



PARALLEL I/O AND PORTABLE DATA FORMATS

HDF5

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What is HDF5?

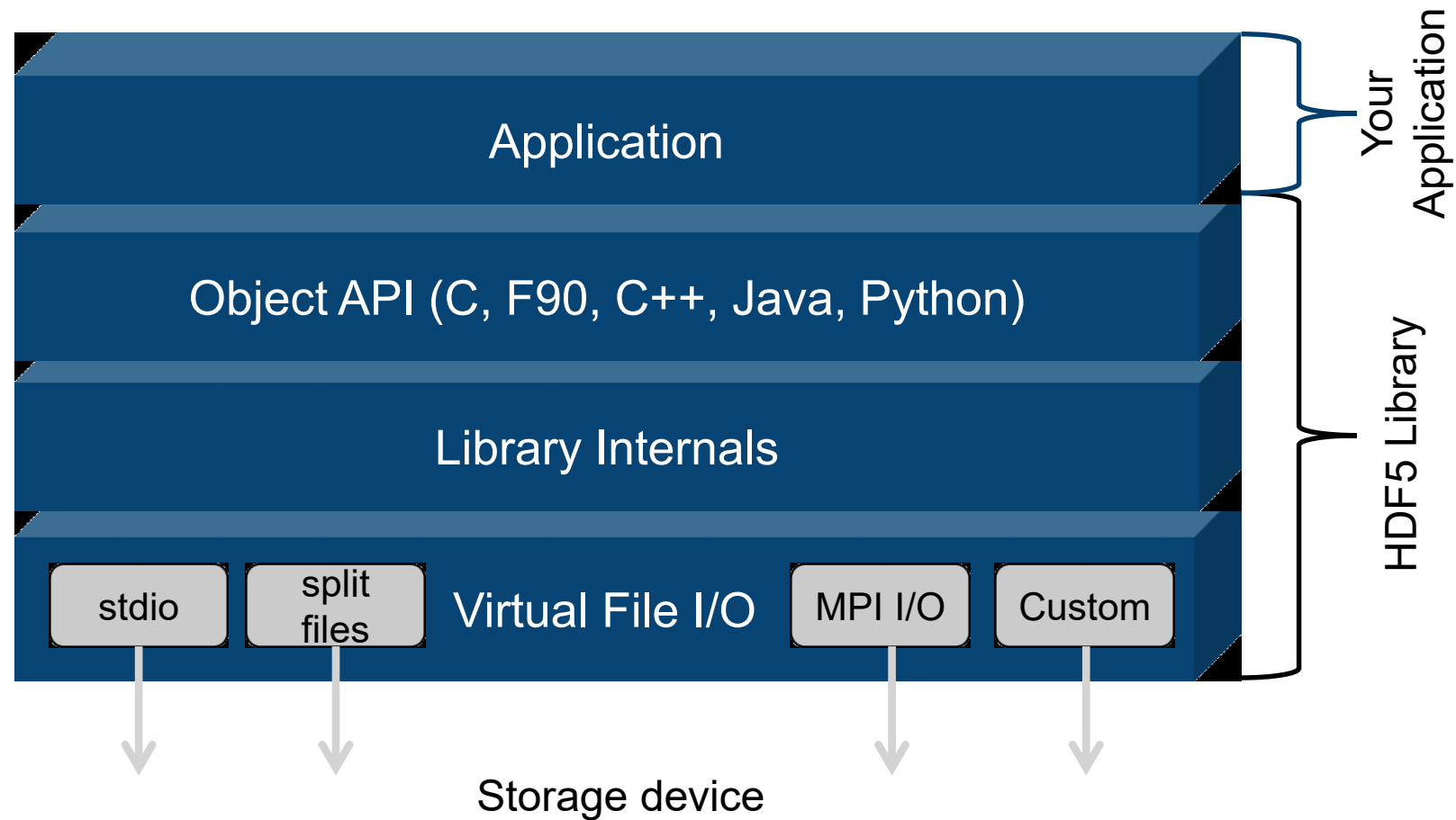
Hierarchical Data Format

- API, data model and file format for I/O management
- Tools suite for accessing data in HDF5 format

HDF5 - Features

- 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

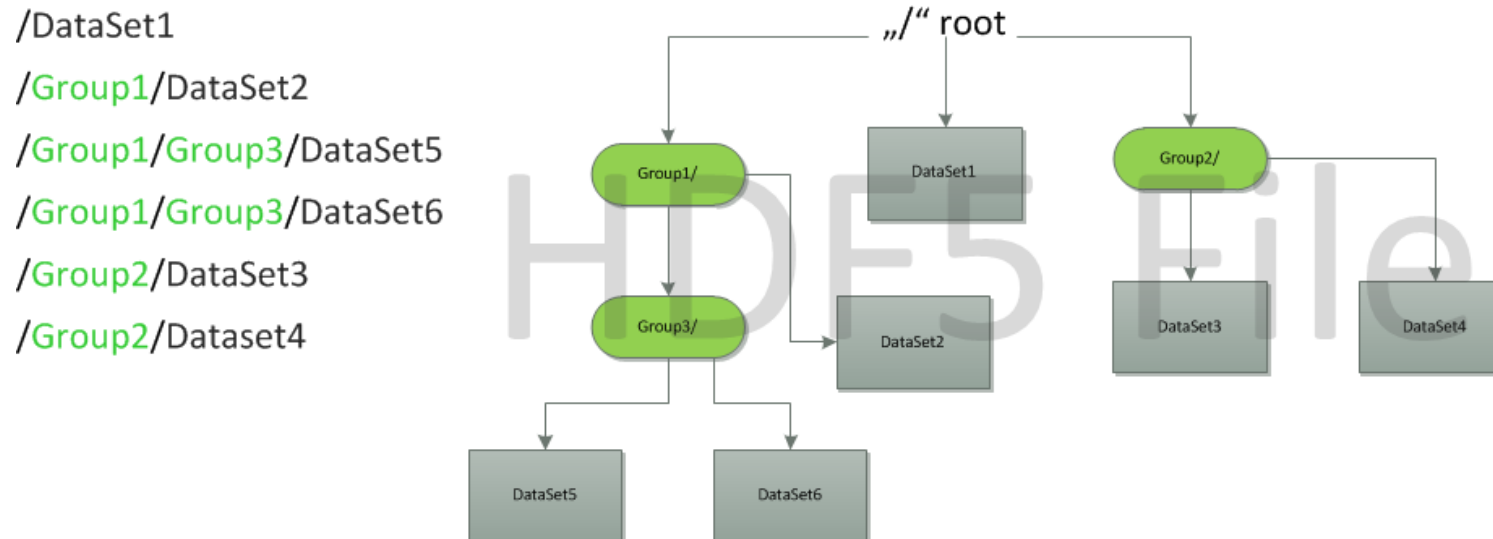
Layers of the HDF5 Library



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



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

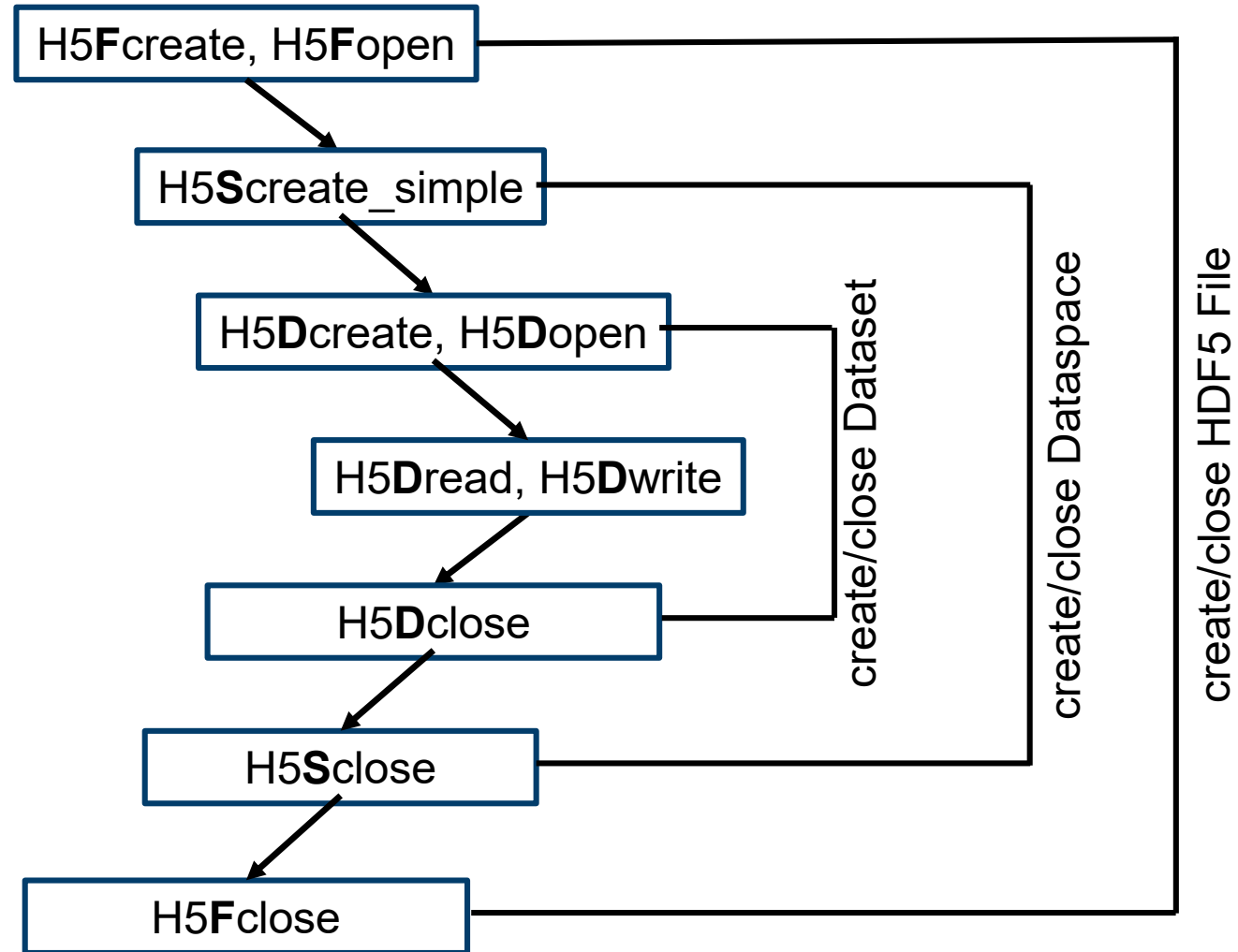
```
H5OPEN_F (STATUS)  
  INTEGER, INTENT (OUT) :: STATUS  
  
H5CLOSE_F (STATUS)  
  INTEGER, INTENT (OUT) :: STATUS
```

- `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

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

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/training2000/hdf5/copy.sh`
 - `cd /p/project/training2000/<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 HDF5/1.10.5 # 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 hid_t H5Screate(H5S_class_t type)
```

```
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

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

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);
```

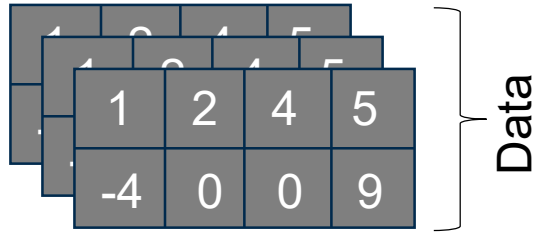
alternative:

```
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

Attributes

- Time = 2.1
- Temp = 122

Storage

- Contiguous

Datatype

- Integer

Creating a Dataset

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

```
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

```
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

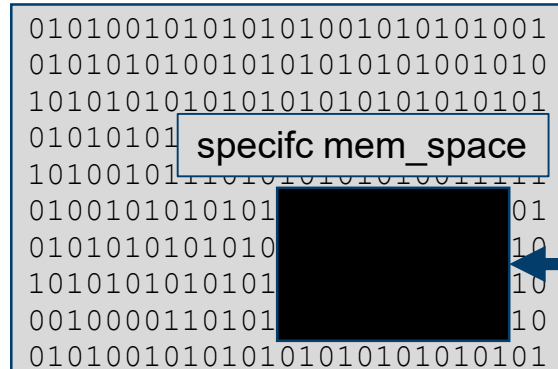
```
H5DWRITE_F(DSET_ID, MEM_TYPE_ID, BUF, DIMS, HDFERR,  
            MEM_SPACE_ID, FILE_SPACE_ID, XFER_PRP)  
INTEGER(HID_T), INTENT(IN) :: DSET_ID, MEM_TYPE_ID  
TYPE, INTENT(IN) :: BUF  
DIMENSION(*), INTEGER(HSIZE_T), INTENT(IN) :: DIMS  
INTEGER, INTENT(OUT) :: HDFERR  
INTEGER(HID_T), OPTIONAL,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

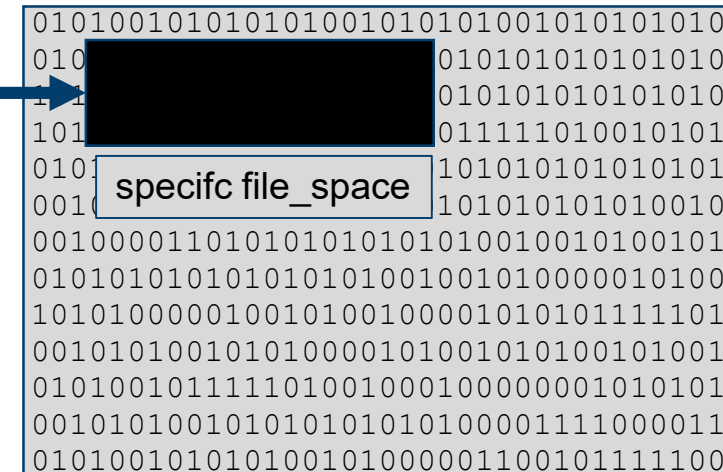
Writing to a dataset

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

Global memory space (ALL selection)



Global default filesystem (given during dataset creation, ALL selection)



Open a existing dataset

C

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

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 hid_t H5Dget_space(hid_t dataset_id)
```

```
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

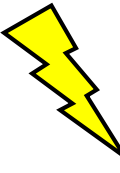
Excursion: row-major / column-major order

- “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

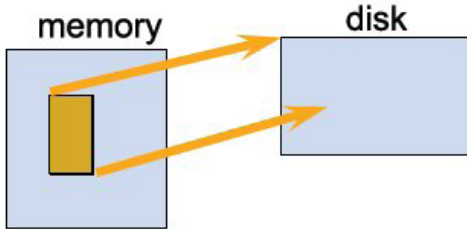
- Storing data in a 3x2 dimensional HDF5 dataset:

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

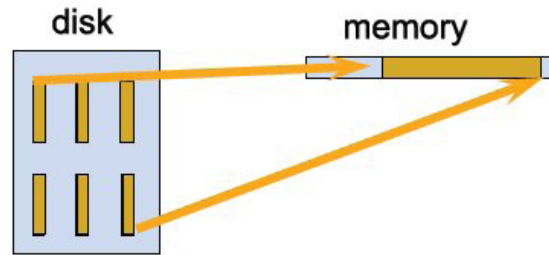
- Storing data in a 2x3 dimensional dataset:

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

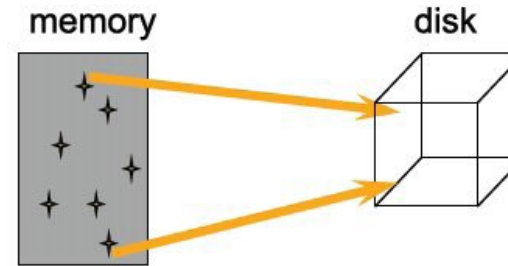
Partial I/O - Hyperslabs



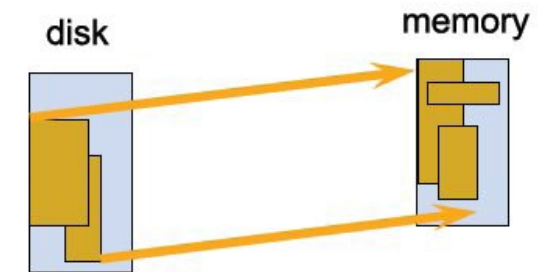
(a) Hyperslab from a 2D array to the corner of a smaller 2D array



(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.

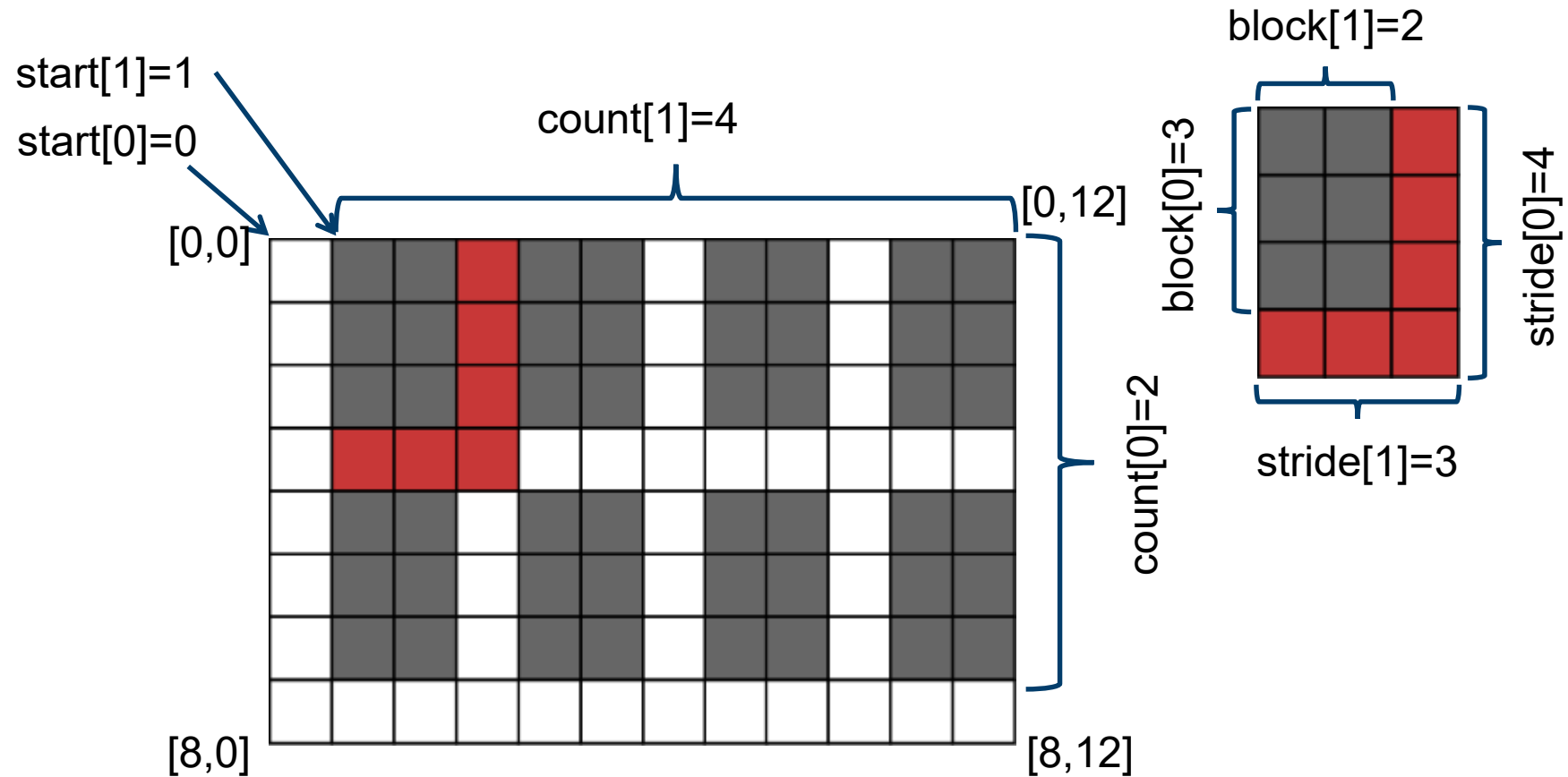


(d) Union of hyperslabs in file to union of hyperslabs in memory.

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

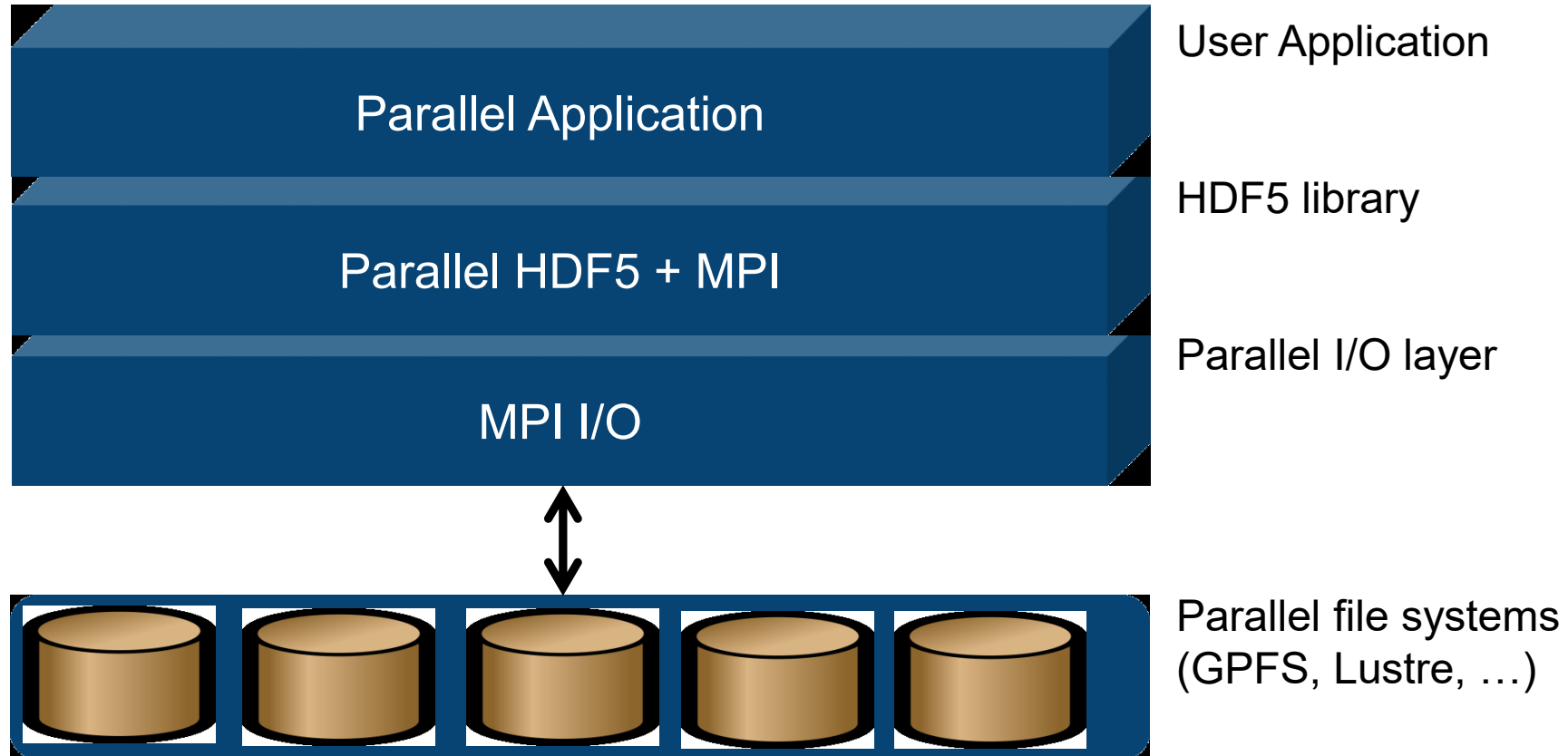
```
H5SSELECT_HYPERSLAB_F(SPACE_ID, OPERATOR, START,  
                        COUNT, HDFERR, STRIDE, BLOCK)  
INTEGER(HID_T), INTENT(IN) :: SPACE_ID  
INTEGER, INTENT(IN) :: OP  
INTEGER(HSIZE_T), DIMENSION(*), INTENT(IN) ::  
    START, COUNT  
INTEGER, INTENT(OUT) :: HDFERR  
INTEGER(HSIZE_T), DIMENSION(*),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



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

```
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

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

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 ...  
...
```

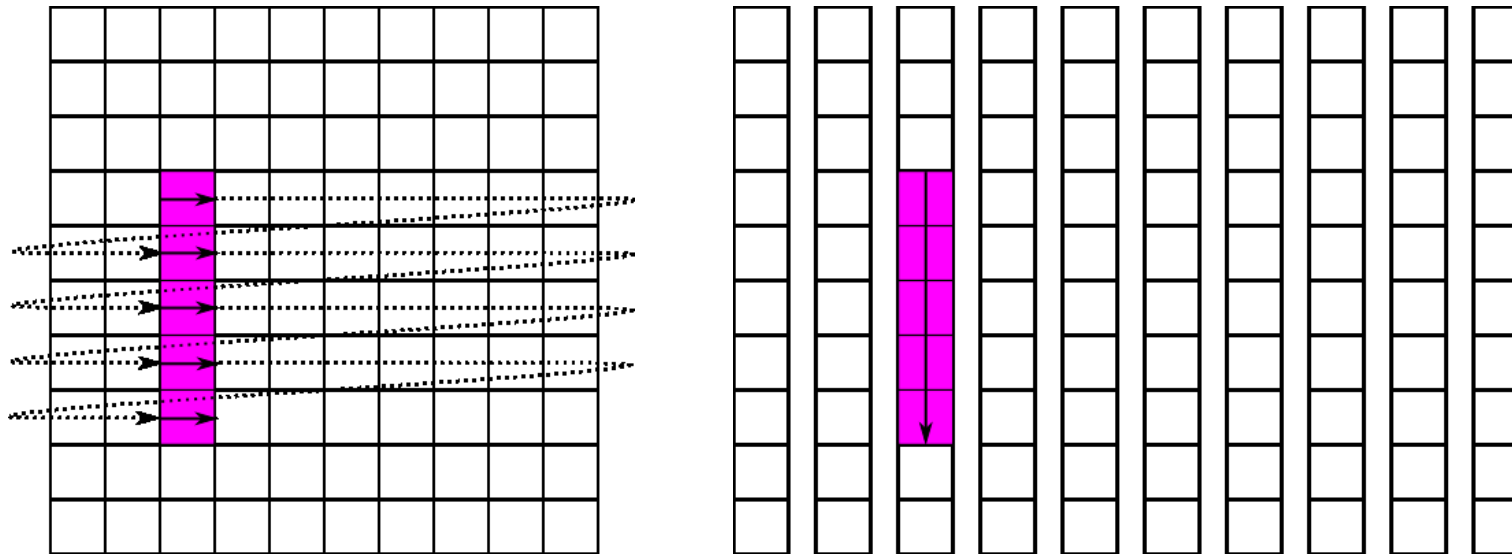
} #cores x 5

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

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



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

Performance hints

Compression

- In-transit compression can help to lower the overall datasize:
- HDF5 allows compression within a parallel, collective write commands for chunked datasets
- NetCDF4 only allows compression within serial programs (so far)
- Gzip (`deflate`) compression available by default (szip can be added on demand)
- Other compression techniques are available by using filters and external plugins:
<https://support.hdfgroup.org/services/filters.html>
- ZFP compression example:

```
H5Pset_zfp_reversible_cdata(cd_nelmts, cd_values);  
nc_def_var_filter(nc_file_id, nc_variable, H5Z_FILTER_ZFP,  
                  cd_nelmts, cd_values);
```

Benchmarking

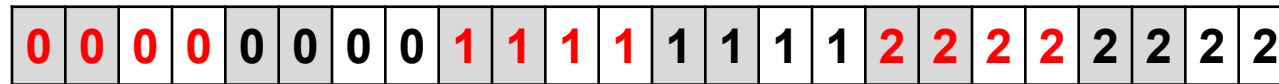
h5perf

- 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`



1 write operation per transfer

- `interleaved`



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`

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

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

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)