Introduction to serial HDF5

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Parallel filesystems and parallel IO libraries PATC@MdS

Training outline

Day 1:

- AM: Serial HDF5 (M. Haefele)
- PM: Parallel IO and parallel HDF5 (M. Haefele)

Day 2:

- AM 1: Luster file system @ TGCC (T. Leibovici)
- AM 2 + PM: XIOS (M-H. Nguyen)

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`https://events.prace-ri.eu/event/569/evaluation/evaluate`

Outline Day 1

Morning:

- HDF5 in the context of Input/Output (IO)
- HDF5 Application Programming Interface (API)
- Playing with Dataspace
- Hands on session

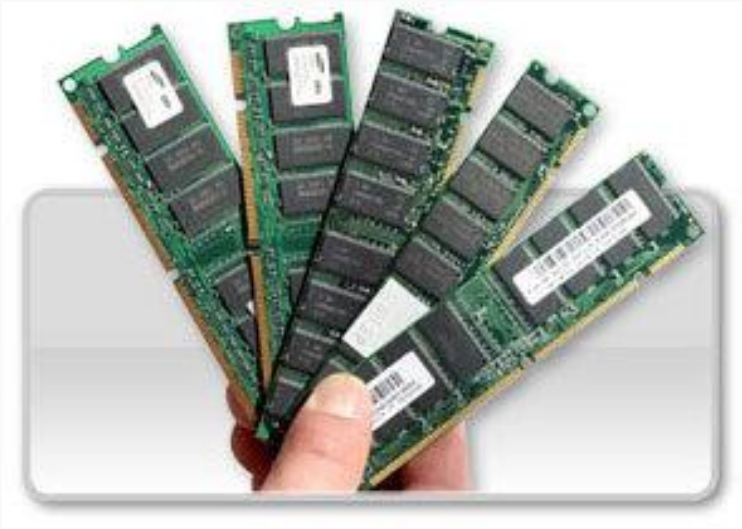
Afternoon:

- Parallel IO issues & concepts
- Basic concepts of MPI-IO
- Parallel HDF5
- Hands on session

IO in a nustshell

Doing Input / Output is about **TRANSPORTING**

Data stored in **memory** to / from Data stored on **disk**

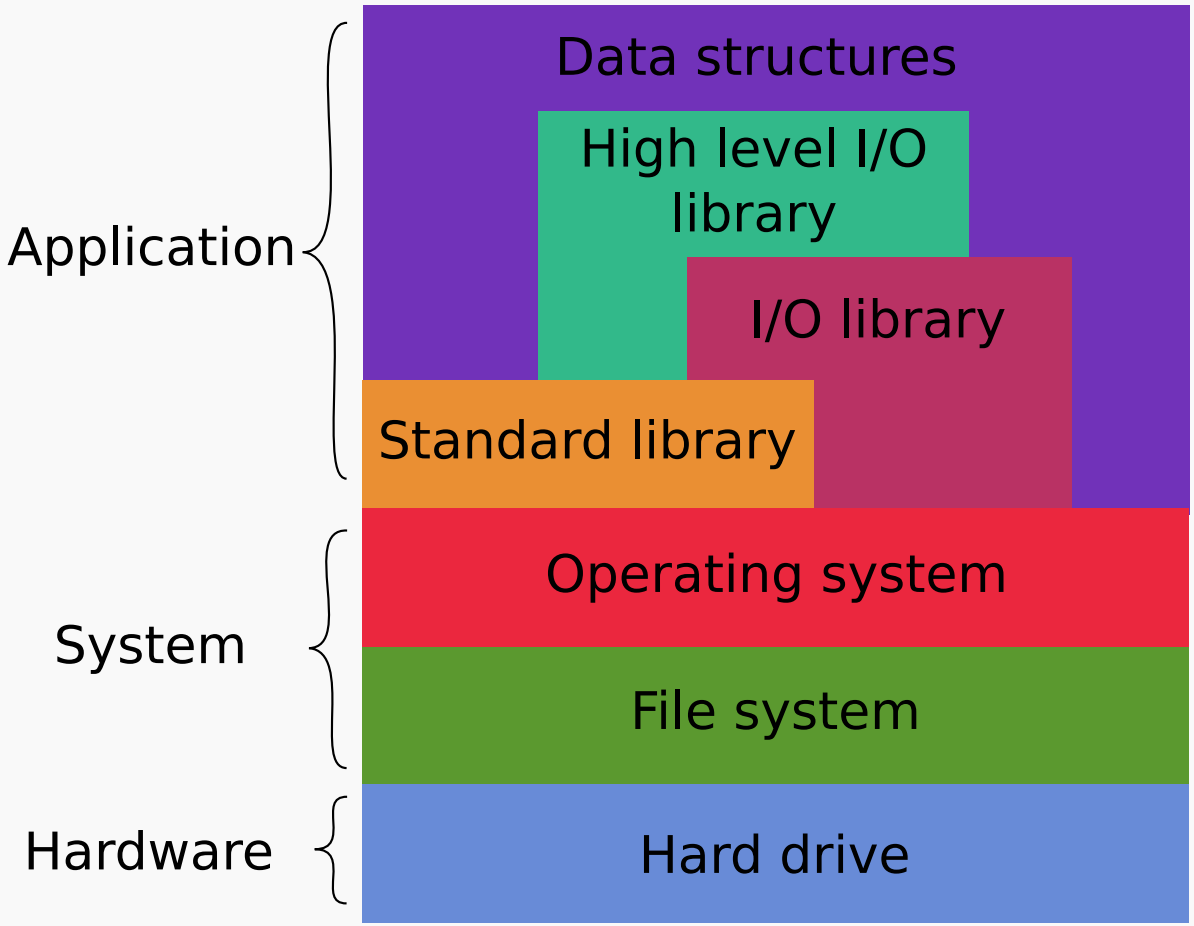


IO in a nustshell

Three criteria / metrics to balance

- Code development / maintenance time
- Performance
- Post-processing requirement

Hardware/Software stack



High level I/O libraries

The purpose of high level I/O libraries is to provide the developer a higher level of abstraction to manipulate computational modeling objects

- Meshes of various complexity (rectilinear, curvilinear, unstructured. . .)
- Discretized functions on such meshes
- Materials
- . . .

Until now, these libraries are mainly used in the context of visualization

Existing libraries

- Silo
  - Wide range of objects
  - Built on top of HDF5
  - “Native” format for VisIt
- Exodus
  - Focused on unstructured meshes and finite element representations
  - Built on top of NetCDF
- Famous/intensively used codes’ output format
- eXtensible Data Model and Format (XDMF)
- **XIOS (XML IO Server)**

I/O libraries

Purpose of I/O libraries:

- Efficient I/O
- Portable binary files
- Higher level of abstraction for the developer

Two main existing libraries:

- Hierarchical Data Format: HDF5
- Network Common Data Form: NetCDF

HDF5 library

HDF5 file:

- HDF5 group: a grouping structure containing instances of zero or more groups or datasets
- HDF5 dataset: a multidimensional array of data elements

HDF5 dataset $\Leftrightarrow$ multidimensional array:

- Name
- Datatype (Atomic, NATIVE, Compound)
- Dataspace (rank, sizes, max sizes)
- Storage layout (contiguous, compact, chunked)

HDF5 High Level APIs

- **Dimension Scale** (H5DS): Enables to attach dataset dimension to scales
- **Lite** (H5LT): Enables to write simple dataset in one call
- **Image** (H5IM): Enables to write images in one call
- **Table** (H5TB): Hides the compound types needed for writing tables
- **Packet Table** (H5PT): Almost H5TB but without record insertion/deletion but supports variable length records
- ...

HDF5 low level API

- **H5F**: File manipulation routines
- **H5G**: Group manipulation routines
- **H5S**: Dataspace manipulation routines
- **H5D**: Dataset manipulation routines
- . . .

Just have a look at the outstanding on-line reference manual for HDF5 !

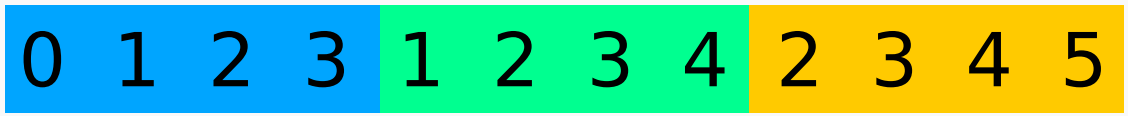
C order versus Fortran order

```c
/* C language */
#define NX 4
#define NY 3
int x,y;
int f[NY][NX];

for (y=0;y<NY;y++)
  for (x=0;x<NX;x++)
    f[y][x] = x+y;
```

```
! Fortran language
integer, parameter :: NX=4
integer, parameter :: NY=3
integer                    :: x,y
integer, dimension(NX,NY) :: f

do y=1,NY
  do x=1,NX
    f(x,y) = (x-1) + (y-1)
  enddo
enddo
```



The memory mapping is identical, the language semantic is different !!

HDF5 first example

```
#define NX      5
#define NY      6
#define RANK    2

int main (void)
{
    hid_t       file, dataset, dataspace;
    hsize_t     dimsf[2];
    herr_t      status;
    int         data[NY][NX];

    init(data);
    file = H5Fcreate("example.h5", H5F_ACC_TRUNC, H5P_DEFAULT,\
                     H5P_DEFAULT);
    dimsf[0] = NY;
    dimsf[1] = NX;
```

HDF5 first example cont.

```
    dataspace = H5Screate_simple(RANK, dimsf, NULL);

    dataset = H5Dcreate(file, "IntArray", H5T_NATIVE_INT, \
        dataspace, H5P_DEFAULT, H5P_DEFAULT, H5P_DEFAULT);

    status = H5Dwrite(dataset, H5T_NATIVE_INT, H5S_ALL, \
                      H5S_ALL,H5P_DEFAULT, data);

    H5Sclose(dataspace);
    H5Dclose(dataset);
    H5Fclose(file);

    return 0;
}
```

HDF5 high level example cont.

```
    status = H5LTmake_dataset_int(file, "IntArray", RANK, dimsf, data);

    H5Fclose(file);

    return 0;
}
```

Variable C type

```
hid_t    file, dataset, dataspace;
hsize_t dimsf[2];
herr_t   status;
```

- hid_t: handler for any HDF5 objects (file, groups, dataset, dataspace, datatypes...)
- hsize_t: C type used for number of elements of a dataset (in each dimension)
- herr_t: C type used for getting error status of HDF5 functions

File creation

```
file = H5Fcreate("example.h5", H5F_ACC_TRUNC, H5P_DEFAULT,\
                 H5P_DEFAULT);
```

- "example.h5": file name
- H5F_ACC_TRUNC: File creation and suppress it if it exists already
- H5P_DEFAULT: file creation property list
- H5P_DEFAULT: file access property list (needed for MPI-IO)

Dataspace creation

```
dimsf[0] = NY;
dimsf[1] = NX;
dataspace = H5Screate_simple(RANK, dimsf, NULL);
```

- RANK: dataset dimensionality
- dimsf: size of the dataspace in each dimension
- NULL: specify max size of the dataset being fixed to the size

Dataset creation

```
dataset = H5Dcreate(file, "IntArray", H5T_NATIVE_INT, \
    dataspace, H5P_DEFAULT, H5P_DEFAULT, H5P_DEFAULT);
```

- file: HDF5 objects where to create the dataset. Should be a file or a group.
- "IntArray": dataset name
- H5T_NATIVE_INT: type of the data the dataset will contain
- dataspace: size of the dataset
- H5P_DEFAULT: default option for property list.

Datatype

- Predefined Datatypes: created by HDF5.
- Derived Datatypes: created or derived from the predefined data types.

There are two types of predefined datatypes:

- **STANDARD**: They defined standard ways of representing data. Ex: H5T_IEEE_F32BE means IEEE representation of 32 bit floating point number in big endian.
- **NATIVE**: Alias to standard data types according to the platform where the program is compiled. Ex: on an Intel based PC, H5T_NATIVE_INT is aliased to the standard predefined type, H5T_STD_32LE.

Datatype cont.

A data type can be:

- ATOMIC: cannot be decomposed into smaller data type units at the API level. Ex: integer
- COMPOSITE: An aggregation of one or more data types. Ex: compound data type, array, enumeration

Dataset writing

```
status = H5Dwrite(dataset, H5T_NATIVE_INT, H5S_ALL, \
                  H5S_ALL,H5P_DEFAULT, data);
```

- dataset: HDF5 objects representing the dataset to write
- H5T_NATIVE_INT: Type of the data in memory
- H5S_ALL: dataspace specifying the portion of memory that needs be read (in order to be written)
- H5S_ALL: dataspace specifying the portion of the file dataset that needs to be written
- H5P_DEFAULT: default option for property list (needed for MPI-IO).
- data: buffer containing the data to write

Closing HDF5 objects

```
H5Sclose(dataspace);
H5Dclose(dataset);
H5Fclose(file);
```

Opened/created HDF5 objects are closed.

Some comments

```
    status = H5LTmake_dataset_int(file, "IntArray", RANK, dimsf, data);

    H5Fclose(file);

    return 0;
}
```

This example is almost a **fwrite**, but:

- The generated file is portable
- The generated file can be accessed with HDF5 tools
- Attributes can be added on datasets or groups
- The type of the data can be fixed
- The storage layout can be modified
- Portion of the dataset can be written
- ...

Concept of start, stride, count block

Considering a *n*-dimensional array, start, stride, count and block are arrays of size *n* that describe a subset of the original array

- **start**: Starting location for the hyperslab (default 0)
- **stride**: The number of elements to separate each element or block to be selected (default 1)
- **count**: The number of elements or blocks to select along each dimension
- **block**: The size of the block (default 1)

Conventions for the examples

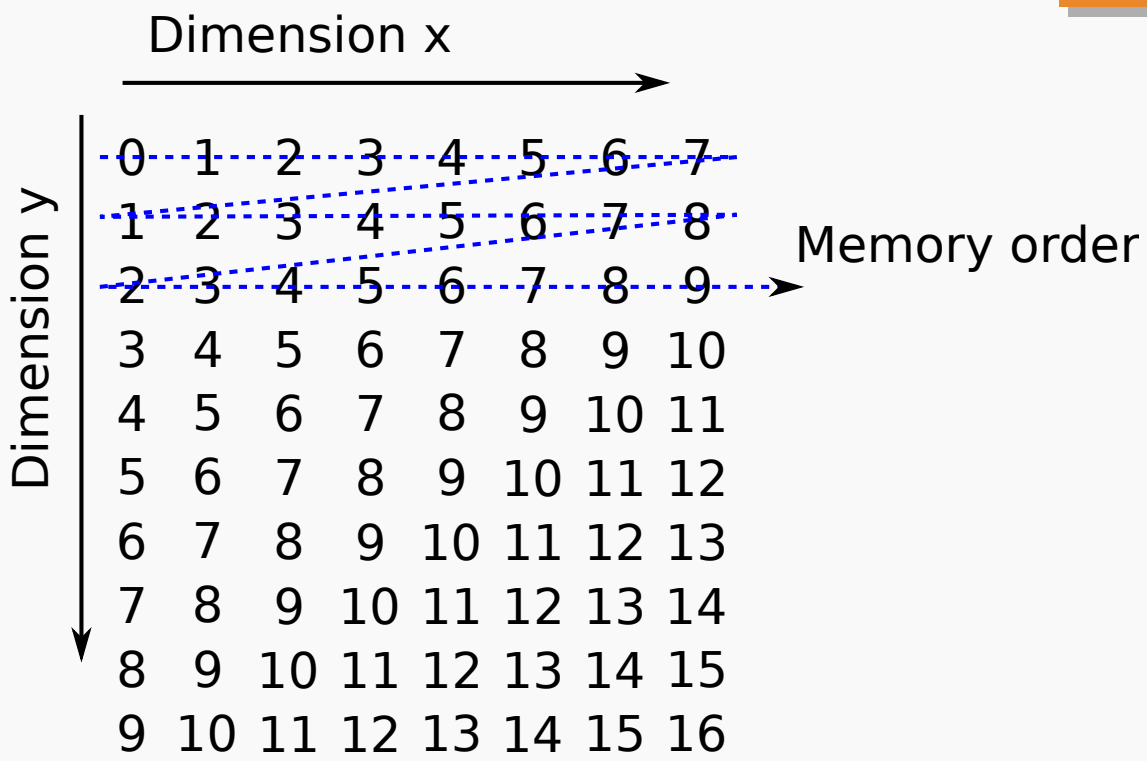
We consider:

- A 2D array $f[N_y][N_x]$ with $N_x = 8, N_y = 10$
- Dimension x is the dimension contiguous in memory
- Graphically, the x dimension is represented horizontal
- Language C convention is used for indexing the dimensions

$\Rightarrow$ Dimension y is index=0

$\Rightarrow$ Dimension x is index=1

Graphical representation



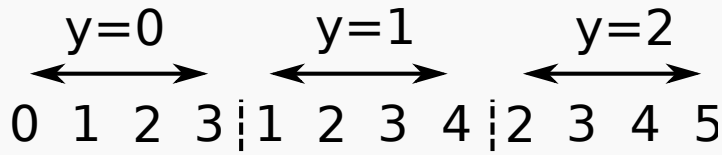

```
int start[2], stride[2], count[2], block[2];
 start[0] = 0;  start[1] = 0;
stride[0] = 1; stride[1] = 1;
 block[0] = 1;  block[1] = 1;
```

Illustration for count parameter

Dimension x

Dimension y

0	1	2	3	4	5	6	7
1	2	3	4	5	6	7	8
2	3	4	5	6	7	8	9
3	4	5	6	7	8	9	10
4	5	6	7	8	9	10	11
5	6	7	8	9	10	11	12
6	7	8	9	10	11	12	13
7	8	9	10	11	12	13	14
8	9	10	11	12	13	14	15
9	10	11	12	13	14	15	16




```
count[0] = 3;   count[1] = 4;
```

Illustration for start parameter

Dimension x

Dimension y

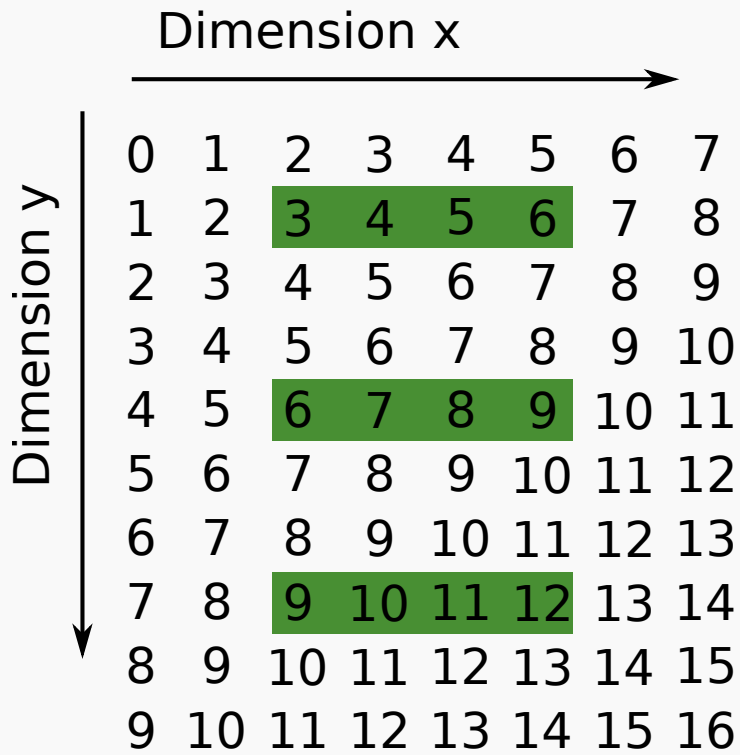
0	1	2	3	4	5	6	7
1	2	3	4	5	6	7	8
2	3	4	5	6	7	8	9
3	4	5	6	7	8	9	10
4	5	6	7	8	9	10	11
5	6	7	8	9	10	11	12
6	7	8	9	10	11	12	13
7	8	9	10	11	12	13	14
8	9	10	11	12	13	14	15
9	10	11	12	13	14	15	16

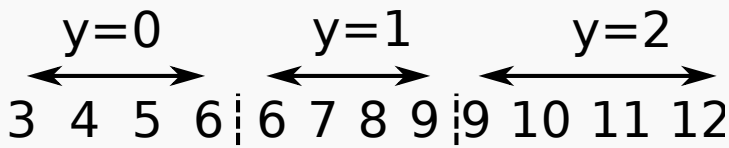
y=0 y=1 y=2

3 4 5 6 | 4 5 6 7 | 5 6 7 8

```
start[0] = 1;   start[1] = 2;
count[0] = 3;   count[1] = 4;
```

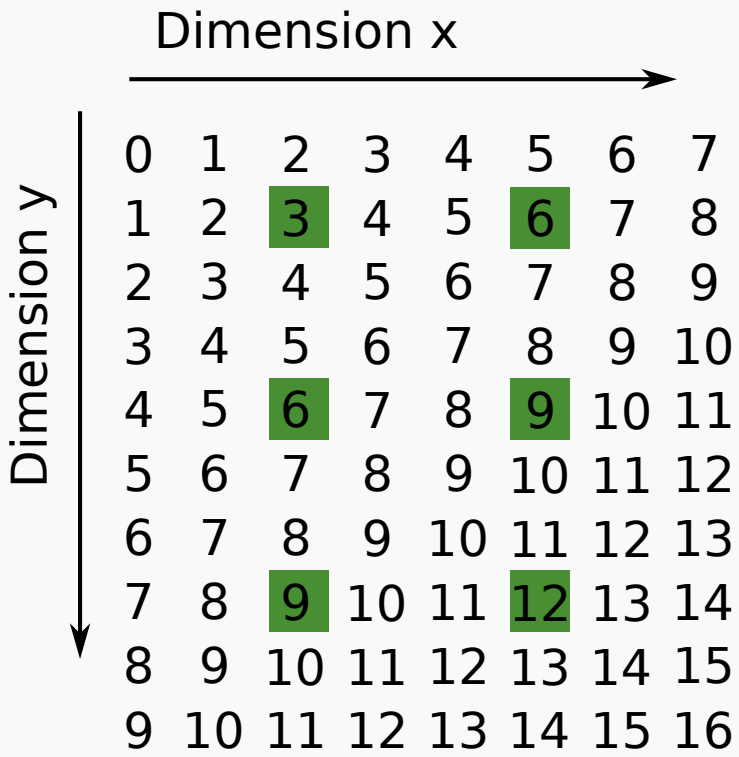
Illustration for stride parameter

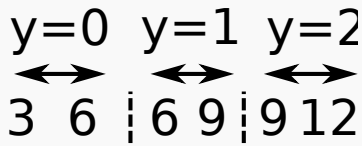





```
start[0] = 1;   start[1] = 2;
count[0] = 3;   count[1] = 4;
stride[0] = 3;  stride[1] = 1;
```

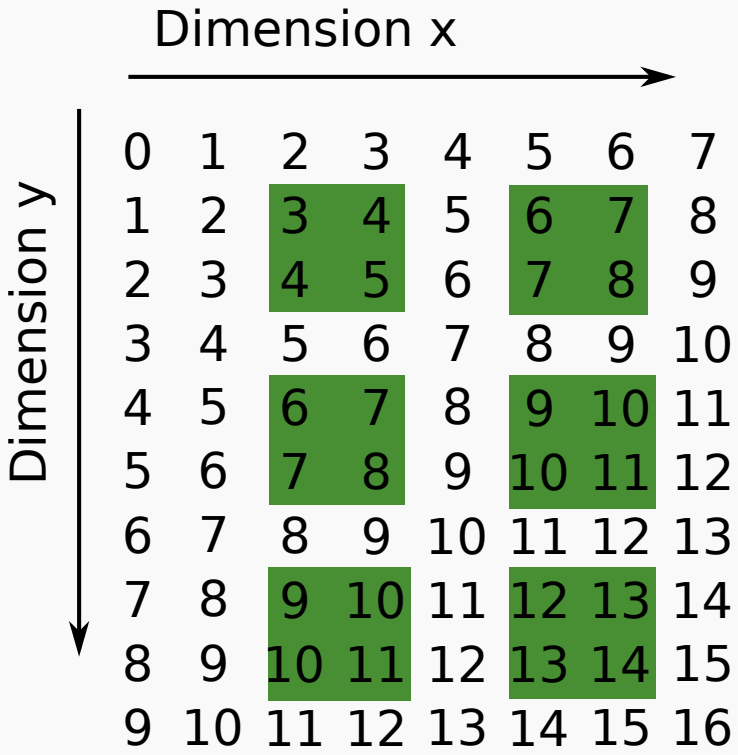
Illustration for stride parameter

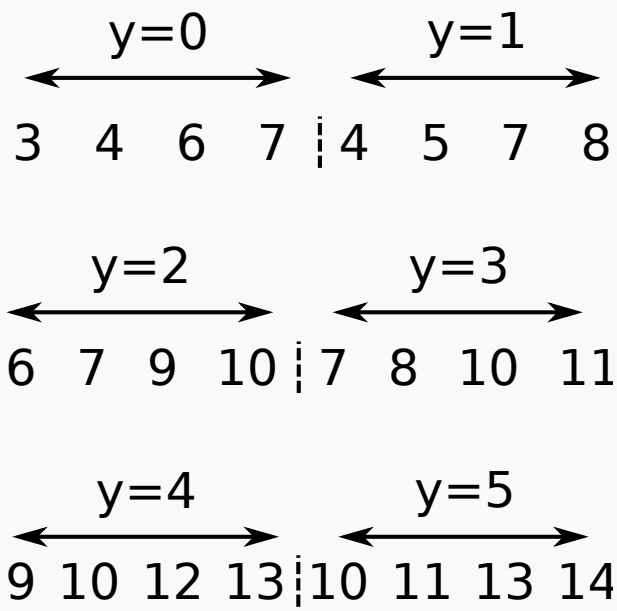





```
start[0] = 1;   start[1] = 2;
count[0] = 3;   count[1] = 2;
stride[0] = 3;  stride[1] = 3;
```

Illustration for block parameter

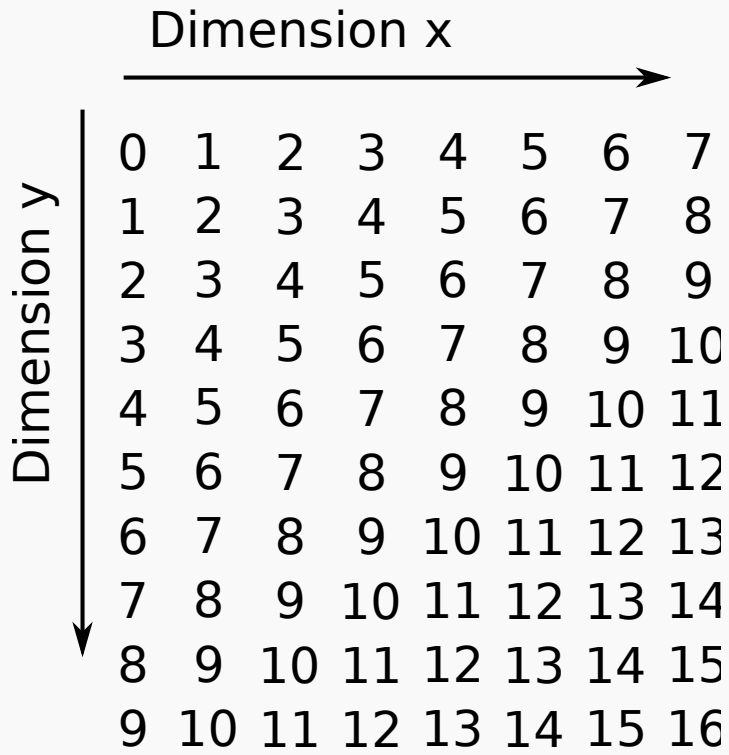





```
start[0] = 1;   start[1] = 2;
count[0] = 3;   count[1] = 2;
stride[0] = 3;  stride[1] = 3;
block[0] = 2;   block[1] = 2;
```

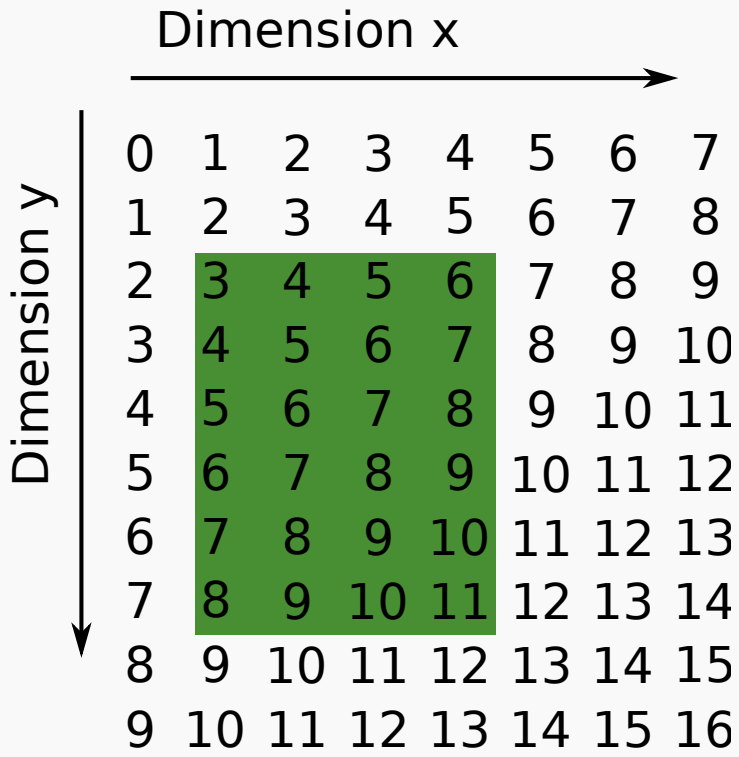
Exercise 1

Please draw the elements selected by the start, stride, count, block set below




```
start[0] = 2;   start[1] = 1;
count[0] = 6;   count[1] = 4;
```

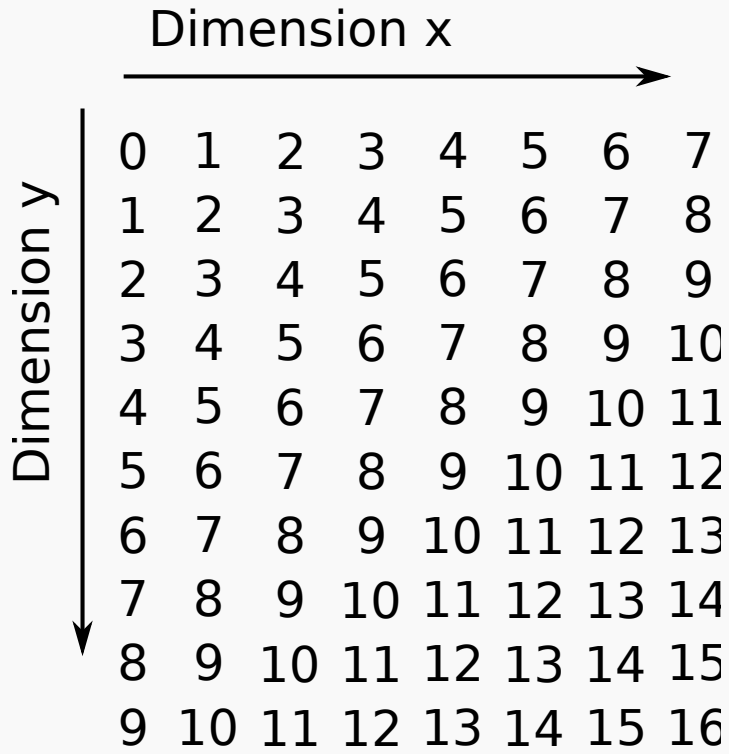
Solution 1




```
start[0] = 2;   start[1] = 1;
count[0] = 6;   count[1] = 4;
```

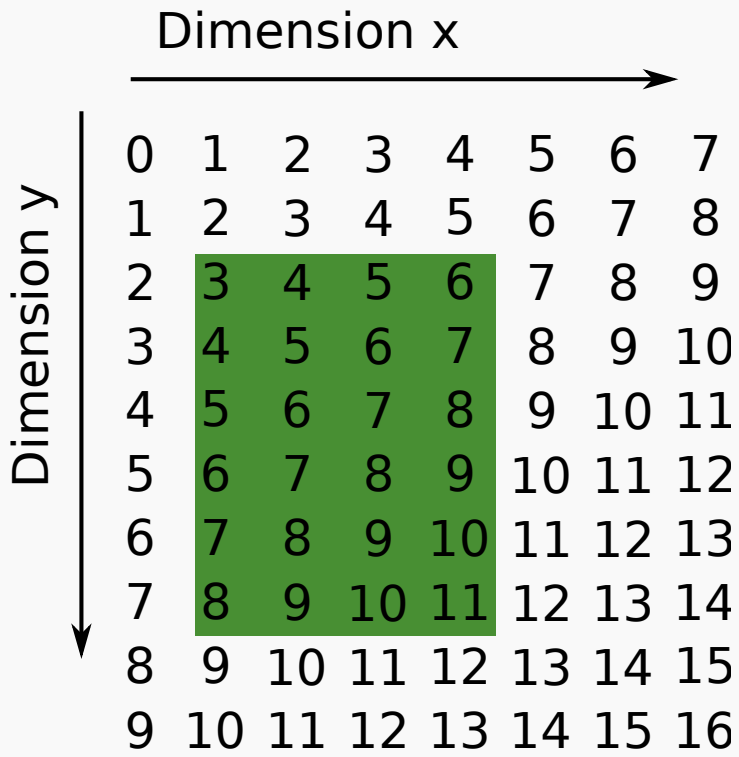
Exercise 2

Please draw the elements selected by the start, stride, count, block set below




```
start[0] = 2;   start[1] = 1;
count[0] = 1;   count[1] = 1;
block[0] = 6;   block[1] = 4;
```

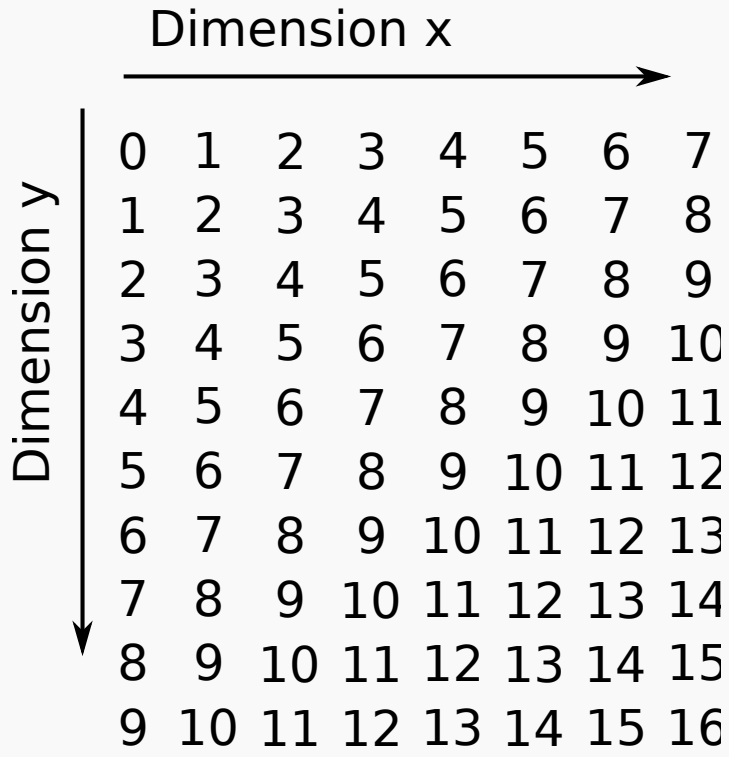
Solution 2




```
start[0] = 2;   start[1] = 1;
count[0] = 1;   count[1] = 1;
block[0] = 6;   block[1] = 4;
```

Exercise 3

Please draw the elements selected by the start, stride, count, block set below




```
 start[0] = 2;   start[1] = 1;
 count[0] = 3;   count[1] = 2;
stride[0] = 2;  stride[1] = 2;
 block[0] = 2;   block[1] = 2;
```

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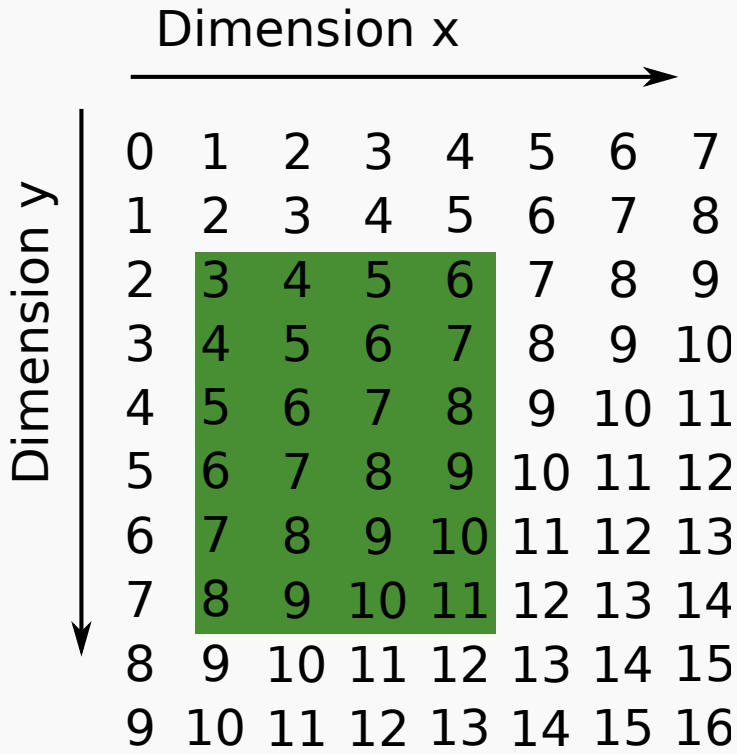
Solution 3




```
 start[0] = 2;   start[1] = 1;
 count[0] = 3;   count[1] = 2;
stride[0] = 2;  stride[1] = 2;
 block[0] = 2;   block[1] = 2;
```

What is a dataspace ?

Dataspace Objects

- Null dataspaces
- Scalar dataspaces
- Simple dataspaces
  - rank or number of dimensions
  - current size
  - maximum size (can be unlimited)

Dataspaces come into play:

- for performing partial IO
- to describe the shape of HDF5 dataset

What is a dataspace for ?

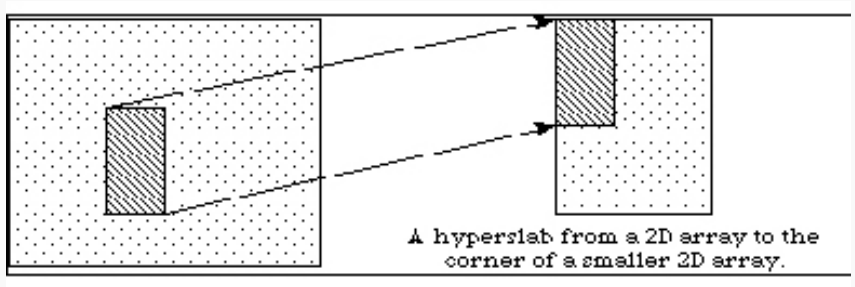


Figure : Access a sub-set of data with a hyperslab[1]

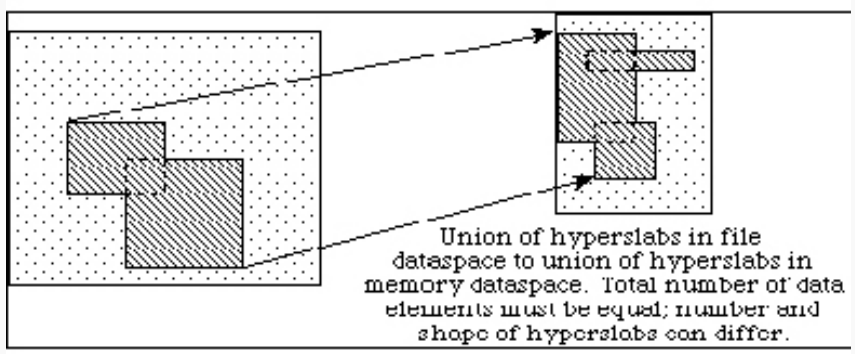


Figure : Build complex regions with hyperslab unions[1]

[1] Figures taken from HDF5 website

What is a dataspace for ?

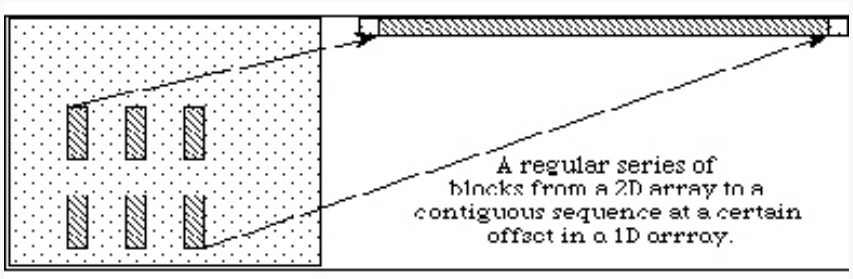


Figure : Use hyper-slabs to gather or scatter data[2]

[2] Figures taken from HDF5 website

How to play with dataspaces

```
hid_t space_id;
hsize_t dims[2], start[2], count[2];
hsize_t *stride=NULL, *block=NULL;

dims[0] = ny; dims[1] = nx;
start[0] = 2;  start[1] = 1;
count[0] = 6;  count[1] = 4;

space_id = H5Screate_simple(2, dims, NULL);

status = H5Sselect_hyperslab(space_id, H5S_SELECT_SET, start,\
stride, count, block);
```

How to play with dataspaces

- *space_id* is modified by *H5Sselect_hyperslab*, so it must exist
- *start, stride, count, block* arrays must be at least the same size as the rank of *space_id* dataspace
- H5S_SELECT_SET replaces the existing selection with the parameters from this call.
- Other operations : H5S_SELECT_OR, AND, XOR, NOTB and NOTA
- *stride, block* arrays are considered as 1 if NULL is passed

Using dataspaces during a partial IO

```
status = H5Sselect_hyperslab(space_id_mem, H5S_SELECT_SET, \
start_mem, stride_mem, count_mem, block_mem);

status = H5Sselect_hyperslab(space_id_disk, H5S_SELECT_SET, \
start_disk, stride_disk, count_disk, block_disk);

status = H5Dwrite(dataset, H5T_NATIVE_INT, space_id_mem, \
                  space_id_disk,H5P_DEFAULT, data);
```

- The two dataspace can describe non contiguous data and can be of different dimension
- But the number of elements must match

HDF5 command line tools

- HDF5 files are non ASCII files
- non human readable files

⇒ Tools provided to manipulate and get information contained in HDF5 files

- Three main ones: **h5ls, h5dump, h5diff**

Hands on HDF5

1. git clone https://github.com/mathaefele/HDF5_hands-on.git
2. cd HDF5_hands-on/hdf5-1
3. Examine the source code, compile and run it
4. Examine the output file example.h5 with h5ls and h5dump command line tools
5. Modify the program to write an additional dataset containing a 3D data of size Nx.Ny.Nz
6. Modify the program to write a single 2D slice of the 3D array instead of the whole array
7. Modify the program to write the previous 2D slice as an extension of the original 2D dataset