to be an “MPI and Lustre pro” to do my research?
  - Where is my checkpoint file?
- HDF5 hides all complexity so you can concentrate on Science
  - Optimized I/O to single shared file

Goal

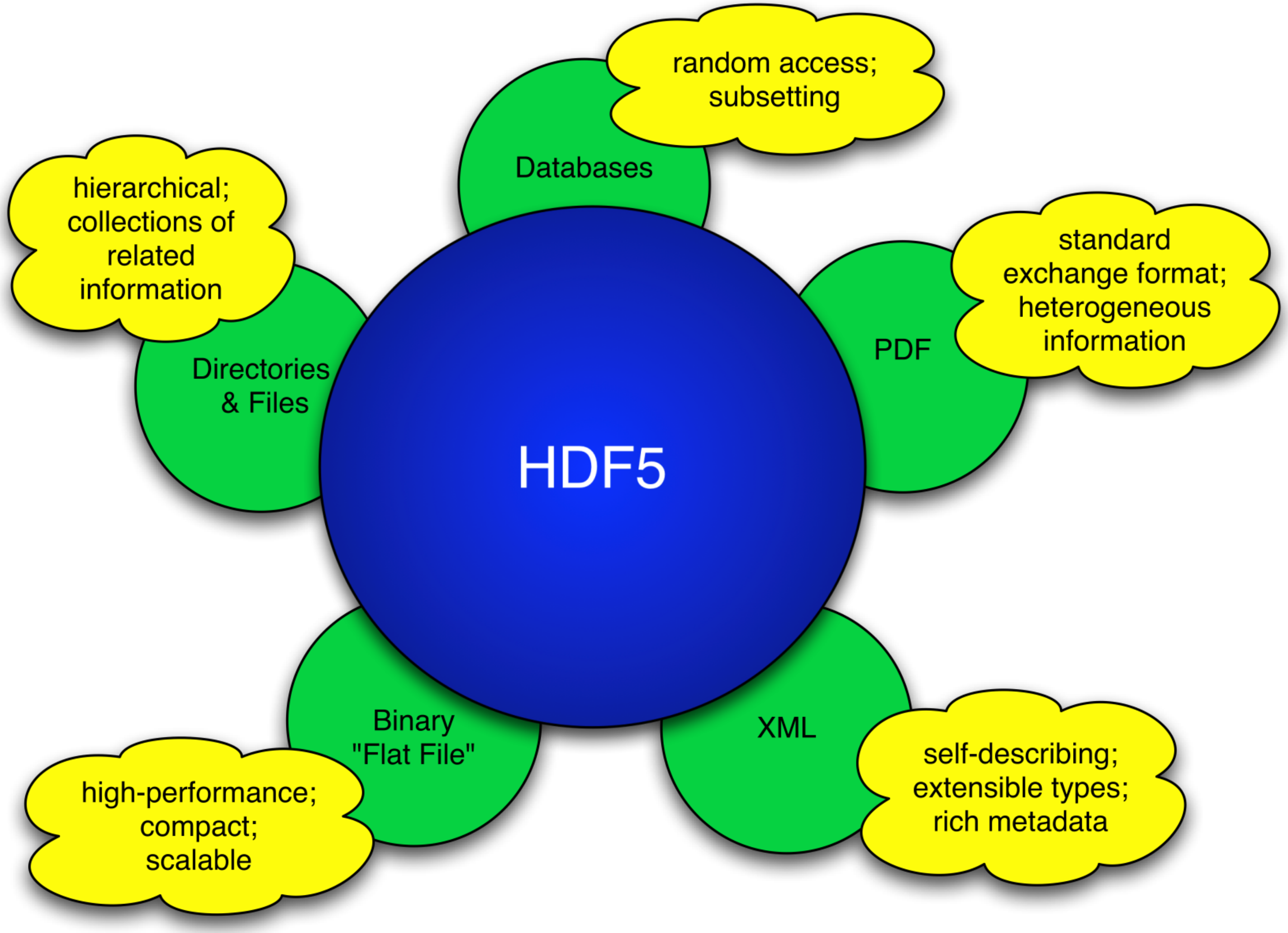
- Introduce you to HDF5
  - HDF5 data model
  - HDF5 programming model
  - Parallel access to HDF5
  - HDF5 performance tuning hints

WHAT IS HDF5?

What is HDF5?

- HDF5 == Hierarchical Data Format, v5
- Open **file format**
  - Designed for high volume or complex data
- Open source **software**
  - Works with data in the format
- A **data model**
  - Structures for data organization and specification

HDF5 is like …


random access; subsetting
Databases
hierarchical; collections of related information
Directories & Files
standard exchange format; heterogeneous information
PDF
HDF5
Binary "Flat File"
high-performance; compact; scalable
XML
self-describing; extensible types; rich metadata

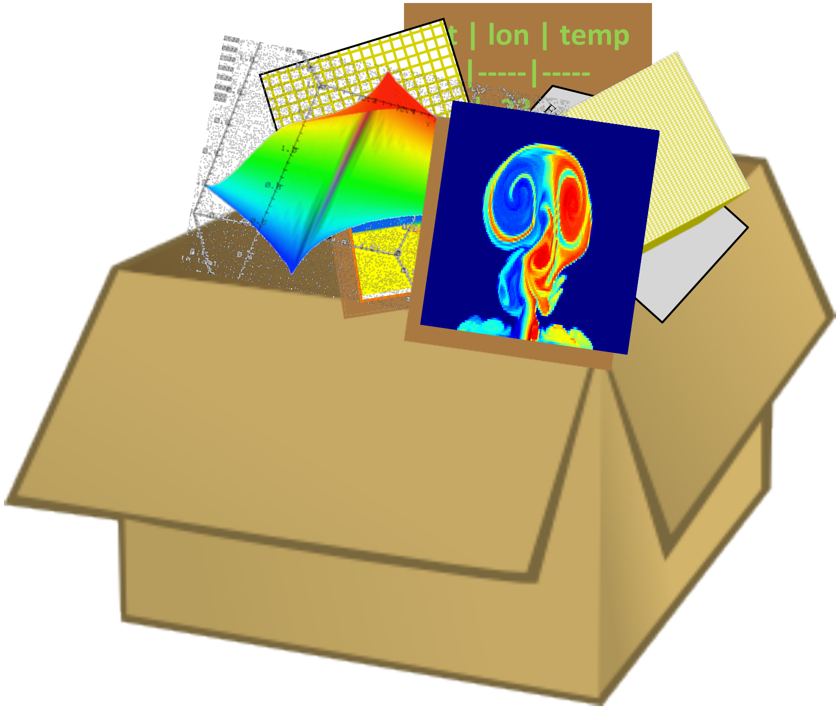
HDF5 is designed …

- for high volume and/or complex data
- for every size and type of system (portable)
- for flexible, efficient storage and I/O
- to enable applications to evolve in their use of HDF5 and to accommodate new models
- to support long-term data preservation

HDF5 DATA MODEL

HDF5 File

An HDF5 file is a **container** that holds data objects.



HDF5 Data Model

Dataset

Group

Attribute

HDF5 Objects

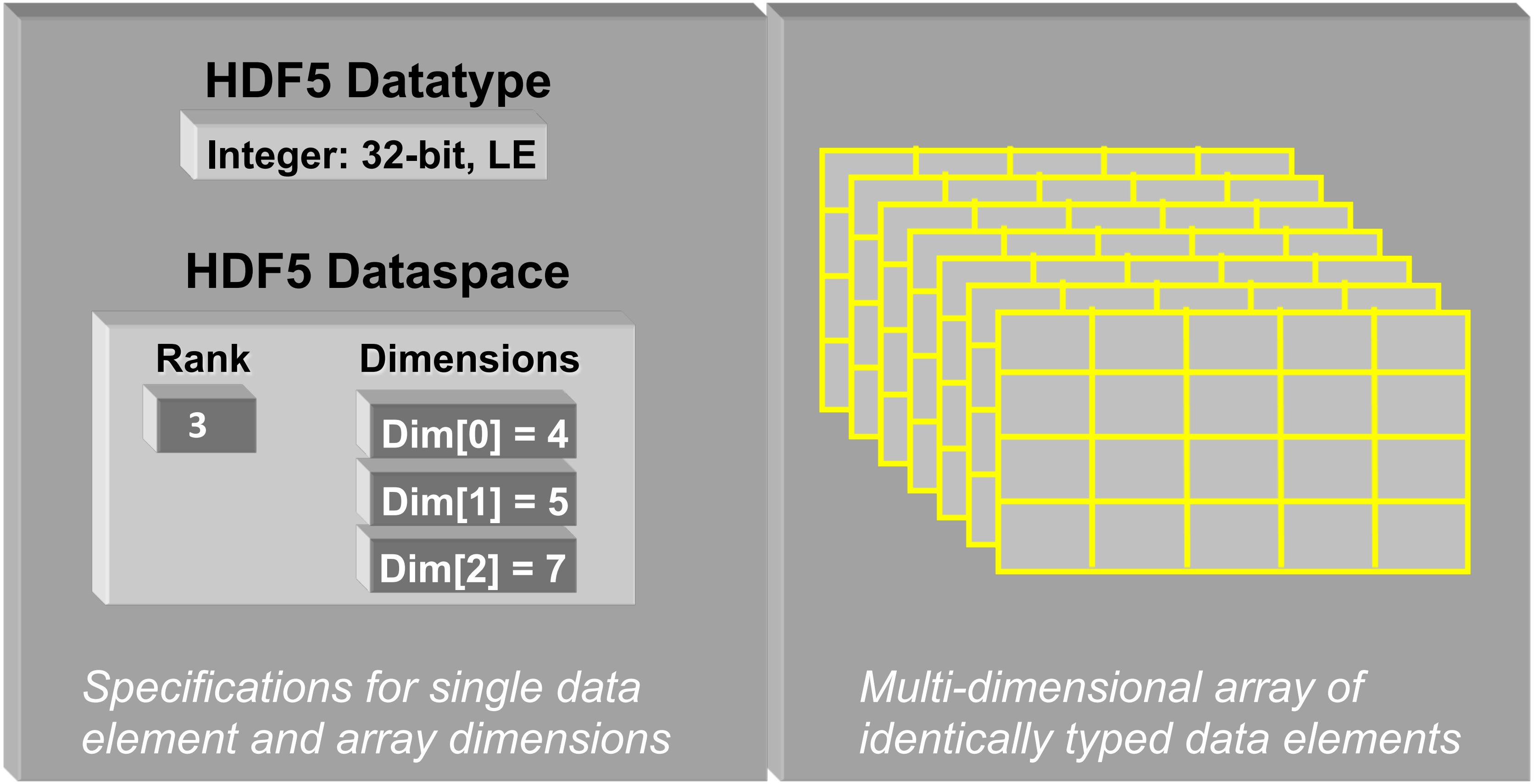
Link

Datatype

Dataspace

File

HDF5 Dataset



HDF5 Datatype

Integer: 32-bit, LE

HDF5 Dataspace

Rank

3

Dimensions

Dim[0] = 4

Dim[1] = 5

Dim[2] = 7

Specifications for single data element and array dimensions

Multi-dimensional array of identically typed data elements

- HDF5 datasets **organize and contain** data elements.
  - HDF5 datatype describes individual data elements.
  - HDF5 dataspace describes the logical layout of the data elements.

HDF5 Dataspace

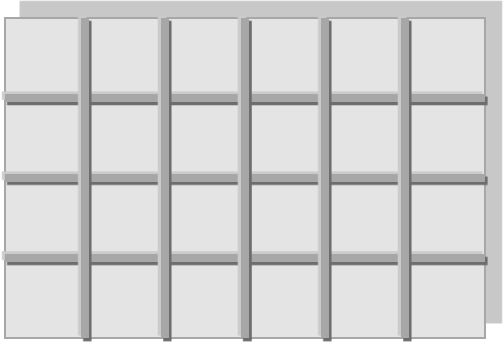
- Describes the logical layout of the elements in an HDF5 dataset
  - NULL
    - no elements
  - Scalar
    - single element
  - Simple array (*most common*)
    - multiple elements organized in a rectangular array
      - rank = number of dimensions
      - dimension sizes = number of elements in each dimension
      - maximum number of elements in each dimension
        - may be fixed or unlimited

HDF5 Dataspace

Two roles:

Dataspace contains spatial information

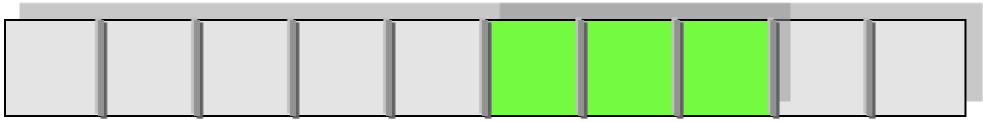
- Rank and dimensions
- Permanent part of dataset definition



Rank = 2

Dimensions = 4x6

Partial I/0: Dataspace describes application's data buffer and data elements participating in I/O



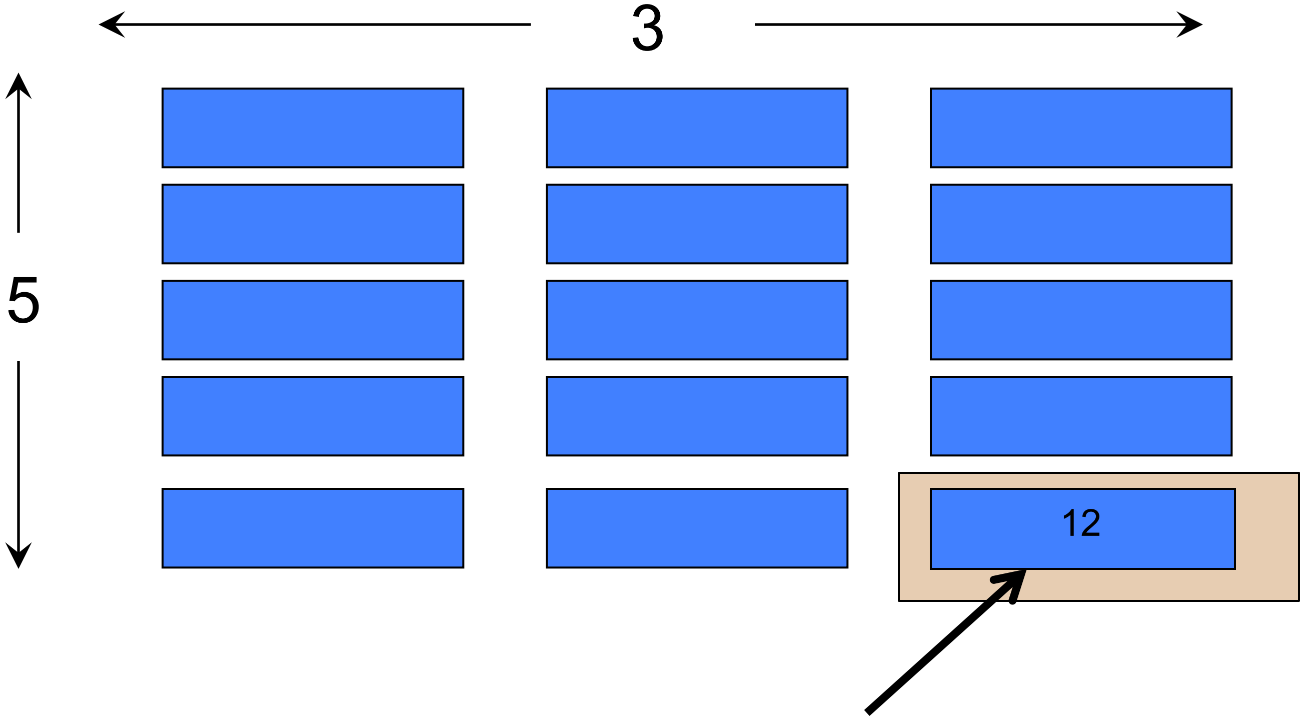
Rank = 1

Dimension = 10

HDF5 Datatypes

- Describe individual data elements in an HDF5 dataset
- Wide range of datatypes supported
  - Integer
  - Float
  - Enum
  - Array
  - User-defined (e.g., 13-bit integer)
  - Variable-length types (e.g., strings, vectors)
  - Compound (similar to C structs)
  - More …

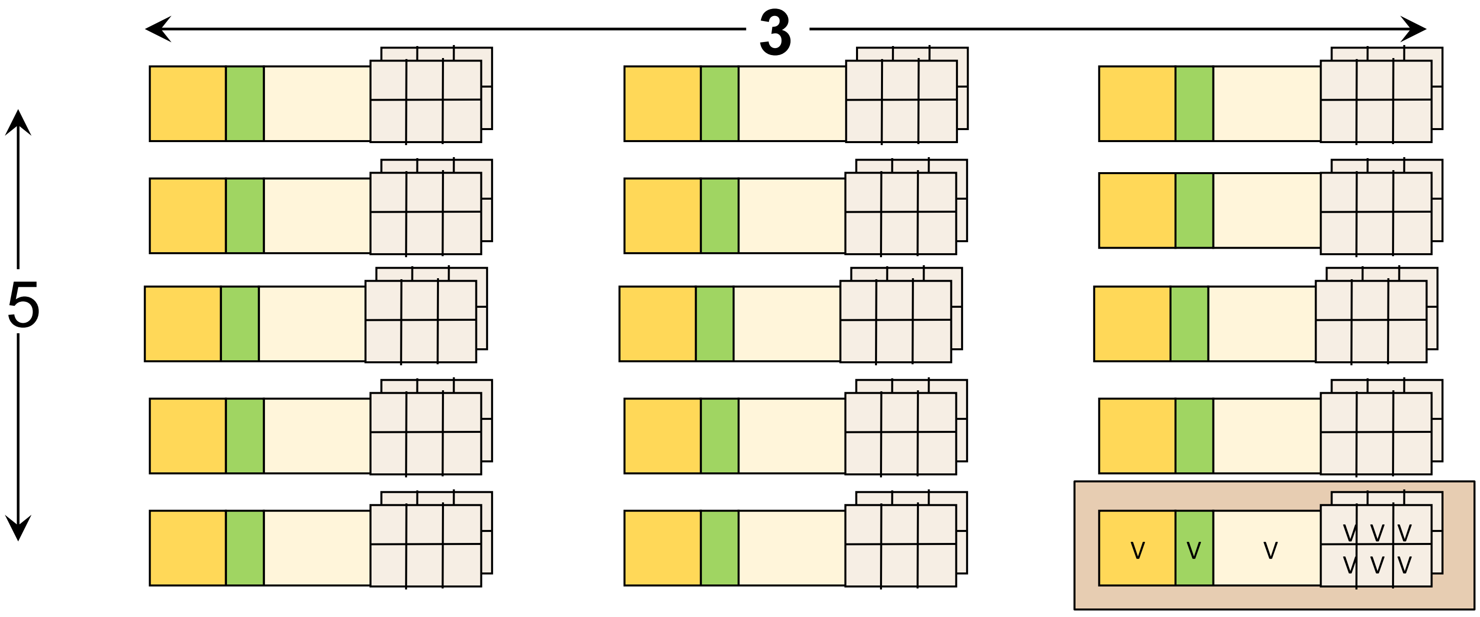
HDF5 Dataset



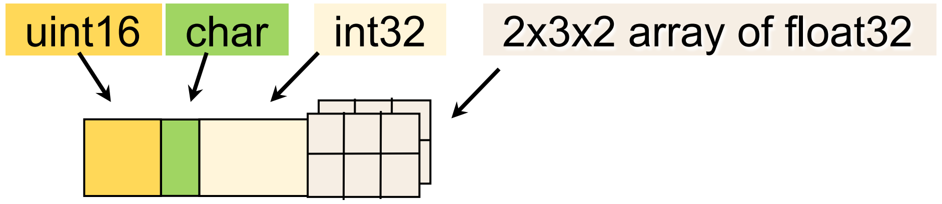
Datatype: 32-bit Integer

Dataspace: Rank = 2
Dimensions = 5 x 3

HDF5 Dataset with Compound Datatype



Compound Datatype:


uint16

char

int32

2x3x2 array of float32

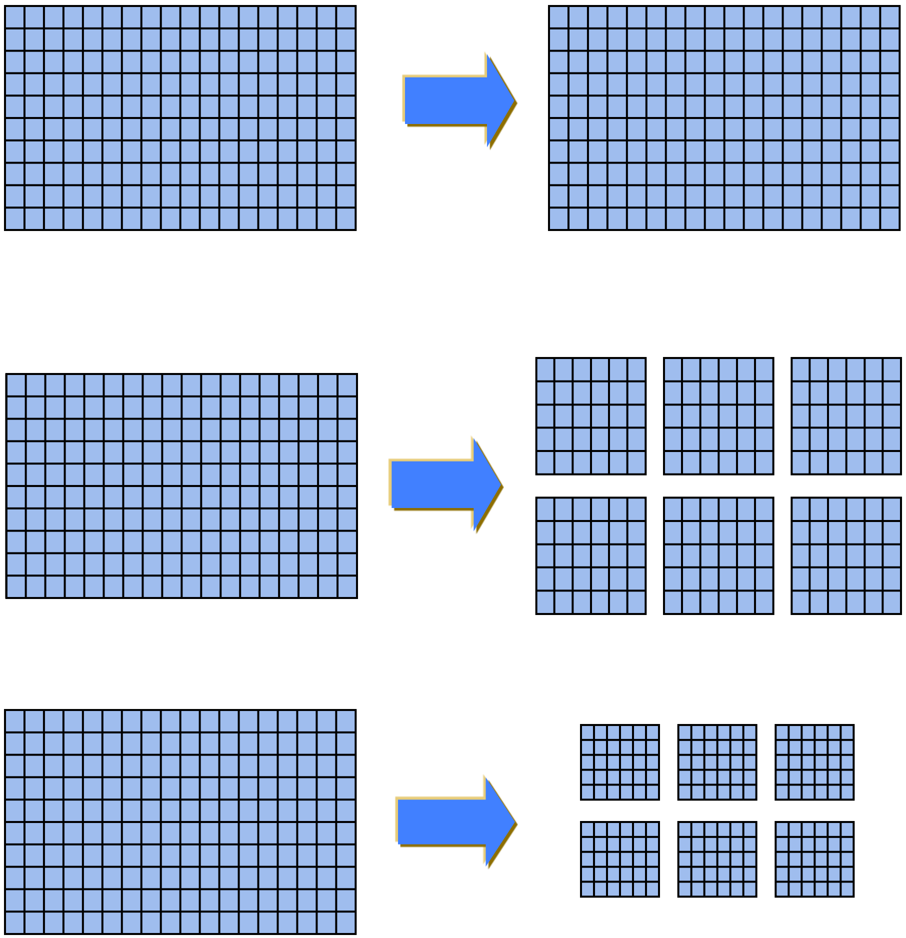
Dataspace: Rank = 2

Dimensions = 5 x 3

How are data elements stored?

Buffer in memory

Data in the file



Contiguous (default)

Data elements stored physically adjacent to each other

Chunked

Better access time for subsets; extendible

Chunked & Compressed

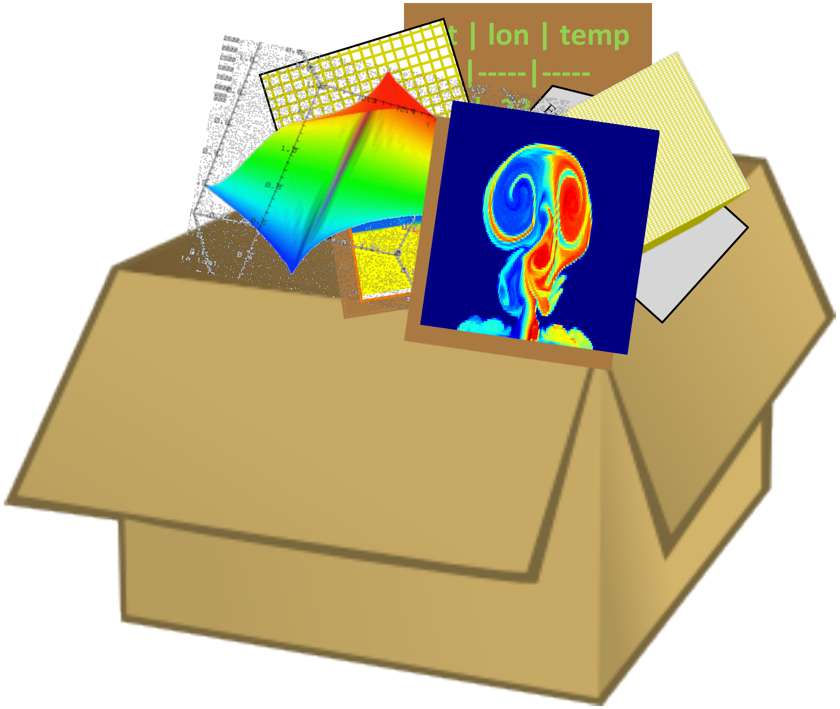
Improves storage efficiency, transmission speed

HDF5 Attributes

- Typically contain user metadata
- Have a name and a value
- Attributes “decorate” HDF5 objects
- Value is described by a datatype and a dataspace
- Analogous to a dataset, but do not support partial I/O operations; nor can they be compressed or extended

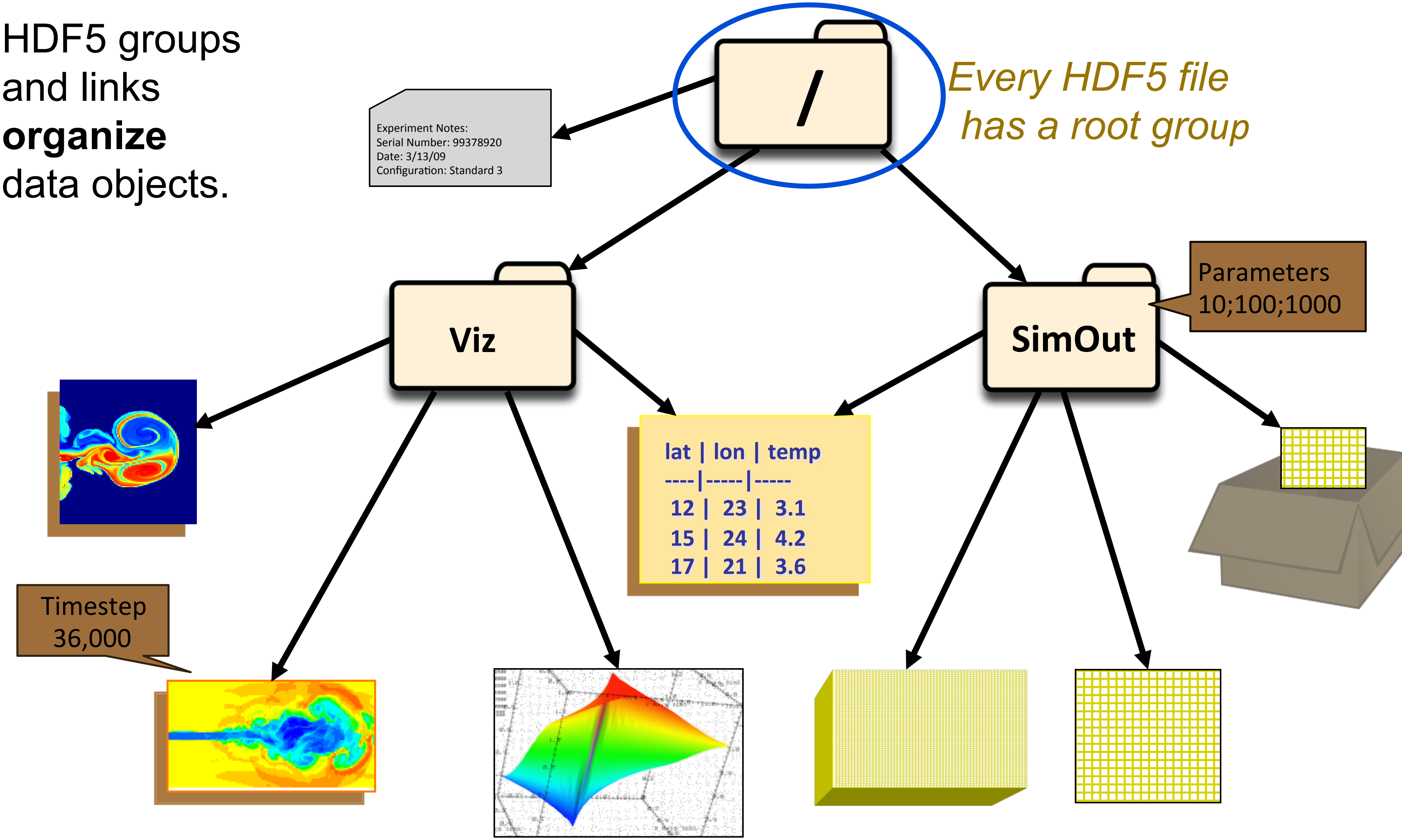
HDF5 File

An HDF5 file is a **smart container** that holds data objects.



HDF5 Groups and Links

HDF5 groups and links **organize** data objects.



Experiment Notes:
Serial Number: 99378920
Date: 3/13/09
Configuration: Standard 3

Every HDF5 file has a root group

```
lat | lon | temp
----|-----|-----
 12 |  23 |  3.1
 15 |  24 |  4.2
 17 |  21 |  3.6
```

HDF5 SOFTWARE

HDF5 Home Page

HDF5 home page: http://hdfgroup.org/HDF5/

- Latest release: HDF5 1.8.13 (1.8.14 coming in November 2014)

HDF5 source code:

- Written in C, and includes optional C++, Fortran 90 APIs, and High Level APIs
- Contains command-line utilities (h5dump, h5repack, h5diff, ..) and compile scripts

HDF5 pre-built binaries:

- When possible, include C, C++, F90, and High Level libraries. Check ./lib/libhdf5.settings file.
- Built with and require the SZIP and ZLIB external libraries

Useful Tools For New Users

`h5dump`:

Tool to "dump" or display contents of HDF5 files

`h5cc, h5c++, h5fc`:

Scripts to compile applications

`HDFView`:

Java browser to view HDF5 files

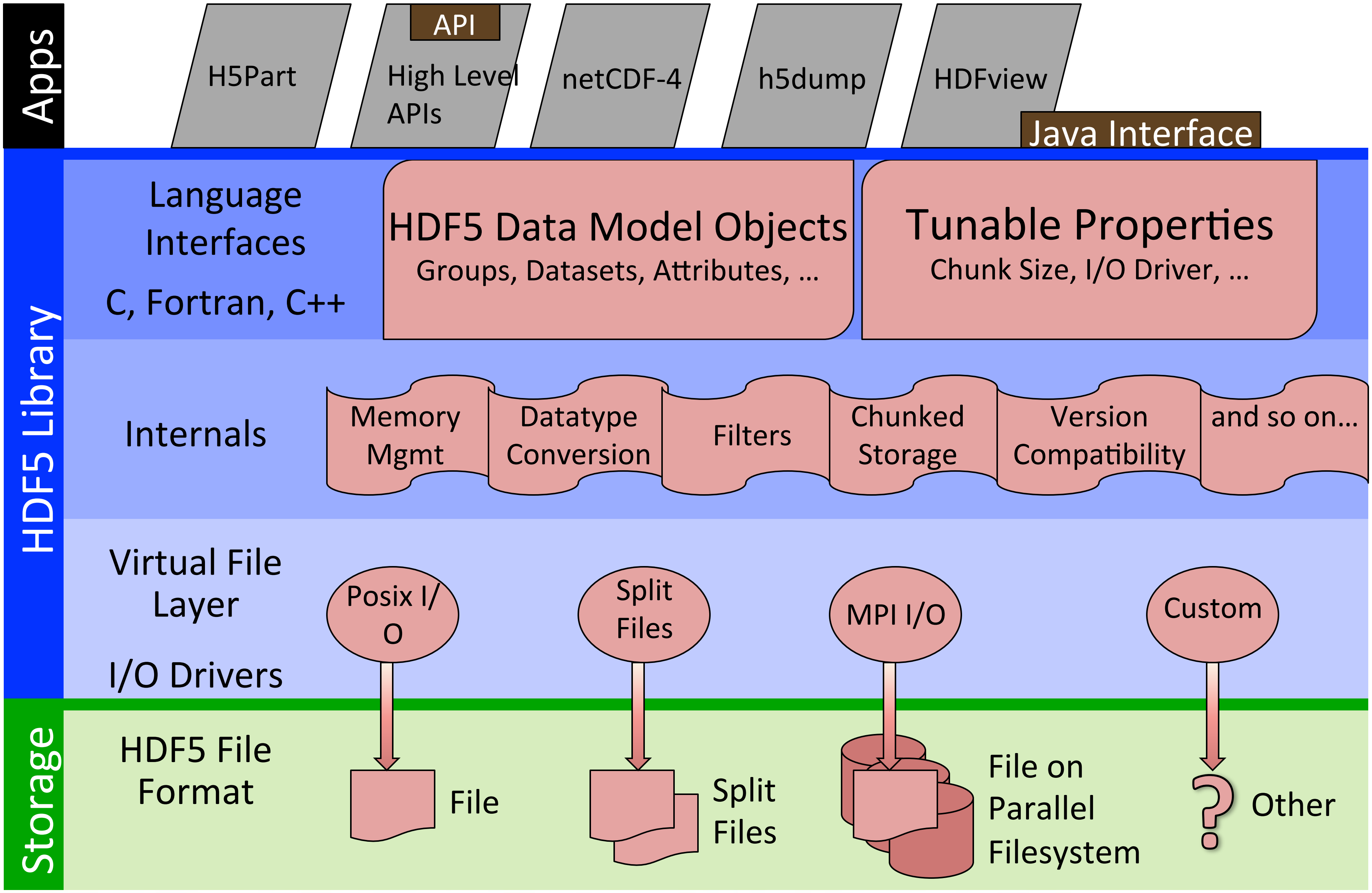
http://www.hdfgroup.org/hdf-java-html/hdfview/

HDF5 Examples (C, Fortran, Java, Python, Matlab)

http://www.hdfgroup.org/ftp/HDF5/examples/

HDF5 PROGRAMMING MODEL AND API

HDF5 Software Layers & Storage



The General HDF5 API

- C, Fortran, Java, C++, and .NET bindings
- IDL, MATLAB, Python (H5Py, PyTables)
- C routines begin with prefix H5*?*

  ? is a character corresponding to the type of object the function acts on

Example Functions:

H5D :	**D**ataset interface	*e.g.,* **H5Dread**
H5F :	**F**ile interface	*e.g.,* **H5Fopen**
H5S :	data**S**pace interface	*e.g.,* **H5Sclose**

The HDF5 API

- For flexibility, the API is extensive
  - ✓ 300+ functions

Victorinox
Swiss Army
Cybertool 34

- This can be daunting… but there is hope
  - ✓ A few functions can do a lot
  - ✓ Start simple
  - ✓ Build up knowledge as more features are needed

General Programming Paradigm

- Object is opened or created
- Object is accessed, possibly many times
- Object is closed

- Properties of object are optionally defined
  - ✓Creation properties (e.g., use chunking storage)
  - ✓Access properties

Basic Functions

H5**F**create (H5**F**open)	*create (open) File*
H5**S**create_simple/H5**S**create	*create dataSpace*
H5**D**create (H5**D**open)	*create (open) Dataset*
H5**D**read, H5**D**write	*access Dataset*
H5**D**close	*close Dataset*
H5**S**close	*close dataSpace*
H5**F**close	*close File*

Other Common Functions

Data**S**paces:	H5Sselect_hyperslab (Partial I/O) H5Sselect_elements (Partial I/O) H5Dget_space
Data**T**ypes:	H5Tcreate, H5Tcommit, H5Tclose H5Tequal, H5Tget_native_type
Groups:	H5Gcreate, H5Gopen, H5Gclose
Attributes:	H5Acreate, H5Aopen_name, H5Aclose, H5Aread, H5Awrite
Property lists:	H5Pcreate, H5Pclose H5Pset_chunk, H5Pset_deflate

C EXAMPLES

How to compile HDF5 applications

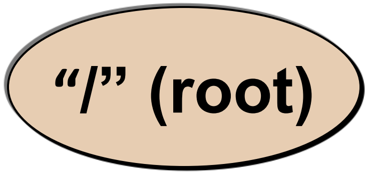
- **`h5cc`** – HDF5 C compiler command
- **`h5fc`** – HDF5 F90 compiler command
- **`h5c++`** - HDF5 C++ compiler command
- To compile:
  - `% h5cc h5prog.c`
  - `% h5fc h5prog.f90`
  - `% h5c++ h5prog.cpp`

Code: Create a File

```
hid_t       file_id;
herr_t      status;

file_id = H5Fcreate("file.h5", H5F_ACC_TRUNC,
                    H5P_DEFAULT, H5P_DEFAULT);

status = H5Fclose (file_id);
```



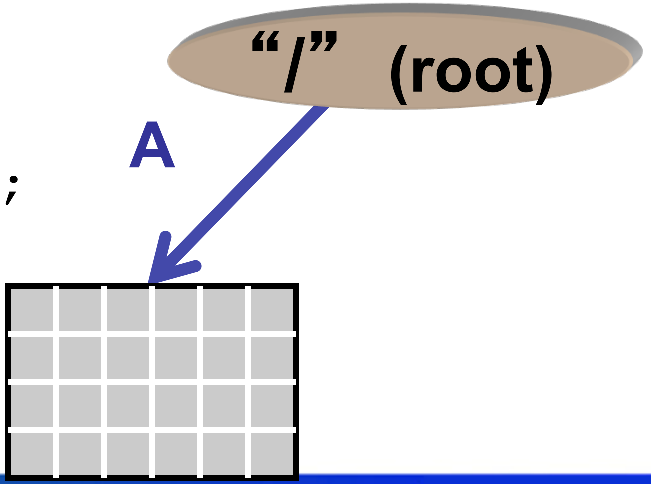
Note: Return codes not checked for errors in code samples.

Code: Create a Dataset

```
hid_t       file_id, dataset_id, dataspace_id;
hsize_t     dims[2];
herr_t      status;

file_id = H5Fcreate (”file.h5", H5F_ACC_TRUNC,
                          H5P_DEFAULT, H5P_DEFAULT);
dims[0] = 4;
dims[1] = 6;
dataspace_id = H5Screate_simple (2, dims, NULL);
dataset_id = H5Dcreate (file_id,”A",H5T_STD_I32BE,
                 dataspace_id, H5P_DEFAULT, H5P_DEFAULT,
                 H5P_DEFAULT);

status = H5Dclose (dataset_id);
status = H5Sclose (dataspace_id);
status = H5Fclose (file_id);
```



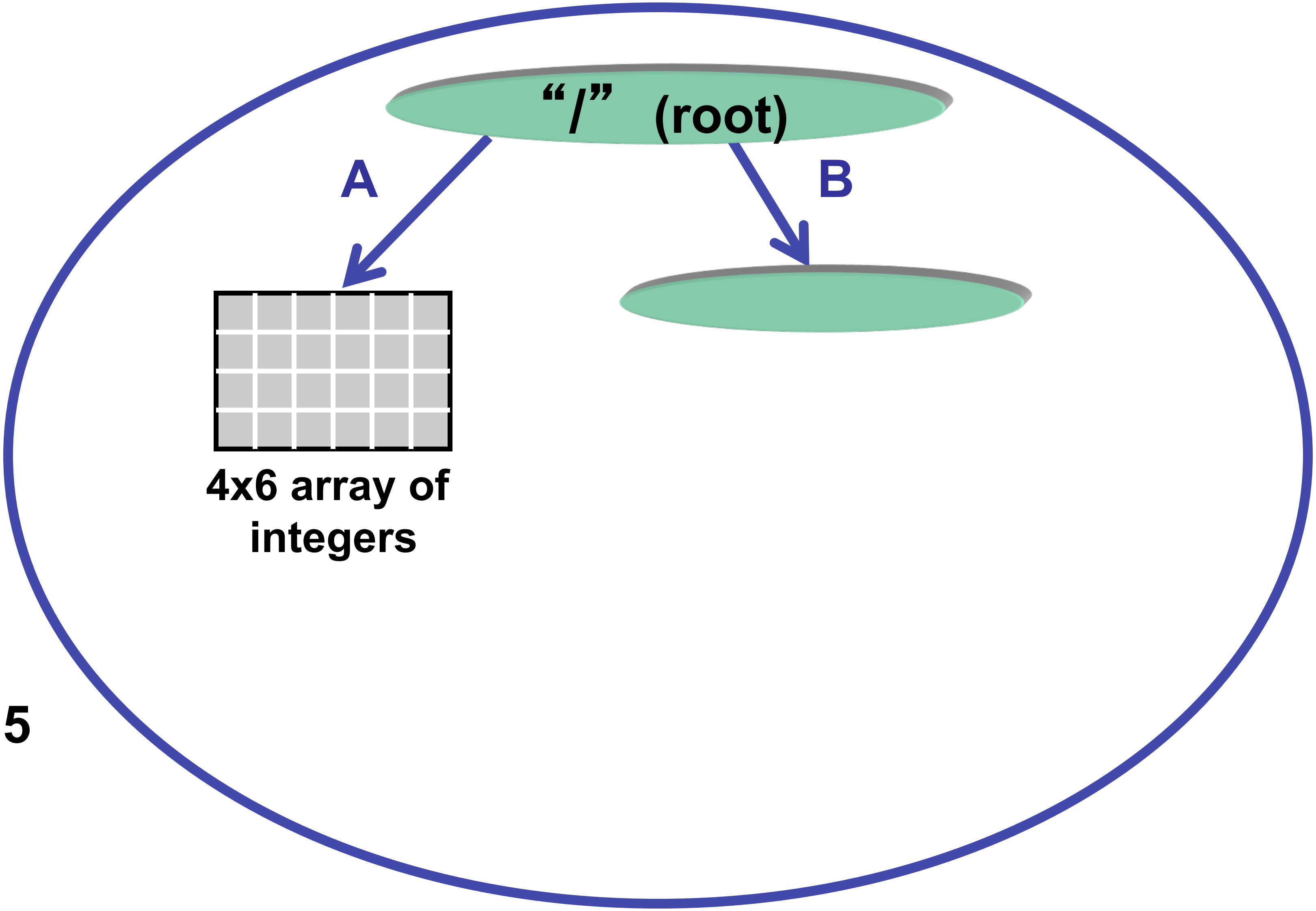
Code: Create a Group

```
hid_t file_id, group_id;
...
/* Open “file.h5” */
file_id = H5Fopen (“file.h5”, H5F_ACC_RDWR,
                         H5P_DEFAULT);

/* Create group "/B" in file. */
group_id = H5Gcreate (file_id,"B", H5P_DEFAULT,
                      H5P_DEFAULT, H5P_DEFAULT);

/* Close group and file. */
status = H5Gclose (group_id);
status = H5Fclose (file_id);
```

Example: Create Dataset & Group



file.h5

Output of h5dump

```
$ h5dump file.h5

HDF5 "file.h5" {
GROUP "/" {
   DATASET "A" {
      DATATYPE  H5T_STD_I32BE
      DATASPACE  SIMPLE { ( 4, 6 ) / ( 4, 6 ) }
      DATA {
      (0,0): 0, 0, 0, 0, 0, 0,
      (1,0): 0, 0, 0, 0, 0, 0,
      (2,0): 0, 0, 0, 0, 0, 0,
      (3,0): 0, 0, 0, 0, 0, 0
      }
   }
   GROUP "B" {
   }
}
}
```

Example Code - H5Dwrite

```
 int  wdata[4][6];

 /* Initialize the dataset. */
 for (i = 0; i < 4; i++)
    for (j = 0; j < 6; j++)
         wdata[i][j] = i * 6 + j + 1;
…. .
status = H5Dwrite (dataset_id, H5T_NATIVE_INT,
           H5S_ALL,H5S_ALL, H5P_DEFAULT, wdata);
```

Output of h5dump after writing

```
$ h5dump file.h5
HDF5 "file.h5" {
GROUP "/" {
   DATASET "A" {
      DATATYPE  H5T_STD_I32BE
      DATASPACE  SIMPLE { ( 4, 6 ) / ( 4, 6 ) }
      DATA {
      (0,0): 1, 2, 3, 4, 5, 6,
      (1,0): 7, 8, 9, 10, 11, 12,
      (2,0): 13, 14, 15, 16, 17, 18,
      (3,0): 19, 20, 21, 22, 23, 24
      }
   }
   GROUP "B" {
   }
}
}
```

PARTIAL I/O IN HDF5

How to write a row?

```
$ h5dump file.h5

HDF5 "file.h5" {
GROUP "/" {
   DATASET "A" {
      DATATYPE  H5T_STD_I32BE
      DATASPACE  SIMPLE { ( 4, 6 ) / ( 4, 6 ) }
      DATA {
      (0,0): 0, 0, 0, 0, 0, 0,
      (1,0): 1, 2, 3, 4, 5, 6,
      (2,0): 0, 0, 0, 0, 0, 0,
      (3,0): 0, 0, 0, 0, 0, 0
      }
   }
   GROUP "B" {
   }
}
}
```

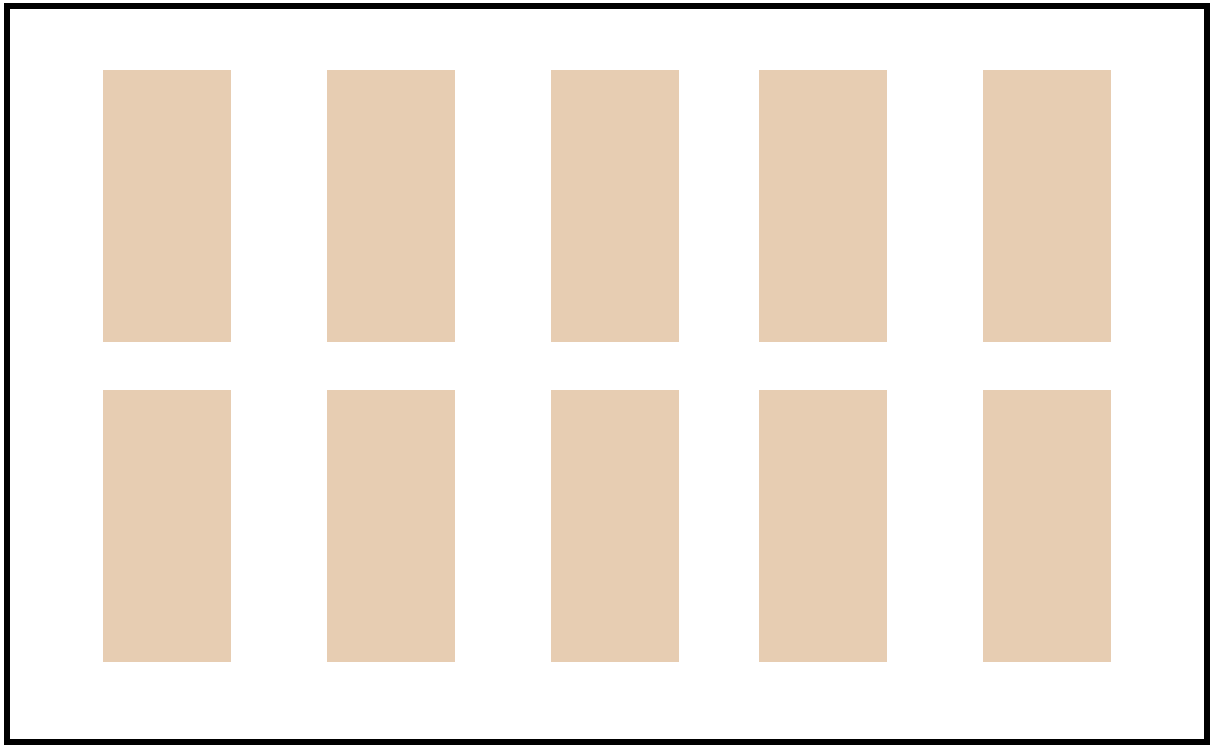
How to Describe a Subset in HDF5?

- Before writing and reading a subset of data one has to describe it to the HDF5 Library.
- HDF5 APIs and documentation refer to a subset as a “selection” or “hyperslab selection”.
- If specified, HDF5 Library will perform I/O on a selection *only* and not on all elements of a dataset.

Types of Selections in HDF5

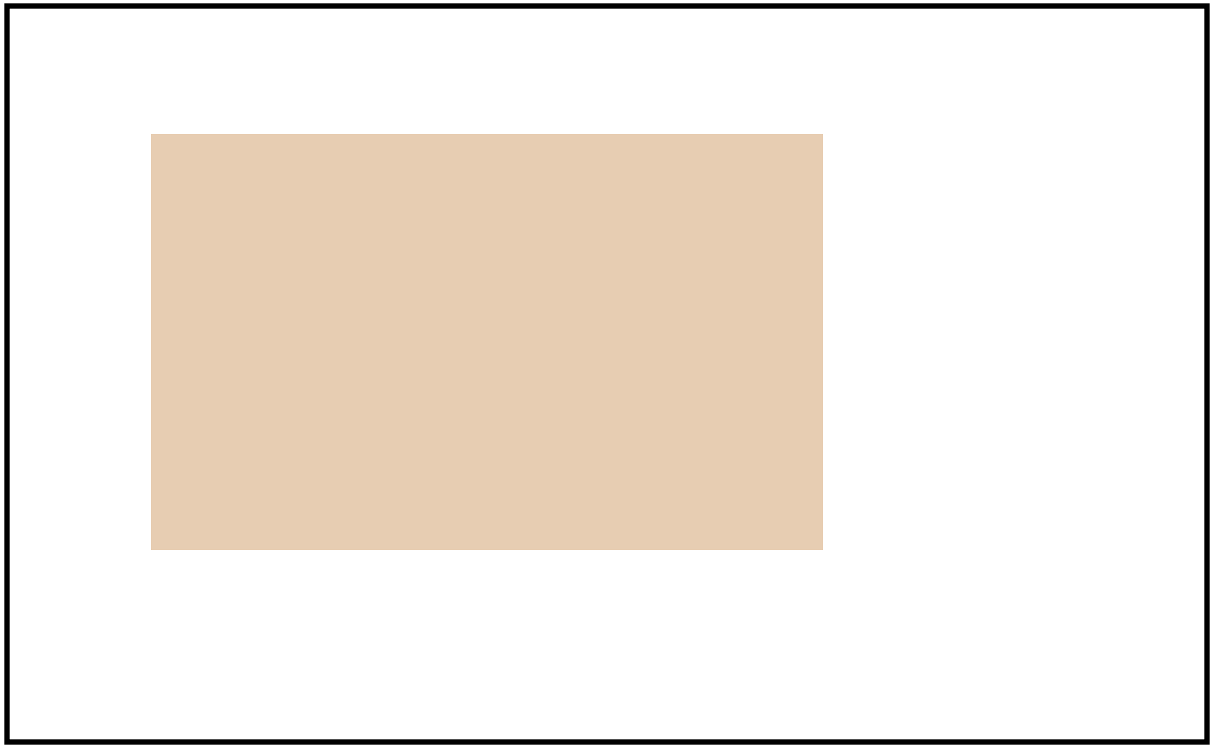
- Two types of selections
  - Hyperslab selection
    - Regular hyperslab
    - Simple hyperslab
    - Result of set operations on hyperslabs (union, difference, …)
  - Point selection
- Hyperslab selection is especially important for doing parallel I/O in HDF5 (See Parallel HDF5 Tutorial)

Regular Hyperslab



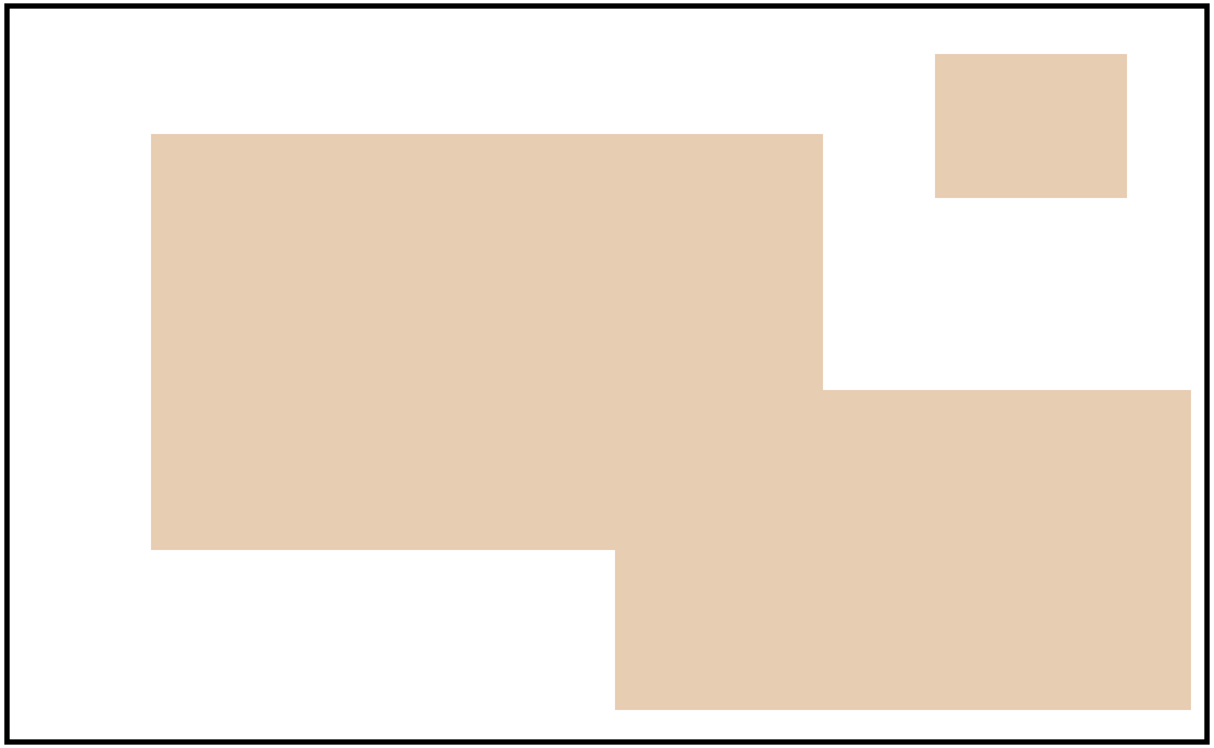
Collection of regularly spaced blocks of equal size

Simple Hyperslab



Contiguous subset or sub-array

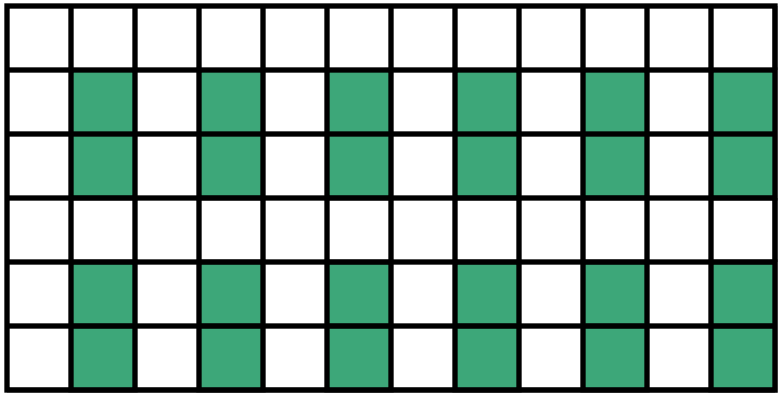
Hyperslab Selection



Result of union operation on three simple hyperslabs

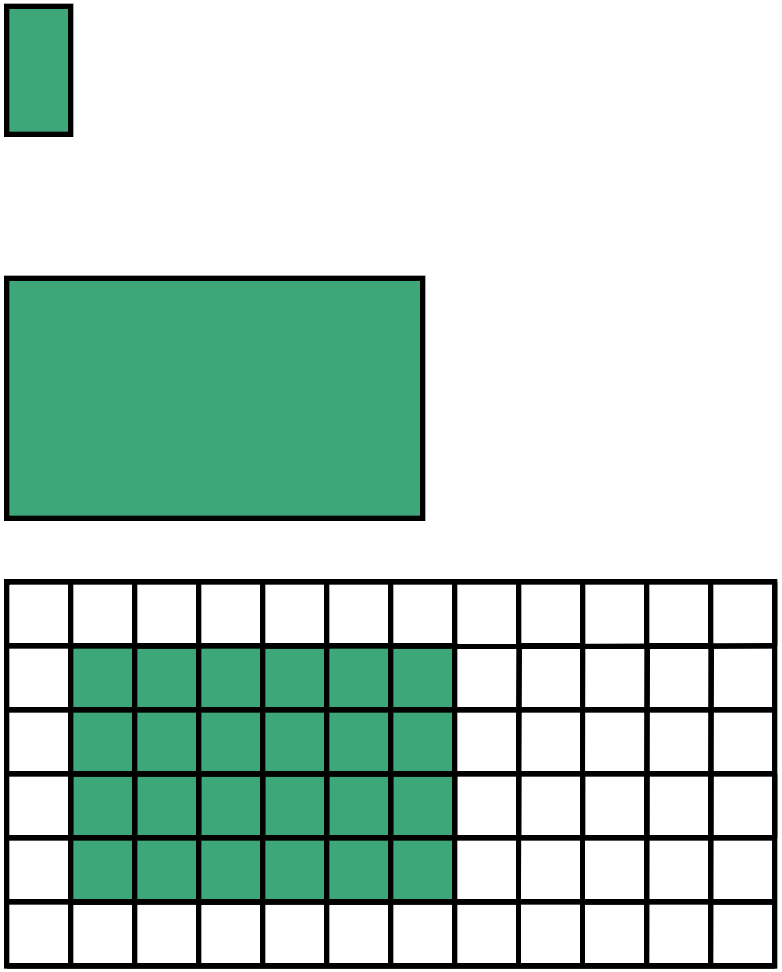
HDF5 Hyperslab Description

- *Everything is "measured" in number of elements*
- Start - starting location of a hyperslab (1,1)
- Stride - number of elements that separate each block (3,2)
- Count - number of blocks (2,6)
- Block - block size (2,1)



Simple Hyperslab Description

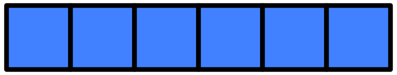
- Two ways to describe a simple hyperslab
- As *several* blocks
  - **Stride – (1,1)**
  - **Count – (2,6)**
  - Block – (2,1)
- As *one* block
  - Stride – (1,1)
  - Count – (1,1)
  - **Block – (4,6)**



No performance penalty for one way or another

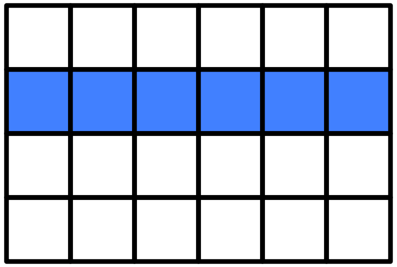
Writing a row

- Memory space selection is 1-dim array of size 6



- File space selection

start = {1,0}, stride = {1,1}, count = {1,6}, block = {1,1}



Number of elements selected in memory should be the same as selected in the file

Writing a row

```
hid_t       mspace_id, fspace_id;
hsize_t     dims[1] = {6};
hsize_t     start[2], count[2];
…..
/* Create memory dataspace */
mspace_id = H5Screate_simple(RANK, dims, NULL);

/* Get file space identifier from the dataset */
fspace_id = H5Dget_space(dataset_id);

/* Select hyperslab in the dataset to write too */
start[0] = 1;
start[1] = 0;
count[0] = 1;
count[1] = 6;
status = H5Sselect_hyperslab(fspace_id, H5S_SELECT_SET,
         start, NULL, count, NULL);
H5Dwrite(dataset_id, H5T_NATIVE_INT, mspace_id, fspace_id,
         H5P_DEFAULT, wdata);
```

HDF5 FILE FORMAT

HDF5 File Format

- Defined by the *HDF5 File Format Specification.*

http://www.hdfgroup.org/HDF5/doc/H5.format.html

- Specifies the bit-level organization of an HDF5 file on storage media.

- HDF5 library adheres to the File Format, users do not need to know the guts of this information.

HDF5 Roadmap

- Concurrency
  - Single-Writer/Multiple-Reader (SWMR)
  - Internal threading
- Virtual Object Layer
- Native HDF5 client/server

- Performance
  - Scalable chunk indices
  - Metadata aggregation and Page buffering
  - Asynchronous I/O
  - Variable-length records
- Fault tolerance
- Parallel I/O
- I/O Autotuning

Thank You!

Questions?