MPI-IO

Parallel Storage Systems

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Outline

- Across how many servers would you distribute a 1 GiB file?
  1. One server
  2. 64 servers
  3. 1,024 servers
  4. As many servers as possible

- Why is the starting server for data distribution often chosen randomly?
  - Easy implementation
  - Even load distribution
  - Fault tolerance

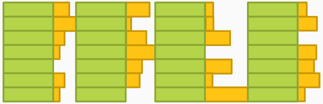
- What is the difference between POSIX and NFS semantics?
    1. POSIX guarantees each write will be synchronized to storage immediately
    2. POSIX guarantees each write will be visible by other processes immediately
    3. NFS guarantees each write will not be visible by other processes until the file is closed
    4. NFS guarantees data will be synchronized to storage when the file is closed

- When would you stripe a directory across multiple servers?
    1. Always
    2. When it contains more than 1,000 files
    3. When it contains more than 1,000,000 files
    4. Never

Outline

Overview

- Parallel applications require efficient parallel I/O
  - Synchronous and serial I/O are bottlenecks
- Synchronous I/O causes all tasks to wait for completion
- Serial I/O requires sending all data to a chosen task
  - One task cannot hold all data, must be done iteratively
- Common scenarios in HPC
  - Reading input data
    - Starting conditions, large data sets
  - Writing output data
    - Result data, checkpoints



[Gorda, 2013]

Overview...

- MPI-IO denotes the I/O part of the MPI standard
  - MPI-IO was introduced with MPI 2.0 in 1997
  - Parallel applications often use MPI anyway
- The most popular implementation is called ROMIO
  - ROMIO is being developed and distributed as part of MPICH
  - It is also being used by OpenMPI and other MPICH derivates
  - Uses the Abstract-Device Interface for I/O (ADIO)
- An alternative implementation in OpenMPI is called OMPIO

Overview...

- MPI-IO provides element-based access
  - POSIX only provides a byte stream
- I/O interface is very similar to the communication interface
  - Reading and writing behave like sending and receiving
  - Collective and non-blocking operations are supported
  - MPI-IO also supports derived datatypes
- MPI-IO is typically not used directly by applications
  - Instead, I/O libraries such as HDF5 use it internally

Outlook

- MPI-IO provides the basis for many I/O libraries
  - HDF5 and NetCDF use MPI-IO for parallel access to shared files
  - ADIOS also supports MPI-IO for parallel I/O
- POSIX can also be used for parallel I/O
  - HDF5 and NetCDF only do serial I/O via POSIX
  - ADIOS also supports parallel I/O via POSIX, but not to a shared file
- ROMIO contains efficient algorithms and implementations for parallel I/O
  - Frees higher layers from having to implement them as well
  - Libraries can focus on their primary tasks

ROMIO

- MPI-IO abstracts from the underlying file systems
  - MPI-IO provides its own syntax and semantics
- ROMIO supports a wide range of architectures
  - IBM SP, Intel Paragon, HP Exemplar, SGI Origin2000, Cray T3E, NEC SX-4 etc.
- ROMIO also supports many file systems
  - IBM PIOFS, Intel PFS, HP/Convex HFS, SGI XFS, NEC SFS, PVFS, Lustre, NFS, NTFS, Unix File System (UFS) etc.

ROMIO…

- MPI-IO's interface can be used by applications and libraries
  - Provides portability across a wide range of file systems and architectures
- File system specifics are contained in ADIO modules
  - Allows providing the best possible performance
    - For instance, data distribution functions are often not portable
  - Also allows hiding different file system syntax and semantics
- It also contains generic optimizations for parallel I/O
  - Optimizations are especially important with growing numbers of processes
  - We will take a look at Data Sieving and Two-Phase I/O later

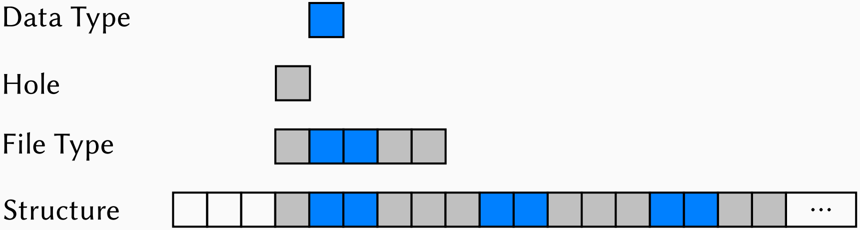
Outline

- File
  - Files are opened collectively by all processes in a communicator
  - Access can be done sequentially or randomly
  - Files are a collection of typed elements
- File pointer
  - File pointer determines position within a file (like POSIX)
  - Individual or shared file pointers are possible

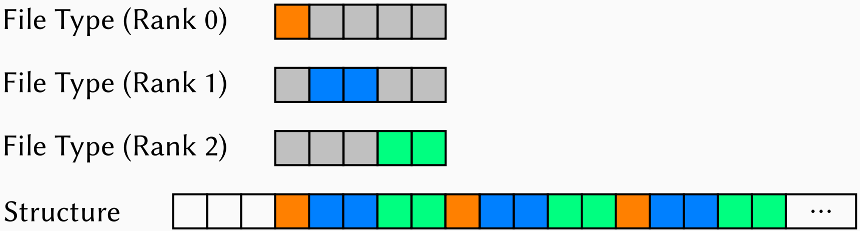
Basics...

- Data type
  - Smallest possible unit used for accessing a file
  - Can also be an elementary type or a derived data type
- Displacement
  - Determines the position a file view begins at
  - Expressed as a byte position relative from the start of a file
    - Can be used for headers etc.

- File type
  - A pattern that describes the structure of a file
  - Consists of data types and holes
  - Pattern is repeated within the file



- File view
  - Process-specific view of the file
  - Determined by displacement, data type and file type



Basics...

- Offset
  - Offset describes a position within a file
  - Given as a number of data types
  - Interpreted relative to the current file view
- File size
  - Size of the file in bytes

Basics…

- File handle
  - Describes an open file, similar to a file descriptor
  - Required for almost all other operations
- Hints
  - Additional information that can be passed to the implementation
  - Typically used to improve performance or reduce overhead

Creating and Opening Files

- MPI_File_open: Opens a file
  - comm: Communicator for collective open
  - filename: Path to the file
  - amode: Access mode used for opening
  - info: Optional hints
  - fh: File handle for further operations
- MPI_File_close: Closes a file
  - fh: File handle

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

int MPI_File_close (MPI_File* fh)
```

Creating and Opening Files…

- MPI_File_open is a collective operation
  - All processes have to open the same file (potentially different names)
  - Process-local files are possible by using MPI_COMM_SELF
- File name is implementation-specific
  - ROMIO allows specifying an ADIO module explicitly
    - For example: pvfs2:/pvfs/path/to/file
- The initial file view is a byte stream (like POSIX)
  - That is, all processes have access to the whole file

Creating and Opening Files...

- `MPI_File_open` offers multiple access modes
  - `MPI_MODE_RDONLY`: Read-only
  - `MPI_MODE_RDWR`: Read and write
  - `MPI_MODE_WRONLY`: Write-only
  - `MPI_MODE_CREATE`: Create file if it does not exist
  - `MPI_MODE_EXCL`: Return error if file exists already
  - `MPI_MODE_DELETE_ON_CLOSE`: Delete file on close

Creating and Opening Files…

- MPI_File_open offers multiple access modes…
  - MPI_MODE_UNIQUE_OPEN: File will not be opened concurrently
  - MPI_MODE_SEQUENTIAL: File will be accessed only sequentially
  - MPI_MODE_APPEND: File pointers will be set to the end of file
- Access modes can also be combined when it makes sense
- Some modes offer potential for optimizations
  - Caching can be enabled for MPI_MODE_UNIQUE_OPEN
  - Read ahead can be used for MPI_MODE_SEQUENTIAL

- What happens if a file opened with `MPI_MODE_UNIQUE_OPEN` is opened elsewhere?
  1. MPI will fall back to regular open
  2. MPI will abort the application
  3. MPI will crash
  4. Undefined behavior

Positioning

- MPI_File_seek: Sets the file pointer
  - fh: File handle
  - offset: Offset within file
  - whence: Positioning mode
  - Behaves like POSIX's lseek

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

Positioning. . .

- MPI supports three modes for positioning
  1. Individual file pointers
  2. Shared file pointers
  3. Explicit offsets

1. Individual file pointers
   - File pointer is process-local and updated with each operation
     - Behaves like POSIX's `read` and `write`
   - Accesses by different processes can lead to conflicts

2. Shared file pointers
    - File pointer is global and updated with each operation
        - Syntax: `MPI_..._shared` and `MPI_..._ordered`
    - Can be used to ensure different processes do not access the same data
    - Support can be limited depending on the used file system
3. Explicit offsets
    - Offset is specified with each operation
        - Behaves like POSIX's `pread` and `pwrite`
        - Syntax: `MPI_..._at`
    - Concurrent access by multiple processes can be done safely
        - Requires calculating the offset manually

Positioning. . .

- `MPI_File_seek` and `MPI_File_seek_shared` set the file pointer
  - Both functions support three positioning modes
    1. `MPI_SEEK_SET`: File pointer is set to specified offset
    2. `MPI_SEEK_CUR`: File pointer is incremented by specified offset
    3. `MPI_SEEK_END`: File pointer is set to end of file plus offset
  - The offset can also be negative (especially useful for `MPI_SEEK_END`)

Shared File Pointers

- Shared file pointers can be used for coordinated access
  - All processes use the same global file pointer
    - Access conflicts can be avoided like this
  - Accesses update the file pointer for all processes
- Can be problematic to implement efficiently
  - Requires some form of (distributed) locks
    - File pointer can only be updated by one process at a time
  - Complicated to scale when using large number of processes
    - Changes have to be announced to all other processes
  - Shared file pointers are not supported by all file systems
    - OrangeFS does not support locks and therefore no shared file pointers

Shared File Pointers...

- `MPI_..._shared` can be used for individual operations
  - Operations can be performed in an arbitrary order
- `MPI_..._ordered` can be used for collective operations
  - Operations are performed according to the processes' ranks
- Useful for several use cases
  - Shared log file, where all processes append new entries
  - Output data to be written to a file in the processes' order

- MPI_File_read: Reads from file
  - fh: File handle
  - buf: Buffer to read into
  - count: Number of elements
  - type: Element type
  - status: Read status
  - Behaves like read
- MPI_File_write: Writes to file
  - fh: File handle
  - buf: Buffer to write from
  - count: Number of elements
  - type: Element type
  - status: Write status
  - Behaves like write

```
int MPI_File_read (MPI_File fh,
                   void* buf,
                   int count,
                   MPI_Datatype type,
                   MPI_Status* status)

int MPI_File_write (MPI_File fh,
                    void* buf,
                    int count,
                    MPI_Datatype type,
                    MPI_Status* status)
```

```
MPI_File fh;
MPI_Offset size;
MPI_Status status;
int nbytes;

MPI_File_open(MPI_COMM_WORLD, "/tmp/mpi-io",
              MPI_MODE_RDWR | MPI_MODE_CREATE | MPI_MODE_DELETE_ON_CLOSE,
              MPI_INFO_NULL, &fh);
MPI_File_write(fh, data, sizeof(data), MPI_BYTE, &status);
MPI_Get_count(&status, MPI_BYTE, &nbytes);
MPI_File_get_size(fh, &size);
MPI_File_close(&fh);
```

- Basic structure is very similary to POSIX
  - Separate call of `MPI_Get_count` necessary (return value is a 32 bit integer)
  - Metadata access is limited to `MPI_File_get_size`

Metadata Operations

- MPI-IO only supports a few operations, especially for metadata
    - Its interface is more akin to an object store than a file system
- There is no support for directory operations at all
    - Full path must be known to open a file
- File management is also very limited
    - Files can only be create via `MPI_File_open`
- Files can be grown and shrunk
    - `MPI_File_set_size` and `MPI_File_preallocate`
- No support for rich metadata like in POSIX
    - No equivalent to `stat`, files size via `MPI_File_get_size`

Non-Contiguous Data Types

- MPI-IO supports non-contiguous data types
  - Enables access to complex structures using a single I/O call
  - Provides convenience for developers but also potential for optimizations
- Accesses are also possible to do manually
  - Would introduce developer and performance overhead
  - Similar to `readv`, `writev`, `aio_read`, `aio_write` and `lio_listio`
    - `readv` and `writev` can only access contiguous areas and are thus not as powerful

- MPI_Type_vector: Create vector type
  - count: Number of blocks
  - blocklength: Number of elements in each block
  - stride: Distance between blocks
  - old: Old data type
  - new: New data type
- Example: 3×3 matrix diagonal

```
int MPI_Type_vector (int count,
                     int blocklength,
                     int stride,
                     MPI_Datatype old,
                     MPI_Datatype* new)

MPI_Type_vector(3, 1, 4,
                MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);
MPI_File_write(fh, buffer,
               1, newtype, &status);
```

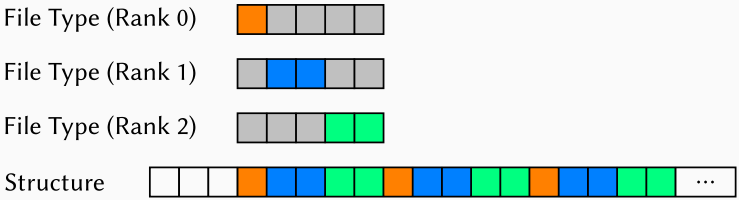
Non-Contiguous Data Types...

```
MPI_Type_vector(3, 1, 4, MPI_DOUBLE, &newtype);
```

1	2	3
4	5	6
7	8	9

- Assumption: Matrix is stored row- or column-wise in memory
  - A 3×3 matrix has three diagonal elements
  - Each diagonal element is a double value
  - Diagonal elements are separated by three elements (have a distance of four)

- MPI-IO supports collective I/O for improved performance
  - All processes perform their access at the same time in a coordinated fashion
    - Syntax: `MPI_..._all`
  - Collective operations provide additional information for potential optimizations
    - Individual operations can result in random access patterns
- Example: Small non-contiguous accesses
  - Each processes accesses several small areas within the file
  - All processes together access the whole file



Non-Blocking Operations

- MPI-IO also supports non-blocking I/O operations
  - Work similar to non-blocking communication operations
    - Syntax: `MPI_..._i...`
  - Allows overlapping I/O and computation (and more)
    - Enables applications to be productive while performing I/O
    - Speedup is limited to 2 with only I/O and computation
- Status can be checked using standard MPI functions
  - For example, `MPI_Wait` and `MPI_Test`

Non-Blocking Operations...

- Non-blocking collective I/O operations are called split collectives
  - Separated due to optimization and implementation reasons
    - Syntax: `MPI_..._begin` and `MPI_..._end`
- Split collectives have several limitations
  - Per process and file only one split collective is allowed at a time
  - Cannot be combined with regular collective operations
  - No collective I/O operations are allowed while a split collective is in progress
  - Implementations are allowed to perform blocking operations internally

- What happens if the buffer of a non-blocking operation is reused before the operation is finished?
    1. MPI will finish the non-blocking operation first
    2. MPI will abort the application
    3. MPI will crash
    4. Undefined behavior

Hints

- Hints can be used to provide implementations with additional information
  - Typically used for optimizations
  - Can be specified for `MPI_File_open` and others
- Examples:
  - Number of devices a file should be distributed across
  - Size used for distributing blocks
  - Information about the data layout
- Hints are optional and do not have to be specified
  - Implementations are also free to ignore hints as they see fit
  - Some implementations allow specifying hints via environment variables

Data Representations

- MPI-IO supports multiple data representations
  - Data portability is an important aspect of MPI-IO
  - Often also handled by I/O libraries based upon MPI-IO
- Three possible representations
  - native: Data is not converted in any way and are stored as in memory
  - internal: Portable data representation across all platforms supported by used implementation
  - external32: Portable data representation across all platforms and implementations, potential loss of precision and performance
- Users can also define their own data representations

Outline

General

- Achievable performance depends on the used operations
  - Large accesses are typically more efficient than small ones
  - Contiguous accesses are usually better than non-contiguous ones
- MPI-IO offers several possibilities of performing I/O
  - Contiguous vs. non-contiguous, individual vs. collective
- Example with a 3×3 matrix:
  - Matrix is stored row-wise in memory
  - Matrix should be read by three processes
  - Each process is responsible for one column

Level 0: Individual Contiguous Accesses

- Each process performs individual accesses
- Contiguous region is read in each iteration

```
for (i = 0; i < 3; i++)
{
    MPI_File_seek(fh, ...);
    MPI_File_read(fh, ...,
        1, MPI_DOUBLE, ...);
}
```

Level 0: Individual Contiguous Accesses

- Each process performs individual accesses
  - One row is read per iteration
- Contiguous region is read in each iteration
  - Individual accesses lead to random pattern

```c
for (i = 0; i < 3; i++)
{
    MPI_File_seek(fh, ...);
    MPI_File_read(fh, ...,
        1, MPI_DOUBLE, ...);
}
```

Level 1: Collective Contiguous Accesses

- Processes perform coordinated collective access
- Contiguous region is read in each iteration

```c
for (i = 0; i < 3; i++)
{
    MPI_File_seek(fh, ...);
    MPI_File_read_all(fh, ...,
        1, MPI_DOUBLE, ...);
}
```

Level 1: Collective Contiguous Accesses

- Processes perform coordinated collective access
    - One row is read per iteration
- Contiguous region is read in each iteration
    - Collective access leads to contiguous pattern

```c
for (i = 0; i < 3; i++)
{
    MPI_File_seek(fh, ...);
    MPI_File_read_all(fh, ...,
        1, MPI_DOUBLE, ...);
}
```

- Each process performs individual accesses
- Non-contiguous column is read by each process

```
MPI_Type_vector(3, 1, 3,
    MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);

MPI_File_seek(fh, ...);
MPI_File_read(fh, ...,
    1, newtype, ...);
```

Level 2: Individual Non-Contiguous Accesses

- Each process performs individual accesses
  - All columns are read
- Non-contiguous column is read by each process
  - Individual accesses lead to random pattern

```
MPI_Type_vector(3, 1, 3,
    MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);

MPI_File_seek(fh, ...);
MPI_File_read(fh, ...,
    1, newtype, ...);
```

Level 3: Collective Non-Contiguous Accesses

- Processes perform coordinated collective access
- Non-contiguous column is read by each process

```
MPI_Type_vector(3, 1, 3,
    MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);

MPI_File_seek(fh, ...);
MPI_File_read_all(fh, ...,
    1, newtype, ...);
```

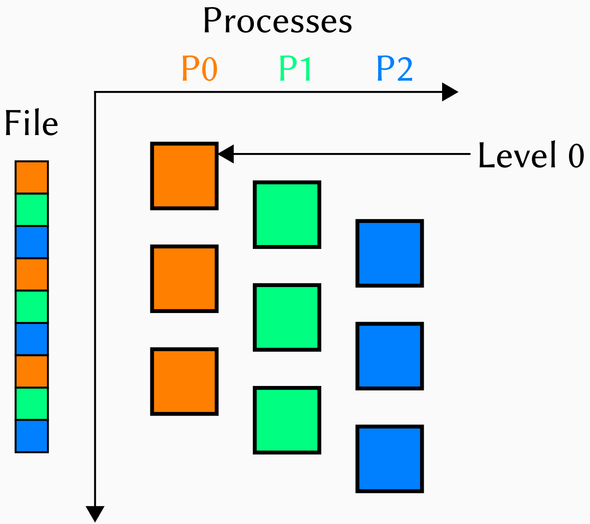
Level 3: Collective Non-Contiguous Accesses

- Processes perform coordinated collective access
  - All columns are read
- Non-contiguous column is read by each process
  - Collective access leads to contiguous pattern

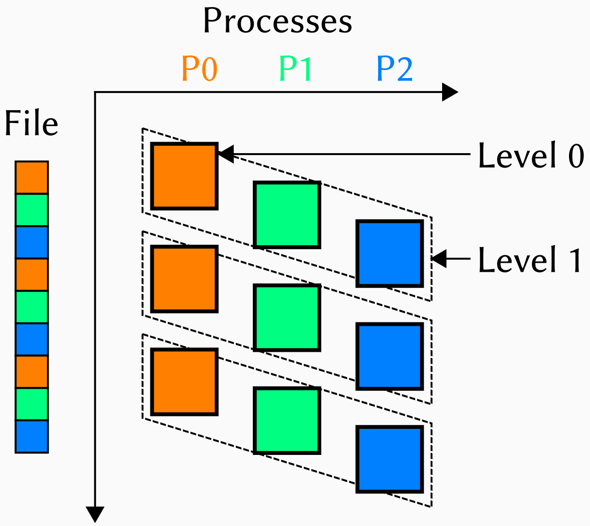
```
MPI_Type_vector(3, 1, 3,
    MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);

MPI_File_seek(fh, ...);
MPI_File_read_all(fh, ...,
    1, newtype, ...);
```

MPI-IO Levels [Thakur et al., 2002]



MPI-IO Levels [Thakur et al., 2002]



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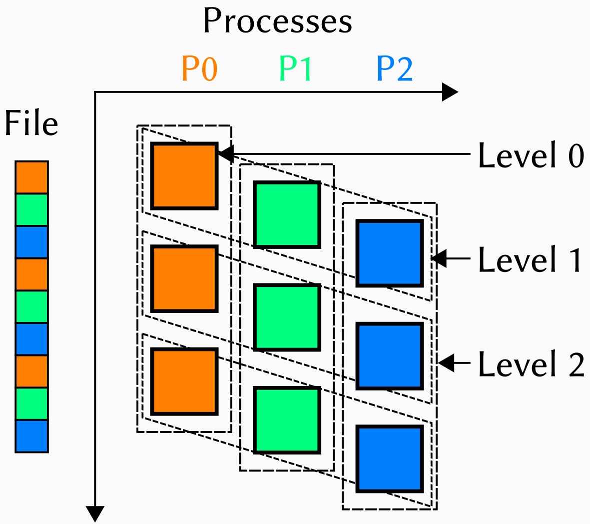
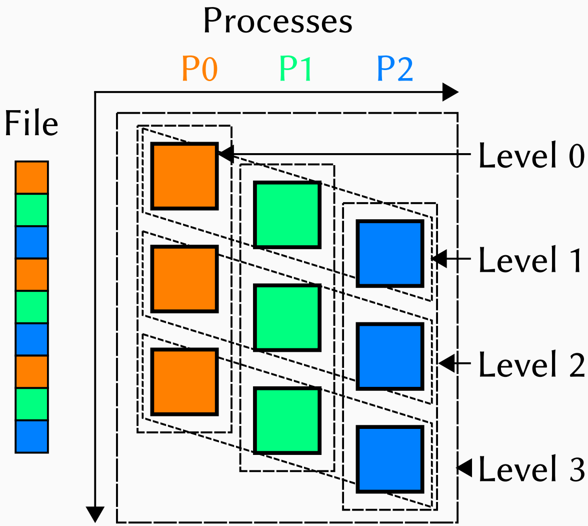


MPI-IO Levels [Thakur et al., 2002]



Semantics

- Reminder: POSIX has strict consistency and coherence requirements
  - Changes have to be visible globally after a `write`
  - I/O should be performed atomically
  - Requirements are relatively easy to support locally
- Efficient parallel I/O is complicated by POSIX semantics
  - Data cannot be cached as effectively due to synchronization
  - Atomicity might require distributed locks

- MPI-IO has less strict requirements than POSIX
  - Changes only have to be visible to the current process
  - Non-overlapping or non-concurrent operations are handled correctly
- Changes do not have to be visible globally immediately after an operation
  - Allows reducing locking overhead and increasing scalability
- MPI-IO semantics is enough for most scientific applications
  - For example, non-overlapping accesses to computed data are common

1. Sync transfers changes to the file system

```
MPI_File_sync(fh);
MPI_Barrier(MPI_COMM_WORLD);
MPI_File_sync(fh);
```

Synchronization

1. Sync transfers changes to the file system
2. Barrier synchronizes all processes

```
MPI_File_sync(fh);
MPI_Barrier(MPI_COMM_WORLD);
MPI_File_sync(fh);
```

Synchronization

1. Sync transfers changes to the file system
2. Barrier synchronizes all processes

```
MPI_File_sync(fh);
MPI_Barrier(MPI_COMM_WORLD);
MPI_File_sync(fh);
```

3. Sync makes changes visible to all processes

Synchronization

1. Sync transfers changes to the file system
2. Barrier synchronizes all processes
    - Necessary for correct synchronization
    - First sync has to be finished for all processes before second sync is called
3. Sync makes changes visible to all processes

```
MPI_File_sync(fh);
MPI_Barrier(MPI_COMM_WORLD);
MPI_File_sync(fh);
```

Synchronization…

- MPI-IO's atomic mode guarantees sequential consistency
  - Has to be enabled explicitly using `MPI_File_set_atomicity`
- Allows MPI-IO to handle overlapping and concurrent accesses correctly
  - Similar to stricter POSIX semantics
- Support depends on file system and is limited
  - ROMIO supports atomic mode, OMPIO does not
  - Typically requires distributed locks
    - Not all file systems implement locks, limiting availability
    - Reminder: OrangeFS does not support locks

Outline

Summary

Positioning	Blocking	Individual	Collective
Explicit Offset	Blocking	read_at write_at	read_at_all write_at_all
	Non-Blocking and Split Collective	iread_at	read_at_all_begin read_at_all_end
		iwrite_at	write_at_all_begin write_at_all_end
Individual File Pointers	Blocking	read write	read_all write_all
	Non-Blocking and Split Collective	iread	read_all_begin read_all_end
		iwrite	write_all_begin write_all_end
Shared File Pointer	Blocking	read_shared write_shared	read_ordered write_ordered
	Non-Blocking and Split Collective	iread_shared	read_ordered_begin read_ordered_end
		iwrite_shared	write_ordered_begin write_ordered_end

Summary...

- MPI-IO is defined similar to MPI's communication operations
  - Supports collectives, derived data types etc.
- Files are a collection of typed elements
  - Each process has its own file view
  - Multiple data representations enable portability
- Positioning can be performed using different modes
  - Explicitly, with individual file pointers or a shared file pointer
- Different access modes allow optimizing parallel I/O
  - Non-contiguous, collective and non-blocking operations can improve performance

References

[Gorda, 2013] Gorda, B. (2013). **HPC Technologies for Big Data.** http://www.hpcadvisorycouncil.com/events/2013/Switzerland-Workshop/Presentations/Day_2/3_Intel.pdf.

[Thakur et al., 2002] Thakur, R., Gropp, W., and Lusk, E. L. (2002). **Optimizing noncontiguous accesses in MPI-IO.** *Parallel Comput.*, 28(1):83–105.