

Advanced Message-Passing Programming

Basic MPI-IO calls



Reusing this material



This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

<http://creativecommons.org/licenses/by-nc-sa/4.0/>

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.

Overview

- Lecture will cover
 - MPI-IO model
 - basic file handling routines
 - setting the file view
 - achieving performance

Comparing MPI-IO and Controller IO

- Controller IO uses a single process for read and write
- This requires a buffer to hold entire file on controller
 - not scalable to many processes due to memory limits
- MPI-IO model
 - each process describes what subsections of the file it owns
 - this is done using standard MPI datatypes
 - these are passed into the MPI-IO routines
 - data is automatically read and transferred directly to local memory
 - there is no single large buffer and no explicit controller process

MPI-IO Approach

- Four stages
 - open file
 - set file view
 - read or write data
 - close file
- All the complexity is hidden in setting the file view
 - this is where the derived datatypes appear
- Write is probably more important in practice than read
 - but exercises concentrate on read
 - makes for an easier progression from serial to parallel IO examples

Opening a File

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

```
MPI_FILE_OPEN(COMM, FILENAME, AMODE, INFO, FH, IERR)  
CHARACTER*(*) FILENAME  
INTEGER COMM, AMODE, INFO, FH, IERR
```

- Attaches a file to the File Handle
 - use this handle in all future IO calls
 - analogous to C file pointer or Fortran unit number
- Routine is collective across the communicator
 - must be called by all processes in that communicator
- Access mode specified by amode
 - common values are: `MPI_MODE_CREATE`, `MPI_MODE_RDONLY`, `MPI_MODE_WRONLY`, `MPI_MODE_RDWR`

Examples

```
MPI_File fh;
int amode = MPI_MODE_RDONLY;
MPI_File_open(MPI_COMM_WORLD, "data.in", amode,
              MPI_INFO_NULL, &fh);

integer fh
integer amode = MPI_MODE_RDONLY
call MPI_FILE_OPEN(MPI_COMM_WORLD, 'data.in', amode,
                  MPI_INFO_NULL, fh, ierr)
```

- Must specify create as well as write for new files

```
int      amode = MPI_MODE_CREATE | MPI_MODE_WRONLY;
integer amode = MPI_MODE_CREATE + MPI_MODE_WRONLY
```

- will return to the `info` argument later

Closing a File

```
MPI_File_close(MPI_File *fh)
```

```
MPI_FILE_CLOSE(FH, IERR)
```

```
INTEGER FH, IERR
```

- Routine is collective across the communicator
 - must be called by all processes in that communicator

Reading Data

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

```
MPI_FILE_READ_ALL(FH, BUF, COUNT, DATATYPE, STATUS, IERR)  
INTEGER FH, COUNT, DATATYPE, STATUS(MPI_STATUS_SIZE), IERR
```

- Reads **count** objects of type **datatype** from the file on each process
 - this is collective across the communicator associated with **fh**
 - similar in operation to C **fread** or Fortran **read**
- No offsets into the file are specified in the read
 - but processes do not all read the same data!
 - actual positions of read depends on the process's own file view
- Similar syntax for write

Setting the File View

```
int MPI_File_set_view(MPI_File fh, MPI_Offset disp,  
                      MPI_Datatype etype, MPI_Datatype filetype,  
                      char *datarep, MPI_Info info);  
  
MPI_FILE_SET_VIEW(FH, DISP, ETYPE, FILETYPE, DATAREP, INFO, IERR)  
INTEGER FH, ETYPE, FILETYPE, INFO, IERR  
CHARACTER*(*) DATAREP  
INTEGER(KIND=MPI_OFFSET_KIND) DISP
```

- **disp** specifies the starting point in the file *in bytes*
- **etype** specifies the elementary datatype which is the building block of the file
- **filetype** specifies which subsections of the global file each process accesses
- **datarep** specifies the format of the data in the file
- **info** contains hints and system-specific information – see later

File Views

- Once set, the process only sees the data in the view
 - different start positions depending on displacement and/or leading gaps in datatype
 - for 2D sections can use MPI vectors or subarray datatypes
 - can then do linear reads – holes in datatype are skipped over

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

rank 1 (0,1)	rank 3 (1,1)
rank 0 (0,0)	rank 2 (1,0)

global file

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

rank 1 filetype

--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

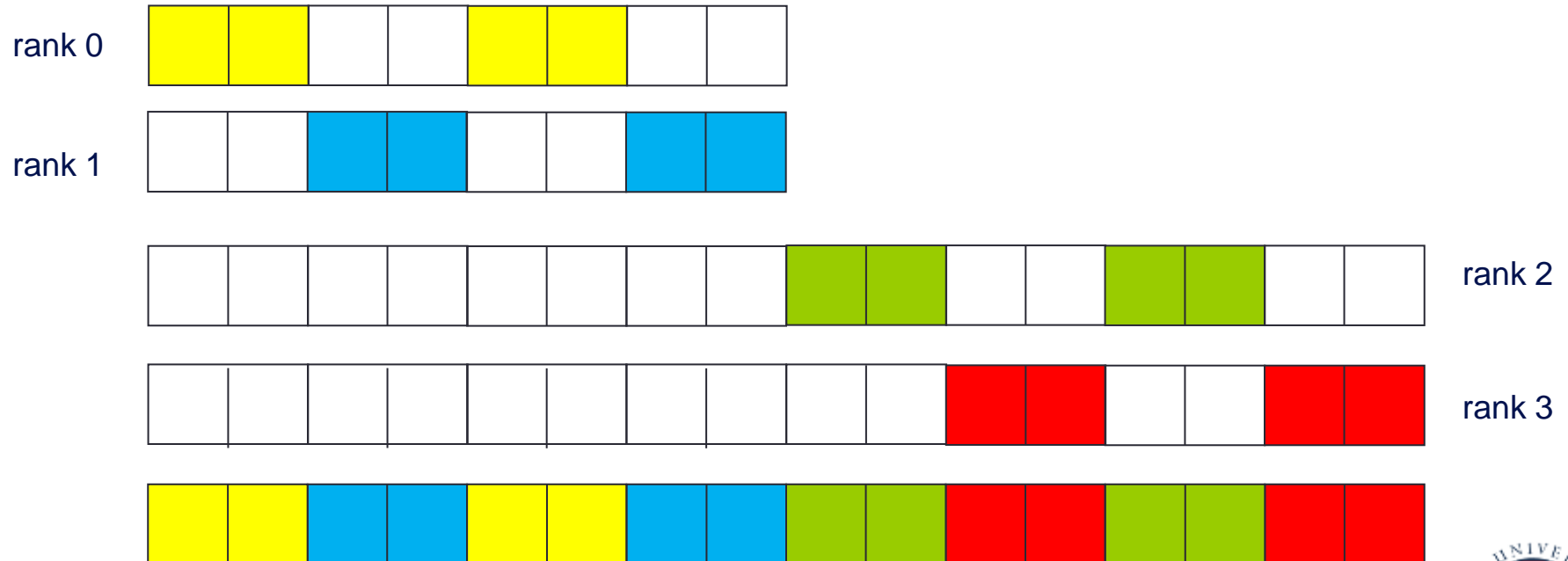
rank 1 view of file

3	4	7	8
---	---	---	---

Filetypes Should Tile the File

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

rank 1 (0,1)	rank 3 (1,1)
rank 0 (0,0)	rank 2 (1,0)



Data Representation

- **datarep** is a string that can be
 - `"native"`
 - `"internal"`
 - `"external32"`
- Fastest is `"native"`
 - raw bytes are written to file exactly as in memory
- Most portable is `"external32"`
 - should be readable by MPI-IO on any platform
- Middle ground is `"internal"`
 - portability depends on the implementation
- I would recommend `"native"`
 - convert file format by hand as and when necessary

Choice of Parameters (1)

- Many different combinations are possible
 - choices of displacements, filetypes, etypes, datatypes, ...
- Simplest approach is to set **disp** = 0 everywhere
 - then specify offsets using datatypes with leading gaps when setting view
 - non-zero **disp** could be useful for skipping global header (eg metadata)
 - **disp** must be of the correct type in Fortran (NOT a default integer)
 - **CANNOT** specify '0' for the displacement: need to use a variable

```
INTEGER(KIND=MPI_OFFSET_KIND) DISP = 0  
CALL MPI_FILE_SET_VIEW(FH, DISP, ...)
```

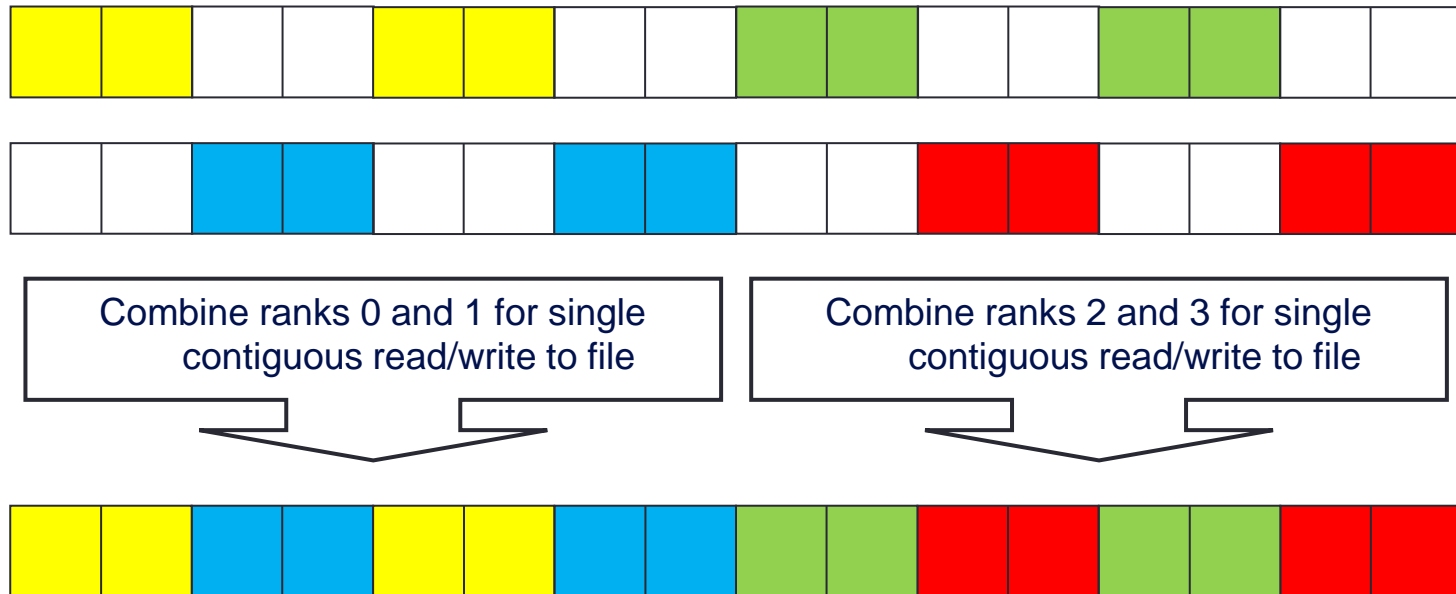
- I would recommend setting the view with subarray types
 - and zero displacements

Choice of Parameters (2)

- Can also use vector datatypes in the view
 - each process then specifies a different, non-zero value of `disp`
- Problems
 - `disp` is specified in bytes so need to know the size of the **etype**
 - files are linear 1D arrays
 - need to do a calculation for displacement of element of 2D array
 - something like $i * NY + j$ (in C) or $j * NX + i$ (in Fortran)
 - then multiply by the number of bytes in a float or REAL
- Using vector types + displacements is one of the exercises
- **etype** normally something like **MPI_REAL** or **MPI_FLOAT**
 - **datatype** in read/write calls is usually the same as the **etype**
 - however, can play some useful tricks (see extra exercises re halos)

Collective IO

- For read and write, “_all” means operation is collective
 - all processes attached to the file are taking part
- Other IO routines exist which are individual (delete “_all”)
 - functionality is the same but performance will be slower
 - collective routines can aggregate reads/writes for better performance



INFO Objects and Performance

- Used to pass optimisation hints to MPI-IO
 - implementations can define any number of allowed values
 - these are portable in as much as they can be ignored!
 - can use the default value `info = MPI_INFO_NULL`
- Info objects can be created, set and freed (see manual for details)
 - `MPI_Info_create`
 - `MPI_Info_set`
 - `MPI_Info_free`
- Using appropriate values may be key to performance
 - e.g. setting buffer sizes, blocking factors, number of IO nodes, ...
 - but is dependent on the system and the MPI implementation
 - need to consult the MPI manual for your machine
 - on ARCHER2, easier to tune Lustre file system than use MPI-IO hints

Summary

- MPI-IO calls deceptively simple
- User must define appropriate filetypes so file view is correct on each process
 - this is the difficult part!
- Use collective calls whenever you can
 - enables IO library to merge reads and writes
 - enables a smaller number of larger IO operations from/to disk