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Parallel I/O: Basics and MPI2

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Introduction

- IO is a crucial issue in the modern high performance codes:
 - 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 trascurable
 - data portability (e.g. endianism)
- Solution to avoid that IO became a bottleneck:
 - HW: parallel file-system available on all the HPC platform
 - SW: high level libraries able to manage parallel accesses to the file in efficient way (e.g. MPI2-IO, HDF5, NetCDF, ...)

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Goals:

- Improve the performance
- Ensure data consistency
- Avoid communication
- Usability

Possible solutions:

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

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Summer School on PARALLEL Parallel IO COMPUTING **Solution 1: Master-Slave Only 1 processor performs IO** Goals: Improve the performance: **NO** Ensure data consistency: **YES** Pe1 Avoid communication: NO Pe0 Data File Pe2 Usability: **YES** Pe3 99444

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Solution 2: Distributed IO

All the processors read/writes their own files



Goals:

Improve the performance: YES (but be careful)

Ensure data consistency: **YES**

Avoid communication: **YES**

Usability: NO

Warning: avoid to parametrize with processors!!!

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Solution 3: Distributed IO on single file

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



Goals:

Improve the performance: **YES** for read, **NO** for write

Ensure data consistency: NO

Avoid communication: **YES**

Usability: YES (portable !!!)





Solution 4: MPI2 IO

MPI functions performs the IO. Asyncronous IO is supported.



Goals:

Improve the performance: YES (strongly!!!)

Ensure data consistency: NO

Avoid communication: **YES**

Usability: **YES**

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I/O Patterns in Parallel applications:

- Different from those in sequential programs, which usually access data in contiguous chunks
- In many parallel programs, each program may need to access several noncontiguous pieces of data from a file
- In addition, groups of processes may need to access the file simulataneously, and the accesses of different processes may be interleaved in the file



MPI-2.x features for Parallel IO

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- MPI-IO: introduced in MPI-2.x standard(1997)
 - Non contiguous access in both memory and file
 - reading/writing a file is like send/receive a message from a MPI buffer
 - optimized access to non-contiguous data
 - collective / non-collective access operations with communicators
 - blocking / non-blocking calls
 - data portability (implementation/system independent)
 - good performance in many implementations

Starting with MPI-IO

- MPI-IO provides basic IO operations:
 - open, seek, read, write, close (ecc.)
- 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 own local pointer to the file (individual file pointer) by 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

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 operations 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 vie 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_CLO	SE 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	

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Open/close a file 3/3

MPI_FILE_CLOSE(fh)

INOUT fh: file handle (handle)

- Collective operation
- This function is called when the file access is finished, to free the file handle.

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Data Access 1/3

MPI-2 provides a large number of routines to read and write data from a file. There are three properties which differentiate the different **data access** routines.

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

- This file 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!



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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

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Data Access 3/3

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

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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.
- 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.
- 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

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 have the following values:

- 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
- It is erroneous to seek to a negative position in the view

Querying the position

MPI_FILE_GET_POSITION (fh, offset)

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

- 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

Using individual file pointers

```
#include ``mpi.h"
#define FILESIZE(1024*1024)
                                                           File offset
int main(int argc, char **argv) {
    int *buf, rank, nprocs, nints, bufsize;
                                                           determined by
    MPI File fh; MPI Status status;
                                                           MPI File_seek
    MPI Init(&argc, &argv);
    MPI Comm rank (MPI COMM WORLD, &rank);
    MPI Comm size (MPI COMM WORLD, &nprocs);
    bufsize = FILESIZE/nprocs;
    nints =bufsize/sizeof(int);
    buf = (int*) malloc(nints);
    MPI File open (MPI COMM WORLD, "/pfs/datafile", MPI MODE RDONLY,
       MPI INFO NULL, & fh);
    MPI File seek(fh, rank*bufsize,MPI SEEK SET);
    MPI File read(fh, buf, nints, MPI INT, &status);
    MPI File close(&fh);
    free(buf);
    MPI Finalize();
    return 0;
}
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```

```
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    Using individual file pointers
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PROGRAM Output
    USE MPI
                                                             File offset
    IMPLICIT NONE
    INTEGER :: err, i, myid, file, intsize
                                                             determined by
    INTEGER :: Status (MPI STATUS SIZE)
                                                             MPI File seek
    INTEGER, PARAMETER :: count=100
    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
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```

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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: source buffer
 IN count: number of written 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 type from begin of view
- The sequence of basic datatypes of **DATATYPE** (= signature of DATATYPE) must match contiguous copies of the etype of the current 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
- The sequence of basic datatypes of **DATATYPE** (= signature of DATATYPE) must match contiguous copies of the etype of the current view



Using explicit offsets

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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
```

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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

Shared file pointer - Write, Read

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

int MPI_File_read_shared (MPI_File fh, void *buf, int count, MPI_Datatype datatype, MPI_Status *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 quering 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

Advanced features of MPI-IO

- Basic MPI-IO features are not useful when
 - Data distibution 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)

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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!





Summer School on **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 ٠ 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, ecc)
 - **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

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Passing hints to Filesystem

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



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







- 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

```
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  Non-contiguous access:
                                                                PARALLEL
                                                              COMPUTING
  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)
99444
```

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Simple Be	rk	Summer School on PARALLEL COMPUTING			
P0 (0,0) m rows P3 (1,0)	- n columns — P1 (0,1) P4 (1,1)	P2 (0,2) P5 (1,2)	gather • MPI-IC MPI_Ty define and pe • local g	ional I/O: mag rs data and pe o: use ype_create_su the view for erform a colle grid (per proce x10000 double	rform I/O ubarray to each process ctive call ess):
processi		2	8	16	32
filesize (Mb) 76		3 1526	6103	12207	24414
Traditional-IO (s)		3 22	86	1738	3570
MPI-IO (s)		1 2	18	33	48

I/O performances are strongly affected by file-system, storage infra-structure, MPI implementation, network,...

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

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- 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 syncronization.

Can be used to overlap IO with computation



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Collective, nonblocking IO

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

...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



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)

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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

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- 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, include I/O!
 - 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

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Useful links

- MPI The Complete Reference vol.2, The MPI Extensions (W.Gropp, E.Lusk et al. 1998 MIT Press)
- Using MPI-2: Advanced Features of the Message-Passing Interface (W.Gropp, E.Lusk, R.Thakur 1999 MIT Press)
- Standard MPI-2.x (or the last 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

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