PARALLEL I/O AND PORTABLE DATA FORMATS

HDF5

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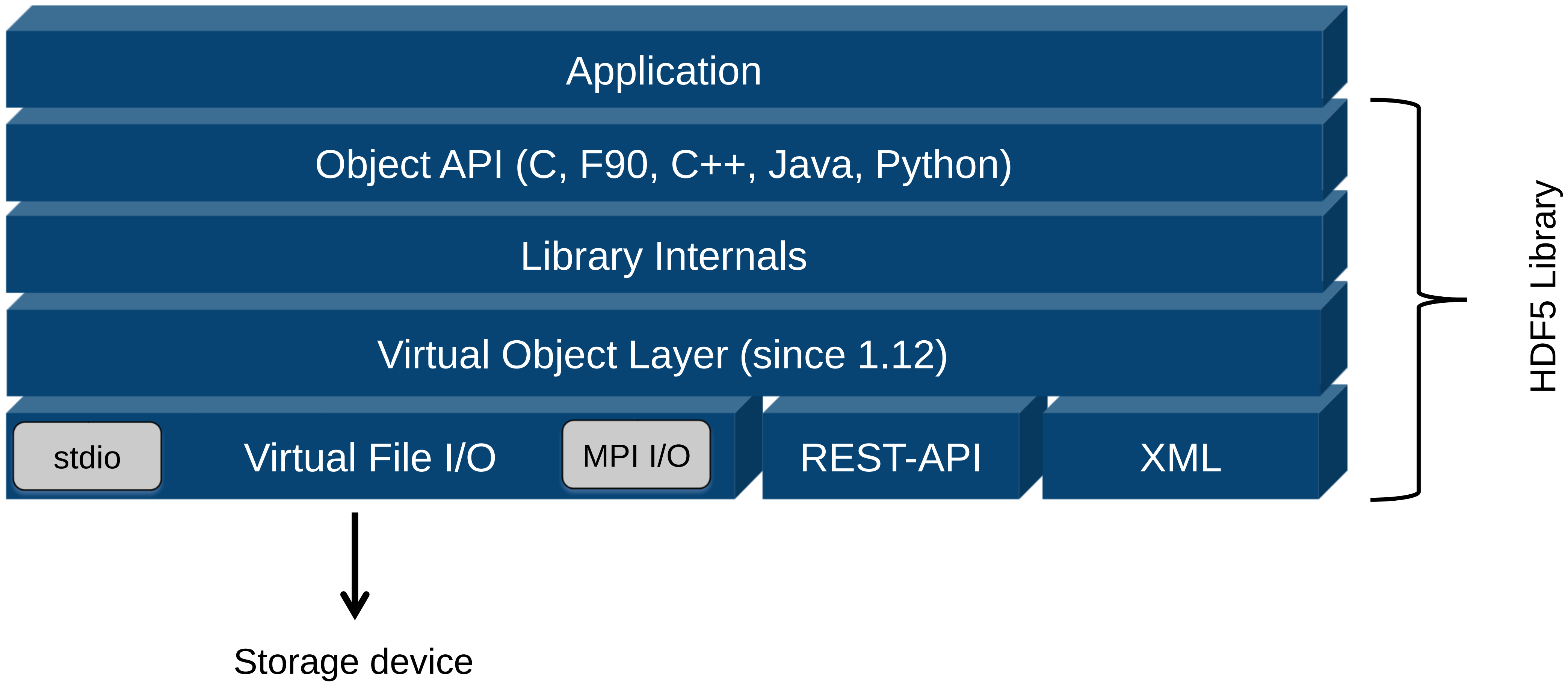
HDF5 - Features

- Hierarchical Data Format
- Supports parallel I/O
- Self describing data model which allows the management of complex data sets
- Portable file format
- Available on a variety of platforms
- Supports C, C++, Fortran 90, Python and Java
- Provides tools to operate on HDF5 files and data

Layers of the HDF5 Library

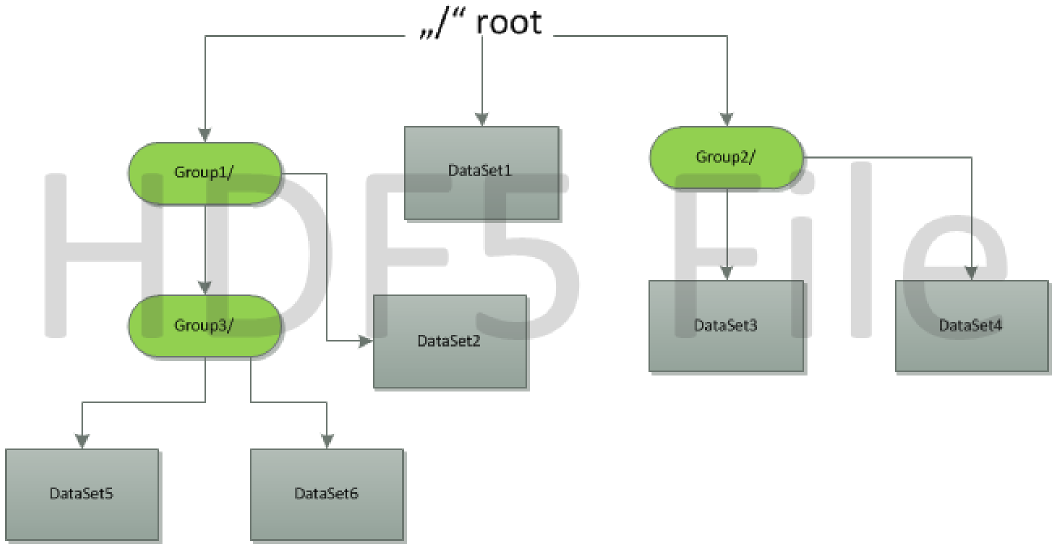


File organization

- HDF5 file structure corresponds in many respects to a Unix/Linux file system (fs)

HDF5		Unix/Linux fs
Group	↔	Directory
Data set	↔	File

/DataSet1
/Group1/DataSet2
/Group1/Group3/DataSet5
/Group1/Group3/DataSet6
/Group2/DataSet3
/Group2/Dataset4



Terminology

File

Container for storing data

Group

Structure which may contain HDF5 objects, e.g. datasets, attributes, datasets

Attribute

Can be used to describe datasets and is attached to them

Dataspace

Describes the dimensionality of the data array and the shape of the data points respectively, i.e. it describes the shape of a dataset

Dataset

Multi-dimensional array of data elements

Library specific types

C

```
#include hdf5.h
hid_t       Object identifier
herr_t      Function return value
hsize_t     Used for dimensions
```

Fortran

```
use hdf5
INTEGER(HID_T)      Object identifier
INTEGER(HSIZE_T)    Used for dimensions
```

- Defined types are integers of different size
- Own defined types ensure portability

Fortran HDF5 open

- The HDF5 library interface needs to be initialized (e.g. global variables) by calling `H5OPEN_F` before it can be used in your code and closed (`H5CLOSE_F`) at the end.

Fortran

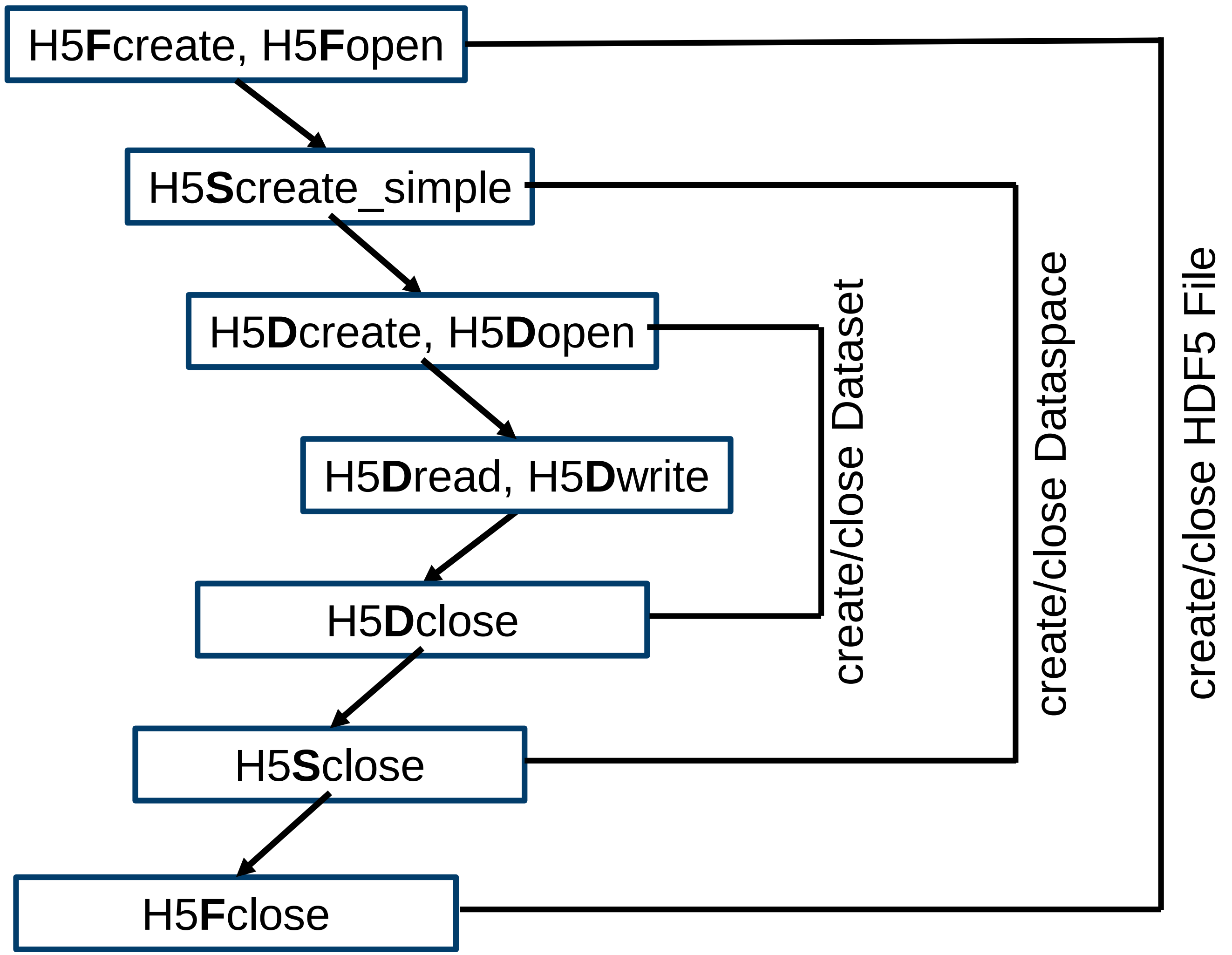
```
H5OPEN_F(STATUS)
  INTEGER, INTENT(OUT) :: STATUS

H5CLOSE_F(STATUS)
  INTEGER, INTENT(OUT) :: STATUS
```

- `status` returns `0` if successful

API naming scheme (excerpt)

- `H5`
  - Library functions: general-purpose functions
- `H5D`
  - Dataset interface: dataset access and manipulation routines
- `H5G`
  - Group interface: group creation and manipulation routines
- `H5F`
  - File interface: file access routines
- `H5P`
  - Property list interface: object property list manipulation routines
- `H5S`
  - Dataspace interface: dataspace definition and access routines

General Procedure



Creating an HDF5 file

C

```
hid_t H5Fcreate(const char *name, unsigned
                access_flag, hid_t creation_prp,
                hid_t access_prp)
```

Fortran

```
H5FCREATE_F(NAME, ACCESS_FLAGS, FILE_ID, HDFERR,
            CREATION_PRP, ACCESS_PRP)
  CHARACTER(*), INTENT(IN) :: NAME
  INTEGER, INTENT(IN) :: ACCESS_FLAGS
  INTEGER(KIND=HID_T), INTENT(OUT) :: FILE_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(KIND=HID_T), OPTIONAL, INTENT(IN) ::
    CREATION_PRP, ACCESS_PRP
```

- `name`: Name of the file
- `access_flags`: File access flags
- `creation_prp` and `access_prp`: File creation and access property list, `H5P_DEFAULT[_F]` if not specified
- Fortran uses `file_id` as return value

Opening an existing HDF5 file

C

```
hid_t H5Fopen(const char *name, unsigned flags,
              hid_t access_prp)
```

Fortran

```
H5FOPEN_F(NAME, FLAGS, FILE_ID, HDFERR,
          ACCESS_PRP)
  CHARACTER(*), INTENT(IN) :: NAME
  INTEGER, INTENT(IN) :: FLAGS
  INTEGER(KIND=HID_T), INTENT(OUT) :: FILE_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(KIND=HID_T), OPTIONAL, INTENT(IN) ::
    ACCESS_PRP
```

- `name`: Name of the file
- `access_prp`: File access property list, `H5P_DEFAULT[_F]` if not specified
- Fortran uses `file_id` as return value
  - Avoid multiple opens of the same file

Access modes

- `H5F_ACC_TRUNC[_F]`: Create a new file, overwrite an existing file
- `H5F_ACC_EXCL[_F]`: Create a new file, `H5Fcreate` fails if file already exists
- `H5F_ACC_RDWR[_F]`: Open file in read-write mode, irrelevant for `H5Fcreate[_f]`
- `H5F_ACC_RDONLY[_F]`: Open file in read-only mode, irrelevant for `H5Fcreate[_f]`
- More specific settings are controlled through file creation property list (`creation_prp`) and file access property lists (`access_prp`) which defaults to `H5P_DEFAULT[_F]`
- `creation_prp` controls file metadata
- `access_prp` controls different methods of performing I/O on files

Group creation

C

```c
hid_t H5Gcreate(hid_t loc_id, const char *name,
                hid_t lcpl_id, hid_t gcpl_id,
                hid_t gapl_id )
```

Fortran

```fortran
H5GCREATE_F(LOC_ID, NAME, GRP_ID, HDFERR,
            SIZE_HINT, LCPL_ID, GCPL_ID, GAPL_ID)
  INTEGER(KIND=HID_T), INTENT(IN) :: LOC_ID
  CHARACTER(LEN=*), INTENT(IN) :: NAME
  INTEGER(KIND=HID_T), INTENT(OUT) :: GRP_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(KIND=SIZE_T), OPTIONAL, INTENT(IN) ::
    SIZE_HINT
  INTEGER(KIND=HID_T), OPTIONAL, INTENT(IN) ::
    LCPL_ID, GCPL_ID, GAPL_ID
```

- `loc_id`: Can be the `file_id` or another `group_id`
- `name` can be an absolute or relative path
- `lcpl_id, gcpl_id, gapl_id`: Property lists for link/group
- use `H5Gclose[_f]` to finalize group access

Closing an HDF5 file

C

```
herr_t H5Fclose(hid_t file_id)
```

Fortran

```
H5FCLOSE_F(FILE_ID, HDFERR)
   INTEGER(KIND=HID_T), INTENT(IN) :: FILE_ID
   INTEGER, INTENT(OUT) :: HDFERR
```

Exercise

Exercise 1 – HDF5 hello world

- Directory preparation:
  - `/p/project/training2202/hdf5/copy.sh`
  - `cd /p/project/training2202/<username>/hdf5`

- Write a serial program in C or Fortran which creates and closes an HDF5 file
- Create a group “data” inside of this file

Check the resulting file using:
`h5dump`

```
module load Intel ParaStationMPI # Load compiler and MPI
module load HDF5/1.12.1 # Load HDF5 libs

mpicc helloworld_hdf5.c -lhdf5 # Compile C style
mpif90 helloworld_hdf5.f90 -lh5df_fortran # Compile Fortran style
```

HDF5 pre-defined datatypes (excerpt)

C	C type	HDF5 file type (pre-defined)	HDF5 memory type (native)
	int	H5T_STD_I32[BE,LE]	H5T_NATIVE_INT
	float	H5T_IEEE_F32[BE,LE]	H5T_NATIVE_FLOAT
	double	H5T_IEEE_F64[BE,LE]	H5T_NATIVE_DOUBLE

Fortran	F type	HDF5 file type (pre-defined)	HDF5 memory type (native)
	integer	H5T_STD_I32[BE,LE]	H5T_NATIVE_INTEGER
	real	H5T_IEEE_F32[BE,LE]	H5T_NATIVE_REAL

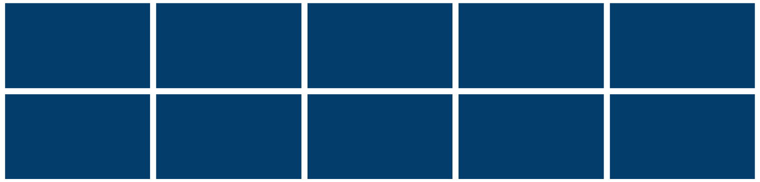
- Native datatype might differ from platform to platform
- HDF5 file type depends on compiler switches and underlying platform
- Native datatypes are not in an HDF file but the pre-defined ones which are referred to by native datatypes appear in the HDF5 files.

Dataspace

- The dataspace is part of the metadata of the underlying dataset
- Metadata are:
  - Dataspace
  - Datatype
  - Attributes
  - Storage info
- The dataspace describes the size and shape of the dataset

Simple dataspace

```
rank: int
current_size: hsize_t[rank]
maximum_size: hsize_t[rank]
```



rank = `2`, dimensions = `2x5`

Creating a dataspace

C

```
hid_t H5Screate_simple(int rank,
                       const hsize_t *current_dims,
                       const hsize_t *maximum_dims)
```

Fortran

```
H5SCREATE_SIMPLE_F(RANK, DIMS, SPACE_ID, HDFERR,
            MAXDIMS)
  INTEGER, INTENT(IN) :: RANK
  INTEGER(KIND=HISIZE_T)(*), INTENT(IN) :: DIMS
  INTEGER(KIND=HID_T), INTENT(OUT) :: SPACE_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(KIND=HISIZE_T)(*), OPTIONAL,
    INTENT(OUT) :: MAXDIMS
```

- `rank`: Number of dimensions
- `maximum_dims` may be `NULL`. Then `maximum_dims` and `current_dims` are the same
- `H5S_UNLIMITED[_F]` can be used as `maximum_dims` to set dimensions to “infinite” size
- use `H5Sclose[_f]` to finalize dataspace access

Creating a dataspace

C

```c
hid_t H5Screate(H5S_class_t type)
```

Fortran

```fortran
H5SCREATE_F(CLASSTYPE, SPACE_ID, HDFERR)
  INTEGER, INTENT(IN) :: CLASSTYPE
  INTEGER(HID_T), INTENT(OUT) :: SPACE_ID
  INTEGER, INTENT(OUT) :: HDFERR
```

- `classtype`: `H5S_SCALAR[_F]` or `H5S_SIMPLE[_F]`

Creating an Attribute

C

```
hid_t H5Acreate(hid_t loc_id, const char *attr_name,
                hid_t type_id, hid_t space_id,
                hid_t acpl_id, hid_t aapl_id)
```

Fortran

```
H5ACREATE_F(LOC_ID, NAME, TYPE_ID, SPACE_ID,
            ATTR_ID, HDFERR, ACPL_ID, AAPL_ID)
  INTEGER(KIND=HID_T), INTENT(IN) :: LOC_ID
  CHARACTER(LEN=*), INTENT(IN) :: NAME
  INTEGER(KIND=HID_T), INTENT(IN) :: TYPE_ID,
    SPACE_ID
  INTEGER(KIND=HID_T), INTENT(OUT) :: ATTR_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(KIND=HID_T), OPTIONAL, INTENT(IN) ::
    ACPL_ID, AAPL_ID
```

- `loc_id` may be any HDF5 object identifier (group, dataset, or committed datatype) or an HDF5 file identifier
- `ACPL_ID, AAPL_ID`: `H5P_DEFAULT[_F]` if not specified
- use `H5Aclose[_f]` to finalize the attribute access

Writing an Attribute

C

```c
herr_t H5Awrite(hid_t attr_id, hid_t mem_type_id,
                const void *buf)
```

Fortran

```fortran
H5AWRITE_F(ATTR_ID, MEMTYPE_ID, BUF, DIMS, HDFERR)
    INTEGER(KIND=HID_T), INTENT(IN) :: ATTR_ID
    INTEGER(KIND=HID_T), INTENT(IN) :: MEMTYPE_ID
    TYPE, INTENT(IN) :: BUF
    INTEGER(KIND=HSIZE_T)(*), INTENT(IN):: DIMS
    INTEGER, INTENT(OUT) :: HDFERR
```

- Fortran: `DIMS` array to hold corresponding dimension sizes of data buffer `buf` (new since 1.4.2)

Writing an Attribute

- StringType Example (C):

```
atype = H5Tcopy(H5T_C_S1);
H5Tset_size(atype, 5);
H5Tset_strpad(atype,H5T_STR_NULLTERM);
…
H5Tclose(atype);
```

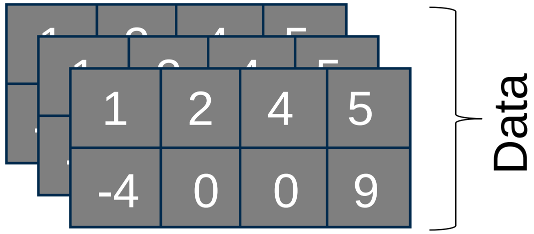
alternative:

```
H5T_STR_SPACEPAD
H5T_STR_NULLPAD
```

- StringType Example (Fortran):

```
call H5Tcopy_f(H5T_C_S1,atype,status)
call H5Tset_size_f(atype, int(5,HSIZE_T),status)
call H5Tset_strpad_f(atype,H5T_STR_NULLTERM_F)
…
call H5Tclose_f(atype, status)
```

Dataset (metadata + data)



Metadata

Dataspace
- rank = 3
- dim[0] = 2
- dim[1] = 4
- dim[2] = 3

Datatype
- Integer

Attributes
- Time = 2.1
- Temp = 122

Storage
- Contiguous

Creating a Dataset

C

```c
hid_t H5Dcreate(hid_t loc_id, const char *name,
                hid_t dtype_id, hid_t space_id,
                hid_t lcpl_id, hid_t dcpl_id,
                hid_t dapl_id)
```

Fortran

```fortran
H5DCREATE_F(LOC_ID, NAME, TYPE_ID, SPACE_ID,
         DSET_ID, HDFERR, DCPL_ID, LCPL_ID, DAPL_ID)
  INTEGER(KIND=HID_T), INTENT(IN) :: LOC_ID
  CHARACTER(LEN=*), INTENT(IN) :: NAME
  INTEGER(KIND=HID_T), INTENT(IN) :: TYPE_ID,
    SPACE_ID
  INTEGER(KIND=HID_T), INTENT(OUT) :: DSET_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(KIND=HID_T), OPTIONAL, INTENT(IN) ::
    DCPL_ID, LCPL_ID, DAPL_ID
```

- use `H5Dclose[_f]` to finalize the dataset access

Creating a Dataset

- `type_id`: Datatype identifier
- `space_id`: Dataspace identifier
- `dcpl_id`: Dataset creation property list
- `lcpl_id`: Link creation property list
- `dapl_id`: Dataset access property list

Property Lists

- Property lists (`H5P`) can be used to change the internal data handling in HDF5
- Default: `H5P_DEFAULT[_F]`
- Creation properties
  - Whether a dataset is stored in a compact, contiguous, or chunked layout
  - Specify filters to be applied to a dataset (e.g. gzip compression or checksum evaluation)
- Access properties
  - The driver used to open a file (e.g. MPI-I/O or Posix)
  - Optimization settings in specialized environments
- Transfer properties
  - Collective or independent I/O

Recipe: Creating an empty dataset

1. Get identifier for dataset location
2. Specify datatype (integer, composite etc.)
3. Define dataspace
4. Specify property lists (or `H5P_DEFAULT[_F]`)
5. Create dataset
6. Close all opened objects

Exercise

Exercise 2 – HDF5 metadata handling

- Extend your serial program
- Create inside the “data” group an empty dataset which should be a two dimensional array (5x20 elements) of integer values
- Add a string attribute connected to this dataset (the string type definition is already available within the template file)
- Write a string value into this attribute

Check the resulting file using:

```
h5dump
```

Writing to a dataset

C

```c
herr_t H5Dwrite(hid_t dataset_id, hid_t mem_type_id,
                hid_t mem_space_id, hid_t
                file_space_id, hid_t xfer_plist_id,
                const void * buf )
```

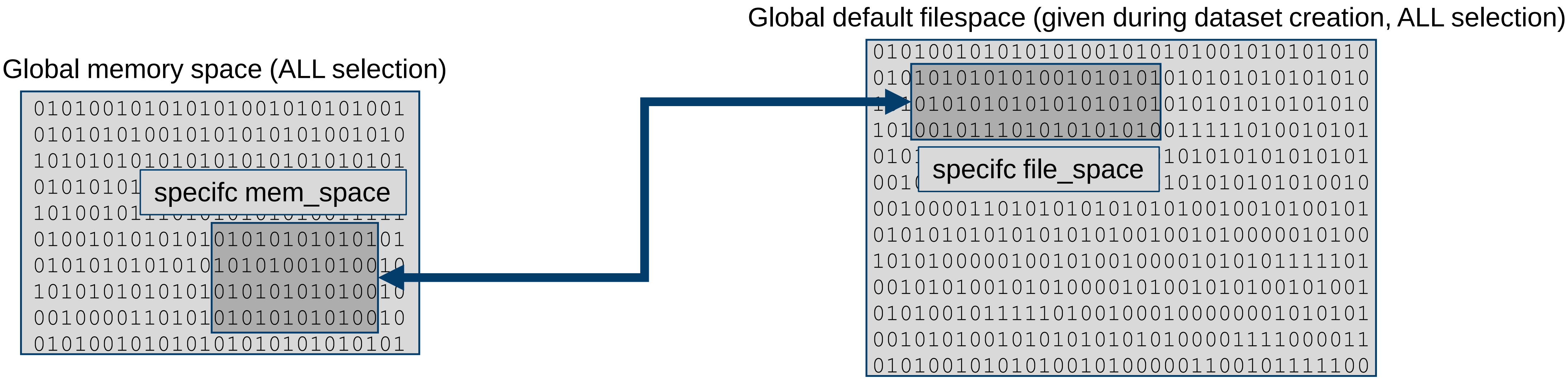
Fortran

```fortran
H5DWRITE_F(DSET_ID, MEM_TYPE_ID, BUF, DIMS, HDFERR,
           MEM_SPACE_ID, FILE_SPACE_ID, XFER_PRP)
  INTEGER(HID_T), INTENT(IN) :: DSET_ID, MEM_TYPE_ID
  TYPE, INTENT(IN) :: BUF
  DIMENSION(*), INTEGER(HSIZE_T), INTENT(IN) :: DIMS
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(HID_T), OPTIONAL, INTENT(IN) ::
    MEM_SPACE_ID, FILE_SPACE_ID, XFER_PRP
```

- `H5S_ALL[_F]` can be used to specify no special `mem_space` or `file_space` identifier
- `xfer_plist_id/xfer_prp` is a transfer property (e.g. to specify collective or independent parallel I/O)

Writing to a dataset

mem_space_id	file_space_id	Behaviour
dataspace id	dataspace id	use dataspaces as is
H5S_ALL	dataspace id	use given file_space dataspace also for mem_space dataspace (including the selection)
dataspace id	H5S_ALL	use *all* selection for default file_space
H5S_ALL	H5S_ALL	use default file_space also for mem_space, set *all* selection for both



Open a existing dataset

C

```c
hid_t H5Dopen(hid_t loc_id, const char *name, hid_t
              dapl_id)
```

Fortran

```fortran
H5DOPEN_F(LOC_ID, NAME, DSET_ID, HDFERR)
  INTEGER(HID_T), INTENT(IN) :: LOC_ID
  CHARACTER(LEN=*), INTENT(IN) :: NAME
  INTEGER(HID_T), INTENT(OUT) :: DSET_ID
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(HID_T), OPTIONAL, INTENT(IN) :: DAPL_ID
```

- `dapl_id`: Dataset access property list

Dataspace inquiry

C

```c
hid_t H5Dget_space(hid_t dataset_id)
```

Fortran

```fortran
H5DGET_SPACE_F(DATASET_ID, DATASPACE_ID, HDFERR)
  INTEGER(HID_T), INTENT(IN) :: DATASET_ID
  INTEGER(HID_T), INTENT(OUT) :: DATASPACE_ID
  INTEGER, INTENT(OUT) :: HDFERR
```

- Returns an identifier for a copy of the dataspace for a dataset.
- `H5Sget_simple_extent_ndims` and `H5Sget_simple_extent_dims` can be used to extract dimension information

Reading a dataset

C

```
herr_t H5Dread(hid_t dataset_id, hid_t mem_type_id,
               hid_t mem_space_id, hid_t
               file_space_id, hid_t xfer_plist_id,
               void * buf)
```

Fortran

```
H5DREAD_F(DSET_ID, MEM_TYPE_ID, BUF, DIMS, HDFERR,
          MEM_SPACE_ID, FILE_SPACE_ID, XFER_PRP)
  INTEGER(HID_T), INTENT(IN) :: DSET_ID, MEM_TYPE_ID
  TYPE, INTENT(IN) :: BUF
  DIMENSION(*), INTEGER(HSIZE_T), INTENT(IN) :: DIMS
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(HID_T), OPTIONAL, INTENT(IN) ::
    MEM_SPACE_ID, FILE_SPACE_ID, XFER_PRP
```

- `H5S_ALL[_F]` can be used to specify no special `mem_space` or `file_space` identifier
- `xfer_plist_id/xfer_prp` is a transfer property (e.g. to specify collective or independent parallel I/O)

Exercise

Exercise 3 – HDF5 write data

- Extend your serial program
- Create a two dimensional array with values 1 up to 100

```
 1  2  3  4  5  6  7 …
21 22 23 24 25 26 27 …
41 42 43 44 45 46 47 …
…
```

- Write this array into the existing empty HD5 dataset

Check the resulting file using:

`h5dump`

Excursion: row-major / column-major order

- “Logical” data view:

  - $M[i,j] = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$

Adress	1	2	3	4	5	6
Value C	1	2	3	4	5	6
Value Fortran	1	3	5	2	4	6

- Storing data in a `3x2` dimensional HDF5 dataset:

  - C: $\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$ Fortran: $\begin{bmatrix} 1 & 3 \\ 5 & 2 \\ 4 & 6 \end{bmatrix}$

- Storing data in a `2x3` dimensional dataset:

  - Fortran: $\begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}$

High-level vs. Low-level APIs

- The HDF5 high-level APIs (`-l hdf5_hl`) can help to write less code for common HDF5 activities
- In the course we only covered the more flexible low-level APIs
- The HDF5 high-level APIs can be used to create quick solution for small HDF5 activities

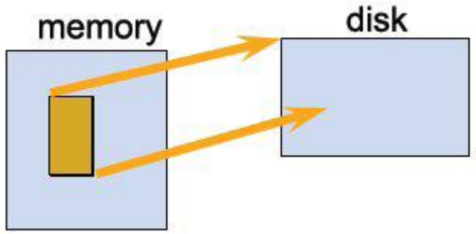
C

```c
herr_t H5LTmake_dataset(hid_t loc_id, const char *dset_name, int rank, const hsize_t *dims, hid_t type_id, const void *buffer)
```

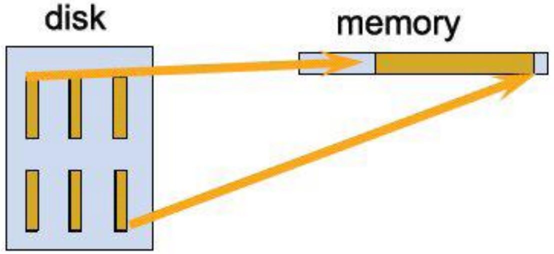
Fortran

```fortran
H5LTMAKE_DATASET_F(loc_id, dset_name, rank, dims, type_id, buf, errcode)
```

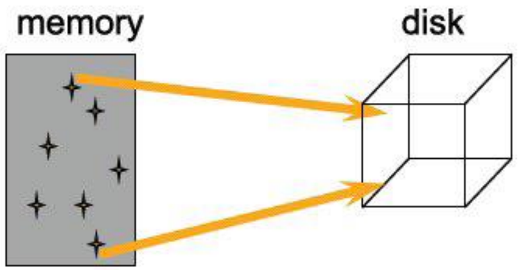
Partial I/O - Hyperslabs



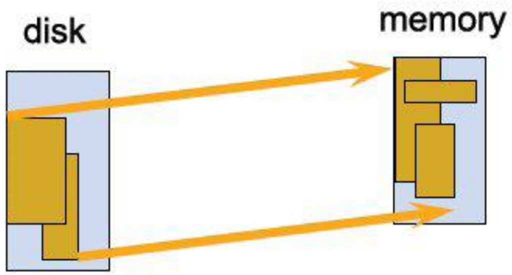
(a) Hyperslab from a 2D array to the corner of a smaller 2D array



(b) Regular series of blocks from a 2D array to a contiguous sequence at a certain offset in a 1D array



(c) A sequence of points from a 2D array to a sequence of points in a 3D array.



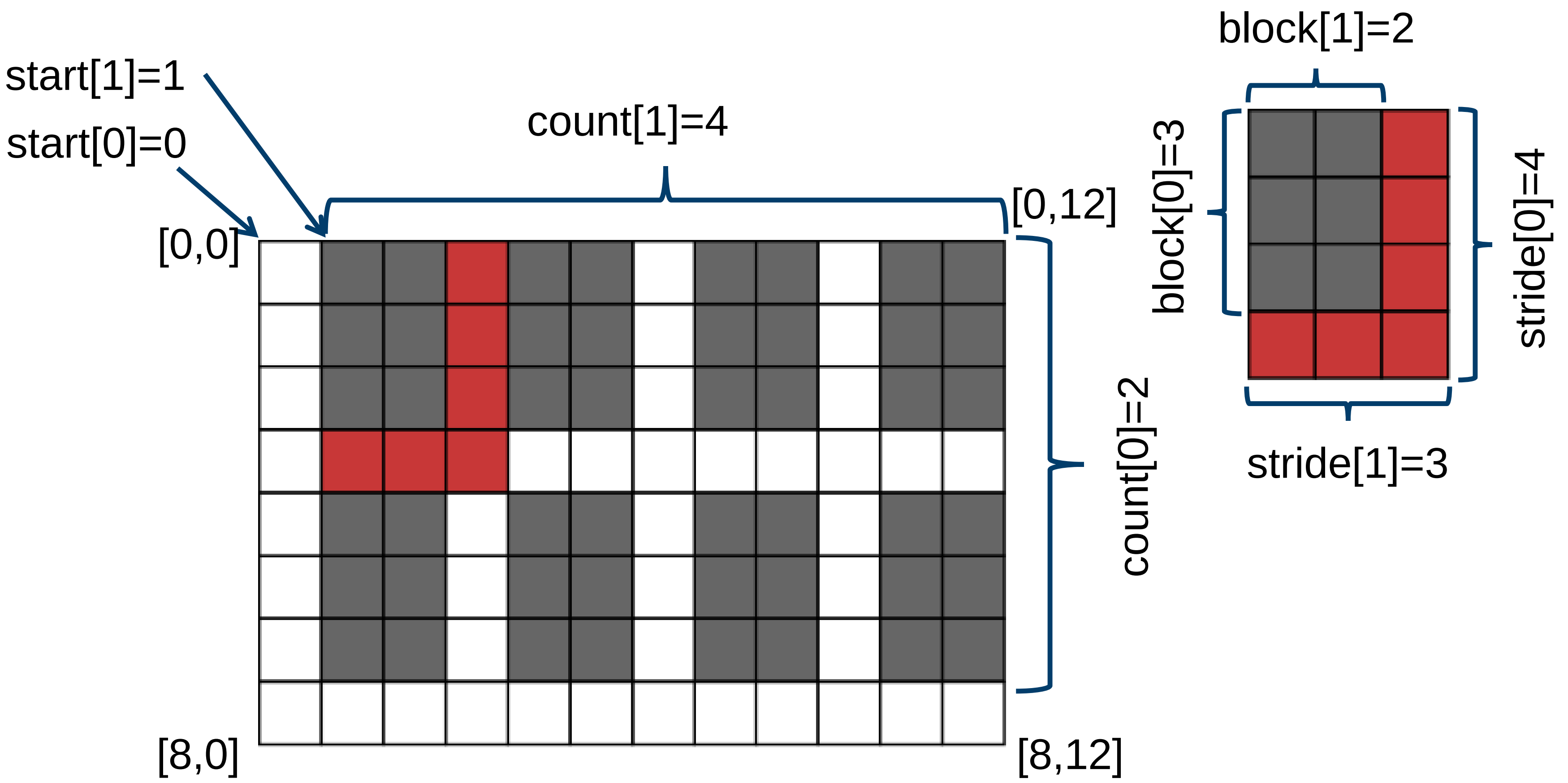
(d) Union of hyperslabs in file to union of hyperslabs in memory.

Partial I/O - Hyperslabs

- Hyperslabs are portions of datasets
  - Contiguous collection of points in a dataspace
  - Regular pattern of points in a dataspace
  - Blocks in a dataspace

- Hyperslabs are described by four parameters:
  - start: (or offset): starting location
  - stride: separation blocks to be selected
  - count: number of blocks to be selected
  - block: size of block to be selected from dataspace
  - **Dimension of these four parameters corresponds to dimension of the underlying dataspace**

Hyperslab example



Creating hyperslabs

C

```
herr_t H5Sselect_hyperslab(hid_t space_id,
             H5S_seloper_t op, const hsize_t *start,
             const hsize_t *stride, const hsize_t
             *count, const hsize_t *block )
```

Fortran

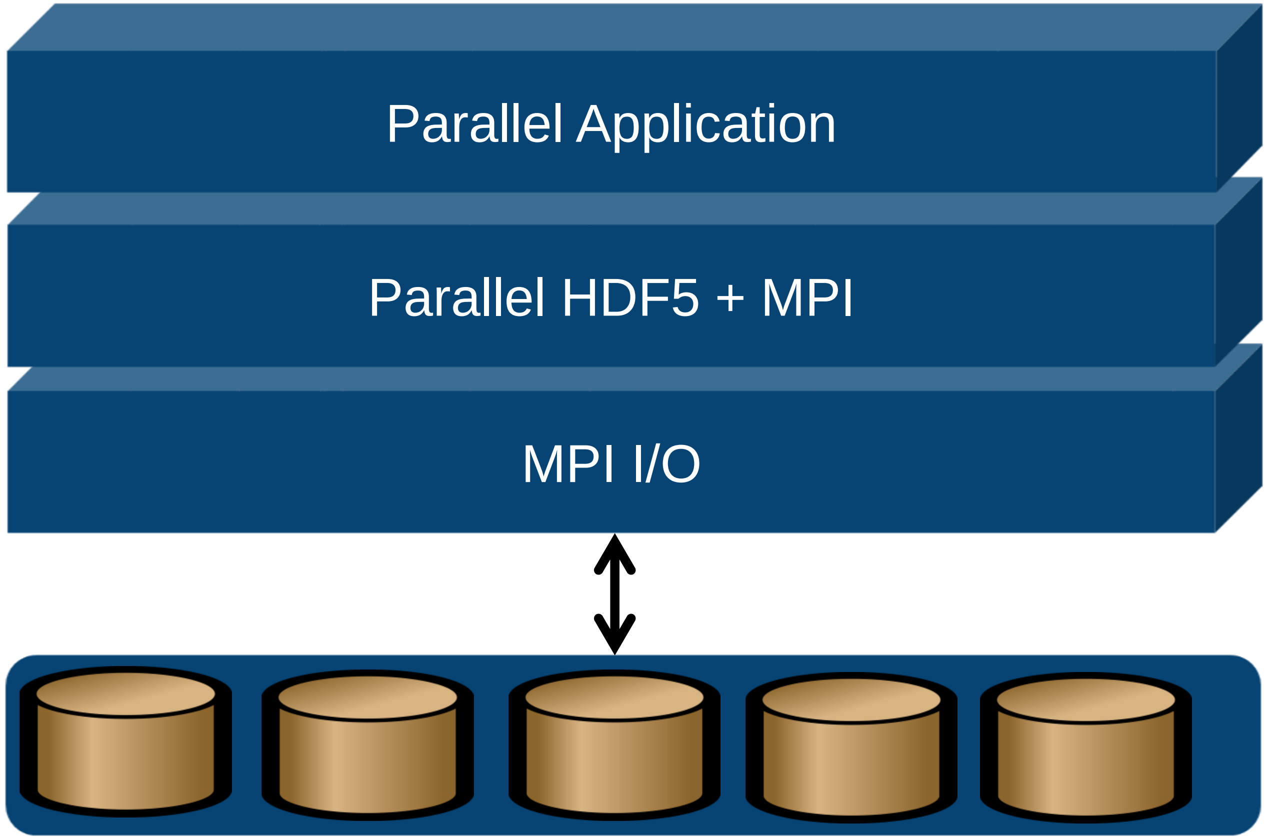
```
H5SSELECT_HYPERSLAB_F(SPACE_ID, OPERATOR, START,
          COUNT, HDFERR, STRIDE, BLOCK)
  INTEGER(HID_T), INTENT(IN) :: SPACE_ID
  INTEGER, INTENT(IN) :: OP
  INTEGER(HSIZE_T), DIMENSION(*), INTENT(IN) ::
    START, COUNT
  INTEGER, INTENT(OUT) :: HDFERR
  INTEGER(HSIZE_T), DIMENSION(*), OPTIONAL,
    INTENT(IN) :: STRIDE, BLOCK
```

Creating hyperslabs

- The following operators (`op`) are supported to combine old and new selections:
- `H5S_SELECT_SET[_F]`: Replaces the existing selection with the parameters from this call. Overlapping blocks are not supported with this operator.
- `H5S_SELECT_OR[_F]`: Adds the new selection to the existing selection.
- `H5S_SELECT_AND[_F]`: Retains only the overlapping portions of the new selection and the existing selection.
- `H5S_SELECT_XOR[_F]`: Retains only the elements that are members of the new selection or the existing selection, excluding elements that are members of both selections.
- `H5S_SELECT_NOTB[_F]`: Retains only elements of the existing selection that are not in the new selection.
- `H5S_SELECT_NOTA[_F]`: Retains only elements of the new selection that are not in the existing selection.

PARALLEL HDF5

Implementation layers



User Application

HDF5 library

Parallel I/O layer

Parallel file systems
(GPFS, Lustre, …)

Important to know

- Most functions of the PHDF5 API are collectives
  - i.e. all processes of the communicator must participate
- PHDF5 opens a parallel file with a communicator
  - Returns a file-handle
  - Future access to the file via the file-handle
  - Different files can be opened via different communicators
- After a file is opened by the processes of a communicator
  - All parts of file are accessible by all processes
  - All objects in the file are accessible by all processes
  - Multiple processes may write to the same data array
  - Each process may write to an individual data array

MPI-IO access template

C

```c
hid_t H5Pcreate(hid_t cls_id);
herr_t H5Pset_fapl_mpio(hid_t fapl_id, MPI_Comm
                        comm, MPI_Info info)
```

Fortran

```fortran
H5PCREATE_F(CLASSTYPE, PRP_ID, HDFERR)
  INTEGER, INTENT(IN) :: CLASSTYPE
  INTEGER(HID_T), INTENT(OUT) :: PRP_ID
  INTEGER, INTENT(OUT) :: HDFERR
H5PSET_FAPL_MPIO_F(PRP_ID, COMM, INFO, HDFERR)
  INTEGER(HID_T), INTENT(IN) :: PRP_ID
  INTEGER, INTENT(IN) :: COMM
  INTEGER, INTENT(IN) :: INFO
  INTEGER, INTENT(OUT) :: HDFERR
```

- `cls_id/classtype` must be `H5P_FILE_ACCESS[_F]`
- Property is used during file creation/access
- Each process of the MPI communicator creates an access template and sets it up with MPI parallel access information

Dataset transfer property

C

```c
hid_t H5Pcreate(hid_t cls_id);
herr_t H5Pset_dxpl_mpio(hid_t dxpl_id,
                        H5FD_mpio_xfer_t xfer_mode )
```

Fortran

```fortran
H5PCREATE_F(CLASSTYPE, PRP_ID, HDFERR)
  INTEGER, INTENT(IN) :: CLASSTYPE
  INTEGER(HID_T), INTENT(OUT) :: PRP_ID
  INTEGER, INTENT(OUT) :: HDFERR
H5PSET_DXPL_MPIO_F(PRP_ID, DATA_XFER_MODE, HDFERR)
  INTEGER(HID_T), INTENT(IN) :: PRP_ID
  INTEGER, INTENT(IN) :: DATA_XFER_MODE
  INTEGER, INTENT(OUT) :: HDFERR
```

- `cls_id/classtype` must be `H5P_DATASET_XFER[_F]`
- `xfer_modes:`
  - `H5FD_MPIO_INDEPENDENT[_F]`: Use independent I/O access (default)
  - `H5FD_MPIO_COLLECTIVE[_F]`: Use collective I/O access

Exercise

Exercise 4 – parallel HDF5

- Extend your serial program to a parallel program
- Fill your two dimensional array with the rank number
- Create a combined dataset of all processes involved
- Logical view:

```
0 0 0 0 0 0 0 0 …
0 0 0 0 0 0 0 0 …
…
1 1 1 1 1 1 1 1 …
1 1 1 1 1 1 1 1 …
…
```

#cores x 5

- Write the data collectively into the file
- Check the resulting file using: `h5dump`

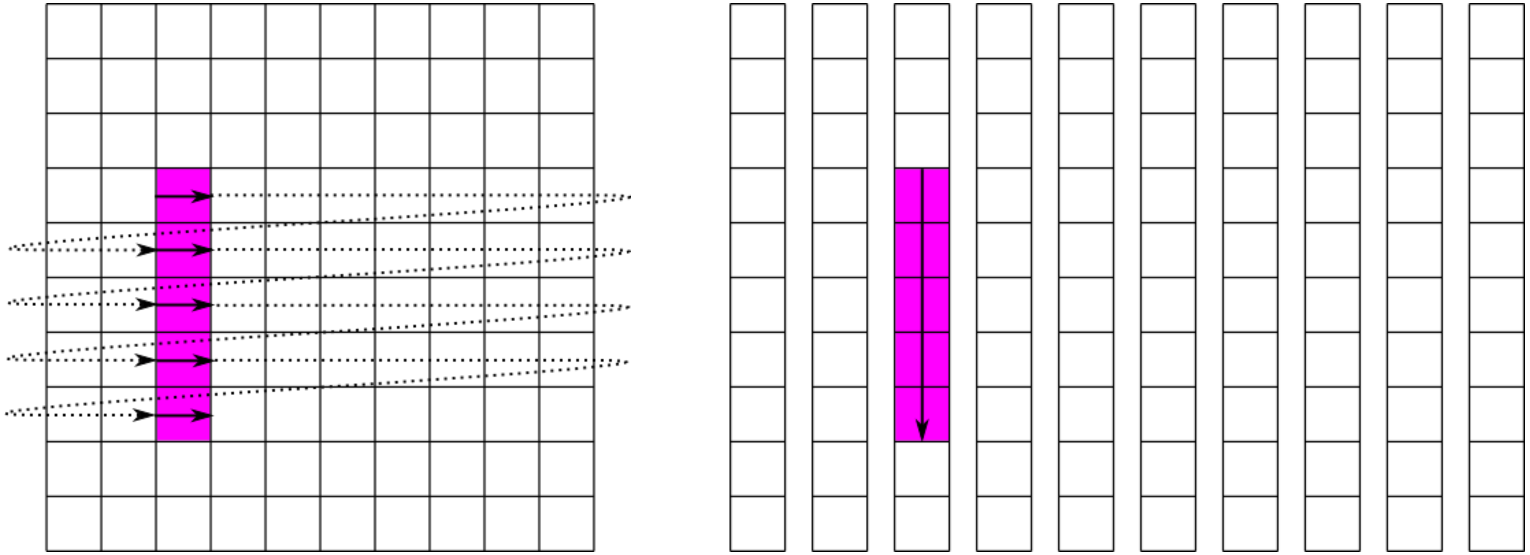
- To start a job on the compute node:

```
srun -N 1 --ntasks-per-node=48 --reservation=pario-2022-02-23
--account=training2202 --time=00:02:00 ./a.out
```

Performance hints

Chunking

- Contiguous datasets are stored in a single block in the file, chunked datasets are split into multiple chunks which are all stored separately in the file.
- Additional chunk cache is possible



C

```c
dcpl_id = H5Pcreate(H5P_DATASET_CREATE);
H5Pset_chunk(dcpl_id, 2, chunk_dims);
```

https://www.hdfgroup.org/HDF5/doc/Advanced/Chunking/

Benchmarking

h5perf

- Simple HDF5 I/O-benchmark application
- 1D or 2D dataset
- Part of the standard HDF5 installation
- Contiguous or interleaved access pattern
- Independent and collective I/O
- Chunking
- Example Options (`h5perf -h`):
  - 1D / 2D (`-g`)
  - Bytes per Process (`-e`)
  - Block size (`-B`)
  - Transfer size (`-x / -X`)
  - Number of datasets (`-d`)

Benchmarking

Example (1D):

- `num-processes = 3`
- `bytes-per-process = 8`
- `block-size = 2`
- `transfer-buffer-size = 4`
- `contiguous`

0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2

1 write operation per transfer

- `interleaved`

0	0	1	1	2	2	0	0	1	1	2	2	0	0	1	1	2	2	0	0	1	1	2	2

2 write operations per transfer

https://www.hdfgroup.org/HDF5/doc/Tools/h5perf_parallel/h5perf_parallel.pdf

Benchmarking

Example (2D):

- `num-processes = 2`
- `bytes-per-process = 4`
- `block-size = 2`
- `transfer-buffer-size = 8`

`contiguous`

0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1

1 write operation per transfer

`interleaved`

0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1
0	0	1	1	0	0	1	1

8 write operations per transfer

https://www.hdfgroup.org/HDF5/doc/Tools/h5perf_parallel/h5perf_parallel.pdf

Exercise

Exercise 5 – Mandelbrot set

- Run the example or implement your own solution for the static decomposition (`type = 1`) of the Mandelbrot example (`mandelhdf5.c` or `mandelhdf5.f90`)
- To implement your own solution copy the `workshop/mandelhdf5.c` or `workshop/mandelhdf5.f90` template file into the main directory
- Time left? Try to run a `h5perf` benchmark (use `h5perf -h` to see all available options)

Hints

Options for running the program:

`-t 1` (static decomposition)

`-f 1` (use HDF5)