





Parallel I/O with MPI IO

Georg Hager, Thomas Zeiser,

Gerhard Wellein, <u>Markus Wittmann</u> (RRZE)

hpc@rrze.fau.de

A. Skjellum, P. Bangalore, S. Herbert,

R. Rabenseifner



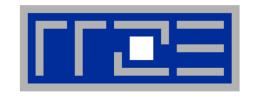






- MPI derived data types
- MPI I/O
 - File open and closing
 - Views
 - Reading and writing
- Examples & Use Cases





Repetition: Derived Data Types in MPI



Derived Datatypes in MPI: Why Do We Need Them?



Root reads configuration and broadcasts it to all others

```
// root: read configuration from
// file into struct config
MPI Bcast(&cfg.nx, 1, MPI INT, ...);
MPI Bcast(&cfg.ny, 1, MPI INT, ...);
MPI Bcast(&cfg.du, 1, MPI DOUBLE,...);
MPI Bcast(&cfg.it, 1, MPI INT, ...);
```

```
MPI Bcast (&cfg, sizeof (cfg),
         MPI BYTE, ..)
is not a solution. Its not portable as
no data conversion can take place
```

MPI Bcast (

```
Send column of matrix (noncontiguous in C):
Send each element alone?
Manually copy elements out into a contiguous
  buffer and send it?
```

&cfg, 1, <type cfg>,...);



Derived Data Types in MPI: Construction



- Create in three steps
- Construct with

Commit new data type with

After use, deallocate the data type with



Derived Data Types in MPI: MPI_TYPE_VECTOR



Create vector-like data type

```
MPI Type vector(count, int blocklength, int stride,
                      MPI Datatype oldtype,
                      MPI Datatype * newtype)
count
                 2
blocklength
                                             MPI Datatype nt;
                 5
stride
                                             MPI Type vector(
                MPI INT
                                               2, 3, 5,
oldtype
                                               MPI INT, &nt);
                  count
                                             MPI Type commit(&nt);
                                             // use nt...
                                             MPI Type free(&nt);
                        size
                              := 6*size(oldtype)
                        extent := 8*extent(oldtype)
  blocklength
                            Caution: Concatenating such types in a SEN
                            operation can lead to unexpected results!
         stride
                            See Sec. 3.12.3 and 3.12.5 of the MPI 1.1 Standard for details.
```

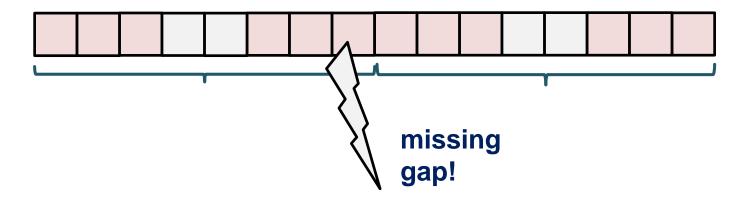


Derived Data Types in MPI: Using a New Type



count argument to send and others must be handled with care:

MPI Send (buf, 2, nt,...) with nt (newtype from prev. slide)

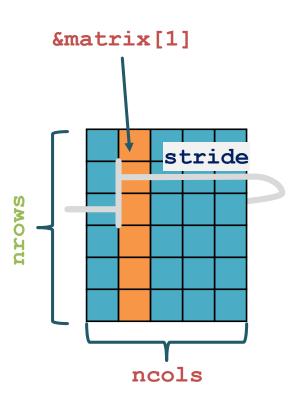




Derived Data Types in MPI: Example for MPI_TYPE_VECTOR



- Create data type describing one column of a matrix
 - assuming row-major layout like in C



```
double matrix[30]
MPI Datatype nt;
// count = nrows, blocklength = 1,
// stride = ncols
MPI Type vector (nrows, 1, ncols,
                MPI DOUBLE, &nt);
MPI_Type_commit(&nt);
// send column
MPI Send(&matrix[1], 1, nt, ...);
MPI Type free(&nt);
```



Derived Data Types in MPI: MPI_Type_create_subarray



Create sub array data type

```
MPI_Type_create_subarray(int dims,
int ar_sizes[], int ar_subsizes[], int ar_starts[],
int order, MPI_Datatype oldtype, MPI_Datatype * newtype)
```

dims:
dimension of the array

ar_sizes: array with sizes of array (dims entries)

ar subsizes: array with sizes of subarray (dims entries)

ar_starts: start indices of the subarray inside array (dims)

entries), start at 0 (also in Fortran)

order

row-major: MPI_ORDER_C

• column-major: MPI ORDER FORTRAN

oldtype: data type the array consist of

newtype: data type describing a subarray



oldtype

Derived Data Types in MPI: MPI_Type_create_subarray



```
dims 2

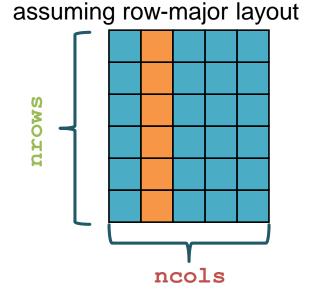
ar_sizes {ncols, nrows}

ar_subsizes {1, nrows}

ar_starts {1, 0}

order MPI_ORDER_C
```

MPI DOUBLE



```
MPI_Type_create_subarray(dims, ar_sizes, ar_subsizes, ar_starts, order, oldtype, &nt)

MPI_Type_commit(&nt);
// use nt...
MPI_Type_free(&nt);
```



Derived Data Types in MPI: MPI_Type_create_subarray



```
dims
               1
ar sizes {5}
ar subsizes {3}
ar starts
          {0}
order
              MPI ORDER C
oldtype
              MPI INT
MPI Type create subarray(dims, ar sizes, ar subsizes, ar starts,
order, oldtype, &nt)
// commit type...
MPI Send(buf, 4, nt, ...)
        nt
                             4 x nt
```



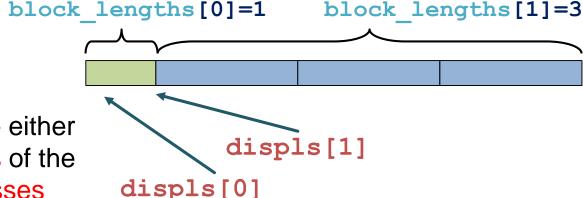
Derived Data Types in MPI: MPI_TYPE_CREATE_STRUCT



- Most general type constructor
 - Describe blocks with arbitrary data types and arbitrary displacements

```
types[0] types[1]
```

```
MPI_Type_create_struct(count,
   int block_lengths[],
   MPI_Aint displs[],
   MPI_Datatype types[],
   MPI_Datatype * newtype)
```



count = 2

The contents of **displs** are either the displacements in bytes of the block bases or MPI addresses



Derived Data Types in MPI: MPI_TYPE_CREATE_STRUCT



What about displacements in Fortran?

```
MPI_GET_ADDRESS(location, address, ierror)
  <type> location
  INTEGER(KIND=MPI_ADDRESS_KIND) address
```

Example:

```
double precision a(100)
integer a1, a2, disp
call MPI_GET_ADDRESS(a(1), a1, ierror)
call MPI_GET_ADDRESS(a(50), a2, ierror)
disp=a2-a1
```

Result would usually be $disp = 392 (49 \times 8)$

When using absolute addresses, set buffer address = MPI_BOTTOM



Derived Data Types in MPI: Summary



- Derived data types provide a flexible tool to communicate complex data structures in an MPI environment
- Most important calls:

```
MPI_Type_vector (second simplest)
MPI_Type_create_subarray
MPI_Type_create_struct (most advanced)
MPI_Type_commit/MPI_Type_free
MPI_GET_ADDRESS
```

Other useful features:

```
MPI_Type_contiguous, MPI_Type_indexed,
MPI_Type_get_extent, MPI_Type_size
```

- Matching rule: send and receive match if specified basic datatypes match one by one, regardless of displacements
 - Correct displacements at receiver side are automatically matched to the corresponding data items





MPI Input/Output

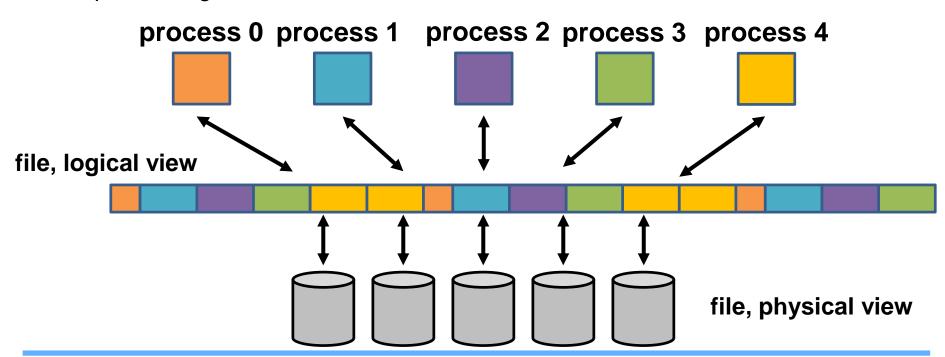


Motivation for MPI I/O



Many parallel applications need ...

- Coordinated parallel access to a file by a group of processes
- Simultaneous access
- All processes read/write many non-contiguous pieces of the file
- i.e. the data may be distributed amongst the processes according to a partitioning scheme

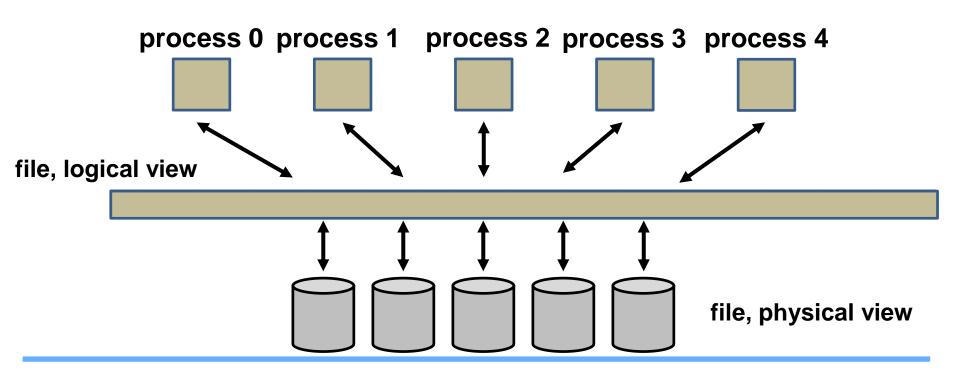




Motivation for MPI I/O



- Many parallel applications need ...
 - all processes may read the same data
- Efficient collective I/O based on
 - fast physical I/O by several processors, e.g. striped
 - distributing (small) pieces by fast message passing





MPI I/O: Features



- Provides a high-level interface to support
 - data file partitioning among processes
 - transfer global data between memory and files ("collective" I/O)
 - asynchronous transfers
 - strided access
- MPI derived data types are used to specify common data access patterns for maximum flexibility and expressiveness



MPI I/O: Principles



- MPI file contains elements of a single MPI data type (etype)
- The file is partitioned among processes using an access template (filetype)
- All file accesses transfer to/from a contiguous or non-contiguous user buffer (MPI data type)
- Several different ways of reading/writing data:
 - non-blocking / blocking
 - collective / individual
 - individual / shared file pointers, explicit offsets
- Automatic data conversion in heterogeneous systems
- File interoperability with external representation





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Open & Closing Files



File Open



- Collective call by all processes which are part of comm
- filename can be different, but must point to the same file
- amode describes access mode (see next slide)
- info object, can be MPI_INFO_NULL (see later)
- fh represents the file handle, associated to it is also comm and the view (see later)
- Process local file I/O is possible by specifying MPI_COMM_SELF as comm



File Access Modes



access mode	description						
MPI_MODE_RDONLY	read only						
MPI_MODE_RDWR	read and write - one of these flags is required						
MPI_MODE_WRONLY	write only						
MPI_MODE_CREATE	create if it does not exist						
MPI_MODE_EXCL	error if file exists						
MPI_MODE_DELETE_ON_CLOSE	file is deleted when closed						
MPI_MODE_UNIQUE_OPEN	file is not concurrently opened by anybody else						
MPI_MODE_SEQUENTIAL	only sequential access will occur (MPI_File_read/write_shared is allowed)						
MPI_MODE_APPEND	all file pointers are located at the end of the file						

- Flags can be or'ed together: MPI_MODE_WRONLY | MPI_MODE_APPEND
- Use or function in Fortran



File Open



All processes in MPI_COMM_WORLD open file collectively

Also possible to open file with only one process



File Close



```
int MPI File close(MPI File *fh)
```

- Collective call by all processes which are part of comm, the file was opened with
- File state is synchronized, i.e. all data is transferred to disk storage
- File handle fh is set to MPI FILE NULL
- File is deleted if MPI_MODE_DELETE_ON_CLOSE was part of access mode
- All outstanding nonblocking requests & split collectives must have been completed

```
MPI_File fh;
...
MPI_File_open(MPI_COMM_WORLD, ..., &fh);
...
MPI_File_close(&fh);
```





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Info Objects



Info Objects I



- Opaque object, storing key/value pairs
- Often used to provide system-specific information
 - via info argument in function calls
 - for MPI IO, process management, memory allocation, ...
- Keys
 - All keys might be ignored
 - MPI defines a set of reserved keys
 - Implementations may provide additional keys
- Keys/values are strings and converted to other types as required
- Use MPI INFO NULL if you do not want to provide additional information

```
MPI_Info info;
```

Generate new, empty info object:

```
int MPI_Info create(MPI_Info *info)
```

Add entry to existing info object:



Info Objects II



Delete entry from info object

```
int MPI Info delete(MPI Info info, const char *key)
```

Retrieve value associated with key

- flag = true: a value is associated with the key and returned in value
- flag = false: no value associated with the key, value is unchanged
- valuelen: size of the buffer value points to,

if associated value is larger, data is truncated

Free info object

```
int MPI Info free(MPI Info *info)
```

Length restriction:

- keys: mpi max info key
- values: mpi max info val



Info Objects for MPI I/O Striping

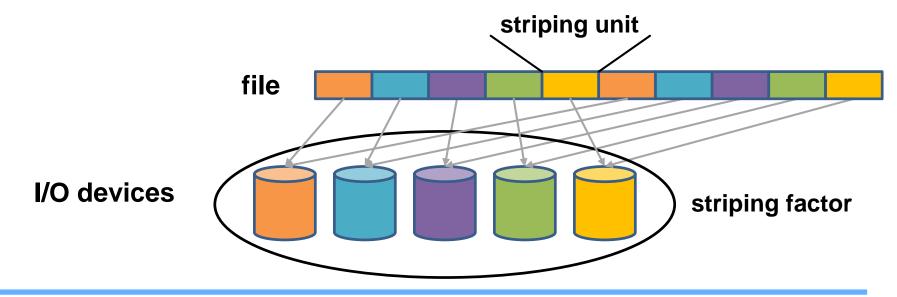


Striping:

- relevant only when file is created, i.e. in MPI File open
- must be the same for all processes
- is only a hint

Keys for info object

striping_factor	int	number of I/O devises the file should be striped across
striping_unit	int	number of consecutive bytes stored on one I/O device before the next is used

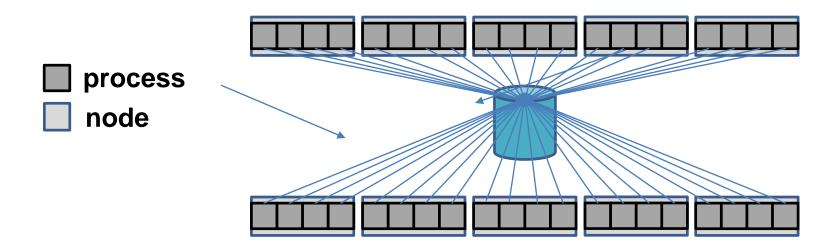




Info Objects for MPI I/O Collective Buffering I



- Each process might access I/O devices
- Can generate high load
- Collective buffering to mitigate this problem





Info Objects for MPI I/O Collective Buffering II



Collective buffering

- Optimization for collective accesses
- Access performed on behalf of all processes by some target nodes
- Key/value pairs must be the same on all processes

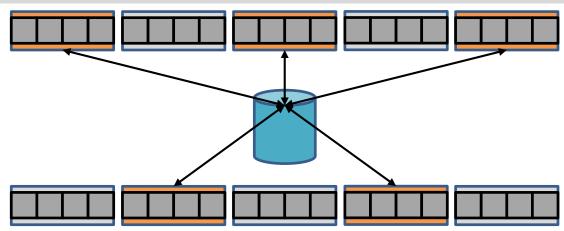
Keys for info object

collective_buffering	bool	true if application might benefit from collective buffering, false if not
cb_block_size	int	target nodes access data in chunks of this size
cb_buffer_size	int	buffer size on target node, that can be used for collective buffering, typically a multiple of the block size
cb_nodes	int	number of target nodes that should be used

process

node

target node





Info Object Example



Example: create MPI info object for MPI_File_open

```
MPI Info info;
MPI Info create(&info);
// Hint: stripe over 10 I/O devices
MPI Info set(info, "striping factor", "10");
// Hint: enable collective buffering
MPI_Info_set(info, "collective buffering", "true");
// Hint: use 4 target nodes for buffering
MPI Info set(info, "cb nodes", "4");
MPI_File_open(comm, filename, amode, info, &fh);
MPI Info free(&info);
```



MPI I/O: Other File Manipulation Routines



Pre-allocating space for a file (may be expensive)

```
int MPI_File_preallocate(MPI_File fh, MPI_Offset size)
```

Resizing a file (may speed up first writing on a file)

```
int MPI_File_set_size(MPI_File fh, MPI_Offset size)
```

Querying file size

```
int MPI File get size(MPI File fh, MPI Offset *size)
```

Querying file access mode

```
int MPI File get amode(MPI File fh, int *amode)
```

File info object

```
int MPI_File_set_info(MPI_File fh, MPI_Info info)
int MPI File get info(MPI File fh, MPI Info *info used)
```



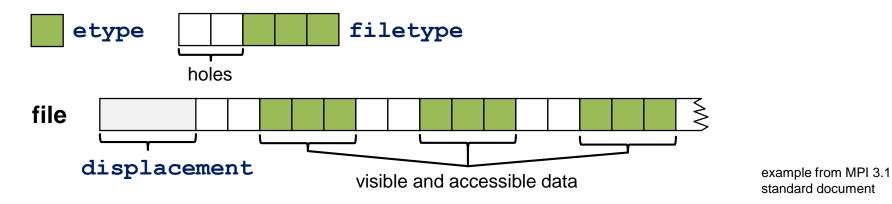


Views



MPI I/O: File Views





- Visible and accessible data from a file
- Each process has its own view
- View is described via (displacement, etype, filetype)
- Pattern of filetype is repeated beginning at displacement
- Views can be changed, but this is a collective operation
- Default view: linear byte stream (0, MPI_BYTE, MPI_BYTE)



MPI I/O: The Default View



- After file open each file has the default view
- Default view: linear byte stream
 - displacement = 0
 - etype = MPI BYTE
 - filetype = MPI BYTE
- MPI BYTE matches with any datatype

file

0	1	2	3	4	5	6	7	8	9	10	11			
0	1	2	3	4	5	6	7	8	9	10	11			process 0
0	1	2	3	4	5	6	7	8	9	10	11	<u></u>	views of	process 1
0	1	2	3	4	5	6	7	8	9	10	11	\S		process 2

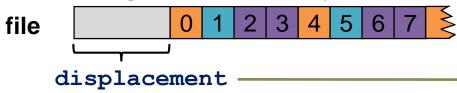


MPI I/O: Definitions

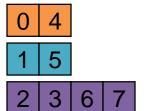




tiling a file with filetypes:



displacement in bytes



view of process 0
view of process 1
view of process 2

example from MPI 3.1 standard document



MPI I/O: Definitions



file	ordered collection of data items
displacement	 position from the beginning of the file marks the start of the view unit: byte
etype	 elementary data type unit of data access and positioning type displacements must be: nonnegative, monot. nondecreasing, and nonabsolut same for all processes
filetype	 single or multiple etypes size of holes must be multiples of etype extent repeated pattern after displacement type displacements must be: nonnegative, monot. nondecreasing, nonabsolut, can be different for all processes
view	 accessible data of a file by a process defined by displacement, etype, filetype
	 position in file relative to current view type MPI_Offset in C, INTEGER(KIND=MPI_OFFSET_KIND) in Fortran uint: etype



MPI I/O: Set/Get File View



- Changes the process's view of the data
- Collective operation
- Local and shared file pointers are reset to zero
- etype and filetype must be committed types
- datarep is a string specifying the format data is written to a file: native, internal, external32, or user-defined
- Same etype extent and same datarep on all processes
- disp: MPI_Offset in C, INTEGER(KIND=MPI_OFFSET_KIND) in Fortran

Returns process's view of the data



MPI I/O: Data Representations



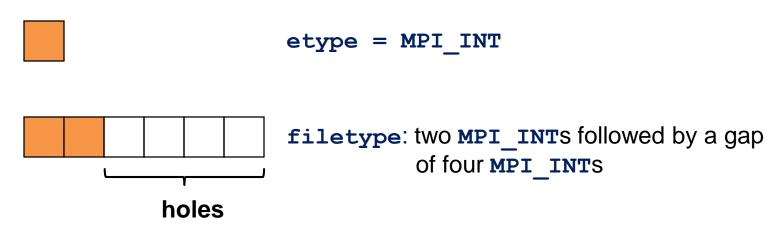
native	 data stored in file identical to memory on homogeneous systems no loss in precision or I/O performance due to type conversions on heterogeneous systems loss of interoperability no guarantee that MPI files accessible from C/Fortran
internal	 data stored in implementation specific format can be used with homogeneous or heterogeneous environments implementation will perform type conversions if necessary no guarantee that MPI files accessible from C/Fortran
external32	 follows standardized representation (big endian IEEE) all input/output operations are converted from/to external32 files can be exported/imported between different MPI environments due to type conversions from (to) native to (from) external32 data precision and I/O performance may be lost internal may be implemented as equal to external32 can be read/written also by non-MPI programs

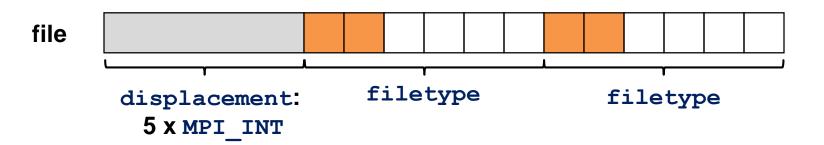


A Simple File View Example



- Basic example: File view for one process
 - View contains holes with respect to original file





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A Simple File View Example: Code (C)



```
subarray
MPI Offset disp;
                                                        filetype
MPI Datatype etype, filetype;
int sizes[] = { 6 };
int sub sizes[] = { 2 };
                                                             2 int
                                                                       holes
int start idxs[] = { 0 };
MPI Type create subarray(1, sizes, sub sizes, start idxs,
                          MPI ORDER C, MPI INT, &filetype);
MPI Type commit(filetype);
disp = 5 * 4; ! 4 = size of MPI INT in bytes
etype = MPI INT;
MPI File open (MPI COMM WORLD, "/pfs/datafile",
              MPI MODE CREATE | MPI MODE RDWR,
              MPI INFO NULL, &fh);
MPI File set view(fh, disp, etype, filetype, "native", MPI INFO NULL);
MPI File write(fh, buf, 1000, MPI INT, MPI STATUS IGNORE);
```

based on © R. Thakur





Reading and Writing



MPI I/O: Aspects of Data Access



- Direction: Read / Write
- Positioning (realized via routine names)
 - explicit offset (_AT)
 - individual file pointer (no positional qualifier)
 - shared file pointer (_shared or _ordered)
 (different names used depending on whether non-collective or collective)

Coordination

- non-collective
- collective (ALL)

Synchronism

- blocking
- non-blocking (_i...) and split collective (_BEGIN, _END)
- Atomicity, (realized with a separate API: MPI_File_set_atomicity)
 - atomic
 - non-atomic



MPI I/O: All Data Access Routines MPI File ...



Positioning	Synchronization	Non-collective	Collective
Explicit offsets	blocking	Reat_at	Read_at_all
		Write_at	Write_at_all
	non-blocking	Iread_at	Iread_at_all
		Iwrite_at	<pre>Iwrite_at_all</pre>
	split collective		Read_at_all_(begin end)
			Write_at_all_(begin end)
	blo akin a	Dood	Dood oll
	blocking	Read	Read_all
		Write	Write_all
Individual file	non-blocking	Iread	Iread_all
pointers		Iwrite	<pre>Iwrite_all</pre>
	split collective		Read_all_(begin end)
	·		Write_all_(begin end)
Shared file pointers	blocking	Read_shared	Read_ordered
		Write_shared	Write_ordered
	non-blocking	Iread_shared	
		Iwrite_shared	
	split collective	_	Read_ordered_(begin end)
			Write_ordered_(begin end)



MPI I/O: Explicit Offsets



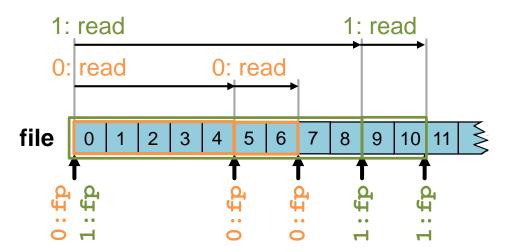
- Read data starting at offset
- Read count elements of datatype
- Starting offset * units of etype from begin of view (displacement)
- Sequence of basic datatypes of datatype (= signature of datatype) must match contiguous copies of the etype of the current view
- EOF can be detected by noting that the amount of data read is less than count
 - i.e. EOF is no error
 - USE MPI_Get_count(&status, datatype, &recv_count)
- Explicit offset routines do not alter file pointer



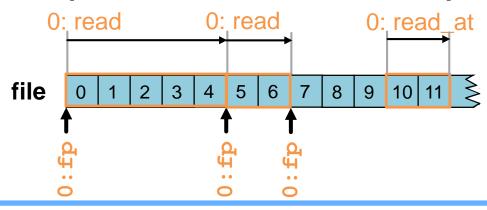
MPI I/O: Individual File Pointer



Each process maintains its own individual file pointer



Explicit offsets do not affect file pointers





MPI I/O: Individual File Pointer



- Arguments have same meaning as for MPI_File_reat_at
- offset is individual file pointer of calling process
- Individual file pointer is automatically incremented by fp = fp + count * elements(datatype)/elements(etype)
- I.e. it points to the next etype after the last one that will be accessed (formula is not valid if EOF is reached)
- Behaves nearly like standard serial file I/O



MPI I/O: Individual File Pointer



Set offset of individual file pointer fp:

whence	description
MPI_SEEK_SET	set fp to offset
MPI_SEEK_CUR	set fp to fp + offset
MPI_SEEK_END	set fp to EOF + offset

Get offset of individual file pointer:

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

Get absolute byte position from offset for current view

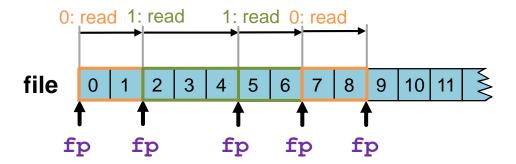
Retrieve offset and convert it into byte displacement, e.g. for usage in new view



MPI I/O: Shared File Pointers



- One shared file pointer per MPI_File_open
- All processes must have the same view
- Individual file pointers are not affected
- Ordering during serialization is not deterministic
- Use ordered (collective call) if determinism is required
- Use *shared routines to get/set file pointer







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Examples & Use Cases



MPI I/O Example: Global Matrix, Subarray I



Task

- read a global matrix from a file
- store a subarray into a local array on each process
- according to a given distribution scheme
- 2-dimensional distribution scheme: (BLOCK,BLOCK)
- garray on the file 20x30:
 - Contiguous indices is language dependent:
 - Fortran: (1,1), (2,1), (3,1), ..., (1,10), (2,10), (3,10), ..., (20,30)
 - in C/C++:[0][0], [0][1], [0][2], ..., [10][0], [10][1], [10][2], ..., [20][30]
- larray = local array in each MPI processsubarray of the global array
- same ordering on file (garray) and in memory (larray)



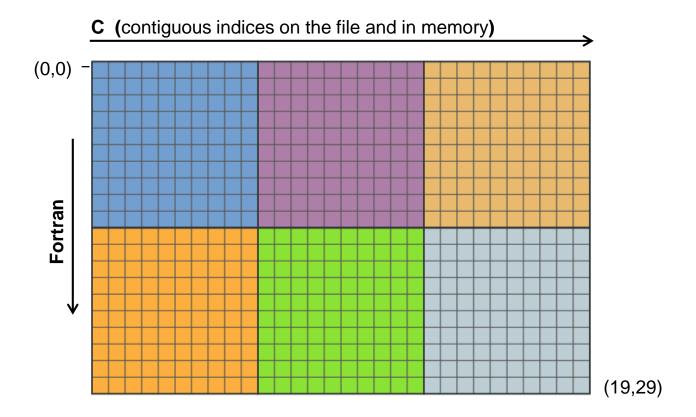
MPI I/O Example: Global Matrix, Subarray II



Process topology: 2x3

global array on the file: 20x30

distributed on local arrays in each processor: 10x10





MPI I/O Example: Global Matrix, Subarray, Reading the file ... III



```
// error handling omitted for brevity
// distribute garray[20,30] onto the processors [2,3]
double larray[10][10];
MPI Offset disp, offset, disp = 0, offset = 0;
ndims=2;
                                                                            Create
psizes[0]=2; period[0]=0;
psizes[1]=3; period[1]=0;
                                                                            topology
MPI Cart create (MPI COMM WORLD, ndims, psizes, period, 1, &comm);
MPI Comm rank(comm, &rank) ;
MPI Cart coords(comm, rank, ndims, coords);
                                                                            Create
gsizes[0]=20; lsizes[0]=10; starts[0]=coords[0]*lsizes[0];
                                                                            custom
gsizes[1]=30; lsizes[1]=10; starts[1]=coords[1]*lsizes[1];
                                                                            datatype
MPI Type create subarray(ndims, gsizes, lsizes, starts,
                          MPI ORDER C, MPI DOUBLE, &stype);
MPI Type commit(&stype);

    Open file

MPI File open (comm, file name, MPI MODE READ, MPI INFO NULL, &fh);
                                                                            create
MPI File set view(fh, disp, MPI DOUBLE, stype, "native", MPI INFO NULL);
                                                                             view
MPI File read at all(fh, offset,

    read data

                      larray, lsizes[0]*lsizes[1], MPI DOUBLE,
                      &status);
```



MPI I/O Example: Global Matrix, Subarray IV



- All MPI coordinates and indices start with 0, even in Fortran, i.e. with MPI ORDER FORTRAN
- MPI indices (here starts) may differ (/) from Fortran indices
- Block distribution on 2*3 processes:

```
rank = 0
                     rank = 1
                                          rank = 2
 coords = (0, 0) coords = (0, 1) coords = (0, 2)
                   starts = (0,10) starts = (0,20)
 starts = ( 0, 0)
 garray( 0:9, 0:9)
                                          garray( 0:9, 20:29)
                     garray( 0:9, 10:19)
= larray(0:9, 0:9)
                    = larray (0:9, 0:9)
                                        = larray(0:9, 0:9)
 rank = 3
                     rank = 4
                                          rank = 5
 coords = (1, 0)
                     coords = (1, 1)
                                          coords = (1, 2)
 starts = 10, 0
                   starts = 10,10
                                          starts = 10,20
                                          garray(10:19, 20:29)
 garray (10:19, 0:9)
                     garray(10:19, 10:19)
= larray(0:9, 0:9)
                    = larray(0:9, 0:9)
                                        = larray(0:9, 0:9)
```



MPI I/O: Application Scenarios I



- Scenery A: Each process has to read the whole file
- Solution 1: MPI File read all

blocking

collective with individual file pointers, with same view (displacement+etype+filetype) on all processes

Solution 2: MPI_File_read_all_begin

nonblocking

collective with individual file pointers, with same view (displacement+etype+filetype) on all processes, then computing some other initialization,

MPI_File_read_all_end.



MPI I/O: Application Scenarios II



 Scenery B: The file contains a list of tasks, each task requires different compute time

Solution: MPI_File_read_shared

non-collective with a shared file pointer (same view is necessary for shared file pointer)

Scenery C: The file contains a list of tasks, each task requires the same compute time

Solution: MPI_File_read_ordered

collective with a shared file pointer

(same view is necessary for shared file pointer)

Of: MPI File read all

collective with individual file pointers,

different views: filetype with

MPI_Type_create_subarray(..., &filetype)



MPI I/O: Error Handling



- File handles have their own error handler
- Default is MPI_ERRORS_RETURN, i.e. non-fatal
 - message passing: mpi_errors_are_fatal
- Default is associated with MPI_FILE_NULL
 - message passing: with MPI_COMM_WOLRD
- Changing the default, e.g., after MPI_Init
 - MPI File set errhandler (MPI FILE NULL, MPI ERRORS ARE FATAL);
 - CALL MPI_FILE_SET_ERRHANDLER(MPI_FILE_NULL, MPI_ERRORS_ARE_FATAL, ierr)
- MPI is undefined after first erroneous MPI call,
- but a high quality implementation will support I/O error handling facilities



MPI-I/O: Summary



- Rich functionality provided to support various data representation and access
- MPI I/O routines provide flexibility as well as portability
- Collective I/O routines can improve I/O performance
- Full implementation of MPI I/O available on / in
 - Intel MPI
 - Open MPI
 - MVAPICH
 - · ..
- Generally, use of MPI I/O is often limited to special file systems;
 do not expect it to work on your average NFS-mounted \$HOME
 - If it works at all data loss might occur!