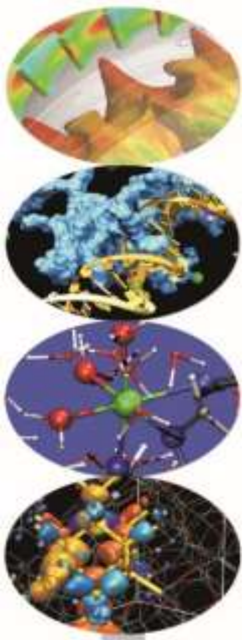
Parallel IO: basics and MPI2-IO

Super Computing Applications and Innovation Department

Courses Edition 2017



Introduction

- IO is a crucial issue in modern HPC applications:
  - deal with very large datasets while running massively parallel applications on supercomputers
  - amount of data saved is increased
  - latency to access to disks is not negligible
  - data portability (e.g. endianness)

- Solutions to avoid that IO become a bottleneck:
  - HW: parallel file-system available on all the HPC platforms
  - SW: high level libraries able to manage parallel accesses to the file in efficient way (e.g. MPI2-IO, HDF5, NetCDF, …)

Data Portability: Data Representation

There are two common different representations of datatypes in computer memory:

Little Endian ⇐ PC (Windows/Linux)

Byte3 Byte2 Byte1 Byte0

will be arranged in memory as follows:

Base Address+0	Byte0
Base Address+1	Byte1
Base Address+2	Byte2
Base Address+3	Byte3

Big Endian

Byte3 Byte2 Byte1 Byte0

will be arranged in memory as follows:

Base Address+0	Byte3
Base Address+1	Byte2
Base Address+2	Byte1
Base Address+3	Byte0

Unix (IBM, SGI, SUN…) ⇒

Data Portability Problem

Endianness is a problem when a binary file created on a computer is read on another computer with different endianness.

This is a subtle problem, because unveils only when you try to use previous data on a different platform.

For example: unformatted data written by an IBM system cannot be read by a Linux/MS Windows PC

Endianness: portability problem

Assuming you will not (or you can't) repeat the simulations:

- you need to write a tool to swap byte order in a proper representation
  - the tool cannot be a general one because depends on the layout of different data type width along the file
- Some compilers have built-in facilities to deal with data written in other formats (i.e: Intel's non-standard specifier CONVERT='BIG_ENDIAN').

Managing IO in Parallel Applications

Solutions to managing IO in parallel applications must take into account different aspects of the application and implementation:

- potential performance improvements
- scaling with respect resources/system size
- ensure data consistency
- avoid communications
- strive for usability

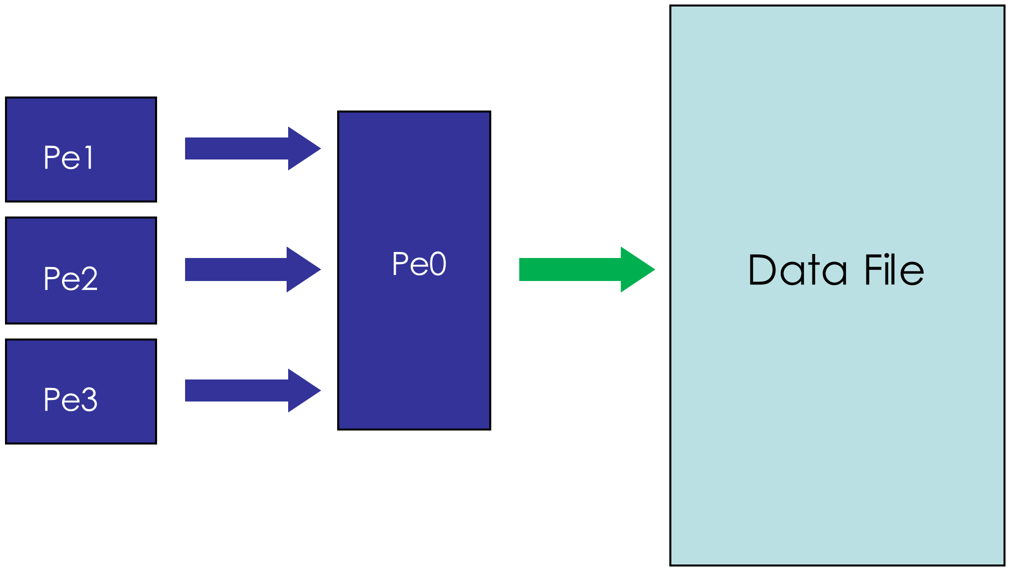
Common approaches:

1. Master-Slave
2. Distributed IO on local files
3. Coordinated controlled accesses
4. MPI-IO or high level libraries
   (e.g. HDF5, NetCDF use MPI-IO as the backbone)

Managing IO in Parallel Applications

Approach 1: Master-Slave

Only 1 processor performs IO



Goals:

Scalable: **NO**

Ensure data consistency: **YES**

Avoid communication: **NO**

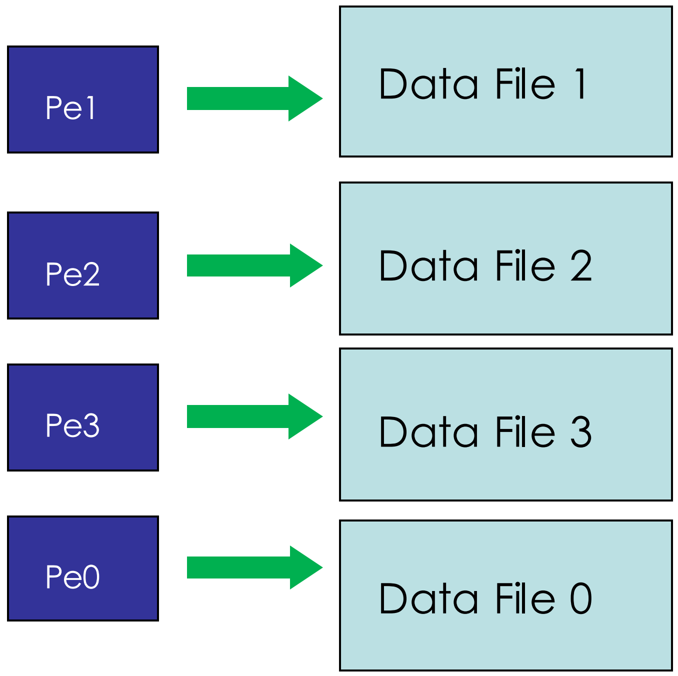
Usability: **YES**

note: no parallel FS needed

Managing IO in Parallel Applications

Approach 2: Distributed IO on local files

All the processors read/writes their own files



Goals:

Scalable: **YES** (... but be careful)

Ensure data consistency: **YES**

Avoid communication: **YES**

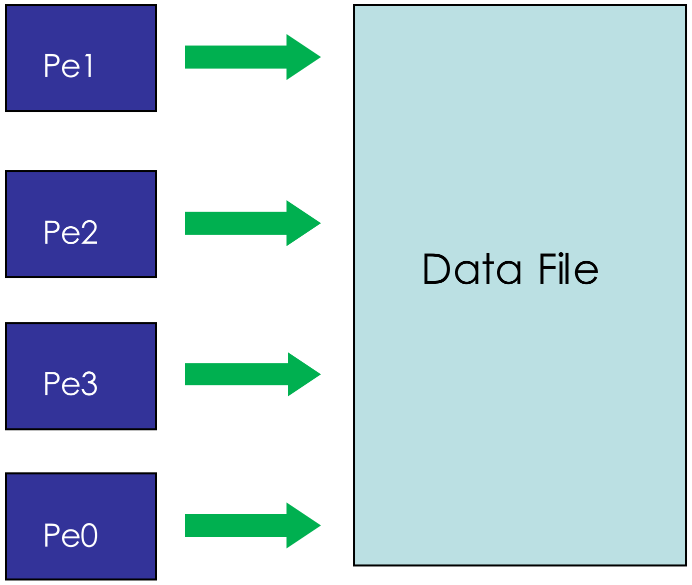
Usability: **NO** **(need extra work later)**

Warning: avoid to parametrize with processors!!!

Managing IO in Parallel Applications

Approach 3: Coordinated controlled accesses

All the processors read/writes on a single ACCESS = DIRECT file



Goals:

Scalable: **YES** (… but be careful)

Ensure data consistency: **NO**

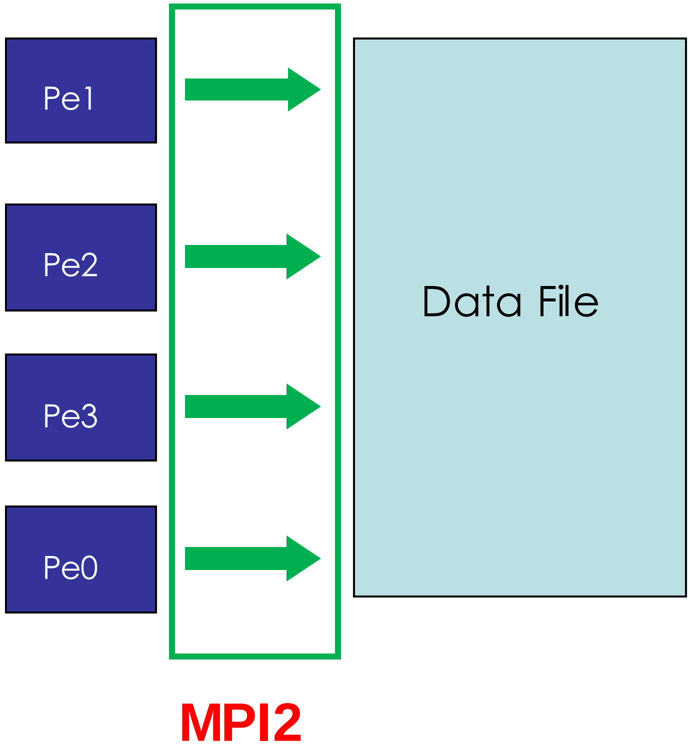
Avoid communication: **YES**

Usability: **YES**

Managing IO in Parallel Applications

Solution 4: MPI2 IO (or other parallel IO libraries)

MPI functions perform the IO. Asynchronous IO is also supported.



Goals:

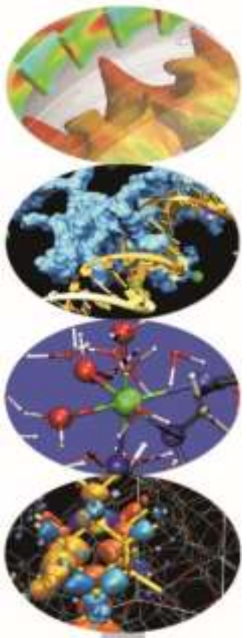
Scalable: **YES (strongly!!!)**

Ensure data consistency: **YES / NO**

Avoid communication: **YES / NO**

Usability: **YES**

MPI2-IO



MPI-2.x features for Parallel IO

- MPI-IO: introduced in MPI-2.x standard (1997)
  - allow non-contiguous access in both memory and file
  - reading/writing a file is like send/receive a message from a MPI buffer
  - optimized access for non-contiguous data
  - collective / non-collective access operations with communicators
  - blocking / non-blocking calls
  - data portability (implementation/system independent)
  - good performance in many implementations
- Why do we start to use it???
  - syntax and semantic are very simple to use
  - performance : 32 MPI processes (4x8) with local grid 50000^2 (sp)
    - MPI-IO: **85**sec vs Traditional master/slave IO: **3200**sec
      - dimension of written file: 305GB
      - measured bandwidth of GPFS (single thread): 65MB/sec
      - measured bandwidth of MPI gather for Master/slave: 900MB/sec
      - MPI_File_write_all (**85**sec) vs MPI_file_write (**320**sec)

Starting with MPI-IO

- MPI-IO provides basic IO operations:
  - open, seek, read, write, close (etc.)
- open/close are collective operations on the same file
  - many modalities to access the file (composable: |,+)
- read/write are similar to send/recv of data to/from a buffer
  - each MPI process has its own local pointer to the file (individual file pointer) for seek, read, write operations
  - offset variable is a particular kind of variable and it is given in elementary unit (etype) of access to file (default in byte)
    - error: declare offset as an integer
  - it is possible to know the exit status of each subroutine/function

Using individual file pointers

```
#include "mpi.h"

int main(int argc, char **argv){
    int rank, nprocs;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

    MPI_File fh; MPI_Status status;
    MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile", MPI_MODE_RDONLY,
       MPI_INFO_NULL, &fh);

    MPI_Offset filesize;
    MPI_File_get_size(fh, &filesize);

    MPI_Offset bufsize = filesize/nprocs;
    int nints = bufsize/sizeof(int);
    int *buf = (int*) malloc(nints);

    MPI_File_seek(fh, rank*bufsize, MPI_SEEK_SET);
    MPI_File_read(fh, buf, nints, MPI_INT, &status);

    MPI_File_close(&fh);
    ...
}
```

File offset determined by MPI_File_seek

Using individual file pointers

```
PROGRAM Output
    USE MPI
    IMPLICIT NONE
    INTEGER :: err, i, myid, file, intsize
    INTEGER :: status(MPI_STATUS_SIZE)
    INTEGER, PARAMETER :: count=10000
    INTEGER DIMENSION(count) :: buf
    INTEGER, INTEGER(KIND=MPI_OFFSET_KIND) :: disp

    CALL MPI_INIT(err)
    CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, err)

    DO i = 1, count
            buf(i) = myid * count + i
    END DO
    CALL MPI_FILE_OPEN(MPI_COMM_WORLD, 'test', MPI_MODE_WRONLY + &
      MPI_MODE_CREATE, MPI_INFO_NULL, file, err)

    CALL MPI_TYPE_SIZE(MPI_INTEGER, intsize, err)
    disp = myid * count * intsize

    CALL MPI_FILE_SEEK(file, disp, MPI_SEEK_SET, err)
    CALL MPI_FILE_WRITE(file, buf, count, MPI_INTEGER, status, err)

    CALL MPI_FILE_CLOSE(file, err)

    CALL MPI_FINALIZE(err)
END PROGRAM Output
```

File offset determined by MPI_File_seek

Open/close a file 1/3

MPI_FILE_OPEN(comm, filename, amode, info, fh)

IN comm: communicator (handle)
IN filename: name of file to open (string)
IN amode: file access mode (integer)
IN info: info object (handle)
OUT fh: new file handle (handle)

- **Collective** operation across processes within a communicator.
- Filename must reference the same file on all processes.
- Process-local files can be opened with **MPI_COMM_SELF**.
- Initially, all processes view the file as a linear byte stream, and each process views data in its own native representation. The file view can be changed via the **MPI_FILE_SET_VIEW** routine.
- Additional information can be passed to MPI environment via the MPI_Info handle. The info argument is used to provide extra information on the file access patterns. The constant **MPI_INFO_NULL** can be specified as a value for this argument.

Open/close a file 2/3

Each process within the communicator must specify the same filename and access mode (amode):

MPI_MODE_RDONLY	read only
MPI_MODE_RDWR	reading and writing
MPI_MODE_WRONLY	write only
MPI_MODE_CREATE	create the file if it does not exist
MPI_MODE_EXCL	error if creating file that already exists
MPI_MODE_DELETE_ON_CLOSE	delete file on close
MPI_MODE_UNIQUE_OPEN	file will not be concurrently opened elsewhere
MPI_MODE_SEQUENTIAL	file will only be accessed sequentially
MPI_MODE_APPEND	set initial position of all file pointers to end of file

Open/close a file 3/3

MPI_FILE_CLOSE(comm)
INOUT fh: file handle (handle)

- Collective operation
- Call this function when the file access is finished to free the file handle.

Passing Info to MPI-IO

- Several parallel file system can benefit from “hints” given to MPI-IO
  - optimization may be possible with performance benefits
- Info to MPI are opaque objects (MPI_Info in C or integer in FORTRAN)
- hints can be provided as (key, value) pairs with MPI_Info_set function

```
MPI_Info info;

MPI_Info_create(&info);

// set number of I/O devices across which the file should be striped
MPI_Info_set(info, “striping_factor”, “4”);

// set the striping unit in bytes
MPI_Info_set(info, “striping_unit”, “65536”);

// buffer size of collective I/O
MPI_Info_set(info, “cb_buffer_size”, “8388608”);

// number of processes that should perform disk accesses during collective I/O
MPI_Info_set(info, “cb_nodes”, “4”);
```

Getting Info from MPI-IO

- Info can also be retrieved from the implementation
  - which hints where used for a file?
  - which default are actually in use?

```
char key[MPI_MAX_INFO_KEY], value[MPI_MAX_INFO_VAL];
MPI_Info info_used;

MPI_File_get_info(fh, &info_used);

int nkeys;
MPI_Info_get_nkeys(info_used, &nkeys);

for (int i=0; i<nkeys; i++) {
  MPI_Info_get_nthkey(info_used, i, key);
  int flag; // return true if key was set
  MPI_Info_get(info_used, key, MPI_MAX_INFO_VAL, value, &flag);
  printf("key = %s, value = %s\n", key, value);
}
```

Individual file pointers - Write

MPI_FILE_WRITE (fh, buf, count, datatype, status)
INOUT fh: file handle (handle)
IN buf: initial address of buffer (choice)
IN count: number of elements in buffer (integer)
IN datatype: datatype of each buffer element (handle)
OUT status: status object (status)

– Write **count** elements of **datatype** from memory starting at **buf** to the file

– Starts writing at the current position of the file pointer

– **status** will indicate how many **bytes** have been written

– Updates position of file pointer after writing

– Blocking, independent (local, not collective) call.

– **Individual file pointers are used:**

Each processor has **its own pointer** to the file

Pointer on a processor **is not influenced** by any other processor

Individual file pointers - Read

MPI_FILE_READ (fh, buf, count, datatype, status)
INOUT fh: file handle (handle)
OUT buf: initial address of buffer (choice)
IN count: number of elements in buffer (integer)
IN datatype: datatype of each buffer element (handle)
OUT status: status object (status)

– Read **count** elements of **datatype** from the file to memory starting at **buf**
– Starts reading at the current position of the file pointer
– **status** will indicate how many **bytes** have been read
– Updates position of file pointer after writing
– Blocking, independent (local, not collective) call.
– **Individual file pointers are used:**
Each processor has **its own pointer** to the file
Pointer on a processor **is not influenced** by any other processor

Get file size

MPI_FILE_GET_SIZE (fh, size)
IN fh: file handle (handle)
OUT size: size of the file in bytes (interger)

- returns the current size in bytes of the fh handle associated file
- size should be a special integer:
  - MPI_Offset in C
  - KIND=MPI_OFFSET_KIND in FORTRAN
- pay attention on overflow when mixing different type of integer in expressions and assignments

MPI-IO Data Access APIs

- MPI-IO provides a large number of routines to read and write data from a file.

- There are three properties which differentiate data access routines:
  - **Positioning:** users can either specify explicitly the offset in the file at which the data access takes place or they can use MPI file pointers
  - **Synchronisation:** as for common communication APIs, we can use both synchronous (blocking) or asynchronous (non-blocking) function calls
  - **Coordination:** data accesses can be local or collective operations

Data Access 1/3

Positioning:

Users can either specify the offset in the file at which the data access takes place or they can use MPI file pointers:

- **Individual file pointers:** each process has its own file pointer that is only altered on accesses of that specific process
- **Shared file pointer:** pointer is shared among all processes in the communicator used to open the file
  - It is modified by any shared file pointer access of any process
  - Shared file pointers can only be used if file type gives each process access to the whole file!
- **Explicit offset:** no file pointer is used or modified
  - An explicit offset is given to determine access position
  - This can not be used with MPI MODE SEQUENTIAL!

Data Access 2/3

Synchronisation:

MPI-2 supports both **blocking** and **non-blocking IO** routines:

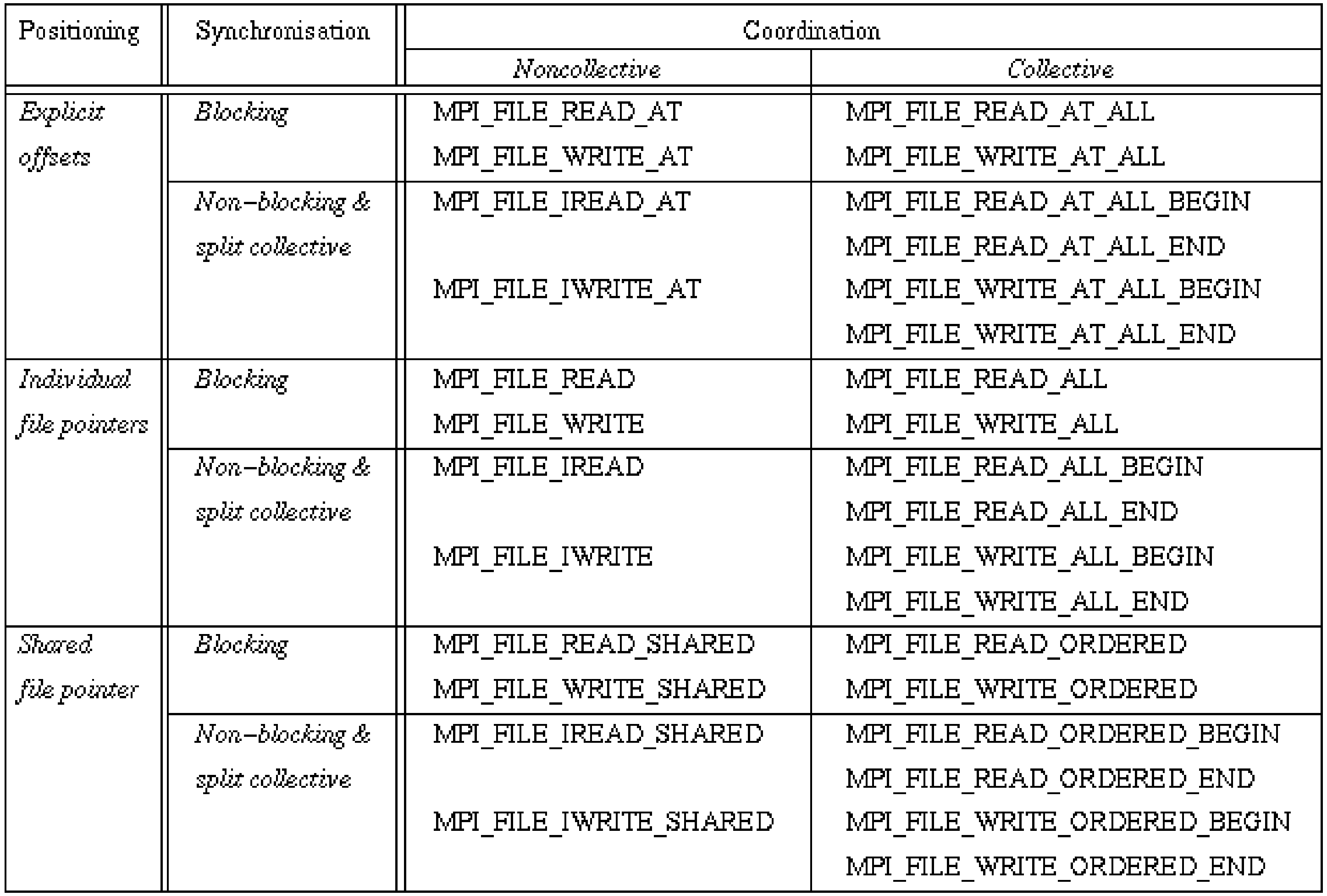
- A **blocking IO call** will not return until the IO request is completed.
- A **nonblocking IO call** initiates an IO operation, but not wait for its completition. It also provides 'split collective routines' which are a restricted form of non-blocking routines for collective data access.

Coordination:

Data access can either take place from individual processes or collectively across a group of processes:

- **collective**: MPI coordinates the reads and writes of processes
- **independent**: no coordination by MPI

Data Access 3/3



Positioning	Synchronisation	Coordination	
		Noncollective	*Collective*
Explicit offsets	*Blocking*	MPI_FILE_READ_AT MPI_FILE_WRITE_AT	MPI_FILE_READ_AT_ALL MPI_FILE_WRITE_AT_ALL
	Non-blocking & split collective	MPI_FILE_IREAD_AT MPI_FILE_IWRITE_AT	MPI_FILE_READ_AT_ALL_BEGIN MPI_FILE_READ_AT_ALL_END MPI_FILE_WRITE_AT_ALL_BEGIN MPI_FILE_WRITE_AT_ALL_END
Individual file pointers	*Blocking*	MPI_FILE_READ MPI_FILE_WRITE	MPI_FILE_READ_ALL MPI_FILE_WRITE_ALL
	Non-blocking & split collective	MPI_FILE_IREAD MPI_FILE_IWRITE	MPI_FILE_READ_ALL_BEGIN MPI_FILE_READ_ALL_END MPI_FILE_WRITE_ALL_BEGIN MPI_FILE_WRITE_ALL_END
Shared file pointer	*Blocking*	MPI_FILE_READ_SHARED MPI_FILE_WRITE_SHARED	MPI_FILE_READ_ORDERED MPI_FILE_WRITE_ORDERED
	Non-blocking & split collective	MPI_FILE_IREAD_SHARED MPI_FILE_IWRITE_SHARED	MPI_FILE_READ_ORDERED_BEGIN MPI_FILE_READ_ORDERED_END MPI_FILE_WRITE_ORDERED_BEGIN MPI_FILE_WRITE_ORDERED_END

Using explicit offsets

```
PROGRAM main
    include 'mpif.h'

    parameter (FILESIZE=1048576, MAX_BUFSIZE=1048576, INTSIZE=4)
    integer buf(MAX_BUFSIZE), rank, ierr, fh, nprocs, nints
    integer status(MPI_STATUS_SIZE), count
    integer (kind=MPI_OFFSET_KIND) offset

    call MPI_INIT(ierr)
    call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
    call MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)

    call MPI_FILE_OPEN(MPI_COMM_WORLD, '/pfs/datafile', &
      MPI_MODE_RDONLY, MPI_INFO_NULL,  fh, ierr)

    nints = FILESIZE/(nprocs*INTSIZE)
    offset = rank * nints * INTSIZE

    call MPI_FILE_READ_AT(fh, offset, buf, nints, MPI_INTEGER, status, ierr)
    call MPI_FILE_CLOSE(fh, ierr)
    call MPI_FINALIZE(ierr)
END PROGRAM main
```

Seeking to a file position

MPI_FILE_SEEK (fh, offset, whence)
INOUT fh: file handle (handle)
IN offset: file offset in byte (integer)
IN whence: update mode (state)

- Updates the individual file pointer according to whence, which can be:
  - MPI_SEEK_SET: the pointer is set to offset
  - MPI_SEEK_CUR: the pointer is set to the current pointer position plus offset
  - MPI_SEEK_END: the pointer is set to the end of the file plus offset
- offset can be negative, which allows seeking backwards
- offset should be a special integer:
  - MPI_Offset in C
  - KIND=MPI_OFFSET_KIND in FORTRAN

Querying the position

MPI_FILE_GET_POSITION (fh, offset)
IN fh: file handle (handle)
OUT offset: offset of the individual file pointer (integer)

- Returns in offset the current position of the individual file pointer
  - offset is in etype units relative to the current view
  - can be used to return to this position later using MPI_FILE_SEEK
- offset should be a special integer:
  - MPI_Offset in C
  - KIND=MPI_OFFSET_KIND in FORTRAN

Explicit offset – Write

MPI_FILE_WRITE_AT (fh, offset, buf, count, datatype, status)
IN fh: file handle (handle)
IN offset: file offset in byte (integer)
IN buf: destination buffer
IN count: number of read elements
IN datatype: MPI type of each element
OUT status: MPI status

- An explicit offset is given to determine access position
- The file pointer is neither used or incremented or modified
- Blocking, independent.

- Writes COUNT elements of DATATYPE from memory BUF to the file
- Starts writing at OFFSET units of etype from begin of view

Explicit offset – Read

MPI_FILE_READ_AT (fh, offset, buf, count, datatype, status)
IN fh: file handle (handle)
IN offset: file offset in byte (integer)
IN buf: destination buffer
IN count: number of read elements
IN datatype: MPI type of each element
OUT status: MPI status

- An explicit offset is given to determine access position
- The file pointer is neither used or incremented or modified
- Blocking, independent.

- reads COUNT elements of DATATYPE from FH to memory BUF
- Starts reading at OFFSET units of etype from begin of view

Shared file pointer – Write, Read

```
MPI_FILE_WRITE_SHARED (fh, buf, count, datatype, status)

MPI_FILE_READ_SHARED (fh, buf, count, datatype, status)
```

- Blocking, independent write/read using the shared file pointer
- Only the shared file pointer will be advanced accordingly
- DATATYPE is used as the access pattern to BUF
- Middleware will serialize accesses to the shared file pointer to ensure collision-free file access

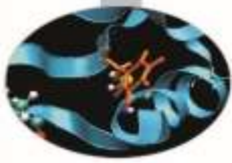
Seeking and querying the shared file pointer position

MPI_FILE_SEEK_SHARED(fh, offset, whence)

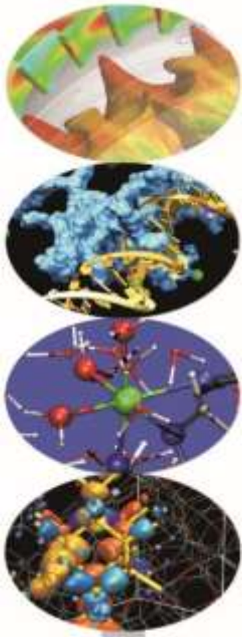
- Updates the individual file pointer according to **WHENCE** (MPI_SEEK_SET, MPI_SEEK_CUR, MPI_SEEK_END)
- **OFFSET** can be negative, which allows seeking backwards
- It is erroneous to seek to a negative position in the view
- The call is collective : all processes with the file handle have to participate

MPI_FILE_GET_POSITION_SHARED(fh, offset)

- Returns the current position of the individual file pointer in **OFFSET**
- The value can be used to return to this position or calculate a displacement
  - Do not forget to convert from offset to byte displacement if needed
- Call is not collective



MPI2-IO
Advanced Features



Advanced features of MPI-IO

- Basic MPI-IO features are not useful when
  - Data distribution is non contiguous in memory and/or in the file
    - e.g., ghost cells
    - e.g., block/cyclic array distributions
  - Multiple read/write operations for segmented data generate poor performances
- MPI-IO allow to access to data in different way:
  - non contiguous access on file: providing the access pattern to file (fileview)
  - non contiguous access in memory: setting new datatype
  - collective access: grouping multiple near accesses in one or more single accesses (decreasing the latency time)

File view

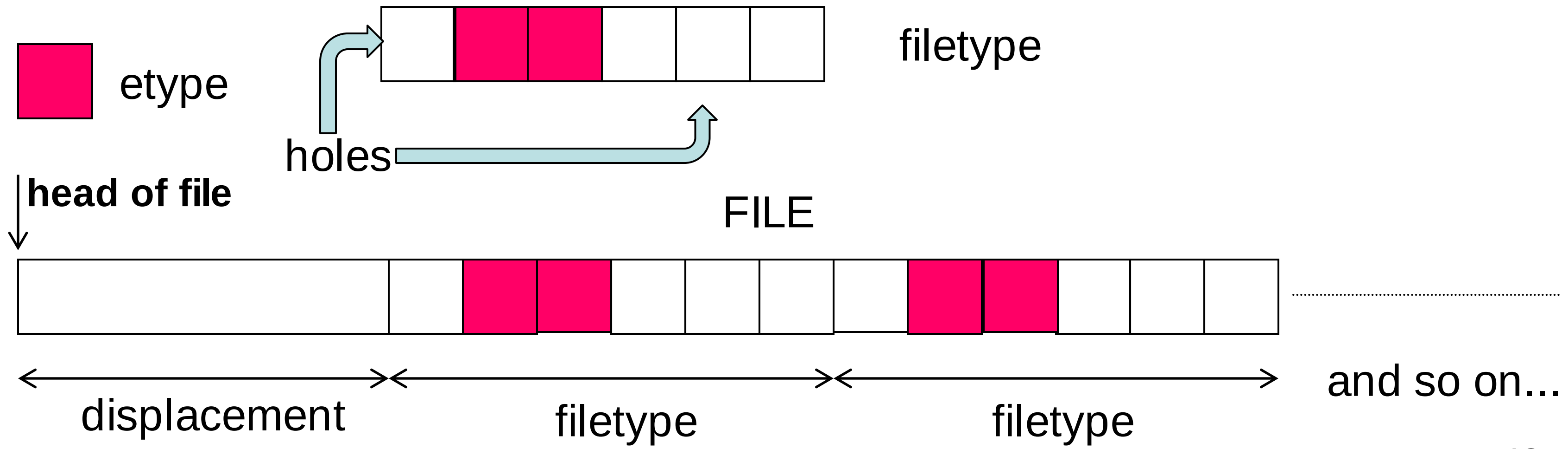
- A file view defines which portion of a file is “visible” to a process
- File view defines also the type of the data in the file (byte, integer, float, …)
- By default, file is treated as consisting of bytes, and process can access (read or write) any byte in the file
- A default view for each participating process is defined implicitly while opening the file
  - No displacement
  - The file has no specific structure (The elementary type is MPI_BYTE)
  - All processes have access to the complete file (The file type is MPI BYTE)

File View

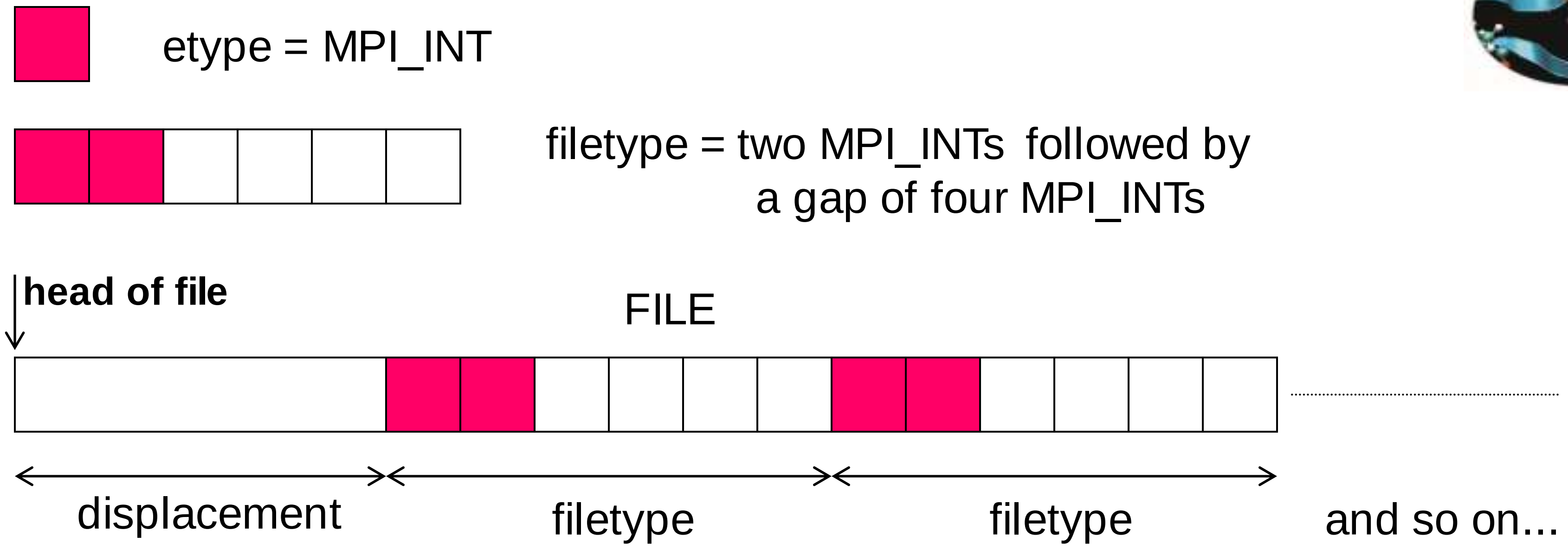
A file view consists of three components

- **displacement** : number of **bytes** to skip from the beginning of file
- **etype** : type of data accessed, defines unit for offsets
- **filetype** : base portion of file visible to process same as etype or MPI derived type consisting of etype

The pattern described by a filetype is repeated, beginning at the displacement, to define the view, as it happens when creating MPI_CONTIGUOUS or when sending more than one MPI datatype element: HOLES are important!



File View Example



- Define a file-view in order to have
  - fundamental access unit (etype) is MPI_INT
  - access pattern (fileytpe) is given by:
    - first 2 fundamental units
    - skips the next 4 fundamental units
  - skips the first part (5 integers) of the file (displacement)

File View

MPI_FILE_SET_VIEW(fh, disp, etype, filetype, datarep, info)

INOUT fh: file handle (handle)

IN disp: displacement from the start of the file, in bytes (integer)

IN etype: elementary datatype. It can be either a pre-defined or a derived datatype but it must have the same value on each process.(handle)

IN filetype: datatype describing each processes view of the file. (handle)

IN datarep: data representation (string)

IN info: info object (handle)

- It is used by each process to describe the layout of the data in the file
- All processes in the group must pass identical values for datarep and provide an etype with an identical extent
- The values for disp, filetype, and info may vary

Data Representation in File View

- Data representation: define the layout and data access modes (byte order, type sizes, etc.)
  - **native:** (default) use the memory layout with no conversion
  - no precision loss or conversion effort
    - not portable
  - **internal:** layout implementation-dependent
    - portable for the same MPI implementation
  - **external32:** standard defined by MPI (32-bit big-endian IEEE)
    - portable (architecture and MPI implementation)
    - some conversion overhead and precision loss
    - not always implemented (e.g. Blue Gene/Q)
- Using or internal and external32, the portability is guaranteed only if using the correct MPI datatypes (not using MPI_BYTE)
- **Note: to be portable the best and widespread choice is to use high-level libraries, e.g. HDF5 or NetCDF**

Passing hints to Filesystem

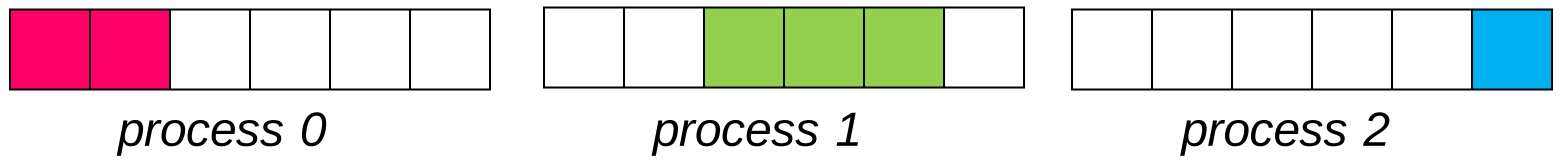
- MPI_File_set_view API allows the user to provide information on the features of the File System employed
  - optional (default: use MPI_INFO_NULL if you are not very expert)
  - may improve performances
    - depend on the MPI implementation

- Infos are objects created by MPI_Info_create
  - elements key-value
  - use MPI_Info_set to add elements

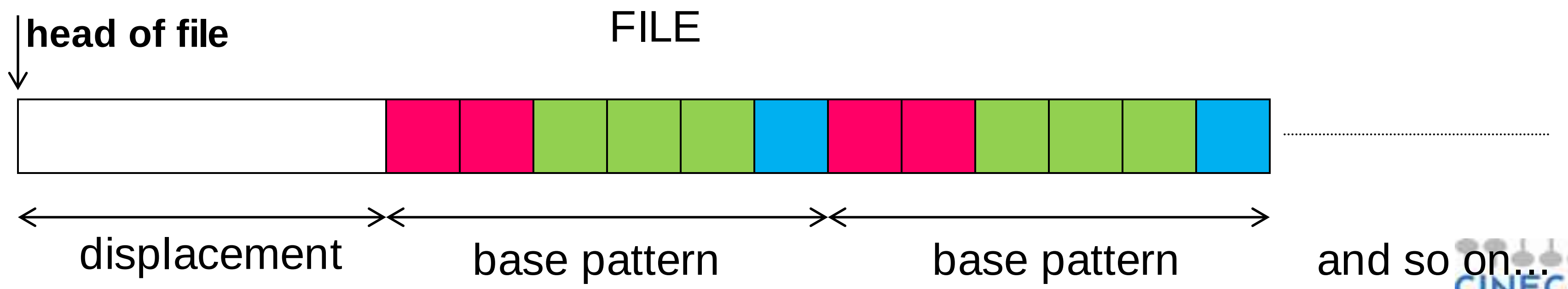
- ... refer to standard for more information and to manuals
  - e.g., consider ROMIO implementation of MPICH
  - specific infos for different file-systems (PFS, PVFS, GPFS, Lustre, ...)

Devising the I/O strategy

- Three main tasks:
  - let each process write to a different area without overlapping
  - repeat (indefinitely?) a certain basic pattern
  - write after an initial displacement
- Consider the following I/O pattern

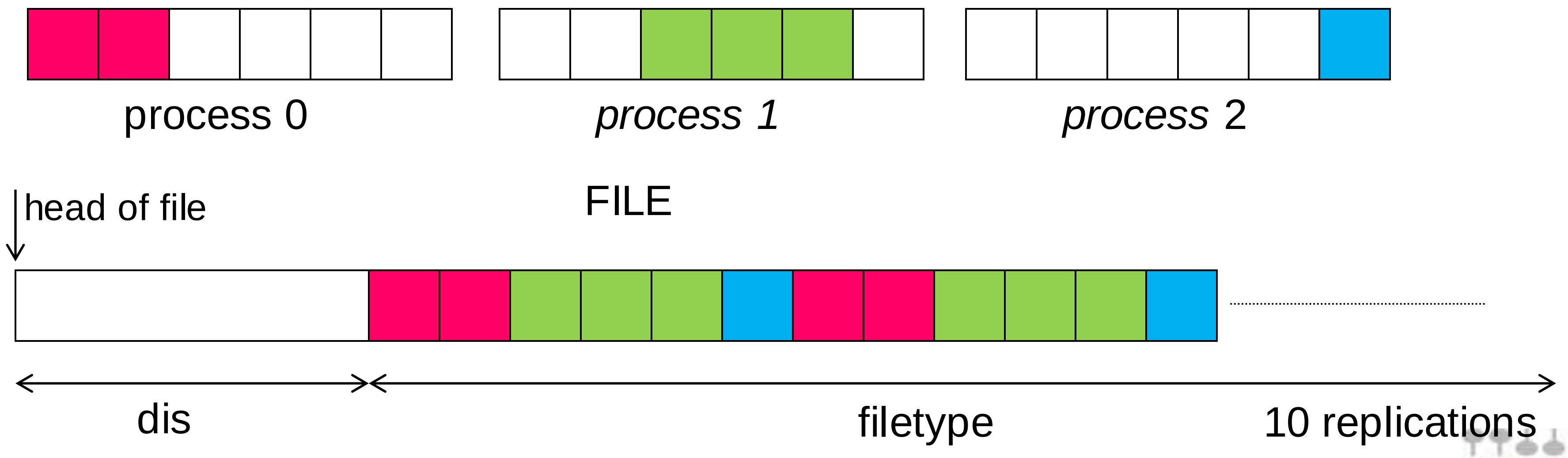


to be replicated a certain amount of (unknown?) times

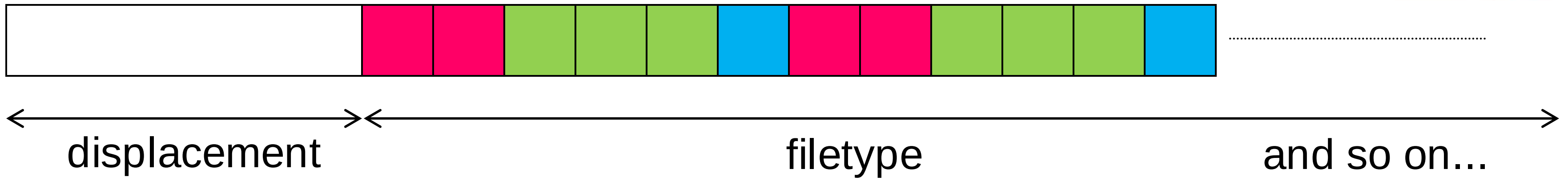


I strategy: data-type replication

- If the whole amount of basic patterns is known (e.g. 10)
  - define MPI vector with count=10, stride=6 and blocklength depending on the process:
    - P0 has 2 elements, P1 has 3 elements, and P2 has 1 element
  - define the file view using different displacements in addition to the base displacement *dis*: *dis*+0, *dis*+2 and *dis*+5



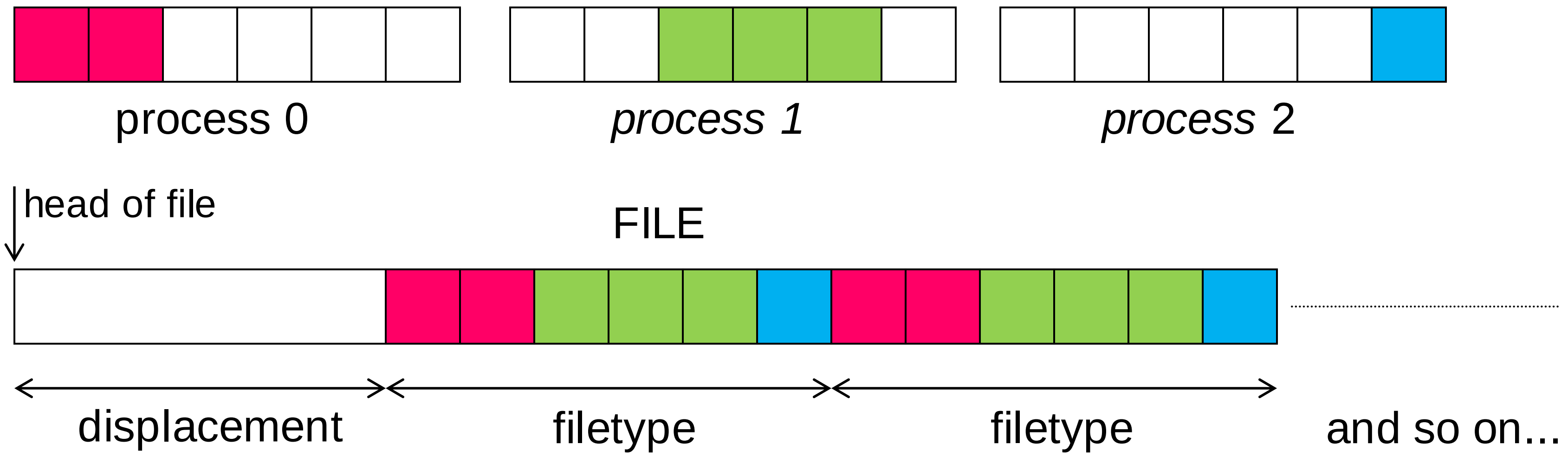
Use data-type replication



```
int count_proc[]={2,3,1};
int count_disp[]={0,2,5};

MPI_Datatype vect_t;
MPI_Type_vector(DIM_BUF, count_proc[myrank], 6, MPI_INT, &vect_t);
MPI_Type_commit(&vect_t);

int size_int;
MPI_Type_size(MPI_INT,&size_int);
offset = (MPI_Offset)count_disp[myrank]*size_int;

MPI_File_set_view(fh,offset,MPI_INT,vect_t, "native",MPI_INFO_NULL);
MPI_File_write(fh, buf, my_dim_buf, MPI_INT, &mystatus);
```

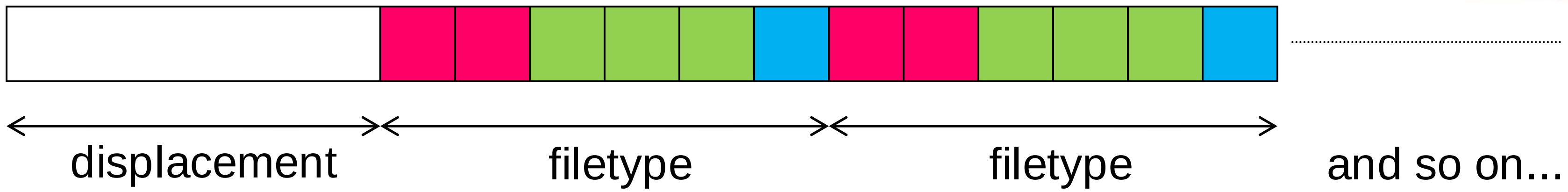
II strategy: file view replication

- If the whole amount of basic patterns is unknown, it is possible to exploit the replication mechanism of the MPI file view
  - define MPI contiguous with lengths 2, 3 and 1, respectively
  - resize the types adding holes (on the right only)
  - set the file view with displacements to balance the left holes



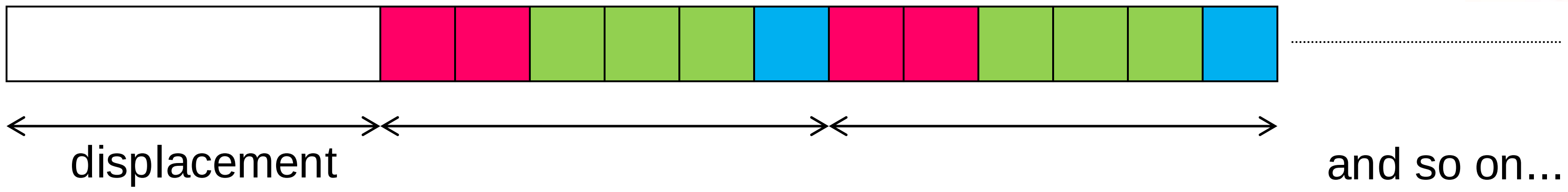
- When writing more than a filetype, a replication occurs; as it happens when sending more than one data, setting the holes is crucial!

Use file view replication



```
MPI_Datatype cont_t;
MPI_Type_contiguous(count_proc[myrank], MPI_INT, &cont_t);
MPI_Type_commit(&cont_t);

int size_int;
MPI_Type_size(MPI_INT,&size_int);

MPI_Datatype filetype;
MPI_Type_create_resized(cont_t, 0, 6*size_int, &filetype);
MPI_Type_commit(&filetype);

offset = (MPI_Offset)count_disp[myrank]*size_int;

MPI_File_set_view(fh, offset, MPI_INT, filetype, "native", MPI_INFO_NULL);

MPI_File_write(fh, buf, my_dim_buf, MPI_INT, &mystatus);
```

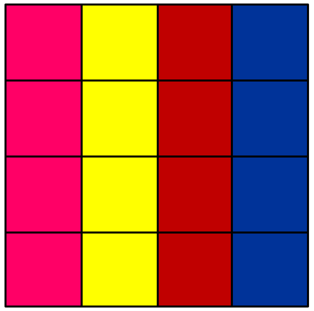
How to replicate patterns?

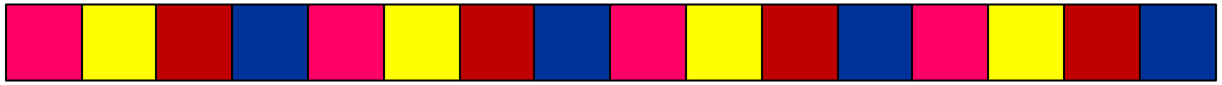


Which is the best replication strategy?

- **If possible, data-type replication is probably better (just one operation)**
- **Surely, easier to be implemented**
- **But exploiting file view replication is mandatory when then number of read/writes is not known *a priori***

Non-contiguous access: with known replication pattern



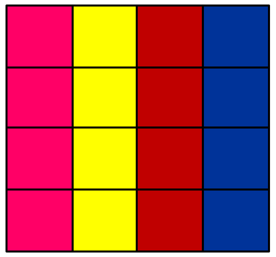


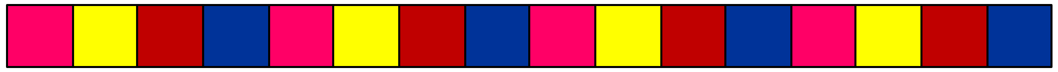
File written per row

2D-array distributed column-wise

- Each process has to access small pieces of data scattered throughout a file
- Very expensive if implemented with separate reads/writes
- Use file type to implement the non-contiguous access
- Again, employ data-type replication mechanism

Non-contiguous access: with known replication pattern





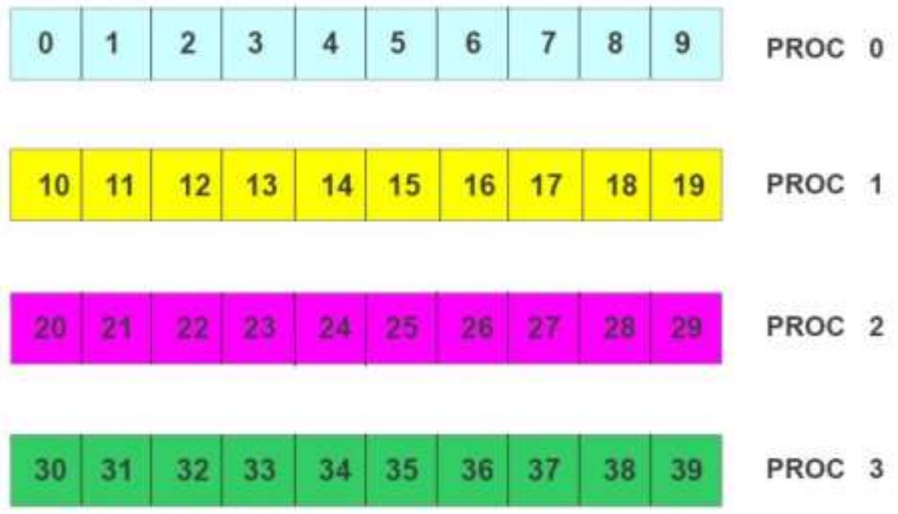
File written per row

2D-array distributed column-wise

```
...
INTEGER :: count = 4
INTEGER, DIMENSION(count) :: buf
...
CALL MPI_TYPE_VECTOR(4, 1, 4, MPI_INTEGER, filetype, err)
CALL MPI_TYPE_COMMIT(&filetype, err)
disp = myid * intsize
CALL MPI_FILE_SET_VIEW(file, disp, MPI_INTEGER, filetype,
   "native", MPI_INFO_NULL, err)
CALL MPI_FILE_WRITE(file, buf, count,MPI_INTEGER, status, err)
```

Hands-on 1: MPI-I/O basics

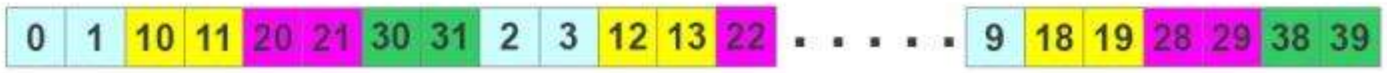
- Write a MPI code where each process stores the following memory layout



- Write a code that writes and reads a binary file in parallel according to the following three steps

Hands-on 1: MPI-I/O basics

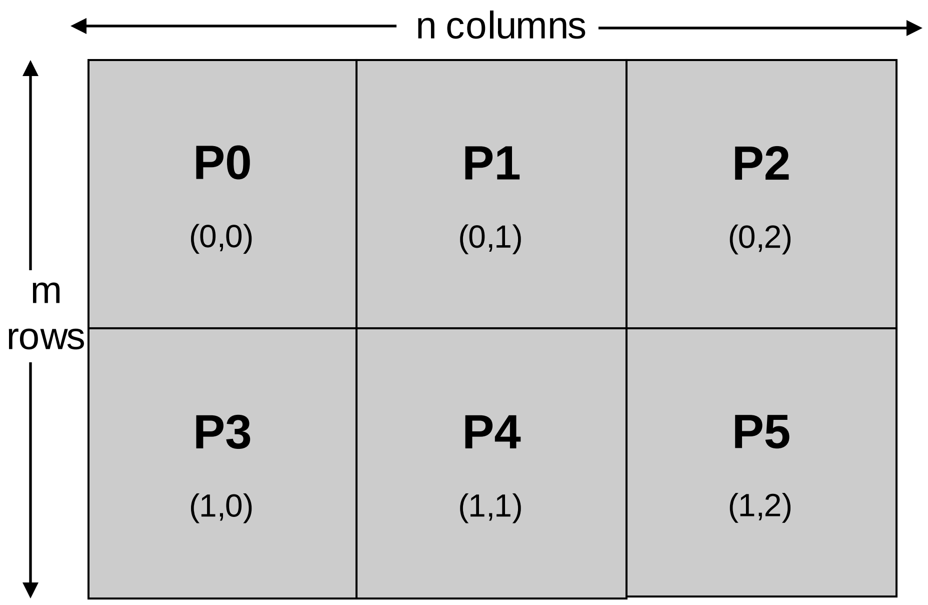
1. First process writes integers 0-9 from the beginning of the file, the second process writes integer 10-19 from the position 10 in the file and so on. Use the individual file pointers.
2. Re-open the file. Each process reads the data just written by using an explicit offset. Check that the reading has been performed correctly.
3. Each process writes the data just read, according to the following pattern (assuming that there are 4 processors):



- Check the result using the shell command:

```
od –i output.dat
```

Non-contiguous access: distributed matrix



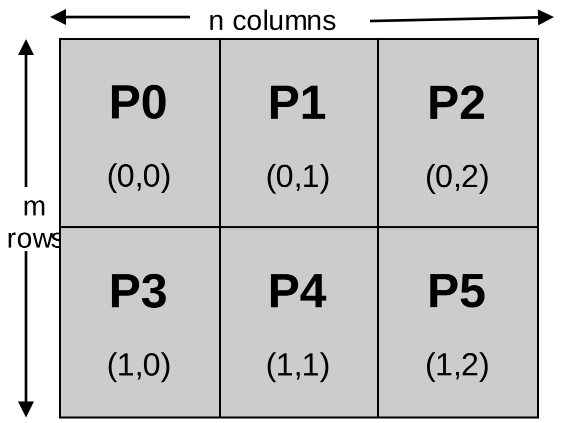
- 2D array, size (m,n) distributed among six processes
- cartesian layout 2x3

- When distributing multi-dimensional arrays among processes, we want to write files which are independent of the decomposition
  - written according to a usual serial order
    in row major order (C) or column major order (Fortran)
- The datatype SUBARRAY may easily handle this situation

Non-contiguous access: distributed matrix

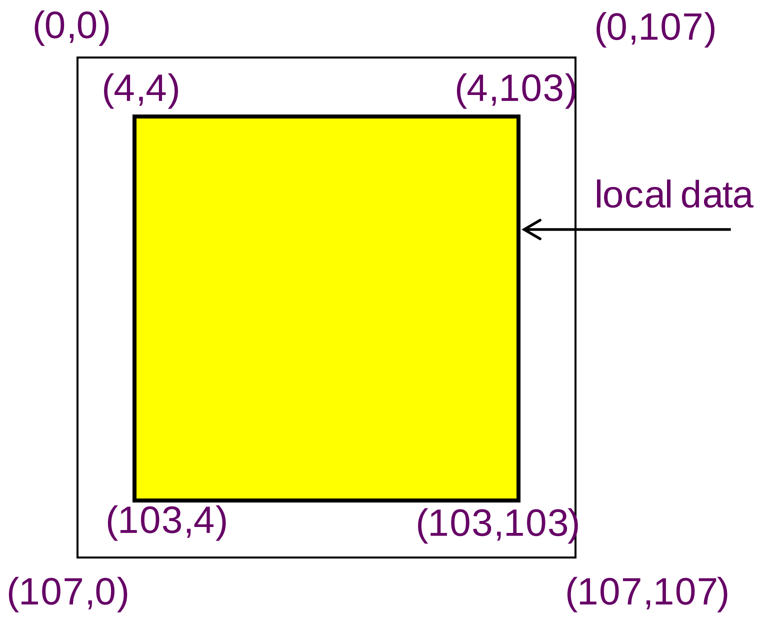
```
gsizes[0] = m;  /* no. of rows in global array */
gsizes[1] = n;  /* no. of columns in global array*/

psizes[0] = 2;  /* no. of procs. in vertical dimension */
psizes[1] = 3;  /* no. of procs. in horizontal dimension */

lsizes[0] = m/psizes[0];   /* no. of rows in local array */
lsizes[1] = n/psizes[1];   /* no. of columns in local array */

MPI_Cart_coords(comm, rank, 2, coords);

/* global indices of first element of local array */
start_indices[0] = coords[0] * lsizes[0];
start_indices[1] = coords[1] * lsizes[1];

MPI_Type_create_subarray(2, gsizes, lsizes, start_indices,
                      MPI_ORDER_C, MPI_FLOAT, &filetype);
MPI_Type_commit(&filetype);
```

Non-contiguous access: distributed matrix



```
/* create filetype and set fileview as in subarray example */
MPI_Type_create_subarray(2, gsizes, lsizes, start_indices,
                      MPI_ORDER_C, MPI_FLOAT, &filetype);
MPI_Type_commit(&filetype);


/* write local data as one big new datatype */
MPI_File_write(fh, local_array, 1, MPI_FLOAT, &status);

...

MPI_File(&fh, &status);
```

Ghost cells, typical case



- local array with sizes (100,100) allocated with sizes (108,108) to store
- ghost areas along edges
- ghost area are filled with neighbouring processes data
- local data are stored from position (4,4)
- non-contiguous memory access is needed

- Local data may be considered as a subarray
- Using MPI_Type_create_subarray we can filter the local data creating a subarray
- This type will be used as access basic type to communicate or to perform I/O

Ghost cells, typical case

```
/* create a derived datatype describing the layout of local array in memory buffer that
     includes ghosts .This is just another sub-array datatype! */
memsizes[0] = lsizes[0] + 8; /* rows in allocated array */
memsizes[1] = lsizes[1] + 8; /* columns in allocated array */

/* indices of first local elements in the allocated array */
start_indices[0] = start_indices[1] = 4;

MPI_Type_create_subarray(2, memsizes, lsizes, start_indices,
        MPI_ORDER_C, MPI_FLOAT, &memtype);
MPI_Type_commit(&memtype);

/* create filetype and set fileview as in subarray example */
...
/* write local data as one big new datatype */
MPI_File_write_all(fh, local_array, 1, memtype, &status);
```

MPI-IO Performance Tests on GALILEO GPFS /gpfs/scratch1

process grid	master/ slave	MPI-IO independent (min / max)	MPI-IO collective	MPI-IO collective (pernode)
1x1		0.5	0.5	0.5
2x1	15,2	0,5 - 1,0	1,2	0,8
2x2	34,4	5,5 - 13,3	3,2	1,5
4x2	74,3	17,2 - 26,2	6,2	2,9
4x4	143,7	44,7 - 62,3	15,6	6,0

MPI-IO raw write performance tests on CINECA GALILEO GPFS filesystem writing a distributed matrix of local size 16384x16384 of floats (1GB per process) on a grid of processes with different IO strategies: master/slave (only master process perform writes), MPI-IO (using independent writes on each process), MPI-IO collective (using collective writes) compiled with openmpi/1.10--gnu--4.9. Reported times are in seconds (less is better). Last column shows performance distributing first grid process dimension among different nodes.

Collective, blocking IO

IO can be performed **collectively** by all processes in a communicator

Same parameters as in independent IO functions (MPI_File_read etc)

- MPI_File_read_all
- MPI_File_write_all

- MPI_File_read_at_all
- MPI_File_write_at_all

- MPI_File_read_oredered
- MPI_File_write_ordered

All processes in communicator that opened file must call function

Performance potentially better than for individual functions

- Even if each processor reads a non-contiguous segment, in total the read is contiguous

Collective, blocking IO

```
int MPI_File_write_all(MPI_File fh, void *buf, int count, MPI_Datatype
datatype, MPI_Status *status)

int MPI_File_read_all( MPI_File mpi_fh, void *buf, int count,
MPI_Datatype datatype, MPI_Status *status )
```

- With collective IO **ALL** the processors defined in a communicator execute the IO operation
- This allows to optimize the read/write procedure
- It is particularly effective for non atomic operations

Independent, nonblocking IO

This is just like non blocking communication.

Same parameters as in blocking IO functions (MPI_File_read etc)

- MPI_File_iread
- MPI_File_iwrite
- MPI_File_iread_at
- MPI_File_iwrite_at
- MPI_File_iread_shared
- MPI_File_iwrite_shared

MPI_Wait must be used for synchronization.

Can be used to overlap IO with computation

Collective, nonblocking IO

For collective IO only a restricted form of nonblocking IO is supported, called Split Collective.

```
MPI_File_read_all_begin( MPI_File mpi_fh, void *buf, int count, MPI_Datatype datatype )

    …computation…

MPI_File_read_all_end( MPI_File mpi_fh, void *buf, MPI_Status *status );
```

- Collective operations may be split into two parts
- Only one active (pending) split or regular collective operation per file handle at any time
- Split collective operations do not match the corresponding regular collective operation
- Same BUF argument in _begin and _end calls

Consistency

- No consistency problems rise when there are no overlapping regions (bytes) accessed by any two processes
- MPI does *not* guarantee that data will automatically read correctly, when accesses of any two processes overlap in the file

```
MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh1)      MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh2)
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ... )     MPI_File_write_at(fh2, 100, buf, 100, MPI_BYTE, ... )
MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ... )    MPI_File_read_at (fh2, 0, buf, 100, MPI_BYTE, ... )
```

- The user must take care of consistency. There are three choices:
  - using *atomic* accesses
  - close and reopen the file
  - ensure that no "*write sequence*" on any process is concurrent with "*any sequence (read/write)*" on another process

Using Atomicity for Consistency

- Change file-access mode to atomic before the write on each process

- MPI guarantees that written data can be read immediately by another process

```
MPI_File_open(MPI_COMM_WORLD, “file”, ....., &fh1)      MPI_File_open(MPI_COMM_WORLD, “file”, ....., &fh2)
MPI_File_set_atomicity(fh1, 1)                          MPI_File_set_atomicity(fh2, 1)
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ... )     MPI_File_write_at(fh2, 100, buf, 100, MPI_BYTE, ... )
MPI_Barrier(MPI_COMM_WORLD)                             MPI_Barrier(MPI_COMM_WORLD)
MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ... )    MPI_File_read_at (fh2, 0, buf, 100, MPI_BYTE, ... )
```

- note: the *barrier* after the writes to ensure each process has completed its write before the read is issued from the other process

Close/Open file for Consistency

- Close the file and reopen just after write operations if other processes need data just written by other processes

```
MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh1)        MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh2)
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ... )       MPI_File_write_at(fh2, 100, buf, 100, MPI_BYTE, ... )
MPI_File_close(&fh1)                                      MPI_File_close(&fh2)
MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh1)        MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh2)
MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ... )      MPI_File_read_at (fh2, 0, buf, 100, MPI_BYTE, ... )
```

- note: each file open operation will create a different MPI context context will be cleared after each close operation

Understanding IO Sequences

- An IO sequence is defined as a set of file operations bracketed by any pair of the functions MPI_File_open, MPI_File_close, MPI_File_sync
- A sequence is a "*write sequence*" if contains *write* operations
- MPI guarantees that the data written by a process can be read by another process if the "*write sequence*" is not concurrent (in time) with any sequence on any other process

```
MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh1)      MPI_File_open(MPI_COMM_WORLD, "file", ....., &fh2)
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ... )
MPI_File_sync(&fh1)                                      MPI_File_sync(&fh2)

MPI_Barrier(MPI_COMM_WORLD)                              MPI_Barrier(MPI_COMM_WORLD)

MPI_File_sync(&fh1)                                      MPI_File_sync(&fh21)
                                                         MPI_File_write_at(fh12, 0, buf, 100, MPI_BYTE, ... )
MPI_File_sync(&fh1)                                      MPI_File_sync(&fh2)

MPI_Barrier(MPI_COMM_WORLD)                              MPI_Barrier(MPI_COMM_WORLD)

MPI_File_sync(&fh1)                                      MPI_File_sync(&fh2)
MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ... )     MPI_File_read_at(fh2, 0, buf, 100, MPI_BYTE, ... )
MPI_File_close(&fh1)                                     MPI_File_close(&fh2)
```

Use cases

1. **Each process has to read in the complete file**
    - Solution: MPI_FILE_READ_ALL
        - Collective with individual file pointers, same view (displacement, etype, filetype) on all processes
        - Internally: read in once from disk by several processes (striped), then distributed broadcast

2. **The file contains a list of tasks, each task requires a different amount of computing time**
    - Solution: MPI_FILE_READ_SHARED
        - Non-collective with a shared file pointer
        - Same view on all processes (mandatory)

Use cases

3. The file contains a list of tasks, each task requires the same amount of computing time

Solution A : MPI_FILE_READ_ORDERED

- Collective with a shared file pointer
- Same view on all processes (mandatory)

Solution B : MPI_FILE_READ_ALL

- Collective with individual file pointers
- Different views: filetype with MPI_TYPE_CREATE_SUBARRAY

Internally: both may be implemented in the same way.

Use cases

4. The file contains a matrix, distributed block partitioning, each process reads a block

Solution: generate different filetypes with MPI_TYPE_CREATE_DARRAY

- The view of each process represents the block that is to be read by this process
- MPI_FILE_READ_AT_ALL with OFFSET=0
- Collective with explicit offset
- Reads the whole matrix collectively
- Internally: contiguous blocks read in by several processes (striped), then distributed with all-to-all.

5. Each process has to read the complete file

Solution: MPI_FILE_READ_ALL_BEGIN/END

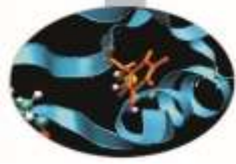
- Collective with individual file pointers
- Same view (displacement, etype, filetype) on all processes
- Internally: asynchronous read by several processes (striped) started, data distributed with bcast when striped reading has finished

Best Practices

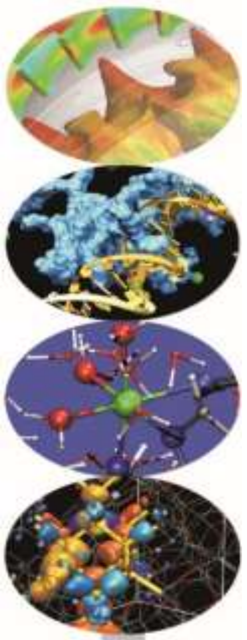
- When designing your code, think I/O carefully!
  - maximize the parallelism
  - if possible, use a single file as restart file and simulation output
  - minimize the usage of formatted output (do you actually need it?)
- Minimize the latency of file-system access
  - maximize the sizes of written chunks
  - use collective functions when possible
  - use derived datatypes for non-contiguous access
- If you are patient, read MPI standards, MPI-2.x or MPI-3.x
- Employ powerful and well-tested libraries based on MPI-I/O:
  - HDF5 or NetCDF

Useful links

- Using Advanced MPI (W.Gropp, T.Hoefler, E.Lusk, R.Thakur - 2014, MIT Press)
- Standard MPI-3.x
(http://www.mpi-forum.org/docs)
- Users Guide for ROMIO (Thakur, Ross, Lusk, Gropp, Latham)
- ... a bit of advertising:
corsi@cineca.it (http://www.hpc.cineca.it)
- ...practice practice practice



QUESTIONS ???



Hands-on 2: MPI-I/O & subarrays

- Write a program which decomposes an integer matrix (m x n) using a 2D MPI Cartesian grid
  - Handle the remainders for non multiple sizes
  - Fill the matrix with the row-linearized indexes

$$A_{ij} = m \cdot i + j$$

11	12	13
14	15	16
17	18	19
20	21	22

  - Reconstruct the absolute indexes from the local ones
  - Remember that in C the indexes of arrays start from 0

- Writes to file the matrix using MPI-I/O collective write and using MPI data-types
  - Which data-type do you have to use?

Hands-on 2: MPI-I/O & subarrays

- Check the results using:
  - Shell Command

    ```
    od -i output.dat
    ```
  - Parallel MPI-I/O read functions (similar to write structure)
  - Serial standard C and Fortran check
    - only rank=0 performs check
    - read row-by-row in C and column-by-column in Fortran and check each element of the row/columns
    - use binary files and fread in C
    - use unformatted and access='stream' in Fortran

- Which one is the most scrupoulous check?
  - is the Parallel MPI-I/O check sufficient?

Rights & Credits

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