PARALLEL I/O WITH MPI

March 14 2018 | Benedikt Steinbusch | Jülich Supercomputing Centre

Part I: Introduction

FEATURES OF MPI I/O

- Standardized I/O API since 1997
- Available in many MPI libraries
- Language bindings for C and Fortran
- Re-uses MPI's concepts for the description of data
- Allows portable and efficient implementation of parallel I/O operations due to support for
  - multiple data representations
  - asynchronous I/O
  - non-contiguous file access patterns
  - collective file access
  - MPI Info Objects

PREREQUISITES

You should be familiar with MPI, especially with

Processes and Ranks	An MPI program is executed by multiple processes in parallel. Processes are identified by ranks (0, 1, …)
Communicator	Combines a group of processes and a context for communication.
Blocking and Nonblocking	Provide different guarantees to the user / different liberties to the MPI library.
P2P and Collective Communication	Communication among pairs or groups of processes
Derived Datatypes	Descriptions of data layouts
MPI Info Objects	Key-value maps that can be used to provide hints

LITERATURE & ACKNOWLEDGEMENTS

Literature

- Message Passing Interface Forum. *MPI: A Message-Passing Interface Standard*. Version 3.1. June 4, 2015. URL: http://mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf
- William Gropp, Ewing Lusk, and Anthony Skjellum. *Using MPI. Portable Parallel Programming with the Message-Passing Interface*. 3rd ed. The MIT Press, Nov. 2014. 336 pp. ISBN: 9780262527392
- William Gropp et al. *Using Advanced MPI. Modern Features of the Message-Passing Interface*. 1st ed. Nov. 2014. 392 pp. ISBN: 9780262527637
- http://www.mpi-forum.org

Acknowledgements

- Rolf Rabenseifner for his comprehensive course on MPI and OpenMP
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LANGUAGE BINDINGS [MPI-3.1, 17, A]

C Language Bindings

C
```
#include <mpi.h>
```

Fortran Language Bindings

Consistent with F08 standard; good type-checking; highly recommended

F08
```
use mpi_f08
```

Not consistent with standard; so-so type-checking; not recommended

F90
```
use mpi
```

Not consistent with standard; no type-checking; strongly discouraged

F77
```
include 'mpif.h'
```

FORTRAN HINTS [MPI-3.1, 17.1.2 – 17.1.4]

This course uses the Fortran 2008 MPI interface (**`use`** `mpi_f08`) which is not available in all MPI implementations. The Fortran 90 bindings differ from the Fortran 2008 bindings in the following points:

- All derived **`type`** arguments are instead **`integer`** (some are arrays of **`integer`** or have a non-default `kind`)
- Argument **`intent`** is not mandated by the Fortran 90 bindings
- The `ierror` argument is mandatory instead of **`optional`**
- Further details can be found in [MPI-3.1, 17.1]

Part II: File Operations

FILE, FILE POINTER & HANDLE [MPI-3.1, 13.1]

File
An MPI file is an ordered collection of typed data items.

File Pointer
A file pointer is an implicit offset into a file maintained by MPI.

File Handle
An opaque MPI object. All operations on an open file reference the file through the file handle.

OPENING A FILE [MPI-3.1, 13.2.1]

C
```
int MPI_File_open(MPI_Comm comm, const char* filename,
↪  int amode, MPI_Info info, MPI_File* fh)
```

F08
```
MPI_File_open(comm, filename, amode, info, fh, ierror)
type(MPI_Comm), intent(in) :: comm
character(len=*), intent(in) :: filename
integer, intent(in) :: amode
type(MPI_Info), intent(in) :: info
type(MPI_File), intent(out) :: fh
integer, optional, intent(out) :: ierror
```

- Collective operation on communicator `comm`
- Filename must reference the same file on all processes
- Process-local files can be opened using `MPI_COMM_SELF`
- `info` object specifies additional information (`MPI_INFO_NULL` for empty)

ACCESS MODE [MPI-3.1, 13.2.1]

`amode` denotes the access mode of the file and must be the same on all processes. It *must* contain exactly one of the following:

`MPI_MODE_RDONLY`	read only access
`MPI_MODE_RDWR`	read and write access
`MPI_MODE_WRONLY`	write only access

and may contain some of the following:

`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 is not opened elsewhere
`MPI_MODE_SEQUENTIAL`	access to the file is sequential
`MPI_MODE_APPEND`	file pointers are set to the end of the file

Combine using bit-wise or (`|` operator in C, `ior` intrinsic in Fortran).

CLOSING A FILE [MPI-3.1, 13.2.2]

C
```
int MPI_File_close(MPI_File* fh)
```

F08
```
MPI_File_close(fh, ierror)
type(MPI_File), intent(out) :: fh
integer, optional, intent(out) :: ierror
```

- Collective operation
- User must ensure that all outstanding nonblocking and split collective operations associated with the file have completed

DELETING A FILE [MPI-3.1, 13.2.3]

C
```
int MPI_File_delete(const char* filename, MPI_Info info)
```

F08
```
MPI_File_delete(filename, info, ierror)
character(len=*), intent(in) :: filename
type(MPI_Info), intent(in) :: info
integer, optional, intent(out) :: ierror
```

- Deletes the file identified by `filename`
- File deletion is a local operation and should be performed by a single process
- If the file does not exist an error is raised
- If the file is opened by any process
  - all further and outstanding access to the file is implementation dependent
  - it is implementation dependent whether the file is deleted; if it is not, an error is raised

FILE PARAMETERS

Setting File Parameters	
MPI_File_set_size	Set the size of a file [MPI-3.1, 13.2.4]
MPI_File_preallocate	Preallocate disk space [MPI-3.1, 13.2.5]
MPI_File_set_info	Supply additional information [MPI-3.1, 13.2.8]

Inspecting File Parameters	
MPI_File_get_size	Size of a file [MPI-3.1, 13.2.6]
MPI_File_get_amode	Acess mode [MPI-3.1, 13.2.7]
MPI_File_get_group	Group of processes that opened the file [MPI-3.1, 13.2.7]
MPI_File_get_info	Additional information associated with the file [MPI-3.1, 13.2.8]

I/O ERROR HANDLING [MPI-3.1, 8.3, 13.7]

Communication, by default, aborts the program when an error is encountered. I/O operations, by default, return an error code.

C
```
int MPI_File_set_errhandler(MPI_File file, MPI_Errhandler
↪  errhandler)
```

F08
```
MPI_File_set_errhandler(file, errhandler, ierror)
type(MPI_File), intent(in) :: file
type(MPI_Errhandler), intent(in) :: errhandler
integer, optional, intent(out) :: ierror
```

- The default error handler for files is `MPI_ERRORS_RETURN`
- Success is indicated by a return value of `MPI_SUCCESS`
- `MPI_ERRORS_ARE_FATAL` aborts the program
- Can be set for each file individually or for all files by setting the error handler on `MPI_FILE_NULL`

FILE VIEW [MPI-3.1, 13.3]

File View
A file view determines what part of the contents of a file is visible to a process. It is defined by a *displacement* (given in bytes) from the beginning of the file, an *elementary datatype* and a *file type*. The view into a file can be changed multiple times between opening and closing.

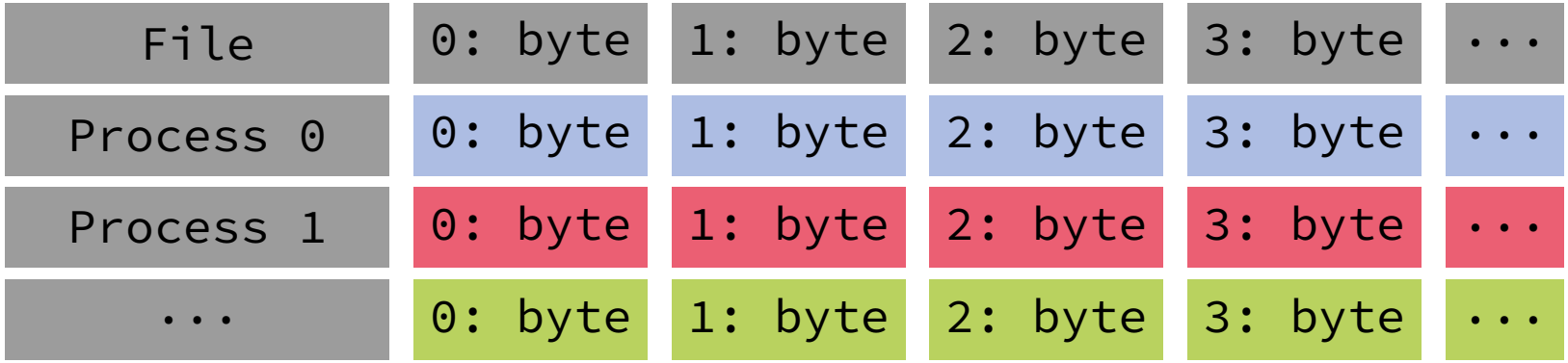
File Types and Elementary Types are Data Types

• Can be predefined or derived
• The usual constructors can be used to create derived file types and elementary types, e.g.
  • `MPI_Type_indexed`,
  • `MPI_Type_create_struct`,
  • `MPI_Type_create_subarray`
• Displacements in their typemap must be non-negative and monotonically nondecreasing
• Have to be committed before use

DEFAULT FILE VIEW [MPI-3.1, 13.3]

When newly opened, files are assigned a default view that is the same on all processes:

- Zero displacement
- File contains a contiguous sequence of bytes
- All processes have access to the entire file



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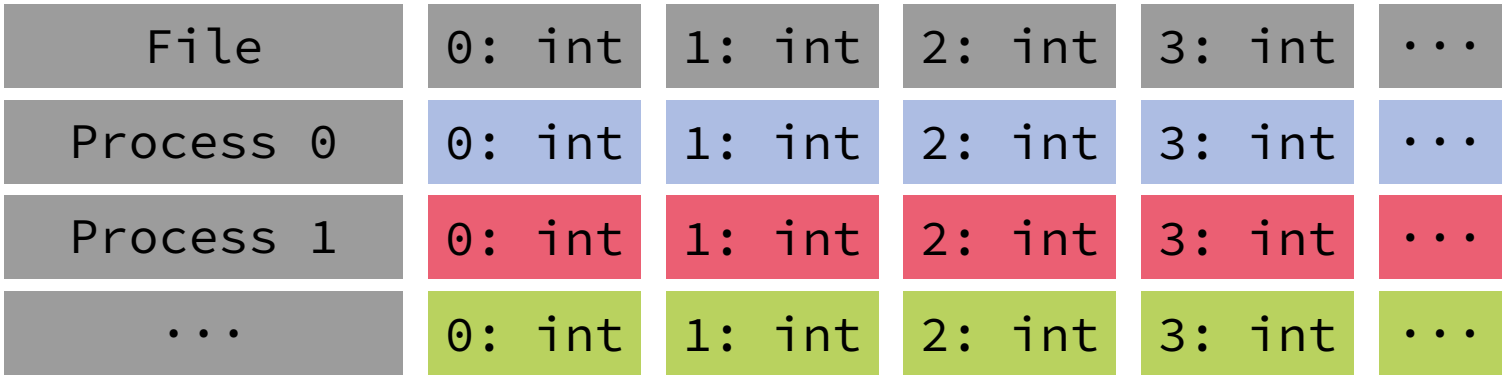
ELEMENTARY TYPE [MPI-3.1, 13.3]

Elementary Type
An elementary type (or *etype*) is the unit of data contained in a file. Offsets are expressed in multiples of etypes, file pointers point to the beginning of etypes. Etypes can be basic or derived.

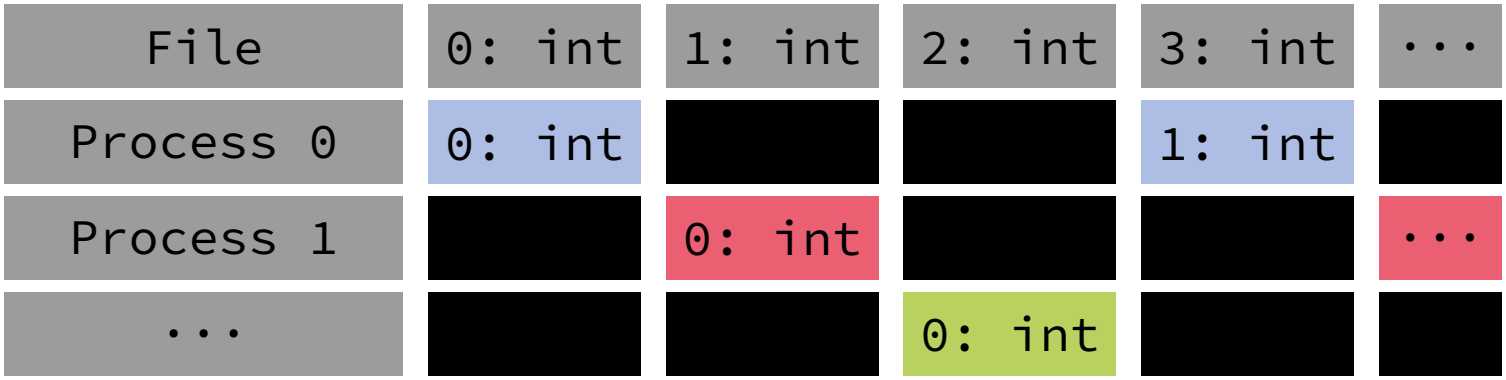
Changing the Elementary Type
E.g. `etype = MPI_INT`:



FILE TYPE [MPI-3.1, 13.3]

File Type
A file type describes an access pattern. It can contain either instances of the *etype* or holes with an extent that is divisible by the extent of the etype.

Changing the File Type
E.g. $\mathit{Filetype}_0 = \{(\mathit{int}, 0), (\mathit{hole}, 4), (\mathit{hole}, 8)\}$, $\mathit{Filetype}_1 = \{(\mathit{hole}, 0), (\mathit{int}, 4), (\mathit{hole}, 8)\}$, ...:



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CHANGING THE FILE VIEW [MPI-3.1, 13.3]

C

```
int MPI_File_set_view(MPI_File fh, MPI_Offset disp,
↪  MPI_Datatype etype, MPI_Datatype filetype, const
↪  char* datarep, MPI_Info info)
```

F08

```
MPI_File_set_view(fh, disp, etype, filetype, datarep,
↪  info, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: disp
type(MPI_Datatype), intent(in) :: etype, filetype
character(len=*), intent(in) :: datarep
type(MPI_Info), intent(in) :: info
integer, optional, intent(out) :: ierror
```

- Collective operation
- `datarep` and extent of `etype` must match
- `disp`, `filetype` and `info` can be distinct
- File pointers are reset to zero
- May not overlap with nonblocking or split collective operations

DATA REPRESENTATION [MPI-3.1, 13.5]

- Determines the conversion of data in memory to data on disk
- Influences the interoperability of I/O between heterogeneous parts of a system or different systems

`"native"`
Data is stored in the file exactly as it is in memory + No loss of precision + No overhead - On heterogeneous systems loss of transparent interoperability

DATA REPRESENTATION [MPI-3.1, 13.5]

`"internal"`
Data is stored in implementation-specific format + Can be used in a homogeneous *and* heterogeneous environment + Implementation will perform conversions if necessary - Can incur overhead - Not necessarily compatible between different implementations

`"external32"`
Data is stored in standardized data representation (big-endian IEEE) + Can be read/written also by non-MPI programs - Precision and I/O performance may be lost due to type conversions between `native` and `external32` representations - Not available in all implementations

DATA ACCESS

Three orthogonal aspects

1. Synchronism
    1. Blocking
    2. Nonblocking
    3. Split collective
2. Coordination
    1. Noncollective
    2. Collective
3. Positioning
    1. Explicit offsets
    2. Individual file pointers
    3. Shared file pointers

POSIX `read()` and `write()`
These are blocking, noncollective operations with individual file pointers.

SYNCHRONISM

Blocking I/O
Blocking I/O routines do not return before the operation is completed.

Nonblocking I/O
• Nonblocking I/O routines do not wait for the operation to finish • A separate completion routine is necessary [MPI-3.1, 3.7.3, 3.7.5] • The associated buffers must not be used while the operation is in flight

Split Collective
• ”Restricted” form of nonblocking collective • Buffers must not be used while in flight • Does not allow other collective accesses to the file while in flight • `begin` and `end` must be used from the same thread

COORDINATION

Noncollective
The completion depends only on the activity of the calling process.

Collective
• Completion may depend on activity of other processes • Opens opportunities for optimization

POSITIONING [MPI-3.1, 13.4.1 – 13.4.4]

Explicit Offset
• No file pointer is used • File position for access is given directly as function argument

Individual File Pointers
• Each process has its own file pointer • After access, pointer is moved to first *etype* after the last one accessed

Shared File Pointers
• All processes share a single file pointer • All processes must use the same file view • Individual accesses appear as if serialized (with an unspecified order) • Collective accesses are performed in order of ascending rank

		coordination	
positioning	**synchronism**	**noncollective**	**collective**
explicit offsets	blocking	`MPI_File_read_at` `MPI_File_write_at`	`MPI_File_read_at_all` `MPI_File_write_at_all`
	nonblocking	`MPI_File_iread_at` `MPI_File_iwrite_at`	`MPI_File_iread_at_all` `MPI_File_iwrite_at_all`

	split collective	N/A	`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`
	nonblocking	`MPI_File_iread` `MPI_File_iwrite`	`MPI_File_iread_all` `MPI_File_iwrite_all`

	split collective	N/A	`MPI_File_read_all_begin`
			`MPI_File_read_all_end`
			`MPI_File_write_all_begin`
			`MPI_File_write_all_end`

shared file pointers	blocking	`MPI_File_read_shared` `MPI_File_write_shared`	`MPI_File_read_ordered` `MPI_File_write_ordered`
	nonblocking	`MPI_File_iread_shared` `MPI_File_iwrite_shared`	N/A

	split collective	N/A	`MPI_File_read_ordered_begin`
			`MPI_File_read_ordered_end`
			`MPI_File_write_ordered_begin`
			`MPI_File_write_ordered_end`

WRITING

blocking, noncollective, explicit offset [MPI-3.1, 13.4.2]

C
```
int MPI_File_write_at(MPI_File fh, MPI_offset offset,
↪  const void* buf, int count, MPI_Datatype datatype,
↪  MPI_Status *status)
```

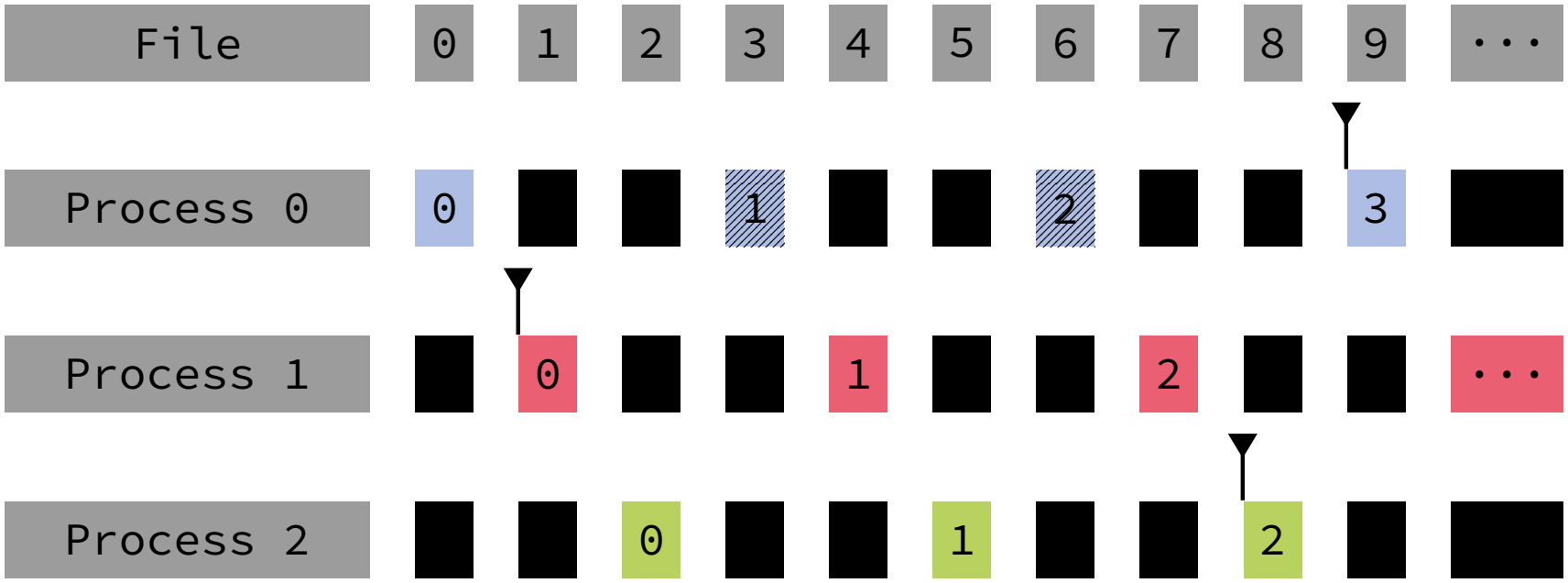
F08
```
MPI_File_write_at(fh, offset, buf, count, datatype,
↪  status, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: offset
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
integer, optional, intent(out) :: ierror
```

- Starting offset for access is explicitly given
- No file pointer is updated
- Writes `count` elements of `datatype` from memory starting at `buf`
- *Typesig*(`datatype`) = *Typesig*(*etype*) . . . *Typesig*(*etype*)
- Writing past end of file increases the file size

EXAMPLE

blocking, noncollective, explicit offset [MPI-3.1, 13.4.2]

Process 0 calls `MPI_File_write_at(offset = 1, count = 2)`:



WRITING

blocking, noncollective, individual [MPI-3.1, 13.4.3]

C

```
int MPI_File_write(MPI_File fh, const void* buf, int
↪  count, MPI_Datatype datatype, MPI_Status* status)
```

F08

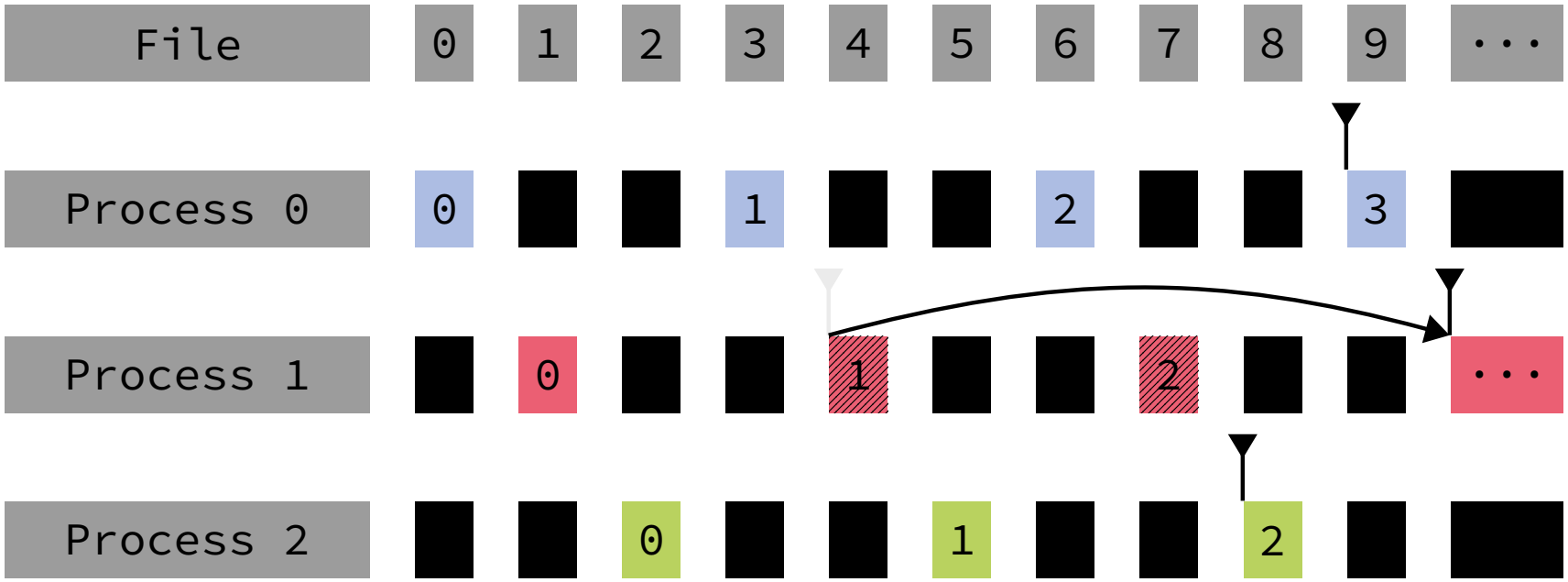
```
MPI_File_write(fh, buf, count, datatype, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Starts writing at the current position of the individual file pointer
- Moves the individual file pointer by the count of *etypes* written

EXAMPLE

blocking, noncollective, individual [MPI-3.1, 13.4.3]

With its file pointer at element 1, process 1 writes `count = 2`:



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WRITING

nonblocking, noncollective, individual [MPI-3.1, 13.4.3]

C

```
int MPI_File_iwrite(MPI_File fh, const void* buf, int
↪  count, MPI_Datatype datatype, MPI_Request* request)
```

F08

```
MPI_File_iwrite(fh, buf, count, datatype, request,
↪  ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Request), intent(out) :: request
integer, optional, intent(out) :: ierror
```

- Starts the same operation as `MPI_File_write` but does not wait for completion
- Returns a `request` object that is used to complete the operation

WRITING

blocking, collective, individual [MPI-3.1, 13.4.3]

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

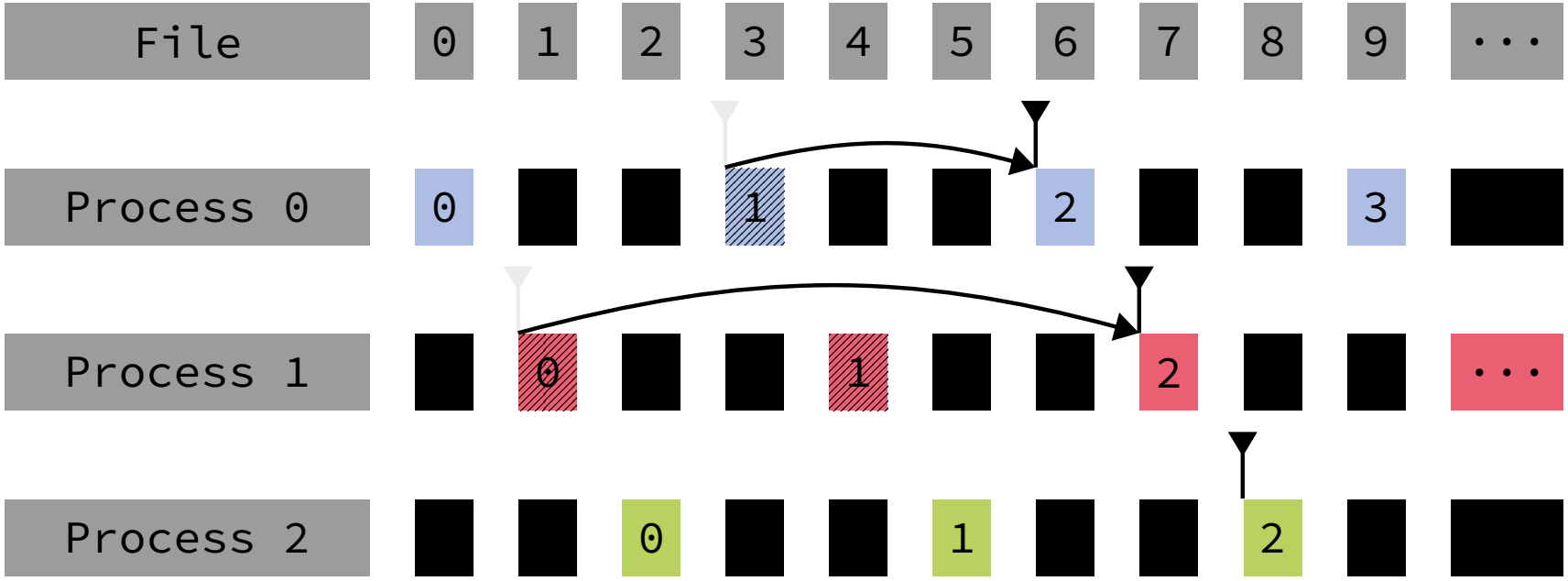
F08
```
MPI_File_write_all(fh, buf, count, datatype, status,
↪  ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Same signature as `MPI_File_write`, but collective coordination
- Each process uses its individual file pointer
- MPI can use communication between processes to funnel I/O

EXAMPLE

blocking, collective, individual [MPI-3.1, 13.4.3]

- With its file pointer at element 1, process 0 writes `count = 1`,
- With its file pointer at element 0, process 1 writes `count = 2`,
- With its file pointer at element 2, process 2 writes `count = 0`:



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WRITING

split-collective, individual [MPI-3.1, 13.4.5]

C

```
int MPI_File_write_all_begin(MPI_File fh, const void* buf,
↪  int count, MPI_Datatype datatype)
```

F08

```
MPI_File_write_all_begin(fh, buf, count, datatype,
↪  ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
integer, optional, intent(out) :: ierror
```

- Same operation as `MPI_File_write_all`, but split-collective
- `status` is returned by the corresponding end routine

WRITING

split-collective, individual [MPI-3.1, 13.4.5]

C
```
int MPI_File_write_all_end(MPI_File fh, const void* buf,
↪  MPI_Status* status)
```

F08
```
MPI_File_write_all_end(fh, buf, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

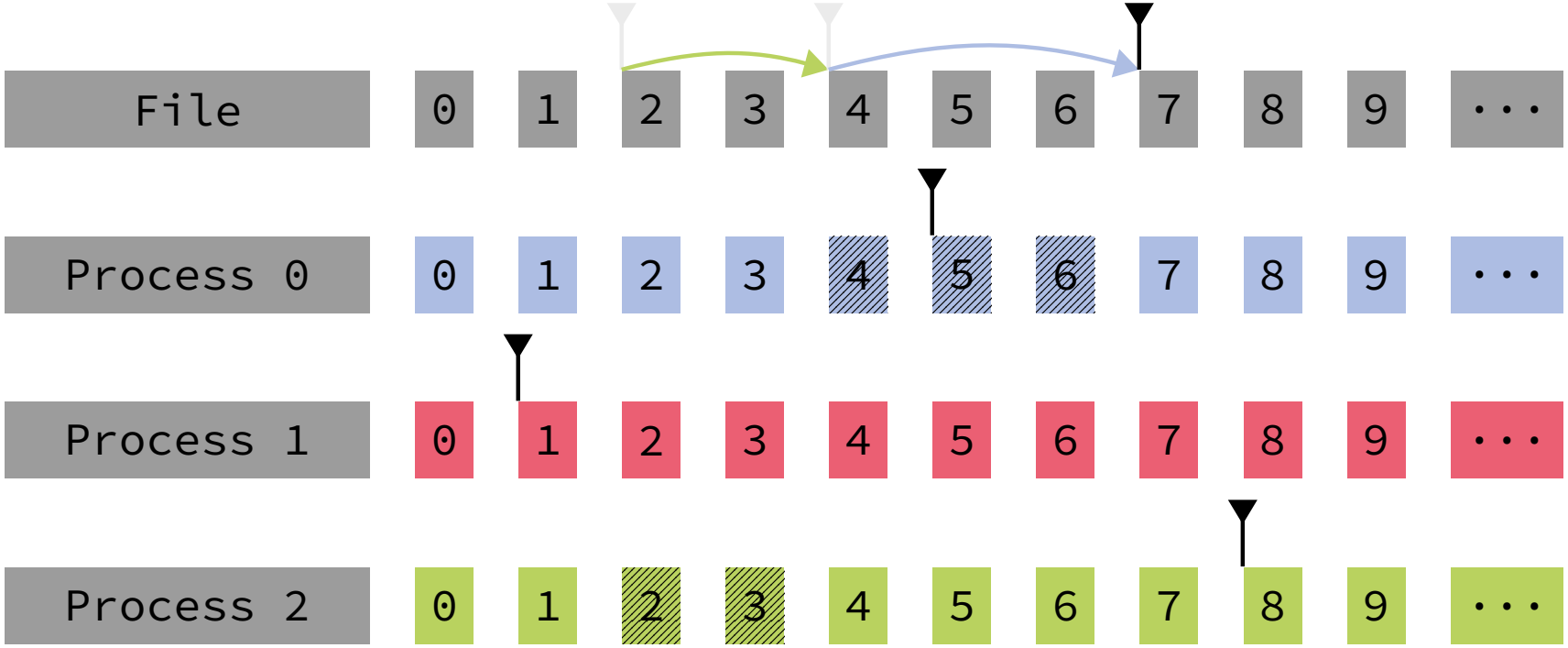
- `buf` argument must match corresponding `begin` routine

EXAMPLE

blocking, noncollective, shared [MPI-3.1, 13.4.4]

With the shared pointer at element 2,

- process 0 writes `count = 3`,
- process 2 writes `count = 2`:



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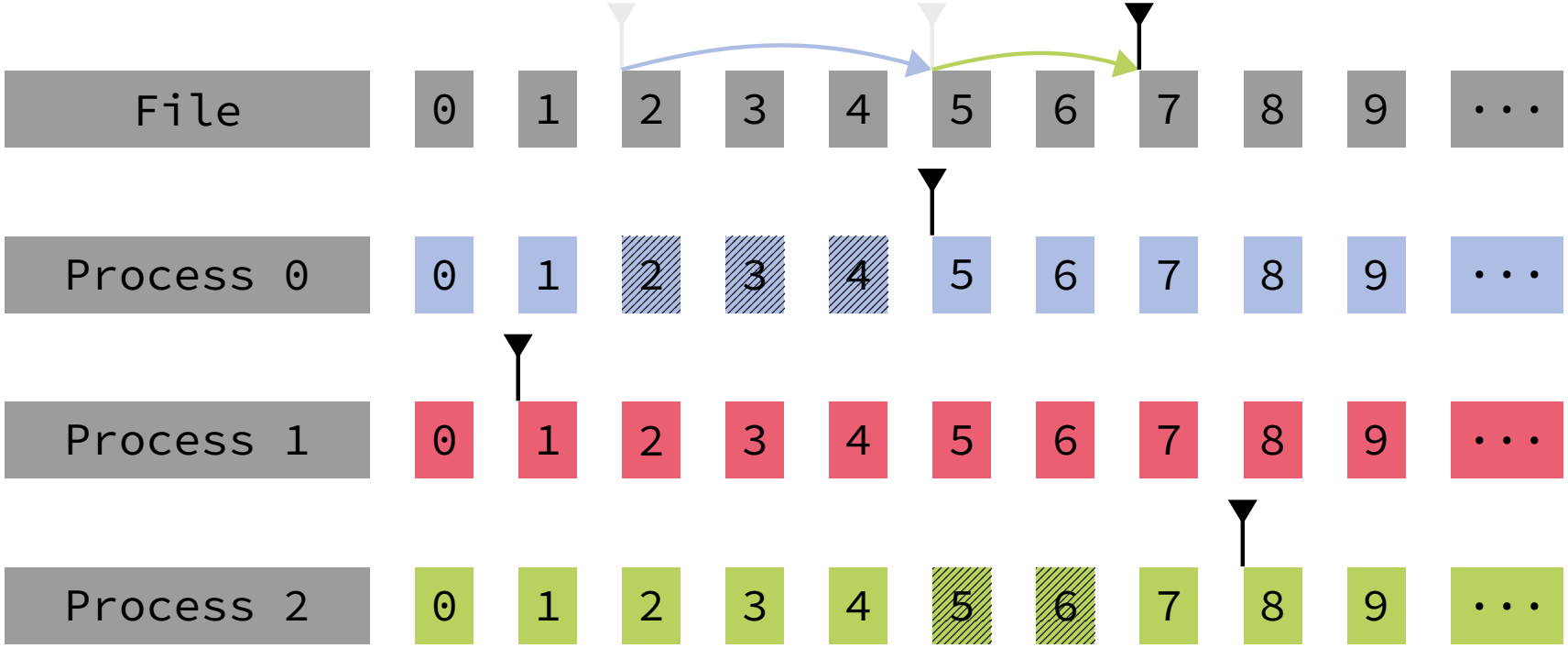
EXAMPLE

blocking, noncollective, shared [MPI-3.1, 13.4.4]

With the shared pointer at element 2,

- process 0 writes `count = 3`,
- process 2 writes `count = 2`:



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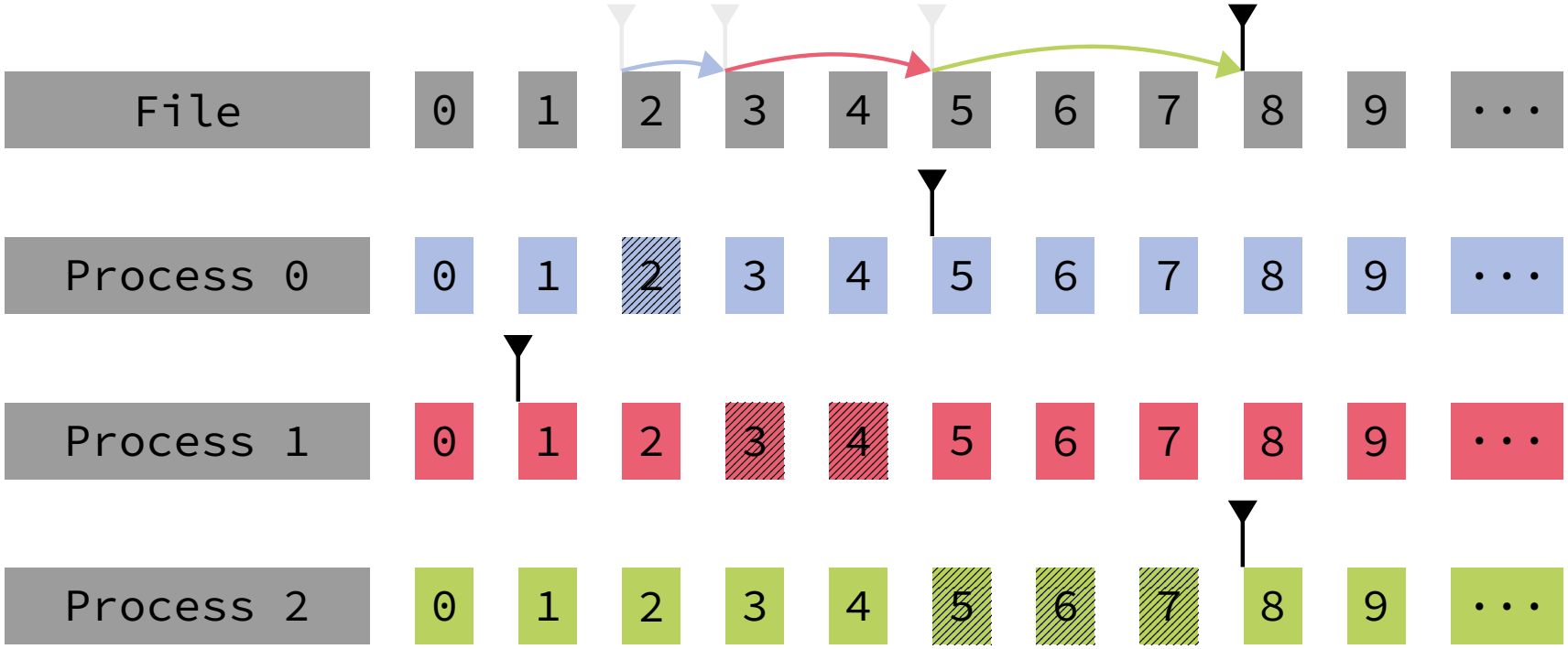
EXAMPLE

blocking, collective, shared [MPI-3.1, 13.4.4]

With the shared pointer at element 2,

- process 0 writes `count = 1`,
- process 1 writes `count = 2`,
- process 2 writes `count = 3`:



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READING

blocking, noncollective, individual [MPI-3.1, 13.4.3]

C
```
int MPI_File_read(MPI_File fh, void* buf, int count,
↪  MPI_Datatype datatype, MPI_Status* status)
```

F08
```
MPI_File_read(fh, buf, count, datatype, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Starts reading at the current position of the individual file pointer
- Reads up to `count` elements of `datatype` into the memory starting at `buf`
- `status` indicates how many elements have been read
- If `status` indicates less than `count` elements read, the end of file has been reached

FILE POINTER POSITION [MPI-3.1, 13.4.3]

C
```
int MPI_File_get_position(MPI_File fh, MPI_Offset*
↪  offset)
```

F08
```
MPI_File_get_position(fh, offset, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(out) :: offset
integer, optional, intent(out) :: ierror
```

- Returns the current position of the individual file pointer in units of *etype*
- Value can be used for e.g.
  - return to this position (via seek)
  - calculate a displacement
- `MPI_File_get_position_shared` queries the position of the shared file pointer

SEEKING TO A FILE POSITION [MPI-3.1, 13.4.3]

C
```
int MPI_File_seek(MPI_File fh, MPI_Offset offset, int
↪ whence)
```

F08
```
MPI_File_seek(fh, offset, whence, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: offset
integer, intent(in) :: whence
integer, optional, intent(out) :: ierror
```

- whence controls how the file pointer is moved:
  - MPI_SEEK_SET sets the file pointer to offset
  - MPI_SEEK_CUR offset is added to the current value of the pointer
  - MPI_SEEK_END offset is added to the end of the file
- offset can be negative but the resulting position may not lie before the beginning of the file
- MPI_File_seek_shared manipulates the shared file pointer

CONVERTING OFFSETS [MPI-3.1, 13.4.3]

C
```
int MPI_File_get_byte_offset(MPI_File fh, MPI_Offset
↪  offset, MPI_Offset* disp)
```

F08
```
MPI_File_get_byte_offset(fh, offset, disp, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: offset
integer(kind=MPI_OFFSET_KIND), intent(out) :: disp
integer, optional, intent(out) :: ierror
```

- Converts a view relative offset (in units of *etype*) into a displacement in bytes from the beginning of the file

CONSISTENCY [MPI-3.1, 13.6.1]

Sequential Consistency
If a set of operations is sequentially consistent, they behave as if executed in some serial order. The exact order is unspecified.

- To guarantee sequential consistency, certain requirements must be met
- Requirements depend on access path and file atomicity

Result of operations that are not sequentially consistent is implementation dependent.

ATOMIC MODE [MPI-3.1, 13.6.1]

Requirements for sequential consistency
Same file handle: always sequentially consistent File handles from same open: always sequentially consistent File handles from different open: not influenced by atomicity, see nonatomic mode

- Atomic mode is not the default setting
- Can lead to overhead, because MPI library has to uphold guarantees in general case

C
```
int MPI_File_set_atomicity(MPI_File fh, int flag)
```

F08
```
MPI_File_set_atomicity(fh, flag, ierror)
type(MPI_File), intent(in) :: fh
logical, intent(in) :: flag
integer, optional, intent(out) :: ierror
```

NONATOMIC MODE [MPI-3.1, 13.6.1]

Requirements for sequential consistency
Same file handle: operations must be either nonconcurrent, nonconflicting, or both File handles from same open: nonconflicting accesses are sequentially consistent, conflicting accesses have to be protected using `MPI_File_sync` File handles from different open: all accesses must be protected using `MPI_File_sync`

Conflicting Accesses
Two accesses are conflicting if they touch overlapping parts of a file and at least one is writing.

C
```
int MPI_File_sync(MPI_File fh)
```

F08
```
MPI_File_sync(fh, ierror)
type(MPI_File), intent(in) :: fh
integer, optional, intent(out) :: ierror
```

NONATOMIC MODE [MPI-3.1, 13.6.1]

The Sync-Barrier-Sync construct

```
   // writing access
    ↪  sequence through one
    ↪  file handle
   MPI_File_sync(fh0);
   MPI_Barrier(
    ↪  MPI_COMM_WORLD);
   MPI_File_sync(fh0);
⏟  // ...
```

```
   // ...
   MPI_File_sync(fh1);
   MPI_Barrier(
    ↪  MPI_COMM_WORLD);
   MPI_File_sync(fh1);
   // access sequence to
    ↪  the same file
    ↪  through a different
⏟   ↪  file handle
```

- `MPI_File_sync` is used to delimit sequences of accesses through different file handles
- Sequences that contain a write access may not be concurrent with any other access sequence

EXERCISES

Exercise 1 – Data Access

1.1 Writing and Reading Data

Write a program:

- Each process writes its own rank to the common file `rank.dat`
- The ranks should be in order in the file $0 \ldots n-1$
- Process 0 reads the whole file and prints the contents to screen

1.2 Accessing Parts of Files

Take the file `rank.dat` from the previous exercise

- The processes read the integers in the file in reverse order, i.e. process 0 reads the last entry, process 1 reads the one before, …
- Each process prints its rank and the integer it read to the screen

Careful: This program might be run on a different number of processes

Part III: The Info Object

THE INFO OBJECT [MPI-3.1, 9]

A Gentle Reminder

Used to pass hints for optimization to MPI

- Consists of (`key`, `value`) pairs, where both `key` and `value` are strings
- Each `key` must appear only once
- `MPI_INFO_NULL` can be used in place of an actual info object
- Keys must not be larger than `MPI_MAX_INFO_KEY`
- Values must not be larger than `MPI_MAX_INFO_VAL`

Info Object API
`MPI_Info_create`, `MPI_Info_dup`, `MPI_Info_free`, `MPI_Info_set`, `MPI_Info_delete`, `MPI_Info_get`, `MPI_Info_get_valuelen`, `MPI_Info_get_nkeys`, `MPI_Info_get_nthkey`

INFO OBJECTS FOR I/O [MPI-3.1, 13.2, 13.2]

Info objects can be associated with files that MPI I/O operates on using several mechanisms:

- When opening a file: the info object is passed to the `MPI_File_open` routine
- While the file is open:
  - When setting a file view using `MPI_File_set_view`
  - Explicitly using `MPI_File_set_info`
- When deleting a file using `MPI_File_delete`
- Globally using a ROMIO hint file

Some info items can only be reasonably used e.g. when opening a file and will be ignored when later used with `MPI_File_set_info`.

FILE INFO OBJECT ACCESSORS [MPI-3.1, 13.2.8]

C
```
int MPI_File_set_info(MPI_File fh, MPI_Info info)
```

F08
```
MPI_File_set_info(fh, info, ierror)
type(MPI_File), intent(in) :: fh
type(MPI_Info), intent(in) :: info
integer, optional, intent(out) :: ierror
```

C
```
int MPI_File_get_info(MPI_File fh, MPI_Info* info)
```

F08
```
MPI_File_get_info(fh, info, ierror)
type(MPI_File), intent(in) :: fh
type(MPI_Info), intent(out) :: info
integer, optional, intent(out) :: ierror
```

PASSING HINTS USING A FILE

Specify Hint File via Environment Variable

```
$ export ROMIO_HINTS=<absolute path>/hintfile
```

- Environment variable must be exported to the compute nodes. Use appropriate mechanisms provided by process starters like `mpiexec` or `runjob`.
- Hints are used for all MPI I/O operations in the application through
  - direct use of MPI I/O routines
  - use of libraries that use MPI I/O

Example Hint File Content

```
collective buffering true
cb_buffer_size       33554432
cb_block_size        4194304
```

RESERVED KEYS FOR I/O [MPI-3.1, 13.2.8]

- An MPI implementation is not required to support these hints
- If a hint is supported by an implementation, it must behave as described by the standard
- Additional keys may be supported

RESERVED KEYS FOR I/O [MPI-3.1, 13.2.8]

`filename: string`	*implementation dependent*
Can be used to inspect the file name of an open file.	

`file_perm: string`	*same, implementation dependent*
Specifies the file permissions to set on file creation.	

`access_style: [string]`	*comma separated*

Specifies the manner in which the file will be accessed until it is closed or this info key is changed. Valid list elements are:

- `read_once`
- `write_once`
- `read_mostly`
- `write_mostly`
- `sequential`
- `reverse_sequential`
- `random`

RESERVED KEYS FOR I/O [MPI-3.1, 13.2.8]

`nb_proc: integer`	*same*
Specifies how many parallel processes usually run the application that accesses this file.	

`num_io_nodes: integer`	*same*
Specifies the number of I/O devices in the system.	

`io_node_list: [string]`	*comma separated, same, implementation dependent*
Specifies a list of I/O devices that should be used to store the file.	

RESERVED KEYS FOR I/O [MPI-3.1, 13.2.8]

`chunked: [integer]`	*comma separated, same*
Specifies that the file consists of a multidimensional array that is often accessed by subarrays. List entries are array dimensions in order of decreasing significance.	

`chunked_item: [integer]`	*comma separated, same*
Specifies the size of one array entry in bytes.	

`chunked_size: [integer]`	*comma separated, same*
Specifies the dimensions of the subarrays.	

RESERVED KEYS FOR I/O [MPI-3.1, 13.2.8]

`collective_buffering: boolean`	*same*
Specifies whether the application may benefit from collective buffering.	

`cb_nodes: integer`	*same*
Specifies the number of target nodes to be used for collective buffering.	

`cb_block_size: integer`	*same*
Specifies the block size to be used for collective buffering. Data access happens in chunks of this size.	

`cb_buffer_size: integer`	*same*
Specifies the size of the buffer space that can be used on each target node.	

RESERVED KEYS FOR I/O [MPI-3.1, 13.2.8]

`striping_factor: integer`	*same*
Specifies the number of I/O devices that the file should be striped across. Relevant only on file creation.	

`striping_unit: integer`	*same*
Specifies the striping unit – the amount of consecutive data assigned to one I/O device – to be used for this file. Only relevant on file creation.	

GOOD CHOICES FOR GPFS

`romio_ds_write: string`	*default: `automatic`*
Specifies whether to use data sieving for write access. Good choice: `enable`	

`romio_ds_read: string`	*default: `automatic`*
Specifies whether to use data sieving for read access. Good choice: `automatic`	

`cb_buffer_size: integer`	*default: `16777216`*
Specifies the size of the buffer space that can be used on each target node. Good choice: `33554432`	

- Default keys already seem to be a good setting
- Collective buffering is switched on by default (`collective_buffering` is ignored, but `romio_cb_read`/`romio_cb_write` are available)
- Data sieving is only important for writing with shared file pointers and for small amounts of data.
- `cb_nodes` is set automatically and cannot be changed by the user

Part IV: Best Practices

GENERAL NOTES

- Choose the file system with the best performance
  - Check file system documentation of HPC centre
  - For JSC:
    - `$WORK` is much faster than `$HOME`
    - Use `$WORK` for I/O, `$HOME` for storage of executables, setups
- Avoid I/O, recalculate if it is faster to do so
- Avoid frequent I/O
- Reduce data/accuracy if possible
- Avoid random access patterns
- Write in large chunks with contiguous data
- Avoid explicit buffer flushes (`MPI_File_sync`)
- Use proper mode for opening files (e.g. read only if data is only read)
- Give proper hints to MPI via info objects

GOOD STRATEGIES FOR GPFS (ON JUQUEEN)

Writing	
MPI I/O routines	Individual file pointers, collective (e.g. `MPI_File_write_all`)
MPI I/O hints	Default values
Environment	`export BGLOCKLESSMPIO_F_TYPE=0x47504653 runjob --env-exp BGLOCKLESSMPIO_F_TYPE`

Reading	
MPI I/O routines	Individual file pointers, collective (e.g. `MPI_File_read_all`)
MPI I/O hints	Default values, or for small amounts of data `romio_ds_write = enable` and `cb_buffer_size = 33554432`
Environment	Do not set `BGLOCKLESSMPIO_F_TYPE`

GOOD STRATEGIES FOR GPFS (ON JUQUEEN)

Shared File Pointers	
MPI I/O routines	`MPI_File_write_ordered`, ...
MPI I/O hints	`romio_ds_write = enable`, `cb_buffer_size = 33554432`, (`16777216` for reading)
Environment	–

Explicit offsets	
MPI I/O routines	`MPI_File_write_at_all`, ...
MPI I/O hints	`romio_ds_write = enable`, `cb_buffer_size = 33554432`
Environment	`export BGLOCKLESSMPIO_F_TYPE=0x47504653 runjob --env-exp BGLOCKLESSMPIO_F_TYPE`

Part V: Mandelbrot Example

SUBARRAY DATA [MPI-3.1, 4.1.3]

C

```
int MPI_Type_create_subarray(int ndims, const int
↪  array_of_sizes[], const int array_of_subsizes[],
↪  const int array_of_starts[], int order, MPI_Datatype
↪  oldtype, MPI_Datatype* newtype)
```

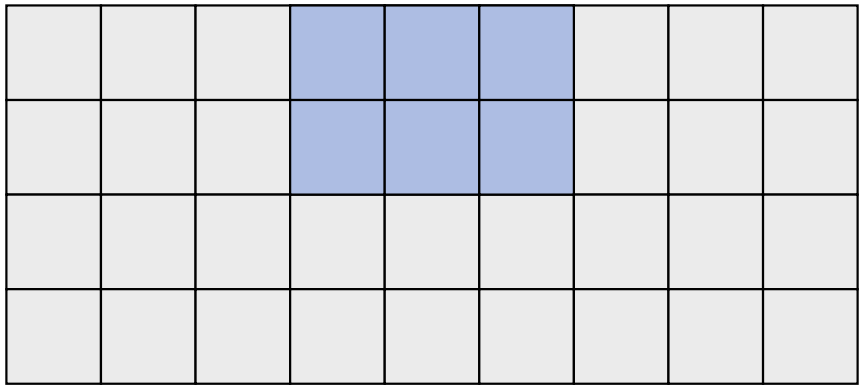
F08

```
MPI_Type_create_subarray(ndims, array_of_sizes,
↪  array_of_subsizes, array_of_starts, order, oldtype,
↪  newtype, ierror)
integer, intent(in) :: ndims, array_of_sizes(ndims),
↪  array_of_subsizes(ndims), array_of_starts(ndims),
↪  order
type(MPI_Datatype), intent(in) :: oldtype
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror
```

EXAMPLE

```
ndims = 2;
array_of_sizes[] = { 4, 9 };
array_of_subsizes[] = { 2, 3 };
array_of_starts[] = { 0, 3 };
order = MPI_ORDER_C;
oldtype = MPI_INT;
```

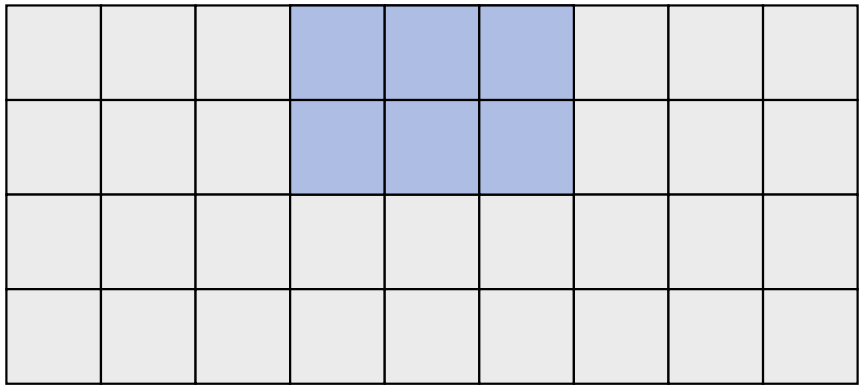
An array with global size 4×9 containing a subarray of size 2×3 at offsets $0, 3$:



EXAMPLE

F08
```
ndims = 2
array_of_sizes(:) = (/ 4, 9 /)
array_of_subsizes(:) = (/ 2, 3 /)
array_of_starts(:) = (/ 0, 3 /)
order = MPI_ORDER_FORTRAN
oldtype = MPI_INTEGER
```

An array with global size 4×9 containing a subarray of size 2×3 at offsets $0, 3$:



COMMIT & FREE [MPI-3.1, 4.1.9]

Before using a derived datatype in communication it needs to be committed

C
```
int MPI_Type_commit(MPI_Datatype* datatype)
```

F08
```
MPI_Type_commit(datatype, ierror)
type(MPI_Datatype), intent(inout) :: datatype
integer, optional, intent(out) :: ierror
```

Marking derived datatypes for deallocation

C
```
int MPI_Type_free(MPI_Datatype *datatype)
```

F08
```
MPI_Type_free(datatype, ierror)
type(MPI_Datatype), intent(inout) :: datatype
integer, optional, intent(out) :: ierror
```

EXERCISES

Exercise 2 – Mandelbrot Set

2.1 Open and Close

Implement a solution for the static decomposition (`type == 1`) of the Mandelbrot set example in the file `mandelmpiio.c` or `mandelmpiio.f90`. Begin by adding appropriate invocations of `MPI_File_open` and `MPI_File_close`.

2.2 File View

Next, construct an MPI datatype (`MPI_Type_create_subarray`) that matches the decomposition type and set a File View accordingly (`MPI_File_set_view`).

2.3 Write Access

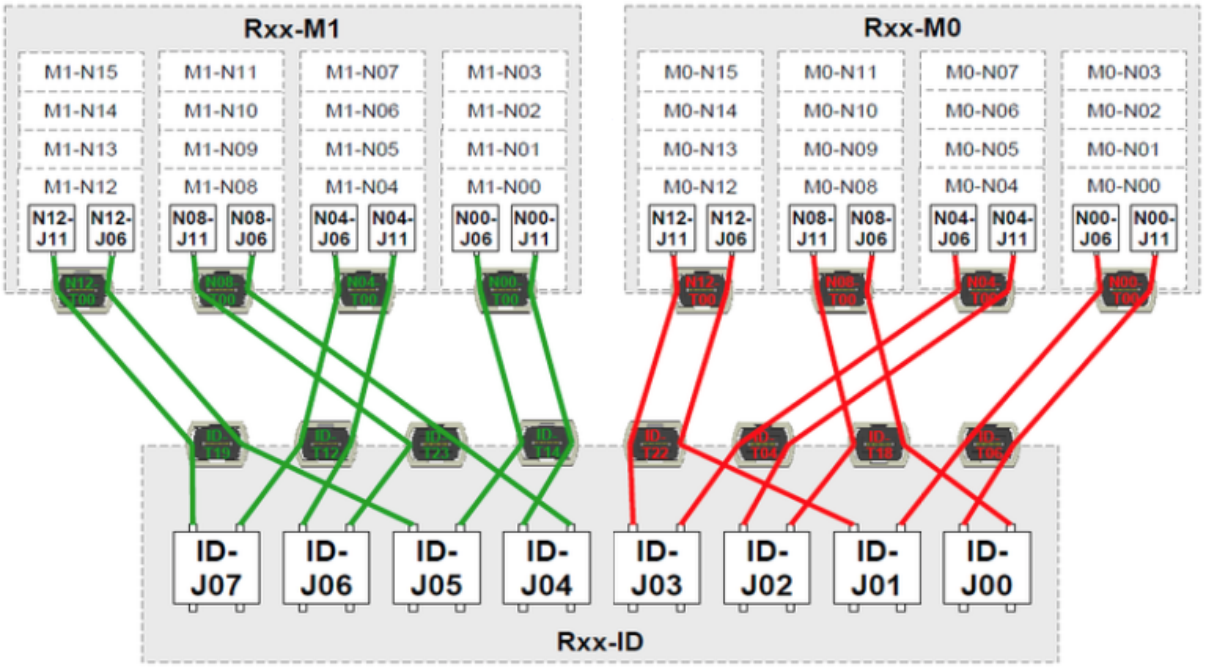
Write to the file using collective routines with individual file pointers (e.g. `MPI_File_write_all`).

Example `mandelmpi` Invocation

```
$ mandelmpi -t 1 -f 2 # static decomposition, MPI I/O format
```

Part VI: MPI Blue Gene/Q Extensions

BLUE GENE/Q: I/O NODE CABLING



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BLUE GENE/Q MPI EXTENSIONS

IBM offers extensions to the MPI standard for Blue Gene/Q

- *Not* part of the MPI standard
- C and Fortran 77 interface for functions
- Functions start with `MPIX_` instead of `MPI_`
- Only those extensions related to I/O are discussed here

Overview over all available extensions:
`http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/UserInfo/MPIextensions.html`

C
```c
#include <mpix.h>
```

F08
```f90
use mpi
```

F77
```f77
include 'mpif.h'
```

PARTITIONING COMM_WORLD ALONG I/O NODES

C
```
int MPIX_Pset_diff_comm_create(MPI_Comm* pset_comm)
int MPIX_Pset_same_comm_create(MPI_Comm* pset_comm)
```

F08
```
MPIX_Pset_diff_comm_create(pset_comm, ierror)
MPIX_Pset_same_comm_create(pset_comm, ierror)
integer:: pset_comm, ierror
```

- Collective operation on `MPI_COMM_WORLD`
- The resulting communicator contains processes which run on nodes associated with different/the same I/O nodes

GENERAL PARTITIONING ALONG I/O NODES

C

```
int MPIX_Pset_diff_comm_create_from_parent(MPI_Comm
↪  parent_comm, MPI_Comm* pset_comm)
int MPIX_Pset_same_comm_create_from_parent(MPI_Comm
↪  parent_comm, MPI_Comm* pset_comm)
```

F08

```
MPIX_Pset_diff_comm_create_from_parent(parent_comm,
↪  pset_comm, ierror)
MPIX_Pset_same_comm_create_from_parent(parent_comm,
↪  pset_comm, ierror)
integer:: parent_comm, pset_comm, ierror
```

Like `MPIX_Pset_diff_comm_create` and `MPIX_Pset_same_comm_create` but works on arbitrary communicator `parent_comm`.

I/O NODE PROPERTIES

C
```
int MPIX_IO_node_id()
```

F08
```
MPIX_IO_node_id(io_node_id)
integer:: io_node_id
```

Returns the ID of the I/O node associated with the node that the current process is running on.

C
```
int MPIX_IO_link_id()
```

F08
```
MPIX_IO_link_id(io_link_id)
integer :: io_link_id
```

Returns the ID of the link to the associated I/O node.

No `ierror` argument on Fortran routines.

DISTANCE TO I/O NODE

C
```
int MPIX_IO_distance()
```

F08
```
MPIX_IO_distance(io_distance)
integer :: io_distance
```

Returns the distance to the associated I/O node in number of network hops.

No `ierror` argument on Fortran routines.