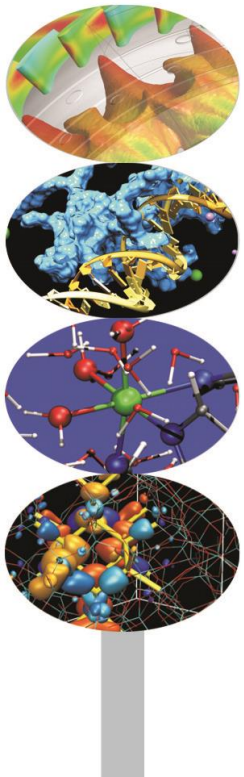
CINECA SCAI
SuperComputing Applications and Innovation

CINECA COURSES High Performance Computing 2014

HDF5: theory & practice



Giorgio Amati
SCAI Dept.

15/16 May 2014

PRACE

CINECA

Agenda

- ✓ HDF5: main issues
- ✓ Using the API (serial)
- ✓ Using the API (parallel)
- ✓ Tools
- ✓ Some comments

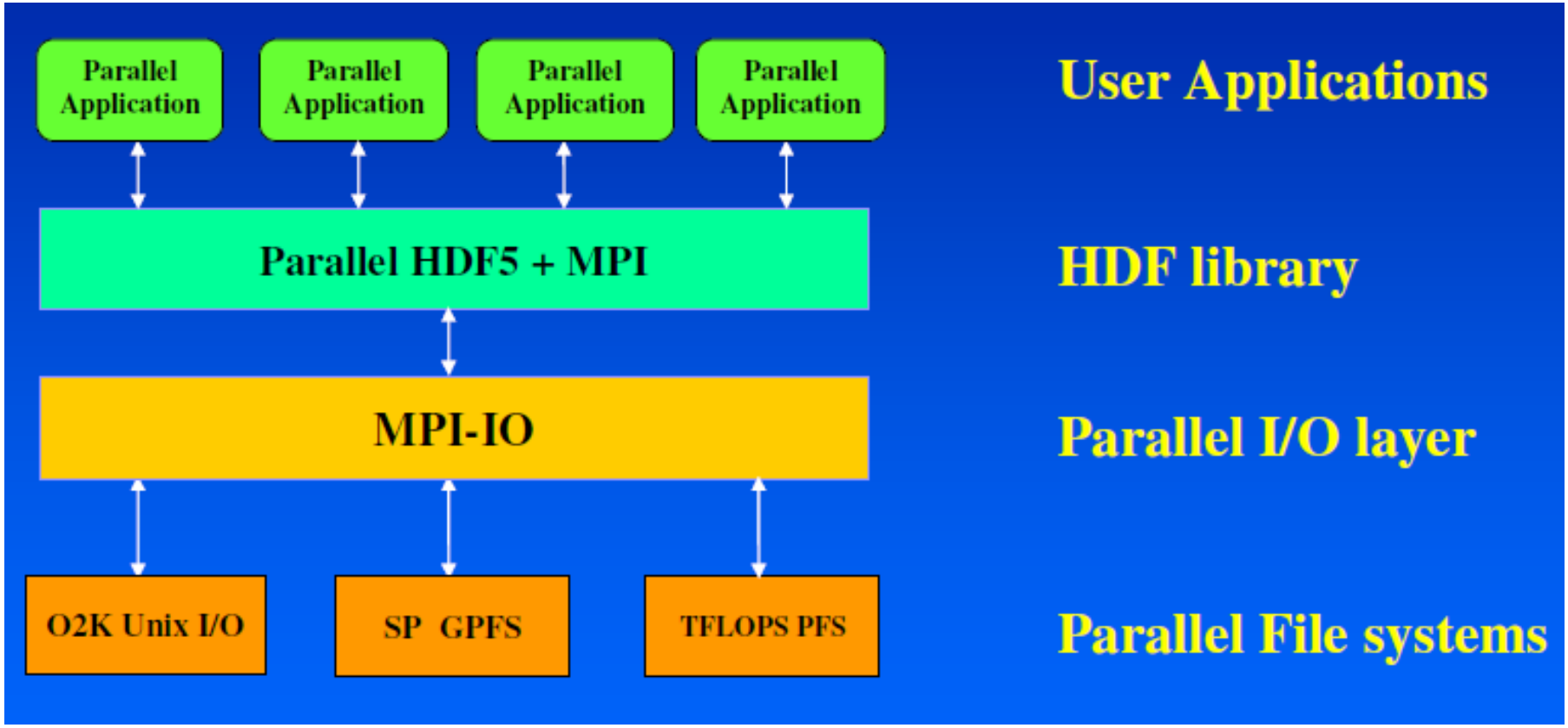
PHDF5 Initial Target

- Support for MPI programming
- Not for shared memory programming
  - Threads
  - OpenMP
- Has some experiments with
  - Thread-safe support for Pthreads
  - OpenMP if called “correctly”

PHDF5 Requirements

- PHDF5 files compatible with serial HDF5 files
  - Shareable between different serial or parallel platforms
- Single file image to all processes
  - One file per process design is undesirable
    - ✓ Expensive post processing
    - ✓ Not useable by different number of processes
- Standard parallel I/O interface
  - Must be portable to different platforms

PHDF5 Implementation Layers



Collective vs. Independent Calls

- MPI definition of collective call
  - All processes of the communicator must participate in the right order
- Independent means not collective
- Collective is not necessarily synchronous

Programming Restrictions

- Most PHDF5 APIs are collective
- PHDF5 opens a parallel file with a communicator
  - ✓ Returns a file-handle
  - ✓ Future access to the file via the file-handle
  - ✓ All processes must participate in collective PHDF5 APIs
  - ✓ Different files can be opened via different communicators

Examples of PHDF5 API

- Examples of PHDF5 collective API
  - ✓ File operations: **`H5Fcreate`**, **`H5Fopen`**, **`H5Fclose`**
  - ✓ Objects creation: **`H5Dcreate`**, **`H5Dopen`**, **`H5Dclose`**
  - ✓ Objects structure: **`H5Dextend`** (increase dimension sizes)

- Array data transfer
  - ✓ Dataset operations: **`H5Dwrite`**, **`H5Dread`**

What Does PHDF5 Support ?

- 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 write to the same data array
  - ✓ Each process writes to individual data array

Programming Model

1. Create or open a Parallel HDF5 file with a collective call to:
   - ✓ **`H5Dcreate, H5Dopen`**
2. Obtain a copy of the file transfer property list and set it to use collective or independent I/O.
   - ✓ First passing a data transfer property list class type to: **`H5Pcreate`**
   - ✓ Set the data transfer mode to either use *independent I/O* access or to use *collective I/O*, with a call to: **`H5Pset_dxpl_mpio`**
3. Access the dataset with the defined transfer property list.
   - ✓ All processes that have opened a dataset may do collective I/O.
   - ✓ Each process may do an independent and arbitrary number of data I/O access calls, using: **`H5Dwrite`** and/or **`H5Dread`**

Setup access template

Each process of the MPI communicator creates an access template and sets it up with MPI parallel access information

Using C:

```
herr_t H5Pset_fapl_mpio(hid_t plist_id, MPI_Comm
   comm, MPI_Info info);
```

UsingF90:

```
integer(hid_t) :: plist_id
integer :: comm, info
h5pset_fapl_mpio_f(plist_id, comm, info);
```

plist_id is a file access property list identifier

Example 1

```
/* Initialize MPI */
MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &mpi_size);
MPI_Comm_rank(MPI_COMM_WORLD, &mpi_rank);
..
/* Set up file access property list for MPI-IO access */
plist_id = H5Pcreate(H5P_FILE_ACCESS);
H5Pset_fapl_mpio(plist_id, MPI_COMM_WORLD, MPI_INFO_NULL);
file_id = H5Fcreate(H5FILE_NAME, H5F_ACC_TRUNC, H5P_DEFAULT, plist_id);

/* release property list identifier */
H5Pclose(plist_id);

/* Close the file. */
H5Fclose(file_id);
```

H5dump: example 1

```
h5dump -H my_first_parallel_file.h5
HDF5 "my_first_parallel_file.h5" {
GROUP "/" {
}
}
```

Creating and Opening Dataset

- All processes of the MPI communicator open/close a dataset by a collective call
  - ✓ C: **`H5Dcreate`** or **`H5Dopen`**; **`H5Dclose`**
  - ✓ F90: **`h5dcreate_f`** or **`h5dopen_f`**; **`h5dclose_f`**

- All processes of the MPI communicator extend dataset with unlimited dimensions before writing to it
  - ✓ C: **`H5Dextend`**
  - ✓ F90: **`h5dextend_f`**

Example 2

```
file_id = H5Fcreate(H5FILE_NAME, H5F_ACC_TRUNC, H5P_DEFAULT,
                    plist_id);

/* Create the dataspace for the dataset.  */
dimsf[0] = NX;
dimsf[1] = NY;
filespace = H5Screate_simple(RANK, dimsf, NULL);

/* Create the dataset with default properties collective */
dset_id = H5Dcreate(file_id,"dataset1",H5T_NATIVE_INT,
                    filespace,H5P_DEFAULT);

H5Dclose(dset_id);
H5Sclose(filespace);
H5Fclose(file_id);
```

H5dump output

```
h5dump my_second_parallel_file.h5
HDF5 "my_second_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (1,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (2,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (3,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (4,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (5,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (6,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (7,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (8,0): 0, 0, 0, 0, 0, 0, 0, 0,
      (9,0): 0, 0, 0, 0, 0, 0, 0, 0
```

…

Accessing a Dataset

- All processes that have opened the dataset may do collective I/O
- Each process may do independent and arbitrary number of data I/O access calls
  - ✓ C: **`H5Dwrite`** and **`H5Dread`**
  - ✓ F90: **`h5dwrite_f`** and **`h5dread_f`**

Accessing a Dataset

- Create and set dataset transfer property
  - C: **`H5Pset_dxpl_mpio`**
    - ✓**`H5FD_MPIO_COLLECTIVE`**
    - ✓**`H5FD_MPIO_INDEPENDENT`** (default)
  - F90: **`h5pset_dxpl_mpio_f`**
    - ✓**`H5FD_MPIO_COLLECTIVE_F`**
    - ✓**`H5FD_MPIO_INDEPENDENT_F`** (default)
- Access dataset with the defined transfer property

Collective write (C)

```
…
/* Create property list for collective dataset write */
plist_id = H5Pcreate(H5P_DATASET_XFER);
H5Pset_dxpl_mpio(plist_id, H5FD_MPIO_COLLECTIVE);

status = H5Dwrite(dset_id, H5T_NATIVE_INT, memspace,
   filespace, plist_id, data);
…
```

Writing Hyperslabs

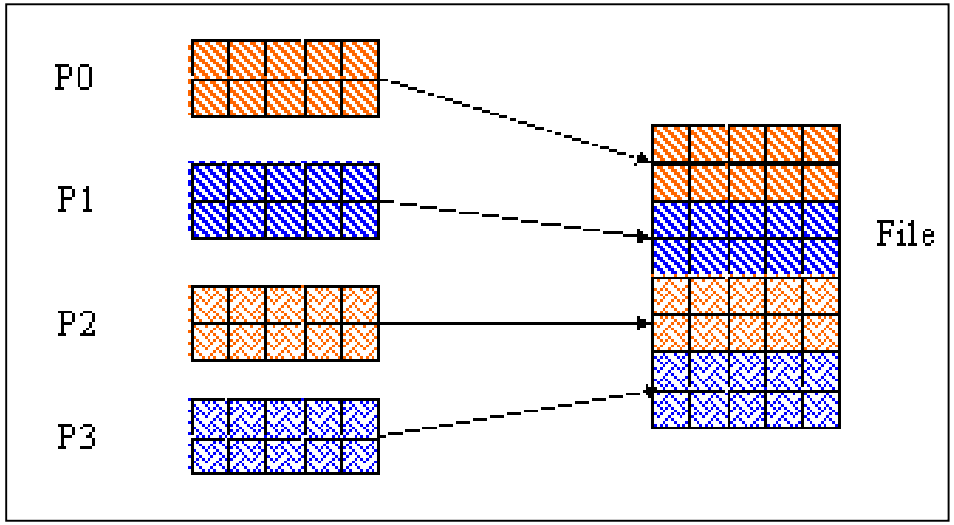
- This is a distributed memory model: data is split among processes
- PHDF5 uses hyperslab model
  - Each process defines memory and file hyperslabs
  - Each process executes partial write/read call
    - ✓ Collective calls
    - ✓ Independent calls

- The memory and file hyperslabs in the first step are defined with the **`H5Sselect_hyperslab`**

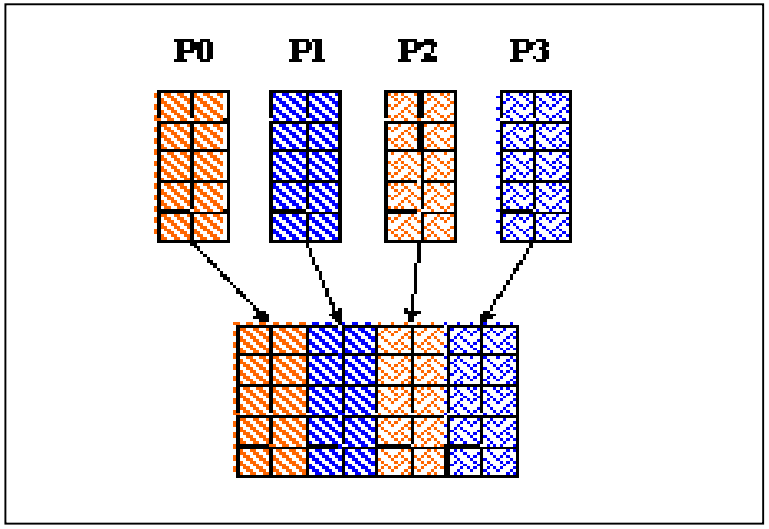
Writing Hyperslabs

- The start (or offset), count, stride, and block parameters define the portion of the dataset to write to.
- By changing the values of these parameters you can write hyperslabs with Parallel HDF5 by
  - ✓ contiguous hyperslab,
  - ✓ regularly spaced data in a column/row,
  - ✓ by patterns,
  - ✓ by chunks.

Contiguous Hyperslab



C example



Fortran 90 example

By rows (C)

```
dimsf[0] = 10; /* set global size */
dimsf[1] = 8;

/* Each task defines dataset in memory and writes it to the
   hyperslab in the file */
count[0] = dimsf[0]/mpi_size;
count[1] = dimsf[1];
memspace = H5Screate_simple(rank, count, NULL);

/* set offset for each task */
offset[0] = mpi_rank * count[0];
offset[1] = 0;

/* Initialize data buffer  */
data = (int *) malloc(sizeof(int)*count[0]*count[1]);
for (i=0; i < count[0]*count[1]; i++) {
     data[i] = mpi_rank*1000 + i;
}
```

Example 3 (by rows)

```
[gamati01@node342 PARALLEL]$ mpirun -np 5 ./a.out
[gamati01@node342 PARALLEL]$ h5dump my_third_parallel_file.h5
HDF5 "my_third_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 1, 2, 3, 4, 5, 6, 7,
      (1,0): 8, 9, 10, 11, 12, 13, 14, 15,
      (2,0): 1000, 1001, 1002, 1003, 1004, 1005, 1006, 1007,
      (3,0): 1008, 1009, 1010, 1011, 1012, 1013, 1014, 1015,
      (4,0): 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007,
      (5,0): 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015,
      (6,0): 3000, 3001, 3002, 3003, 3004, 3005, 3006, 3007,
      (7,0): 3008, 3009, 3010, 3011, 3012, 3013, 3014, 3015,
      (8,0): 4000, 4001, 4002, 4003, 4004, 4005, 4006, 4007,
      (9,0): 4008, 4009, 4010, 4011, 4012, 4013, 4014, 4015
      }
```

….

Example 3 (by row)

```
[gamati01@node342 PARALLEL]$ mpirun -np 10 ./a.out
[gamati01@node342 PARALLEL]$ h5dump my_third_parallel_file.h5
HDF5 "my_third_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 1, 2, 3, 4, 5, 6, 7,
      (1,0): 1000, 1001, 1002, 1003, 1004, 1005, 1006, 1007,
      (2,0): 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007,
      (3,0): 3000, 3001, 3002, 3003, 3004, 3005, 3006, 3007,
      (4,0): 4000, 4001, 4002, 4003, 4004, 4005, 4006, 4007,
      (5,0): 5000, 5001, 5002, 5003, 5004, 5005, 5006, 5007,
      (6,0): 6000, 6001, 6002, 6003, 6004, 6005, 6006, 6007,
      (7,0): 7000, 7001, 7002, 7003, 7004, 7005, 7006, 7007,
      (8,0): 8000, 8001, 8002, 8003, 8004, 8005, 8006, 8007,
      (9,0): 9000, 9001, 9002, 9003, 9004, 9005, 9006, 9007
      }
```

By columns (C)

```
dimsf[0] = 10; /* set global size */
dimsf[1] = 8;

/* Each task defines dataset in memory and writes it to the
   hyperslab in the file */
count[0] = dimsf[0];
count[1] = dimsf[1]/mpi_size;
memspace = H5Screate_simple(rank, count, NULL);

/* set offset for each task */
offset[1] = 0;
offset[1] = mpi_rank * count[1];

/* Initialize data buffer  */
data = (int *) malloc(sizeof(int)*count[0]*count[1]);
for (i=0; i < count[0]*count[1]; i++) {
     data[i] = mpi_rank*1000 + i;
}
```

Example 3 (by Column)

```
[gamati01@node342 PARALLEL]$ mpirun -np 2 ./a.out
[gamati01@node342 PARALLEL]$ h5dump my_forth_parallel_file.h5
HDF5 "my_forth_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 1, 2, 3, 1000, 1001, 1002, 1003,
      (1,0): 4, 5, 6, 7, 1004, 1005, 1006, 1007,
      (2,0): 8, 9, 10, 11, 1008, 1009, 1010, 1011,
      (3,0): 12, 13, 14, 15, 1012, 1013, 1014, 1015,
      (4,0): 16, 17, 18, 19, 1016, 1017, 1018, 1019,
      (5,0): 20, 21, 22, 23, 1020, 1021, 1022, 1023,
      (6,0): 24, 25, 26, 27, 1024, 1025, 1026, 1027,
      (7,0): 28, 29, 30, 31, 1028, 1029, 1030, 1031,
      (8,0): 32, 33, 34, 35, 1032, 1033, 1034, 1035,
      (9,0): 36, 37, 38, 39, 1036, 1037, 1038, 1039
      }
   }
```

Example 3 (by Column)

```
[gamati01@node342 PARALLEL]$ mpirun -np 8 ./a.out
[gamati01@node342 PARALLEL]$ h5dump my_forth_parallel_file.h5
HDF5 "my_forth_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 1000, 2000, 3000, 4000, 5000, 6000, 7000,
      (1,0): 1, 1001, 2001, 3001, 4001, 5001, 6001, 7001,
      (2,0): 2, 1002, 2002, 3002, 4002, 5002, 6002, 7002,
      (3,0): 3, 1003, 2003, 3003, 4003, 5003, 6003, 7003,
      (4,0): 4, 1004, 2004, 3004, 4004, 5004, 6004, 7004,
      (5,0): 5, 1005, 2005, 3005, 4005, 5005, 6005, 7005,
      (6,0): 6, 1006, 2006, 3006, 4006, 5006, 6006, 7006,
      (7,0): 7, 1007, 2007, 3007, 4007, 5007, 6007, 7007,
      (8,0): 8, 1008, 2008, 3008, 4008, 5008, 6008, 7008,
      (9,0): 9, 1009, 2009, 3009, 4009, 5009, 6009, 7009
      }
```

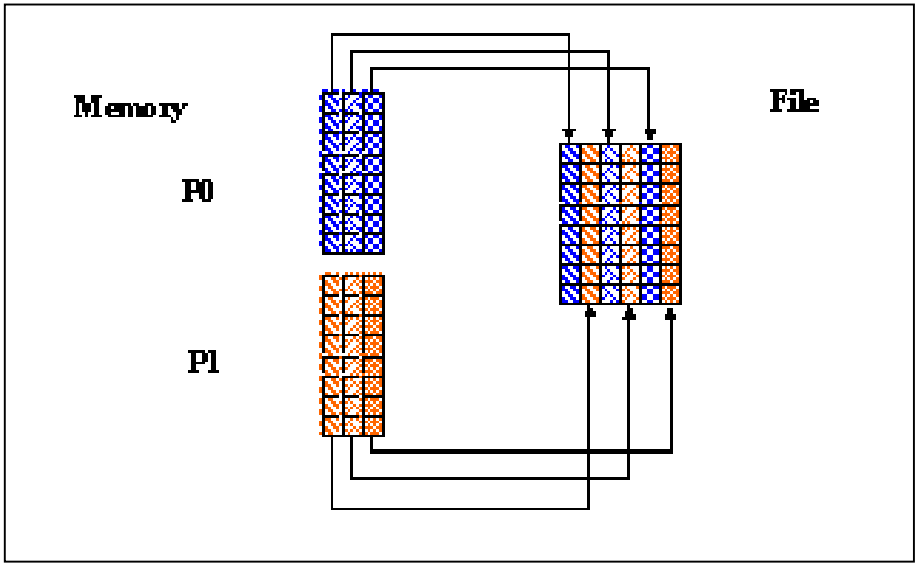
Example 4 (2D decomposition)

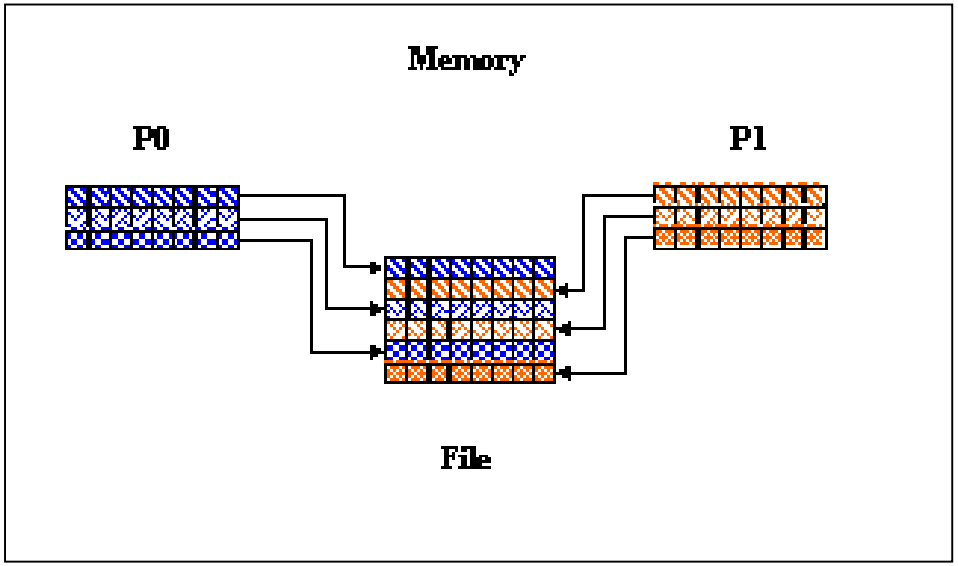
```
count[0] = dimsf[0]/proc_x;
count[1] = dimsf[1]/proc_y;

/* set coordinates... */
if(mpi_rank == 0) { x = 0; y = 0;}
if(mpi_rank == 1) { x = 1; y = 0;}
if(mpi_rank == 2) { x = 0; y = 1;}
if(mpi_rank == 3) { x = 1; y = 1;}

memspace = H5Screate_simple(rank, count, NULL);

/* set offset for each task */
offset[0] = x*count[0];
offset[1] = y*count[1];
```

2D Decomposition

```
[gamati01@node342 PARALLEL]$ mpirun -np 4 ./a.out
[gamati01@node342 PARALLEL]$ h5dump my_fifth_parallel_file.h5
HDF5 "my_third_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 1, 2, 3, 2000, 2001, 2002, 2003,
      (1,0): 4, 5, 6, 7, 2004, 2005, 2006, 2007,
      (2,0): 8, 9, 10, 11, 2008, 2009, 2010, 2011,
      (3,0): 12, 13, 14, 15, 2012, 2013, 2014, 2015,
      (4,0): 16, 17, 18, 19, 2016, 2017, 2018, 2019,
      (5,0): 1000, 1001, 1002, 1003, 3000, 3001, 3002, 3003,
      (6,0): 1004, 1005, 1006, 1007, 3004, 3005, 3006, 3007,
      (7,0): 1008, 1009, 1010, 1011, 3008, 3009, 3010, 3011,
      (8,0): 1012, 1013, 1014, 1015, 3012, 3013, 3014, 3015,
      (9,0): 1016, 1017, 1018, 1019, 3016, 3017, 3018, 3019
      }
   }
```

Regularly spaced data

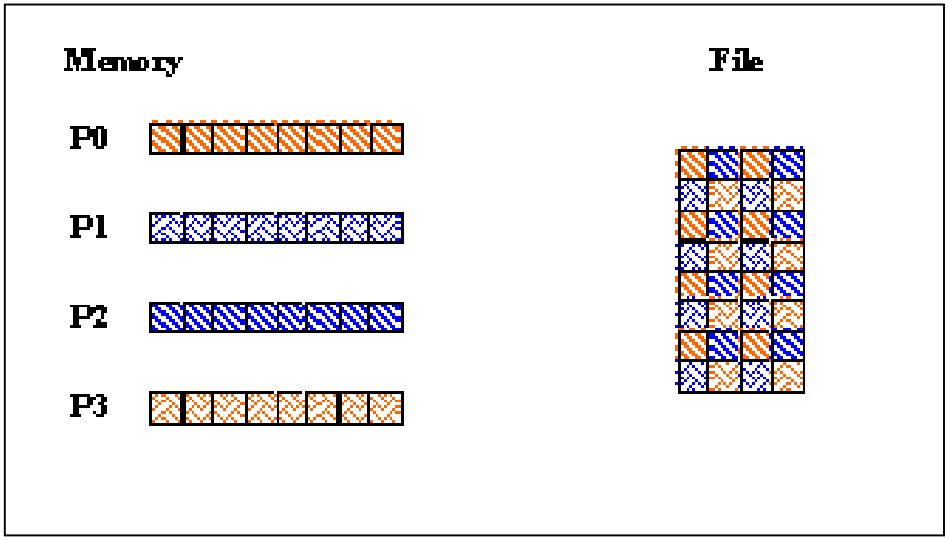




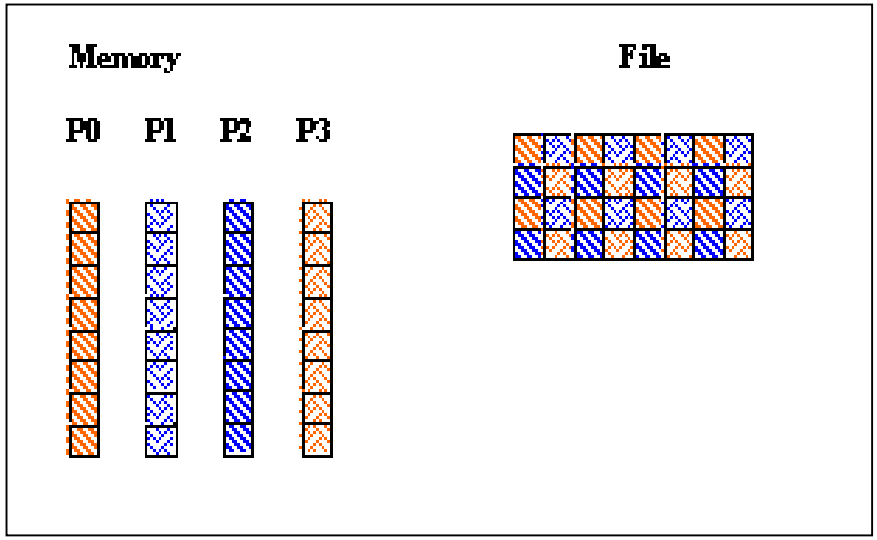
C example

Fortran 90 example

By patterns



C example



Fortran 90 example

Reading Hyperslabs

- The start (or offset), count, stride, and block parameters define the portion of the dataset to read from

Example 5 (1D decomposition)

```
proc_x = mpi_size; proc_y = 1;
dimsf[0] = 10; dimsf[1] = 8;
count[0] = dimsf[0]/proc_x; count[1] = dimsf[1];
offset[0] = x*count[0]; offset[1] = y*count[1];

/* Set up file access property list for MPI-IO access */
plist_id = H5Pcreate(H5P_FILE_ACCESS);
status = H5Pset_fapl_mpio(plist_id, MPI_COMM_WORLD,
   MPI_INFO_NULL);
file_id = H5Fopen(H5FILE_NAME, H5F_ACC_RDWR, plist_id);

/* Create property list for collective dataset read */
plist2_id = H5Pcreate(H5P_DATASET_XFER);
status = H5Pset_dxpl_mpio(plist2_id, H5FD_MPIO_COLLECTIVE);

status = H5Dread(dset_id, H5T_NATIVE_INT, memspace, filespace1,
   plist2_id, data);
```

The file to read…

```
[gamati01@node342 PARALLEL]$ h5dump my_fifth_parallel_file.h5
HDF5 "my_third_parallel_file.h5" {
GROUP "/" {
   DATASET "dataset1" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 10, 8 ) / ( 10, 8 ) }
      DATA {
      (0,0): 0, 1, 2, 3, 2000, 2001, 2002, 2003,
      (1,0): 4, 5, 6, 7, 2004, 2005, 2006, 2007,
      (2,0): 8, 9, 10, 11, 2008, 2009, 2010, 2011,
      (3,0): 12, 13, 14, 15, 2012, 2013, 2014, 2015,
      (4,0): 16, 17, 18, 19, 2016, 2017, 2018, 2019,
      (5,0): 1000, 1001, 1002, 1003, 3000, 3001, 3002, 3003,
      (6,0): 1004, 1005, 1006, 1007, 3004, 3005, 3006, 3007,
      (7,0): 1008, 1009, 1010, 1011, 3008, 3009, 3010, 3011,
      (8,0): 1012, 1013, 1014, 1015, 3012, 3013, 3014, 3015,
      (9,0): 1016, 1017, 1018, 1019, 3016, 3017, 3018, 3019
      }
   }
```

Output

```
[gamati01@node342 PARALLEL]$ cat RUN/task.0.dat
i =  0, value --> 0
i =  1, value --> 1
i =  2, value --> 2
i =  3, value --> 3
i =  4, value --> 2000
i =  5, value --> 2001
i =  6, value --> 2002
i =  7, value --> 2003
i =  8, value --> 4
i =  9, value --> 5
i = 10, value --> 6
i = 11, value --> 7
i = 12, value --> 2004
i = 13, value --> 2005
i = 14, value --> 2006
i = 15, value --> 2007
```

Agenda

- ✓ HDF5: main issues
- ✓ Using the API (serial)
- ✓ Using the API (parallel)
- ✓ Tools
- ✓ Some comments

HFD5: Tools/1

- The are many tools usefull
  - ✓ h5ls
  - ✓ h5dump
  - ✓ h5debug
  - ✓ h5repart
  - ✓ h5mkgrp
  - ✓ h5redeploy
  - ✓ h5import
  - ✓ h5repack
  - ✓ …

HFD5: Tools/2

- The are many tools usefull
  - ✓ h5jam
  - ✓ h5unjam
  - ✓ h5copy
  - ✓ h5stat
  - ✓ gif2h5
  - ✓ h52gif
  - ✓ h5perf_serial
  - ✓ h5perf
  - ✓ hdfview

Agenda

- ✓ HDF5: main issues
- ✓ Using the API (serial)
- ✓ Using the API (parallel)
- ✓ Tools
- ✓ Some comments

API 1.6 vs API 1.8

- Moving from release 1.6.x to 1.8.0 some interfaces were modified
  - ✓ If your program uses 1.6/1.8 API and HDF5 library was compiled using 1.6/1.8 API → no problem
  - ✓ If your program uses 1.8 API and HDF5 library was compiled using 1.6 API → no way
  - ✓ If your program uses 1.6 API and HDF5 library was compiled using 1.8 API → use "**-DH5_USE_16_API**"

```
[amati@droemu PARALLEL]$ h5pcc -showconfig  | grep Mapping
            Default API Mapping: v18
[amati@droemu PARALLEL]$ h5pcc -showconfig  | grep Deprecated
 With Deprecated Public Symbols: yes
```

API 1.6 vs API 1.8

```
[amati@droemu PARALLEL]$ h5pcc parallel_ex4.c
parallel_ex4.c: In function 'main':
parallel_ex4.c:97: error: too few arguments to function 'H5Dcreate2'
[amati@droemu PARALLEL]$ h5pcc parallel_ex5.c
parallel_ex5.c: In function 'main':
parallel_ex5.c:64: error: too few arguments to function 'H5Dopen2'
[amati@droemu PARALLEL]$ h5pcc -DH5_USE_16_API parallel_ex4.c
[amati@droemu PARALLEL]$ h5pcc -DH5_USE_16_API parallel_ex5.c
```

- 1.6 API

```
H5Dcreate(file_id,"dset",H5T_NATIVE_INT,filespace,H5P_DEFAULT);
H5Dopen(file_id, "dataset1");
```

- 1.8 API

```
H5Dcreate(file_id,"dset",H5T_NATIVE_INT,filespace,H5P_DEFAULT,
          H5P_DEFAULT,H5P_DEFAULT);
H5Dopen(file_id, "dataset1",H5P_DEFAULT);
```

Bug or a Feature?

- Try to read a single precision restart from a double precision simulation.
  - ✓ It gives no error
  - ✓ The simulation runs "correctly"
  - ✓ But now it is a single precision simulation (form a numerical point of view)!!!
  - ✓ But as memory occupation (in RAM) is a double precision simulation!!!

HFD5: some (final) comments

- HDF5 as “robust” API.
  - ✓ It works but take care of warning
  - ✓ Check with h5dump the results
  - ✓ Use the error handle (**`herr_t`**) to verify that everthing is ok

Usefull links

The HDF Group Page: http://hdfgroup.org/

HDF5 Home Page: http://hdfgroup.org/HDF5/

HDF Helpdesk: help@hdfgroup.org

HDF Mailing Lists: http://hdfgroup.org/services/support.html

Parallel tutorial: http://hdf.ncsa.uiuc.edu/HDF5/doc/Tutor

1.8 vs 1.6:
http://www.hdfgroup.org/HDF5/doc/ADGuide/WhatsNew180.html
http://www.hdfgroup.org/HDF5/doc/ADGuide/Changes.html

That's all folks!!!!