Introduction to HDF5

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The HDF Group
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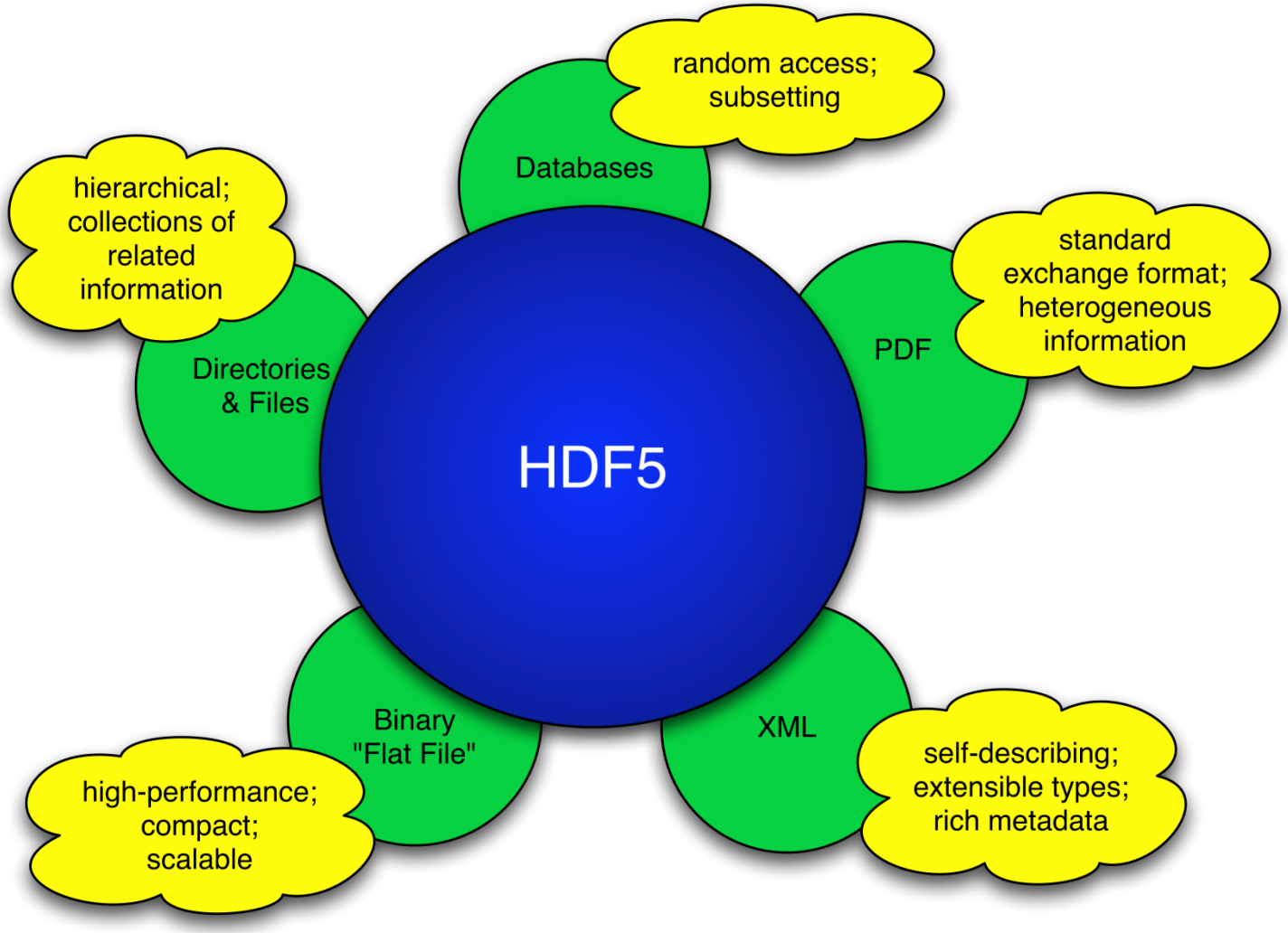
What is HDF5?

- 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

HDF = Hierarchical Data Format

- HDF4 is the first HDF
  - Originally called HDF; last major release was version 4
- HDF5 benefits from lessons learned with HDF4
  - Changes to file format, software, and data model
  - HDF5 and HDF4 are *different*
- No plans for an HDF6!

HDF5 is like …


HDF5
Databases
random access; subsetting
hierarchical; collections of related information
Directories & Files
PDF
standard exchange format; heterogeneous information
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 Technology Platform

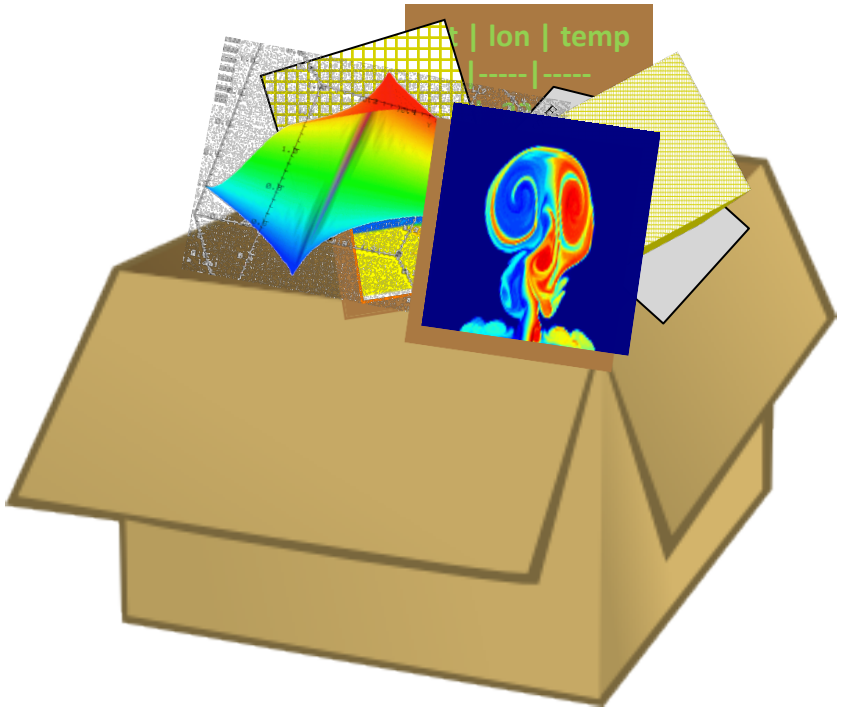
- HDF5 **data model**
  - The "building blocks" for data organization and specification
- HDF5 **software**
  - Library, language interfaces, tools
- HDF5 **file format**
  - Bit-level organization of HDF5 file

HDF5 Data Model

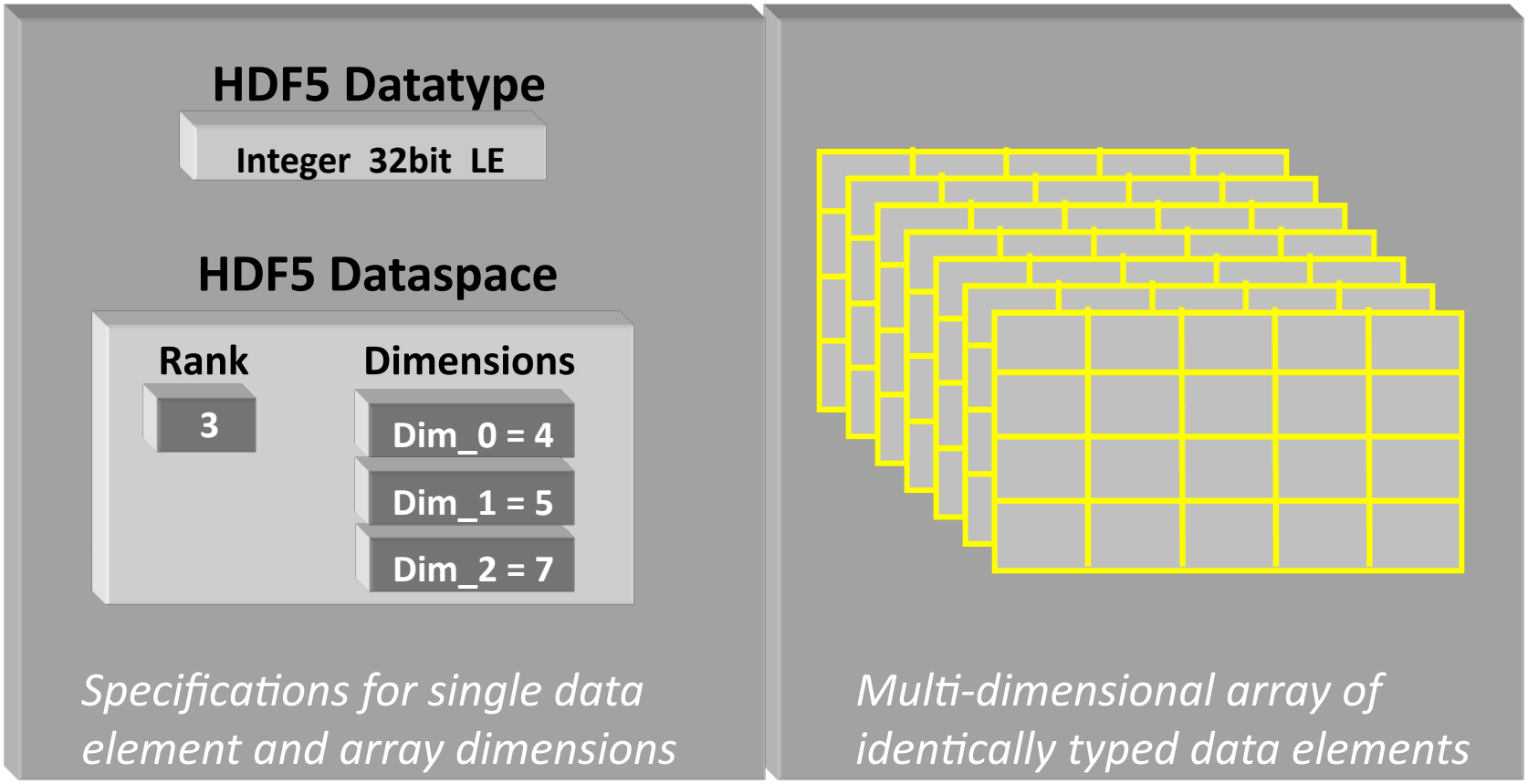
a.k.a. HDF5 Abstract Data Model
a.k.a. HDF5 Logical Data Model

HDF5 File

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



HDF5 Dataset



- HDF5 datasets **organize and contain** "raw data values".
  - HDF5 datatypes describe individual data elements.
  - HDF5 dataspaces describe the logical layout of the data elements.

HDF5 Dataspaces

- Describe 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

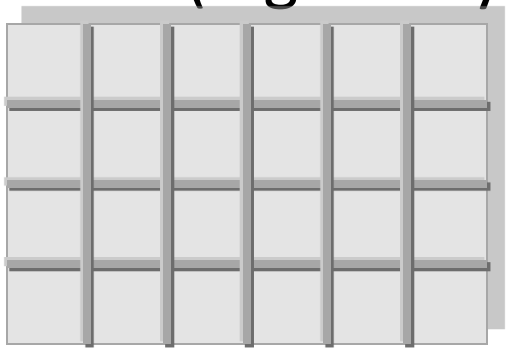
HDF5 Dataspaces

Two roles:

Dataspace contains spatial information (logical layout) about a dataset

stored in a file

- Rank and dimensions
- Permanent part of dataset definition



Rank = 2

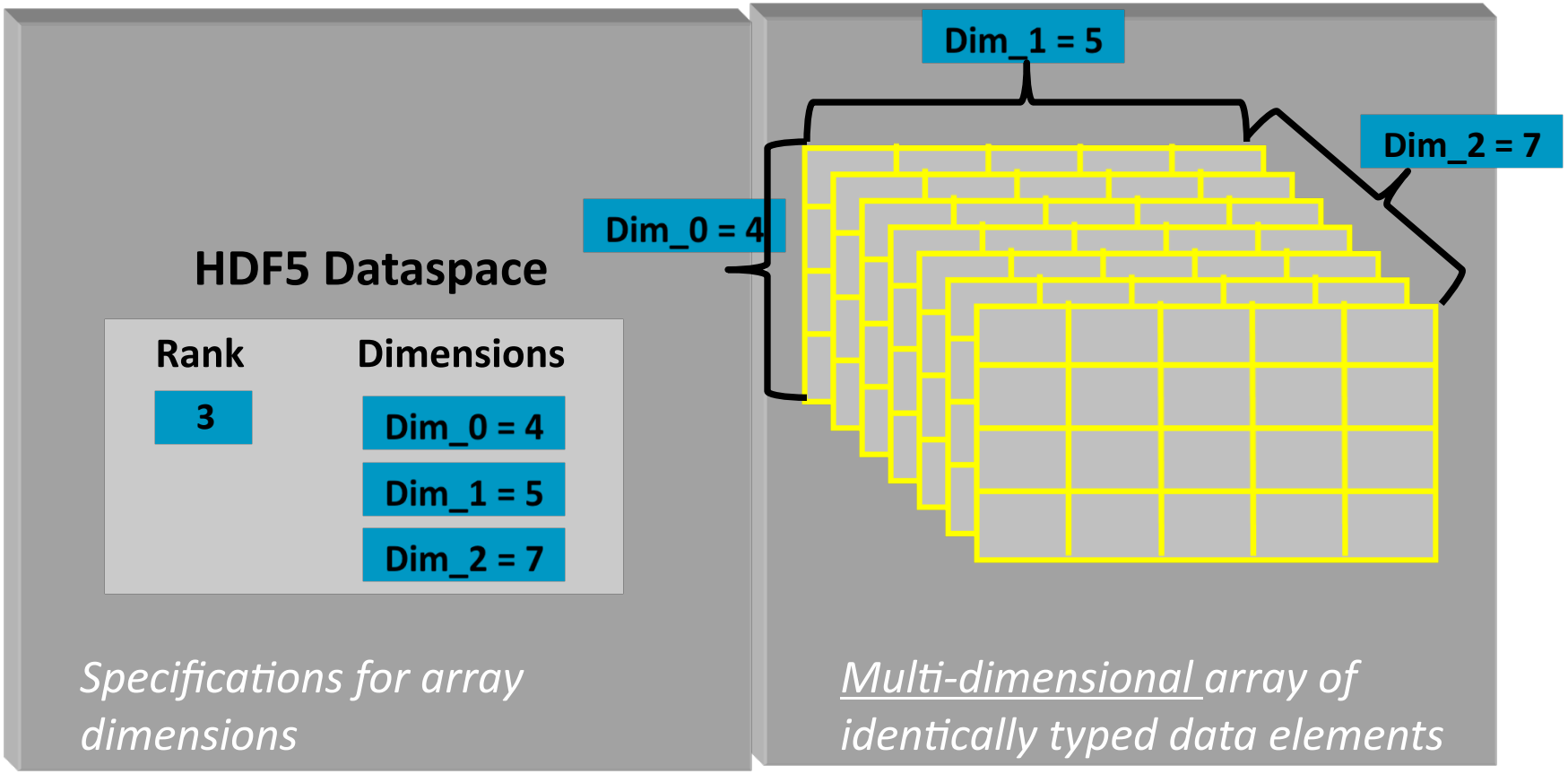
Dimensions = 4x6

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

Rank = 1

Dimension = 10

HDF5 Dataset & Dataspace

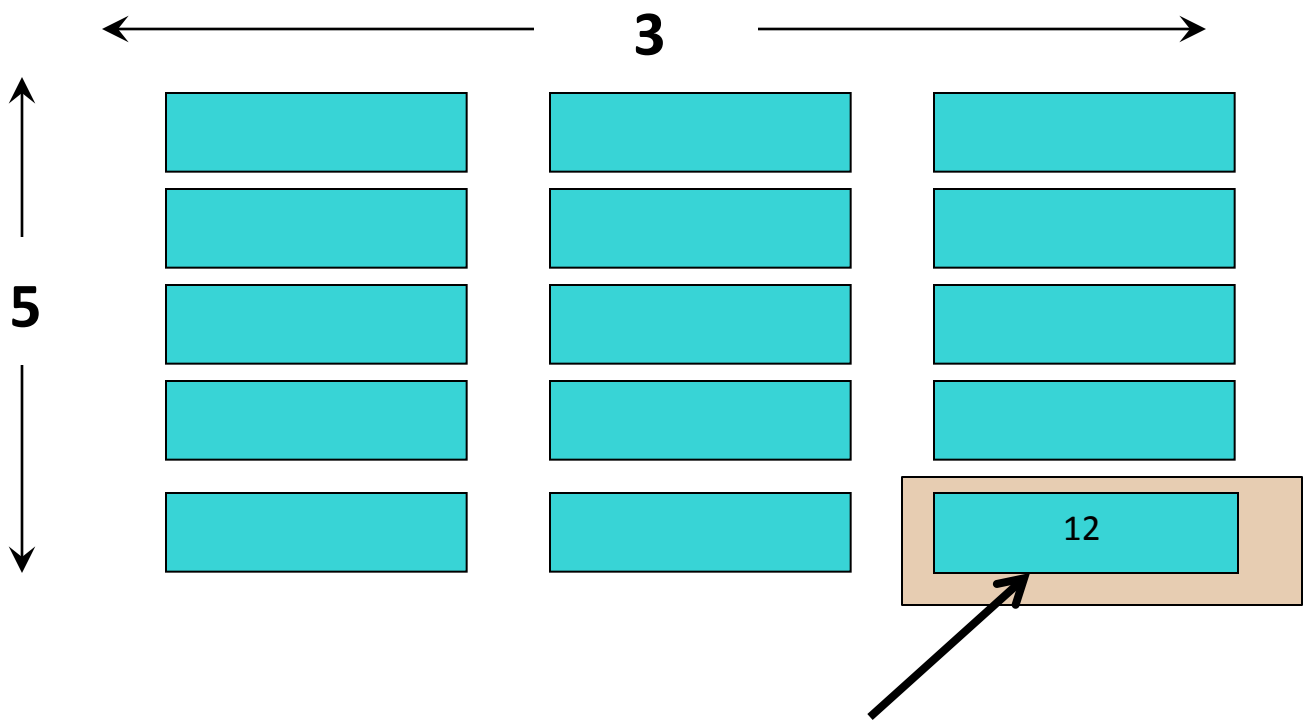


- HDF5 datasets organize and contain "raw data values".
  - HDF5 dataspaces **describe the logical layout of the data elements**.

HDF5 Datatypes

- Describe individual data elements in an HDF5 dataset
- Wide range of datatypes supported
  - Signed/unsigned Integer
  - Float
  - User-defined (e.g., 13-bit integer)
  - Fixed and variable-length strings
  - Variable length sequences
  - Arrays
  - Compound (similar to C structs)
  - Enumerated
  - Many more …

HDF5 Dataset

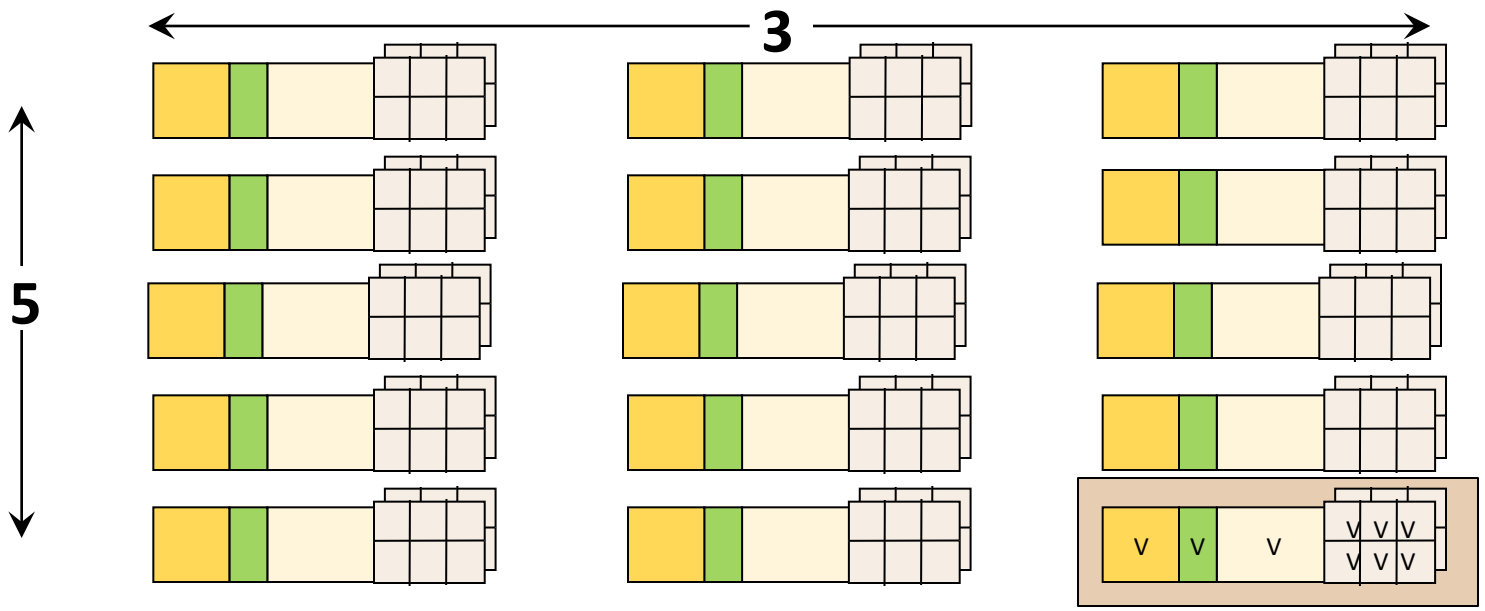


Datatype: 32-bit Integer

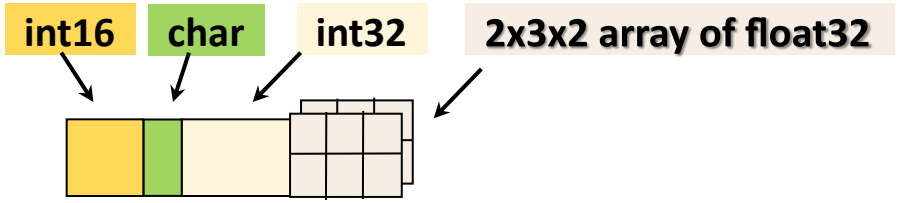
Dataspace: Rank = 2

Dimensions = 5 x 3

HDF5 Dataset with Compound Datatype



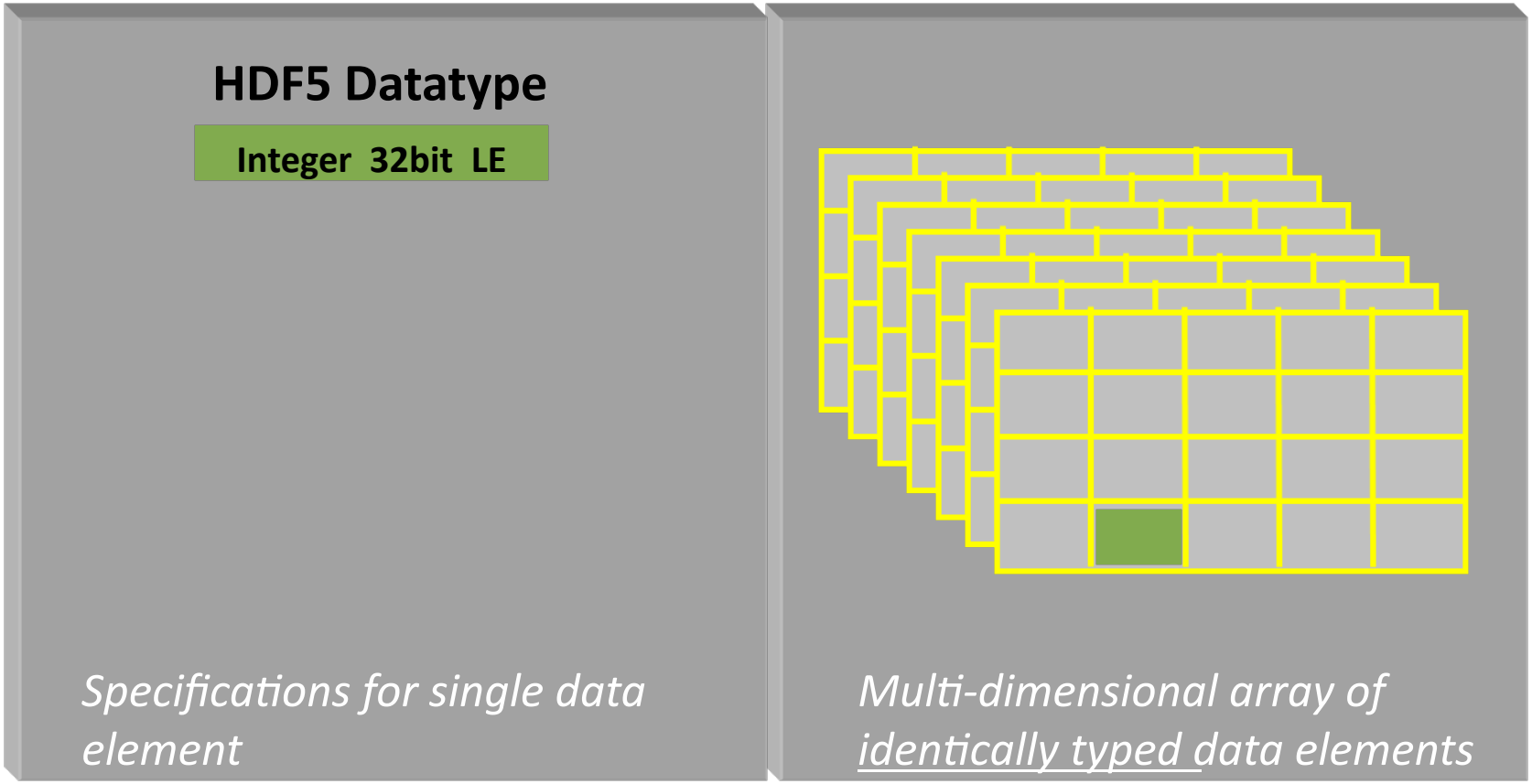
Compound Datatype:



Dataspace: Rank = 2

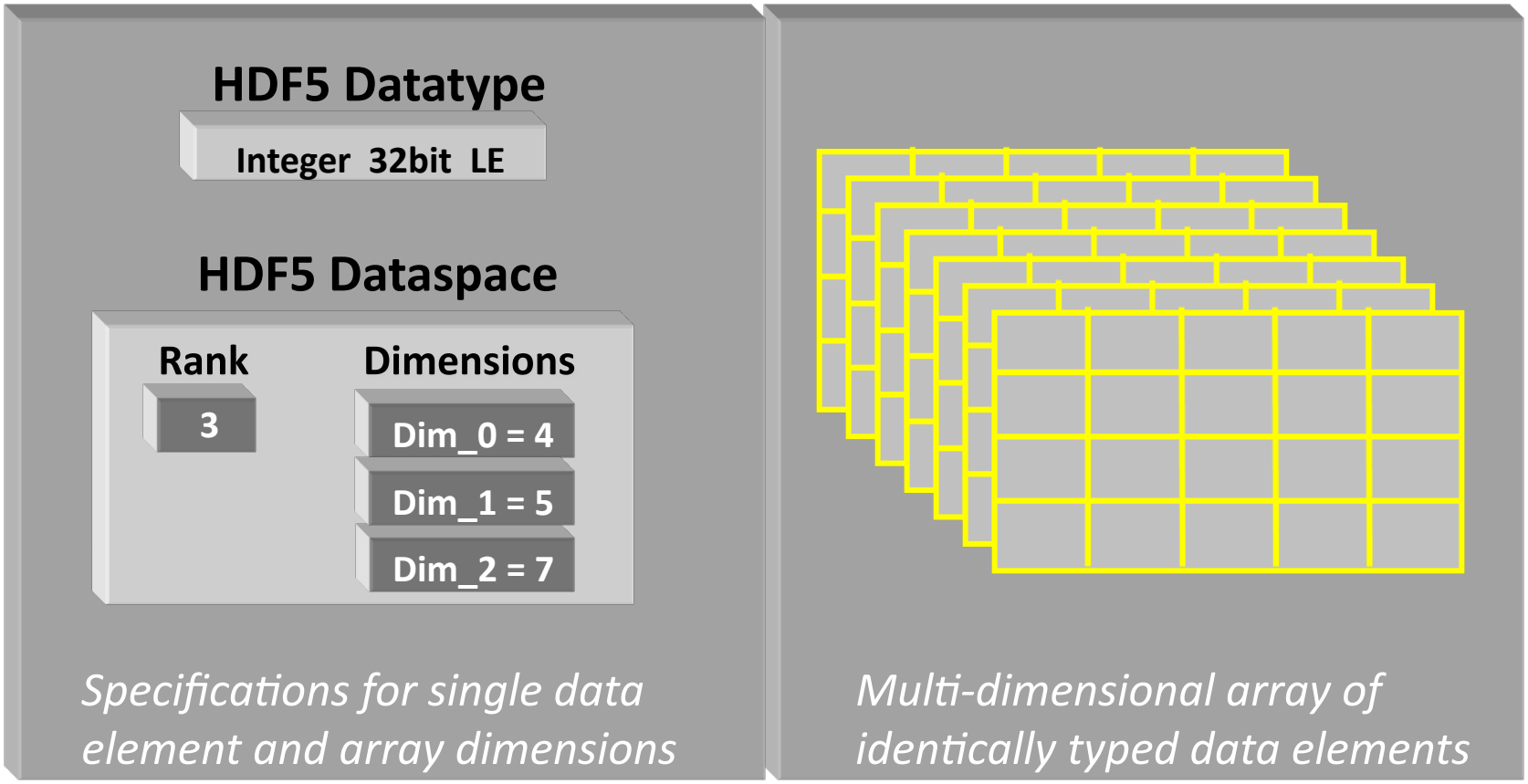
Dimensions = 5 x 3

HDF5 Dataset & Datatype



- HDF5 datasets organize and contain “raw data values”.
  - HDF5 datatypes **describe individual data elements.**

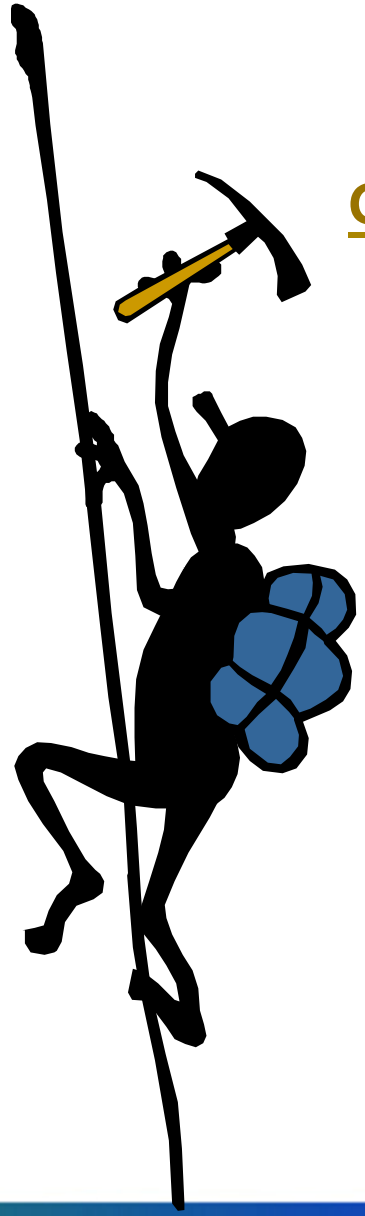
HDF5 Dataset



- HDF5 datasets organize and contain "raw data values".
  - HDF5 datatypes describe individual data elements.
  - HDF5 dataspaces describe the logical layout of the data elements.

HDF5 Data Model: Are we there yet?

HDF5 Objects



Group and **Link**

Attribute

Dataspace ✓

Datatype ✓

Dataset ✓

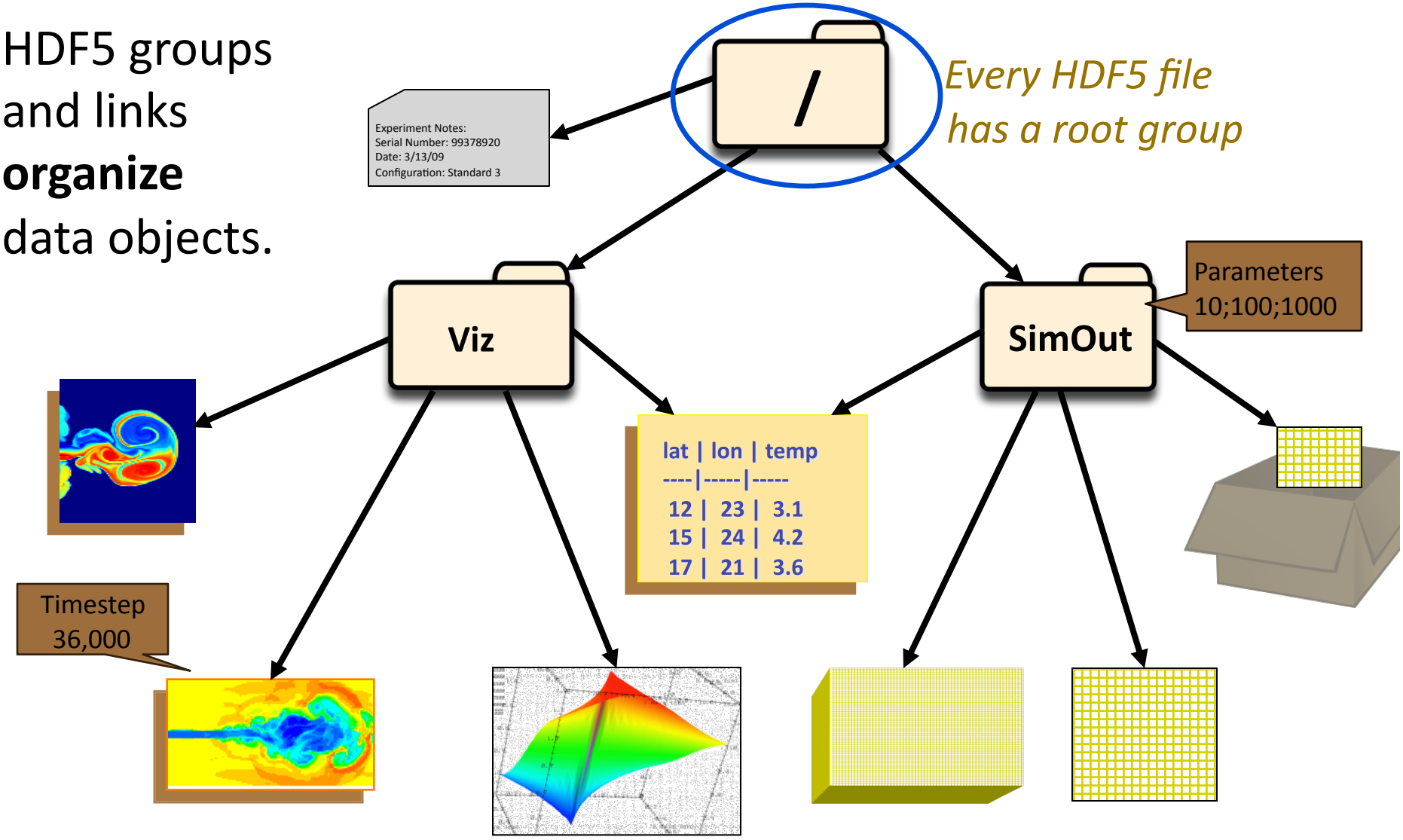
File ✓

HDF5 Attributes

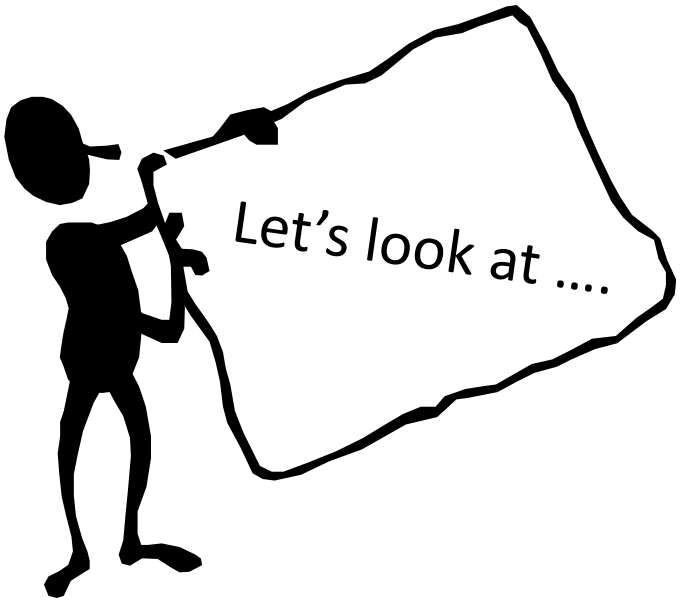
- Typically contain user metadata
- Have a name and a value
- Are associated with HDF5 objects.
- Value is described by a datatype and a dataspace
  - analogous to a dataset

HDF5 Groups and Links

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



HDF5 Technology Platform



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  - The "building blocks" for data organization and specification
- HDF5 **software**
  - Library, language interfaces, tools

HDF5 Home Page

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

- Latest release: HDF5 1.8.5 (1.8.6 coming in November!)

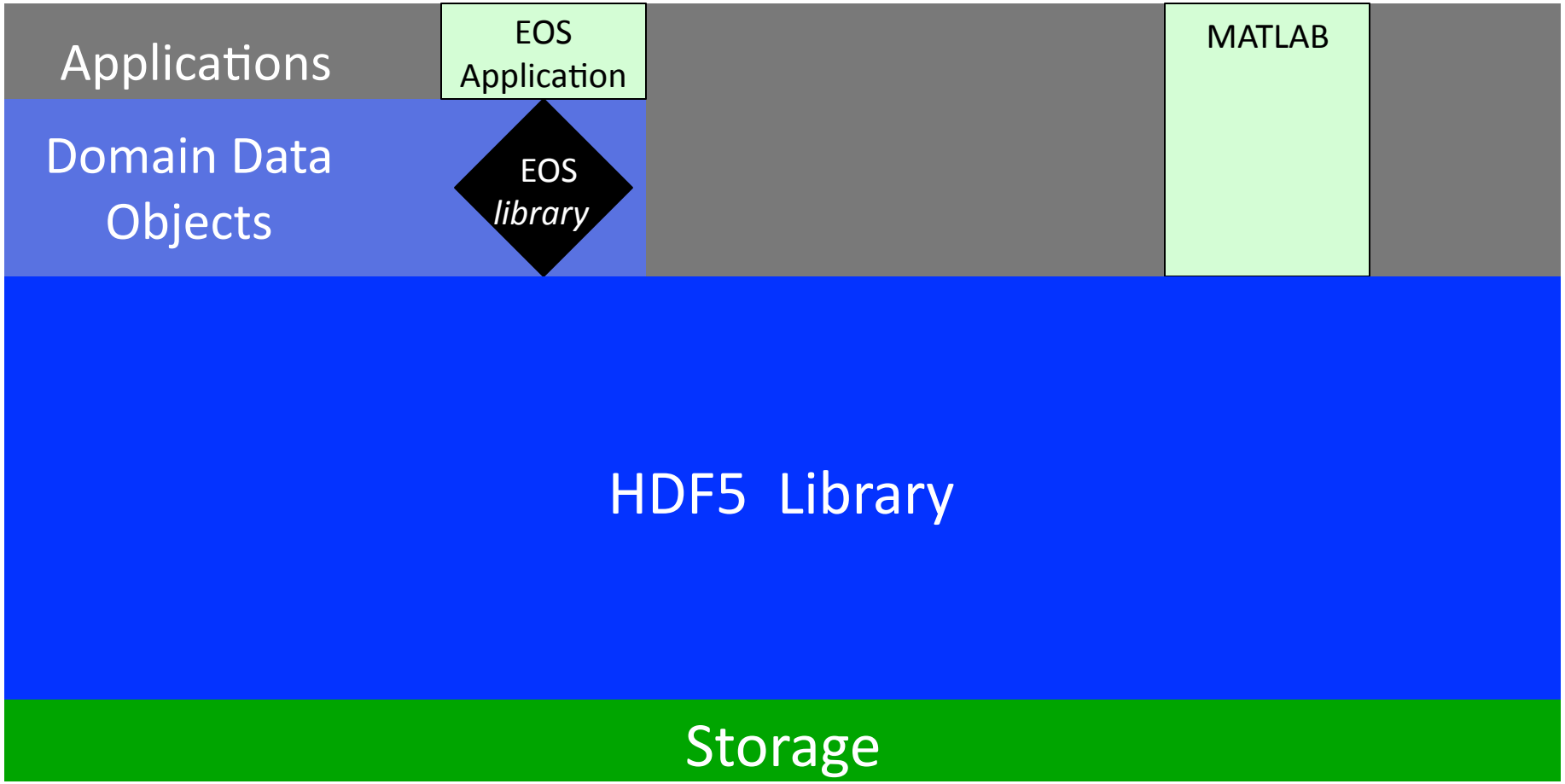
HDF5 source code:

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

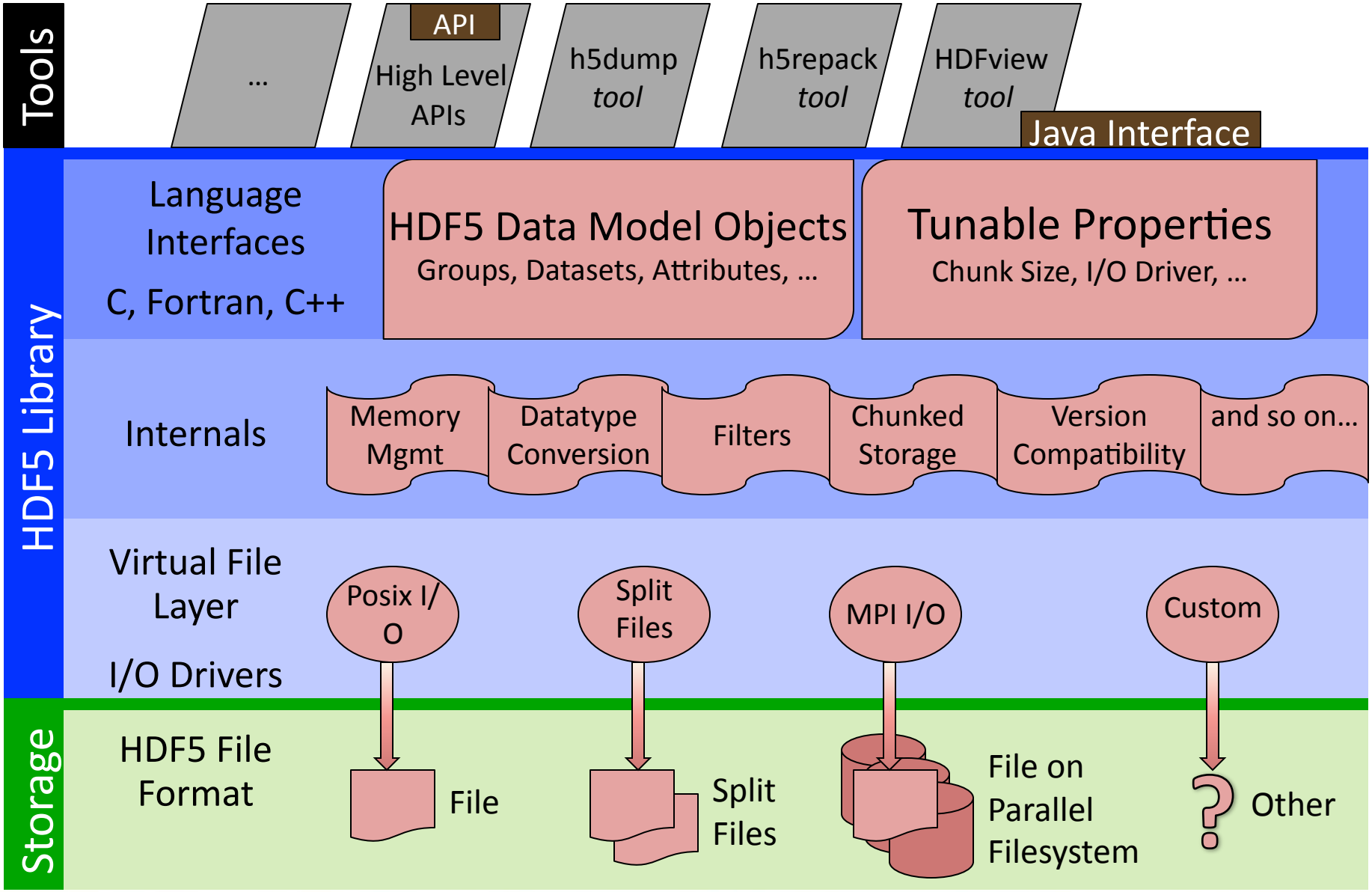
HDF5 pre-built binaries:

- 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

HDF5 API and Applications



HDF5 Software Layers & Storage



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 HDF4 and HDF5 files

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

Introduction to HDF5 Programming Model and APIs

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
  - ✓Access properties

Order of Operations

- An order is imposed on operations by argument dependencies

  For Example:

  A file must be opened before a dataset

  -because-

  the dataset open call requires a file handle as an argument.

- Objects can be closed in any order.

The General HDF5 API

- Currently C, Fortran 90, Java, and C++ bindings.
- 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**

HDF5 Defined Types

For portability, the HDF5 library has its own defined types:

hid_t: object identifiers (native *integer*)

hsize_t: size used for dimensions (*unsigned long* or *unsigned long long*)

herr_t: function return value

hvl_t: variable length datatype

Note: This is not an exhaustive list!

For **C**, include hdf5.h in your HDF5 application.

The HDF5 API

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

Victronix
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

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

DataSpaces:	H5Sselect_hyperslab (Partial I/O) H5Sselect_elements (Partial I/O) H5Dget_space
Groups:	H5Gcreate, H5Gopen, H5Gclose
Attributes:	H5Acreate, H5Aopen_name, H5Aclose, H5Aread, H5Awrite
Property lists:	H5Pcreate, H5Pclose H5Pset_chunk, H5Pset_deflate

High Level APIs

- Included along with the HDF5 library
- Simplify steps for creating, writing, and reading objects.
- Do not entirely ‘wrap’ HDF5 library

Example HDF5 Code

Steps to Create a File

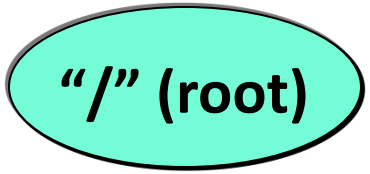
1. Decide on properties the file should have and create them if necessary:
   - Creation properties
   - Access properties
   - We will use Default properties.

2. Create the file

3. Close the file and the property lists, as needed

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);
```

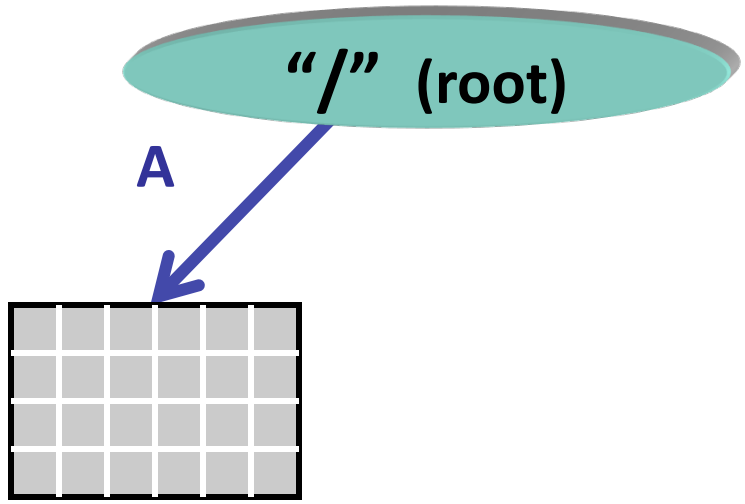


Note: Return codes not checked for errors in code samples.

Steps to Create a Dataset

1. Define dataset characteristics
   a) Datatype – integer
   b) Dataspace - 4x6
   c) Properties if needed, or use H5P_DEFAULT

2. Decide where to put it
   2. Group or root group
3. Create dataset in file
4. Close everything



HDF5 Pre-defined Datatype Identifiers

HDF5 defines* set of Datatype Identifiers per HDF5 session.

For example:

C Type	HDF5 File Type	HDF5 Memory Type
int	H5T_STD_I32BE H5T_STD_I32LE	H5T_NATIVE_INT
float	H5T_IEEE_F32BE H5T_IEEE_F32LE	H5T_NATIVE_FLOAT
double	H5T_IEEE_F64BE H5T_IEEE_F64LE	H5T_NATIVE_DOUBLE

*** Value of datatype is NOT fixed**

Pre-defined File Datatype Identifiers

Examples:

H5T_IEEE_F64LE	Eight-byte, little-endian, IEEE floating-point
H5T_STD_I32LE	Four-byte, little-endian, signed two's complement integer

NOTE: What you see in the file. Name is the same everywhere and explicitly defines a datatype.

***STD= "An architecture with a semi-standard type like 2's complement integer, unsigned integer…"**

Pre-defined Native Datatypes

Examples of predefined native types in C:

H5T_NATIVE_INT	(int)
H5T_NATIVE_FLOAT	(float)
H5T_NATIVE_UINT	(unsigned int)
H5T_NATIVE_LONG	(long)
H5T_NATIVE_CHAR	(char)

NOTE: Memory types.
Different for each machine.
Used for reading/writing.

Code: Create a Dataset

```
1   hid_t       dataspace_id;
2   hsize_t     dims[2];

.
.
.
5   dims[0] = 4;
6   dims[1] = 6;
7   dataspace_id = H5Screate_simple (2, dims, NULL);
```

Define a dataspace

rank

current dims

Code: Create a Dataset

```
1   hid_t       file_id, dataset_id, dataspace_id;

    .
    .
    .

8   dataset_id = H5Dcreate (file_id,"A",H5T_STD_I32BE,
                    dataspace_id, H5P_DEFAULT,H5P_DEFAULT,
                     H5P_DEFAULT);
```

Where to put it

Datatype

Size & shape

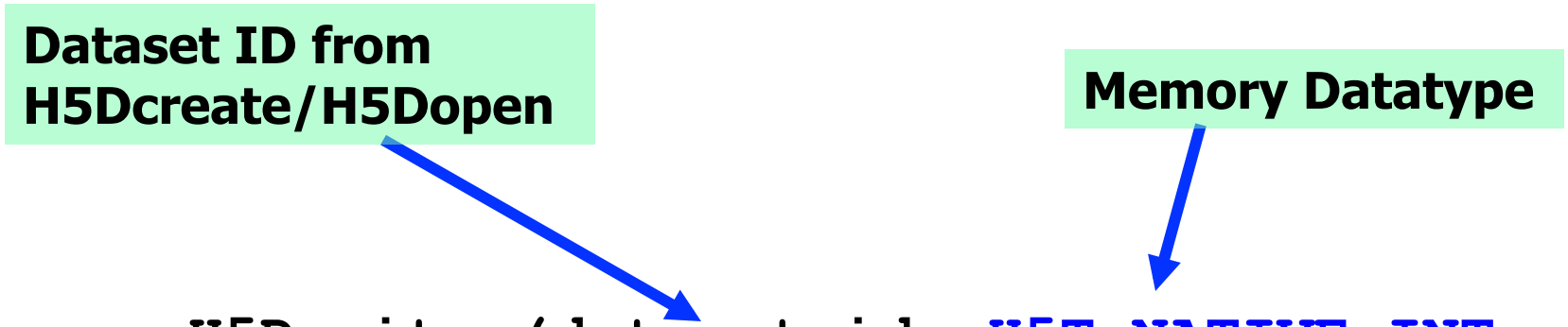
Properties (Link Creation, Dataset Creation and Access)

Code: Create a Dataset

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

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

5   dims[0] = 4;
6   dims[1] = 6;
7   dataspace_id = H5Screate_simple (2, dims, NULL);

8   dataset_id = H5Dcreate (file_id,”A",H5T_STD_I32BE,
                    dataspace_id, H5P_DEFAULT, H5P_DEFAULT,
                    H5P_DEFAULT);

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

Terminate access to dataspace, dataset, file

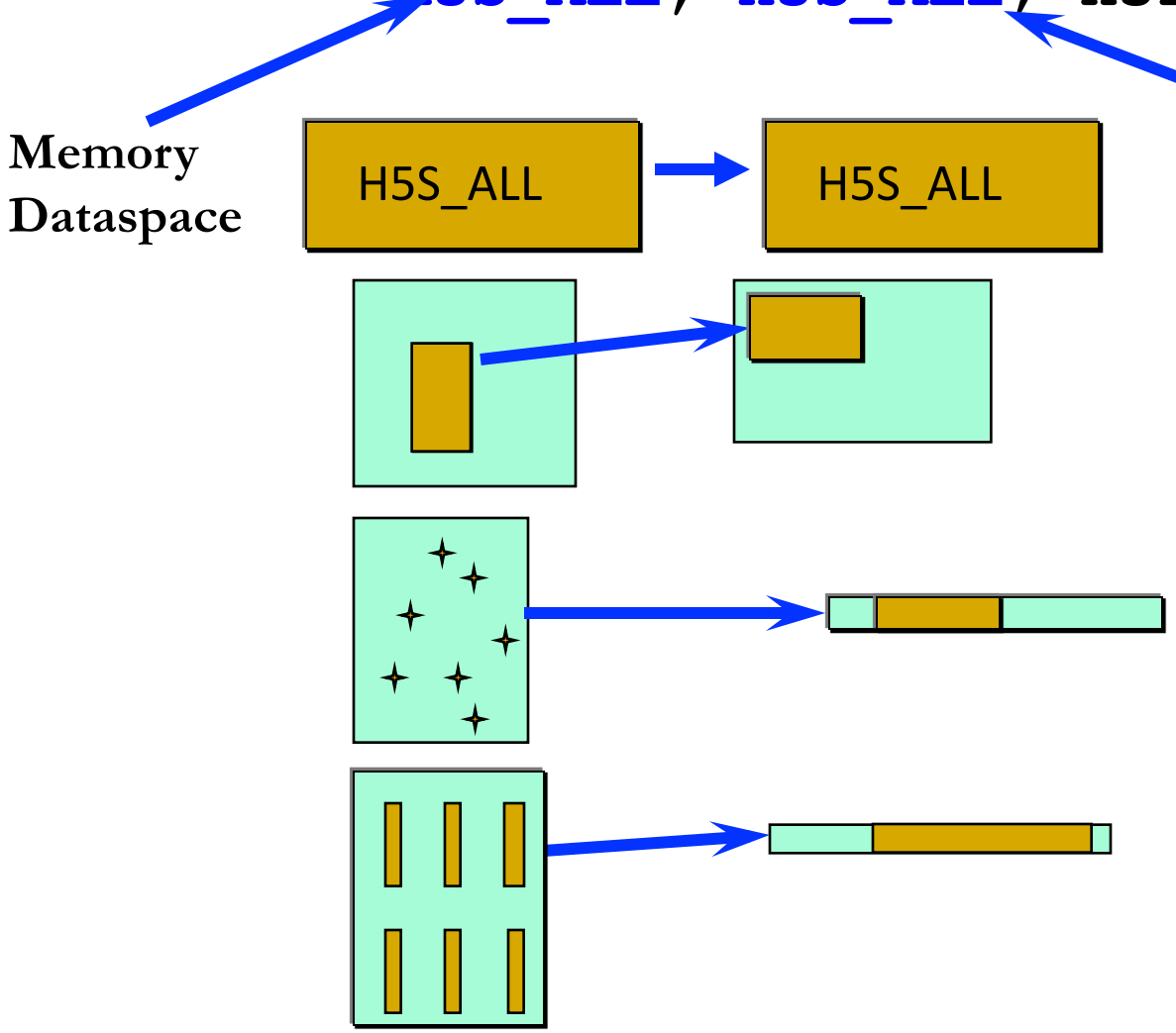
Example Code - H5Dwrite




```
status = H5Dwrite (dataset_id, H5T_NATIVE_INT,
                   H5S_ALL,H5S_ALL, H5P_DEFAULT, wdata);
```

Partial I/O

```
status = H5Dwrite (dataset_id, H5T_NATIVE_INT,
                   H5S_ALL, H5S_ALL, H5P_DEFAULT,wdata);
```



To Modify Dataspace:

H5Sselect_hyperslab

H5Sselect_elements

Example Code – H5Dwrite

```
status = H5Dwrite (dataset_id, H5T_NATIVE_INT,
                   H5S_ALL, H5S_ALL, H5P_DEFAULT, wdata);
```

Data Transfer Property List
(MPI I/O, Transformations,…)

Example Code – H5Dread

```
status = H5Dread (dataset_id, H5T_NATIVE_INT,
                  H5S_ALL, H5S_ALL, H5P_DEFAULT, rdata);
```

High Level APIs: HDF5 Lite (H5LT)

```
#include "hdf5_hl.h"
.
.

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

  status = H5LTmake_dataset (file_id,"A",2,dims,
                      H5T_STD_I32BE, data);

  status = H5Fclose (file_id);
```

High Level APIs

- HDF5 Lite
- HDF5 Image
- HDF5 Table
- HDF5 Dimension Scales
- HDF5 Packet Table

Steps to Create a Group

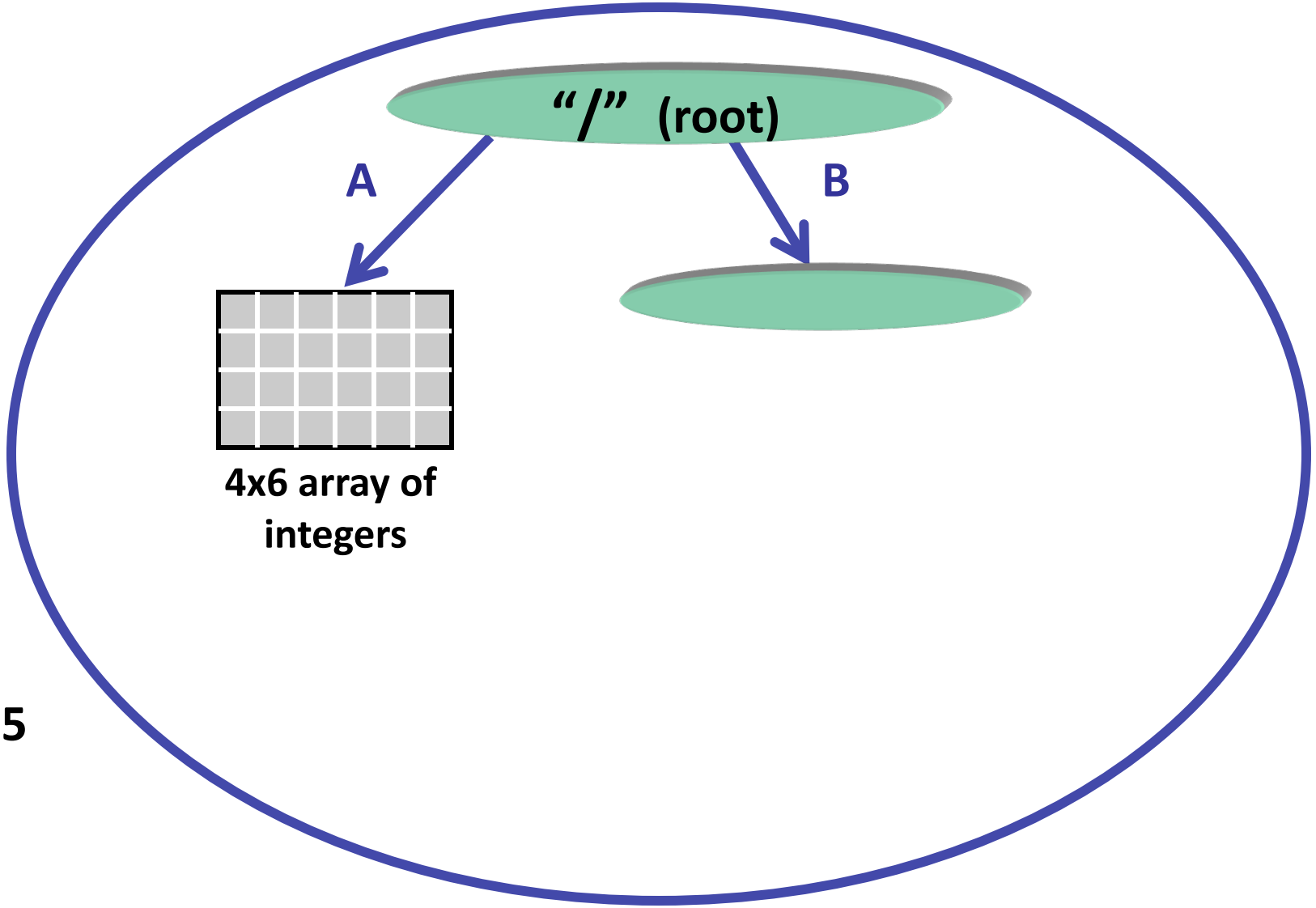
1. Decide where to put it – “root group”

2. Define properties or use H5P_DEFAULT

5. Create group in file.

4. Close the group.

Example: Create a Group



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);
```

HDF5 Tutorial and Examples

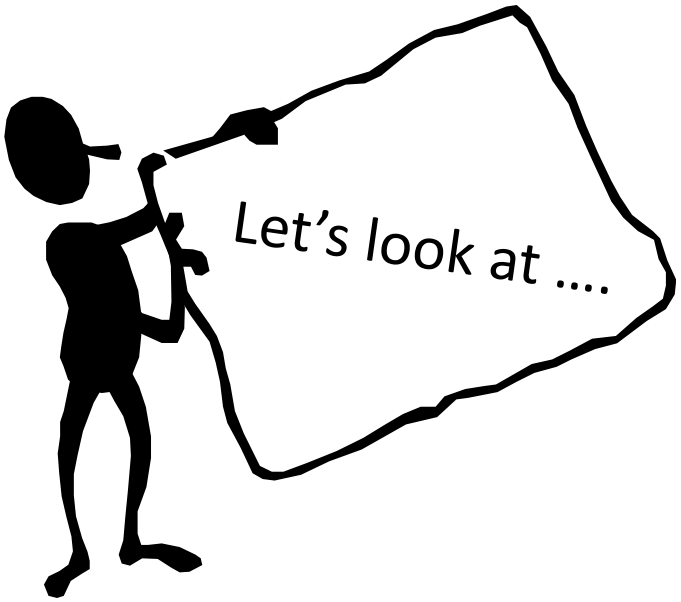
HDF5 Tutorial:

http://www.hdfgroup.org/HDF5/Tutor/

HDF5 Example Code:

http://www.hdfgroup.org/ftp/HDF5/examples/examples-by-api/

HDF5 Technology Platform



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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, so for the most part basic users do not need to know the guts of this information.

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Thank You!

Questions/comments?