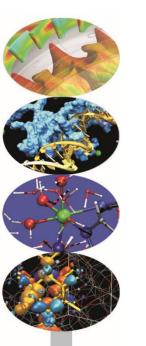


Parallel IO: basics and MPI2-IO



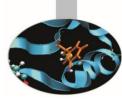
Super Computing Applications and Innovation Department

Courses Edition 2016





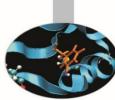
Introduction



- IO is a crucial issue in modern HPC applications:
 - 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 negligible
 - data portability (e.g. endianness)
- Solutions to avoid that IO become a bottleneck:
 - HW: parallel file-system available on all the HPC platforms
 - SW: high level libraries able to manage parallel accesses to the file in efficient way (e.g. MPI2-IO, HDF5, NetCDF, ...)







Solutions to managing IO in parallel applications must take into account different aspects of the application and implementation:

- potential performance improvements
- scaling with respect resources/system size
- ensure data consistency
- avoid communications
- strive for usability

Common approaches:

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

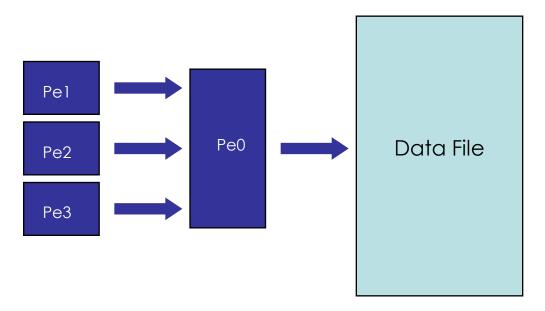






Approach 1: Master-Slave

Only 1 processor performs IO



Goals:

Scalable: NO

Ensure data consistency: YES

Avoid communication: NO

Usability: **YES**

note: no parallel FS needed

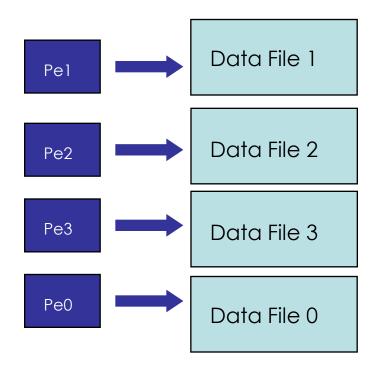






Approach 2: Distributed IO on local files

All the processors read/writes their own files



Goals: Scalable: <mark>YES</mark>

Ensure data consistency: YES

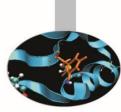
Avoid communication: **YES**

Usability: NO (need extra work later)

Warning: avoid to parametrize with processors!!!

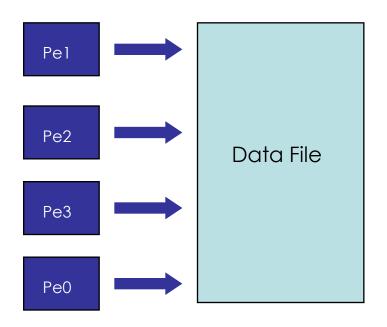






Approach 3: Coordinated controlled accesses All the processors read/writes on a single file

offsets to access data must be explicitly specified



Goals:

Scalable: **YES**

Ensure data consistency: NO

Avoid communication: **YES**

Usability: **YES**

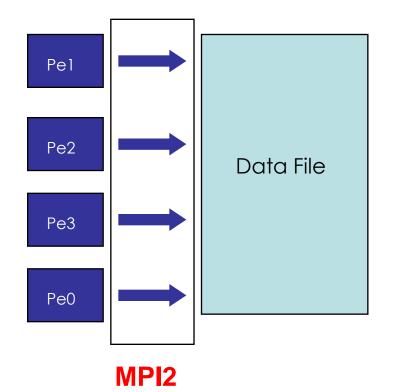






Solution 4: MPI2 IO (or other parallel IO libraries)

MPI functions perform the IO. Asynchronous IO is also supported.



Goals:

Scalable: **YES**

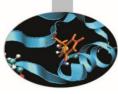
Ensure data consistency: YES

Avoid communication: **YES**

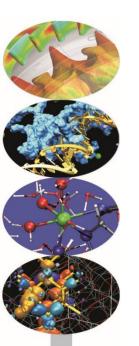
Usability: **YES**







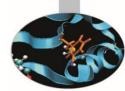
MPI2-IO







MPI-2.x features for Parallel IO

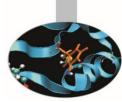


- MPI-IO: introduced in MPI-2.x standard (1997)
 - allow non-contiguous access in both memory and file
 - reading/writing a file is like send/receive a message from a MPI buffer
 - optimized access for non-contiguous data
 - collective / non-collective access operations with communicators
 - blocking / non-blocking calls
 - data portability (implementation/system independent)
 - good performance in many implementations
- Why do we start to use it???
 - syntax and semantic are very simple to use
 - performance : 32 MPI processes (4x8) with local grid 50000² (sp)
 - MPI-IO: **85**sec vs Traditional master/slave IO: **5200**sec
 - dimension of written file: 305GB
 - measured bandwidth of GPFS (single thread): 65MB/sec
 - measured bandwidth of MPI gather for Master/slave: 900MB/sec
 - MPI_File_write_all (85sec) vs MPI_file_write (320sec)





Starting with MPI-IO



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





Using individual file pointers

#include ``mpi.h"

```
int main(int argc, char **argv){
    int rank, nprocs;
```

MPI_Init(&argc, &argv); MPI_Comm_rank(MPI_COMM_WORLD, &rank); MPI_Comm_size(MPI_COMM_WORLD, &nprocs); File offset determined by MPI_File_seek

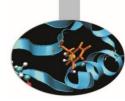
```
MPI_File fh; MPI_Status status;
MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile", MPI_MODE_RDONLY,
MPI_INFO_NULL, &fh);
```

```
int filesize;
MPI_File_get_size(fh, &filesize);
int bufsize = filesize/nprocs;
int nints = bufsize/sizeof(int);
int *buf = (int*) malloc(nints);
```

```
MPI_File_seek(fh, rank*bufsize, MPI_SEEK_SET);
MPI_File_read(fh, buf, nints, MPI_INT, &status);
```

```
MPI_File_close(&fh);
```

. . .

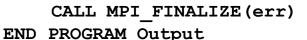


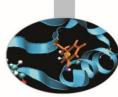


Using individual file pointers

PROGRAM Output

```
USE MPI
IMPLICIT NONE
INTEGER :: err, i, myid, file, intsize
INTEGER :: status (MPI STATUS SIZE)
INTEGER, PARAMETER :: count=10000
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)
```



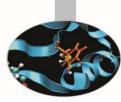


File offset determined by MPI File seek





Open/close a file 1/3



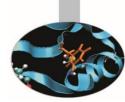
MPI_FILE_OPEN(comm, filename, amode, info, fh)
IN comm: communicator (handle)
IN filename: name of file to open (string)
IN amode: file access mode (integer)
IN info: info object (handle)
OUT fh: new file handle (handle)

- **Collective** operation 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 via 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



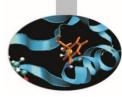
Each process within the communicator must specify the same filename and access mode (amode):

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 delete file on close MPI_MODE_DELETE_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





Open/close a file 3/3



MPI_FILE_CLOSE (comm) INOUT fh: file handle (handle)

- Collective operation
- Call this function when the file access is finished to free the file handle.





Passing Info to MPI-IO



- Several parallel file system can benefit from "hints" given to MPI-IO
 - optimization may be possible with performance benefits
- Info to MPI are opaque objects (MPI_Info in C or integer in FORTRAN)
- hints can be provided as (key, value) pairs with MPI_Info_set function

```
MPI_Info info;
MPI_Info_create(&info);
// set number of I/O devices across which the file should be striped
MPI_Info_set(info, "striping_factor", "4");
// set the striping unit in bytes
MPI_Info_set(info, "striping_unit", "65536");
// h. fformain and antheration I/O
```

// buffer size of collective I/0
MPI_Info_set(info, "cb_buffer_size", "8388608");

// number of processes that should perform disk accesses during collective I/O
MPI_Info_set(info, "cb_nodes", "4");



Getting Info from MPI-IO

- Info can also be retrieved from the implementation
 - which hints where used for a file?
 - which default are actually in use?

```
char key[MPI_MAX_INFO_KEY], value[MPI_MAX_INFO_VAL];
MPI_Info info_used;
MPI_File_get_info(fh, &info_used);
int nkeys;
MPI_Info_get_nkeys(info_used, &nkeys);
for (int i=0; i<nkeys; i++) {
    MPI_Info_get_nthkey(info_used, i, key);
    int flag; // return true if key was set
    MPI_Info_get(info_used, key, MPI_MAX_INFO_VAL, value, &flag);
    printf("key = %s, value = %s\n", key, value);
}
```



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 (local, not collective) call.
- Individual file pointers are used:

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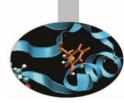
Each processor has its own pointer to the file

Pointer on a processor is not influenced by any other processor



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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 (local, not collective) call.
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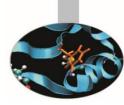
Each processor has its own pointer to the file

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 be:
 - 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 in offset the current position of the individual file pointer
 - offset is in etype units relative to the current view
- 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 MPI_FILE_GET_BYTE_OFFSET





Querying file size



MPI_FILE_GET_SIZE (fh, size)
IN fh: file handle (handle)
OUT size: file size in bytes (integer)

- Returns the file size in bytes
- The value is returned in a variable type of proper kind:
 - integer MPI_KIND_OFFSET in FORTRAN
 - MPI_Offset in C





MPI-IO Data Access APIs

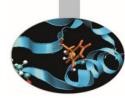


- MPI-IO provides a large number of routines to read and write data from a file.
- There are three properties which differentiate data access routines:
 - **Positioning:** users can either specify explicitly the offset in the file at which the data access takes place or they can use MPI file pointers
 - **Synchronisation:** as for common communication APIs, we can use both synchronous (blocking) or asynchronous (non-blocking) function calls
 - **Coordination:** data accesses can be local or collective operations





Data Access 1/3



Positioning:

Users can either specify the offset in the file at which the data access takes place or they can use MPI file pointers:

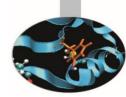
- Individual file pointers: each process has its own file pointer that is only altered on accesses of that specific process
- Shared file pointer: pointer is shared among all processes in the communicator used to open the file
 - It is modified by any shared file pointer access of any process
 - Shared 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.

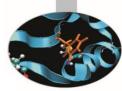
Coordination:

- 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





Data Access 3/3

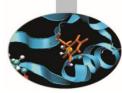


Positioning	Synchronisation	Coordination	
		Noncollective	Collective
Explicit	Blocking	MPI_FILE_READ_AT	MPI_FILE_READ_AT_ALL
offsets		MPI_FILE_WRITE_AT	MPI_FILE_WRITE_AT_ALL
	Non-blocking &	MPI_FILE_IREAD_AT	MPI_FILE_READ_AT_ALL_BEGIN
	split collective		MPI_FILE_READ_AT_ALL_END
		MPI_FILE_IWRITE_AT	MPI_FILE_WRITE_AT_ALL_BEGIN
			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





Using explicit offsets



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)
```

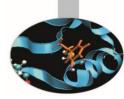
END PROGRAM main



30



Explicit offset - Write



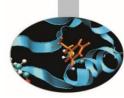
MPI_FILE_WRITE_AT (fh, offset, buf, count, datatype, status)
IN fh: file handle (handle)
IN offset: file offset in byte (integer)
IN buf: destination buffer
IN count: number of read elements
IN datatype: MPI type of each element
OUT status: MPI status

- An explicit offset is given to determine access position
- The file pointer is neither used or incremented or modified
- Blocking, independent.
- Writes COUNT elements of DATATYPE from memory BUF to the file
- Starts writing at OFFSET units of etype from begin of view





Explicit offset - Read

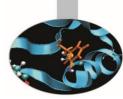


MPI_FILE_READ_AT (fh, offset, buf, count, datatype, status)
IN fh: file handle (handle)
IN offset: file offset in byte (integer)
IN buf: destination buffer
IN count: number of read elements
IN datatype: MPI type of each element
OUT status: MPI status

- 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







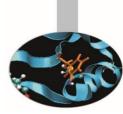
MPI_FILE_WRITE_SHARED (fh, buf, count, datatype, status)
MPI_FILE_READ_SHARED (fh, buf, count, datatype, status)

- 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





Seeking and querying the shared file pointer position



MPI_FILE_SEEK_SHARED(fh, offset, whence)

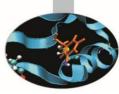
- Updates the individual file pointer according to WHENCE (MPI_SEEK_SET, MPI_SEEK_CUR, MPI_SEEK_END)
- OFFSET can be negative, which allows seeking backwards
- It is erroneous to seek to a negative position in the view
- The call is collective : all processes with the file handle have to participate

MPI_FILE_GET_POSITION_SHARED(fh, offset)

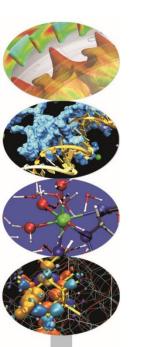
- Returns the current position of the individual file pointer in OFFSET
- The value can be used to return to this position or calculate a displacement
 - Do not forget to convert from offset to byte displacement if needed
- Call is not collective







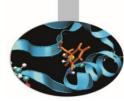
MPI Derived Datatypes







Derived datatypes

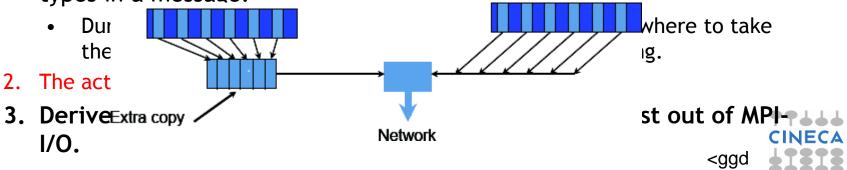


You may need to send messages that contain

- 1. non-contiguous data of a single type (e.g. a sub-block of a matrix)
- 2. contiguous data of mixed types (e.g., an integer count, followed by a sequence of real numbers)
- 3. non-contiguous data of mixed types

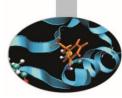
Datatype solution:

1. The idea of MPI derived datatypes is to provide a simple, portable, elegant and efficient way of communicating non-contiguous or mixed types in a message.





Definition



A **general datatype** is an **opaque object** able to describe a buffer layout in memory by specifing:

- A sequence of basic datatypes
- A sequence of integer (byte) displacements.

Typemap = {(type 0, displ 0), ... (type n-1, displ n-1)}

- pairs of basic types and displacements (in byte)

Type signature = {type 0, type 1, ... type n-1}

- list of types in the typemap
- gives size of each elements
- tells MPI how to interpret the bits it sends and received

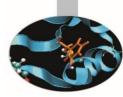
Displacement:

- tells MPI where to get (when sending) or put (when receiving)





Typemap



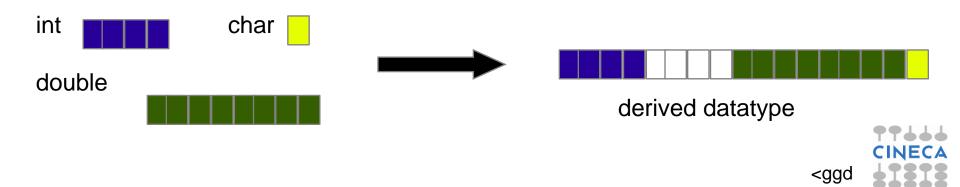
Example:

Basic datatypes are particular cases of a general datatype, and are predefined:

MPI_INT = {(int, 0)}

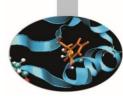
```
General datatype with typemap
```

Typemap = {(int,0), (double,8), (char,16)}





How to use



General datatypes are created and destroyed at run-time through calls to MPI library routines.

Implementation steps are:

- 1. Creation of the datatype from existing ones with a **datatype constructor**.
- 2. Allocation (committing) of the datatype before using it.
- 3. Usage of the derived datatype for MPI communications and/or for MPI-I/O
- 4. Deallocation (**freeing**) of the datatype after that it is no longer needed.

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Some derived datatype constructors



- MPI_TYPE_CONTIGUOUS
- MPI_TYPE_VECTOR
- MPI_TYPE_CREATE_HVECTOR
- MPI_TYPE_INDEXED
- MPI_TYPE_CREATE_HINDEXED
- ... (many other)
- MPI_TYPE_CREATE_SUBARRAY
- MPI_TYPE_CREATE_STRUCT

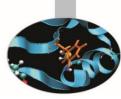
contiguous datatype regularly spaced datatype like vector, but the stride is specified in byte variably spaced datatype like indexed, but the stride is specified in byte

subarray within a multidimensional array fully general datatype





MPI_TYPE_CONTIGUOUS



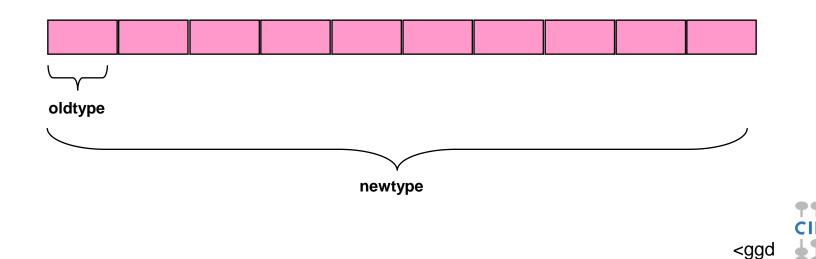
MPI_TYPE_CONTIGUOUS (count, oldtype, newtype)

IN count: replication count (non-negative integer)

IN oldtype: old datatype (handle)

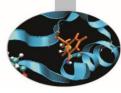
OUT newtype: new datatype (handle)

- MPI_TYPE_CONTIGOUS constructs a typemap consisting of the **replication** of a **datatype** into contiguous locations.
- newtype is the datatype obtained by concatenating count copies of oldtype.



Example

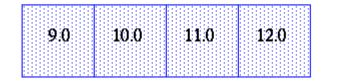




count = 4; MPI_Type_contiguous(count, MPI_FLOAT, &rowtype);

1.0	2.0	3.0	4.0
5.0	6.0	7.0	8.0
9.0	10.0	11.0	12.0
13.0	14.0	15.0	16.0

MPI_Send(&a[2][0], 1, rowtype, dest, tag, comm);



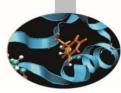
1 element of rowtype

a[4][4]

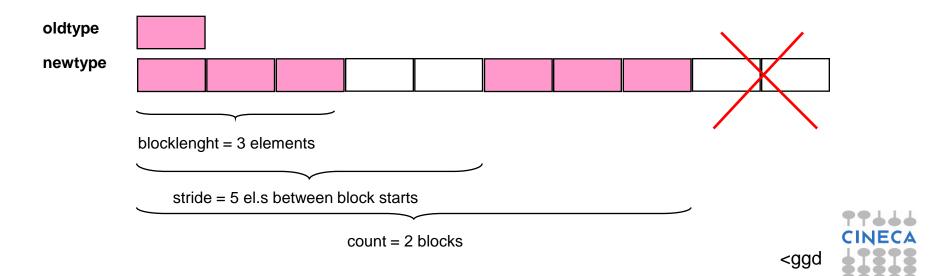




MPI_TYPE_VECTOR

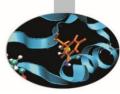


Consist of a number of elements of the same datatype repeated with a certain stride





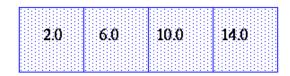
Example



count = 4; blocklength = 1; stride = 4; MPI_Type_vector(count, blocklength, stride, MPI_FLOAT, &columntype);

1.0	2.0	3.0	4.0	
5.0	6.0	7.0	8.0	a[4][4]
9.0	10.0	11.0	12.0	~r .jr .j
13.0	14.0	15.0	16.0	

MPI_Send(&a[0][1], 1, columntype, dest, tag, comm);

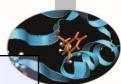


1 element of columntype

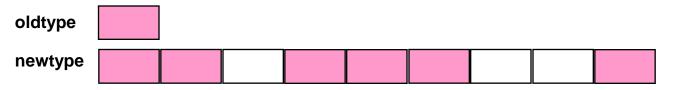




MPI_TYPE_INDEXED



- Creates a new type from blocks comprising identical elements
- The size and displacements of the blocks can vary



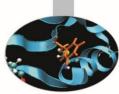
count=3, array_of_blocklenghths=(/2,3,1/), array_of_displacements=(/0,3,8/)

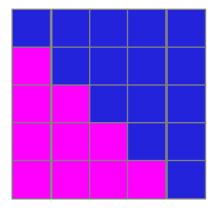


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Example 2







```
/* upper triangular matrix */
double a[100][100];
int displ[100], blocklen[100], int i;
MPI_Datatype upper;
/* compute start and size of the rows */
for (i=0; i<100; i++) {
    displ[i] = 100*i+i;
    blocklen[i] = 100-i;
}</pre>
```

/* create and commit a datatype for upper triangular matrix */
MPI_Type_indexed (100, blocklen, disp, MPI_DOUBLE, &upper);
MPI_Type_commit (&upper);
/* ... send it ...*/
MPI_Send (a, 1, upper, dest, tag, MPI_COMM_WORLD);
MPI_Type_free (&upper);





Size vs. extent of a datatype

Basic datatypes:

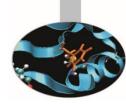
• size = extent = number of bytes used by the compiler

Derived datatypes:

- extent include holes but...
- ... final holes are a figment of our imagination MPI_TYPE_VECTOR (3, 2, 4, old_type, new_type)

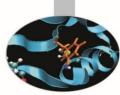
old type							•
new type						K	
							>

- size = 6 x size of "old type"
- extent = 10 x extent of "old type"





SCA Query size and extent of datatype



MPI_TYPE_SIZE (datatype, size)

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IN datatype: datatype (handle)
OUT size: datatype size (integer)

• Returns the total number of bytes of the entry datatype

MPI_TYPE_GET_EXTENT (datatype, lb, extent)
IN datatype: datatype to get information on(handle)
OUT lb: lower bound of datatype (integer)
OUT extent: extent of datatype (integer)

• Returns the lower bound and the extent of the entry datatype

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Use of Datatype in Communications



 The extent of a datatype controls how the datatype is used with the count > 1 field in MPI communications

call MPI_Send(buf,count,datatype,...)

• What does actually send?

do i=0,count-1
 call MPI_Send(bufb(1+i*extent(datatype)),1,datatype,...)
enddo

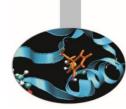
where *bufb* is a byte type like *integer*1*

- extent is used to decide where to send from or receive to for count>1 datatype communications
 - Normally, this is right after the last byte used for (i-1)

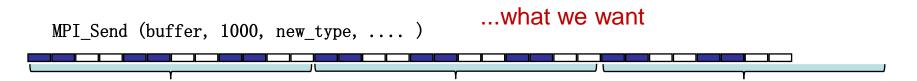




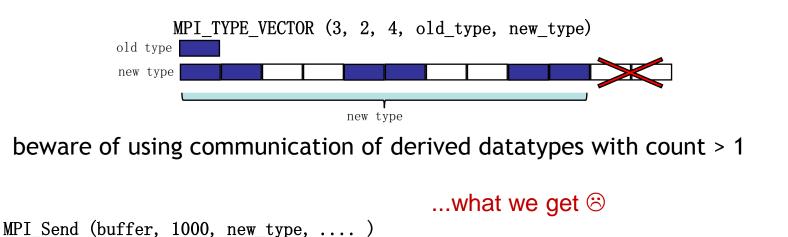
Use of Datatype in Communications

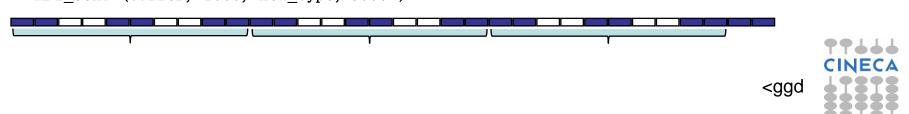


 Were we to use a derived datatype (i.e: MPI_TYPE_VECTOR) in a communication with count>1 of this derived datatype



• Remember that trailing holes are discarded in datatype creation:







Resizing datatypes

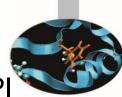
MPI_TYPE_CREATE_RESIZED (oldtype, newlb, newextent, newtype)
IN oldtype: input datatype (handle)
IN newlb: new lower bound of datatype (integer, in terms of bytes)
IN newextent: new extent of datatype (integer, in term of bytes)
OUT newtype: output datatype (handle)

- Returns in newtype a handle to a new datatype that is identical to oldtype, except that the lower bound of this new datatype is set to be "lb", and its upper bound is set to be "lb + extent".
- Modifying extent is useful to handle alignments of the last items of structs
 - crucial when communicating more than one derived data-type
- Modifying also the lower bound can be confusing, use with particular care

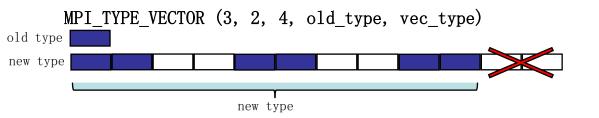




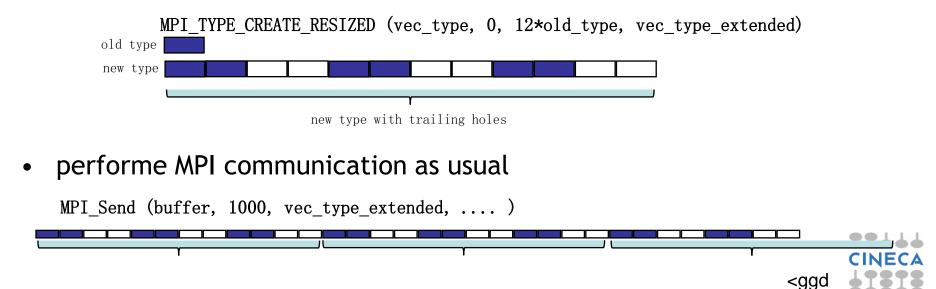
Extend Datatype for Communications



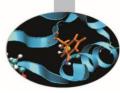
- If you want to use a derived datatype as a basic template in MPI communications, remember to take extent into account
 - trailing holes are discarded in datatype creation



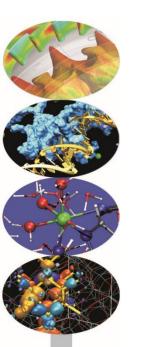
• extend the created datatype with the MPI_TYPE_CREATE_RESIZED







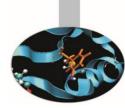
MPI2-IO Advanced Features







Advanced features of MPI-IO



- Basic MPI-IO features are not useful when
 - Data distribution 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 MPI derived datatype
 - collective access: grouping multiple near accesses in one or more single accesses (decreasing the latency time)





MPI-IO: File view

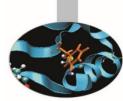


- A file view defines which portion of a file is "visible" to a process
- File view defines also the type of the data in the file (byte, integer, float, ...)
- By default, file is treated as consisting of bytes, and process can access (read or write) any byte in the file
- A default view for each participating 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)





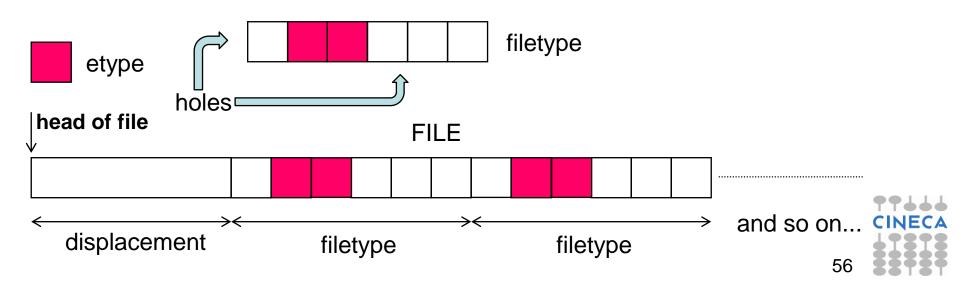
MPI-IO: File View



A file view consists of three components

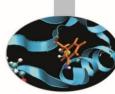
- displacement : number of bytes to skip from the beginning of file
- etype : type of data accessed, defines unit for offsets
- filetype : base portion of file visible to a process

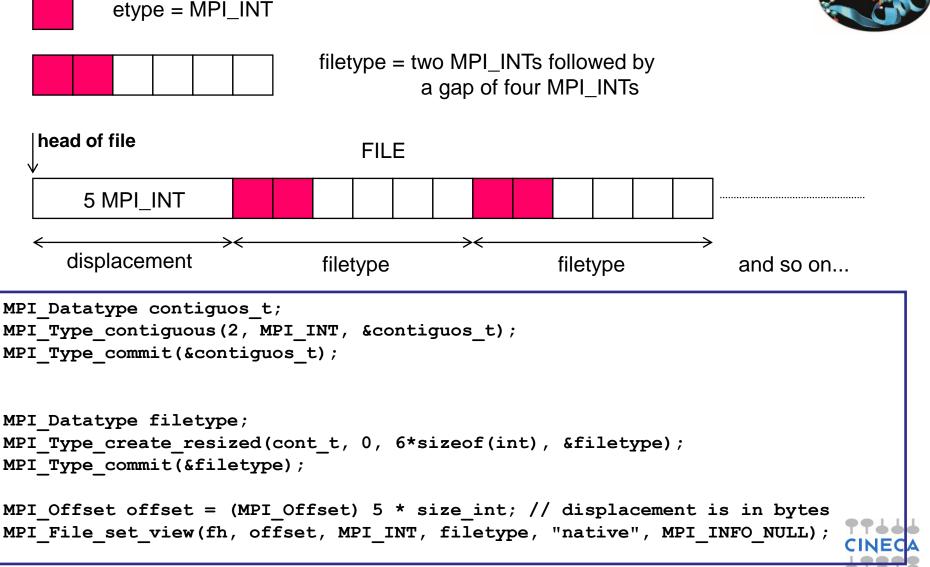
The pattern described by a filetype is repeated, beginning at the displacement, to define the view, as it happens when creating MPI_CONTIGUOUS or when sending more than one MPI datatype element: HOLES are important!





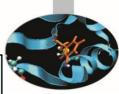
File View Example







File View



MPI_FILE_SET_VIEW(fh, disp, etype, filetype, datarep, info) INOUT fh: file handle (handle)

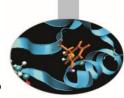
- IN disp: displacement from the start of the file, in bytes
 (integer)
- IN etype: elementary datatype. It can be either a pre-defined or a derived datatype but it must have the same value on each process. (handle)
- IN filetype: datatype describing each processes view of the
 file. (handle)
- IN datarep: data representation (string)

IN info: info object (handle)

- It is used by each process to describe the layout of the data in the file
- 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, etc.)
 - native: (default) use the memory layout with no conversion
 - no precision loss or conversion effort
 - not portable

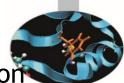
Computing Applications and Innovation

- 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





Passing hints to Filesystem



- MPI_File_set_view API allows the user to provide information on the features of the File System employed
 - optional (default: use MPI_INFO_NULL if you are not very expert)
 - may improve performances
 - depend on the MPI implementation
- 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 implementation of MPICH
 - specific infos for different file-systems (PFS, PVFS, GPFS, Lustre, ...)



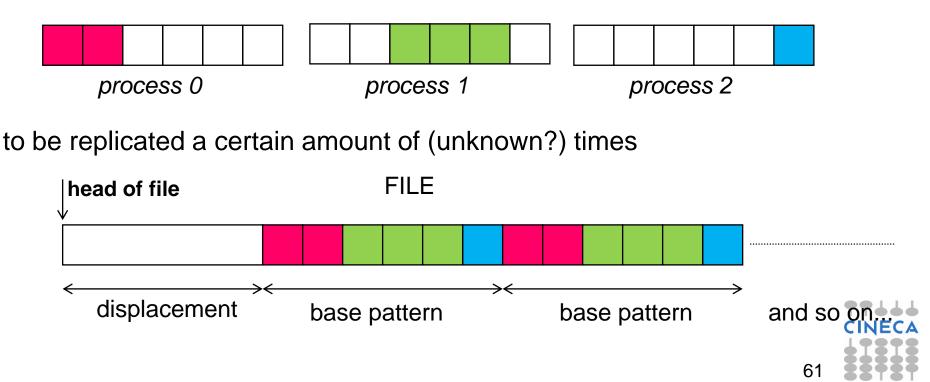
60



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

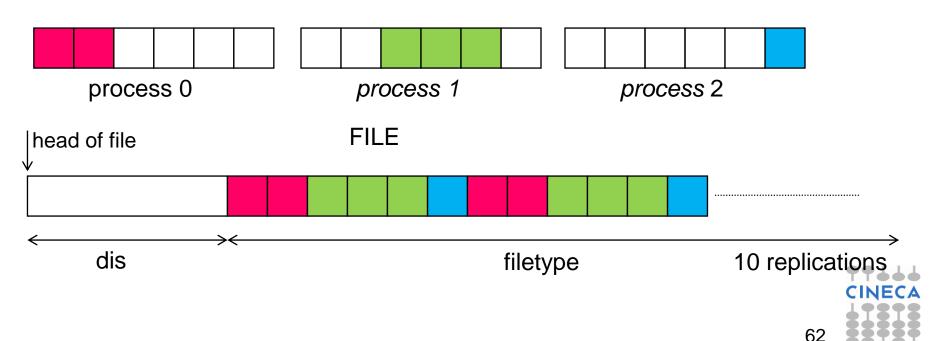


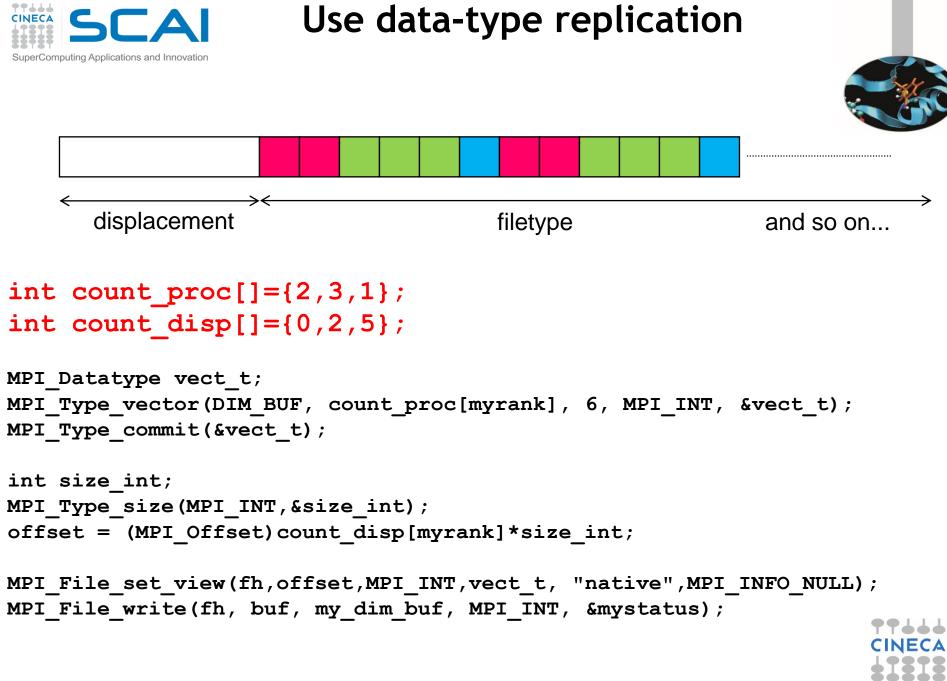


I strategy: data-type replication



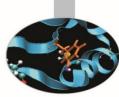
- If the whole amount of basic patterns is known (e.g. 10)
 - define MPI vector with count=10, stride=6 and blocklength depending on the process:
 - P0 has 2 elements, P1 has 3 elements, and P2 has 1 element
 - define the file view using different displacements in addition to the base displacement *dis*:
 - dis+0, dis+2, dis+5



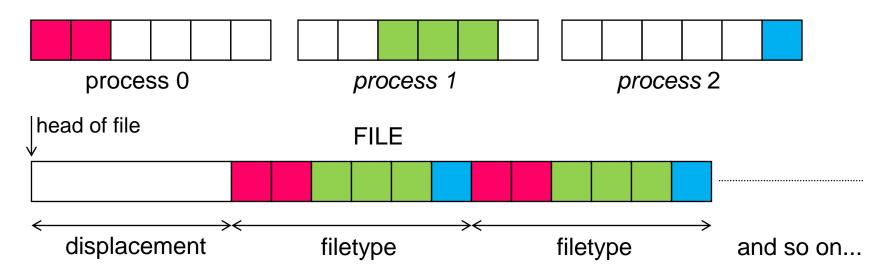




Il strategy: file view replication



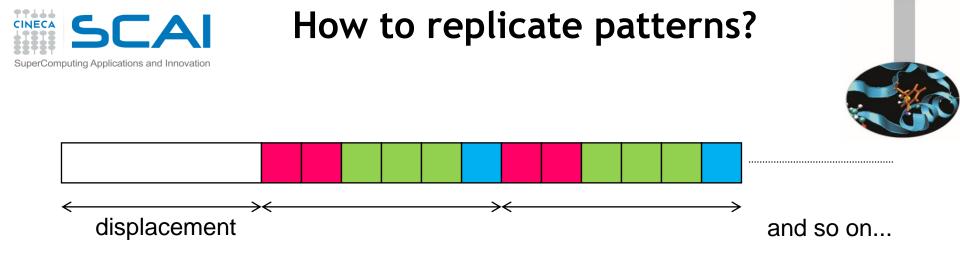
- If the whole amount of basic patterns is unknown, it is possible to exploit the replication mechanism of the MPI file view
 - define MPI contiguous with lengths 2, 3 and 1, respectively
 - resize the types adding holes (on the right only)
 - set the file view with displacements to balance the left holes



 When writing more than a filetype, a replication occurs; as it happens when sending more than one data, setting the holes is crucial!



```
77666
                            Use file view replication
CINECA
SuperComputing Applications and Innovation
                                                                     displacement
                               filetype
                                                     filetype
                                                                      and so on...
MPI Datatype cont t;
MPI Type contiguous (count proc[myrank], MPI INT, &cont t);
MPI Type commit(&cont t);
int size int;
MPI Type size (MPI INT, & size int) ;
MPI Datatype filetype;
MPI Type create resized(cont t, 0, 6*size int, &filetype);
MPI Type commit(&filetype);
offset = (MPI Offset)count disp[myrank]*size int;
MPI File set view(fh, offset, MPI INT, filetype, "native", MPI INFO NULL);
MPI File write(fh, buf, my dim buf, MPI INT, &mystatus);
```

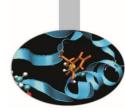


Which is the best replication strategy?

- If possible, data-type replication is probably better
 - Surely, easier to be implemented
- But exploiting file view replication is mandatory when then number of read/writes is not known a priori

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•	n columns ———					
↑						
	P0	P1	P2			
	(0,0)	(0,1)	(0,2)			
m						
rows						
	P3	P4	P5			
	(1,0)	(1,1)	(1,2)			
↓						

- 2D array, size (m,n) distributed among six processes
- cartesian layout 2x3

- When distributing multi-dimensional arrays among processes, we want to write files which are independent of the decomposition
 - written according to a usual serial order
 in row major order (C) or column major order (Fortran)
- The datatype SUBARRAY may easily handle this situation



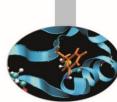


MPI_TYPE_CREATE_SUBARRAY

The subarray type constructor creates an MPI datatype describing an n-dimensional subarray of an n-dimensional array. The subarray may be situated anywhere within the full array, and may be of any nonzero size up to the size of the larger array as long as it is confined within this array.

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	r r	n columns -		►
Ī	P0	P1	P2	
m	(0,0)	(0,1)	(0,2)	
rows	P3	P4	P5	
	(1,0)	(1,1)	(1,2)	
• •				

The subarray type constructor creates an MPI datatype describing an n-dimensional subarray of an n-dimensional array. The subarray may be situated anywhere within the full array, and may be of any nonzero size up to the size of the larger array as long as it is confined within this array.







gsizes[0] = m; /* no. of rows in global array */
gsizes[1] = n; /* no. of columns in global array*/
psizes[0] = 2; /* no. of procs. in vertical dimension */
psizes[1] = 3; /* no. of procs. in horizontal dimension */

```
lsizes[0] = m/psizes[0]; /* no. of rows in local array */
lsizes[1] = n/psizes[1]; /* no. of columns in local array */
```

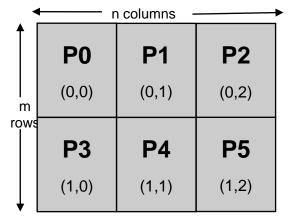
MPI_Cart_coords(comm, rank, 2, coords);

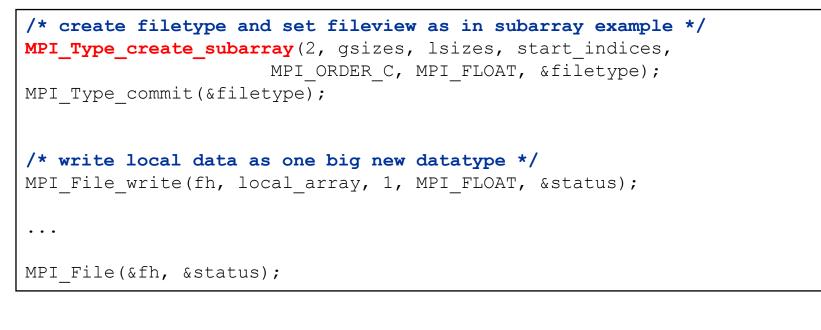
```
/* global indices of first element of local array */
start_indices[0] = coords[0] * lsizes[0];
start indices[1] = coords[1] * lsizes[1];
```

70 **CINECA**







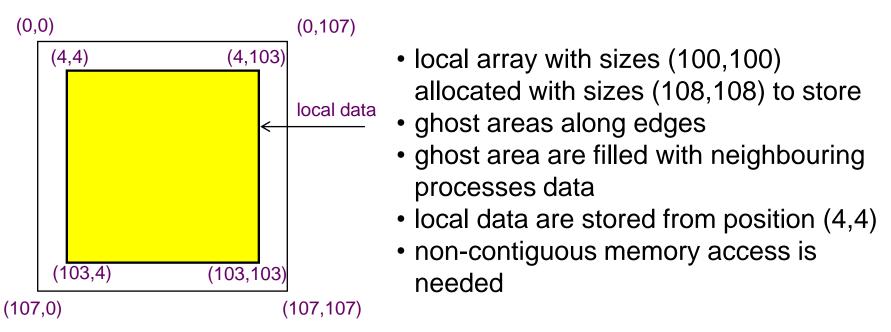


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SuperComputing Applications and Innovation

Ghost cells, typical case





- Local data may be considered as a subarray
- Using MPI_Type_create_subarray we can filter the local data creating a subarray for accesing only required data to be taken from memory
- This type will be used as access basic type to communicate or to CINECA perform I/O



Ghost cells, typical case



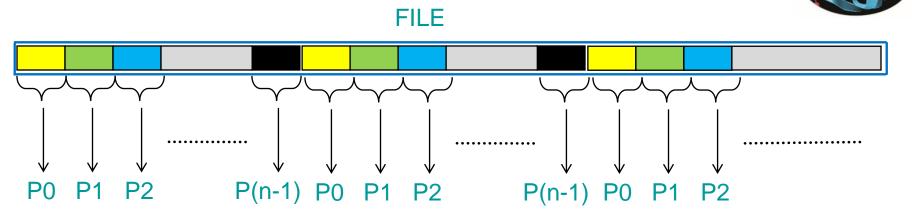
/* create a derived datatype describing the layout of local array in memory
 buffer that includes ghosts .This is just another sub-array datatype! */
memsizes[0] = lsizes[0] + 8; /* rows in allocated array */
memsizes[1] = lsizes[1] + 8; /* columns in allocated array */

/* indices of first local elements in the allocated array */
start_indices[0] = start_indices[1] = 4;

/* create filetype and set fileview as in subarray example */
...
/* write local data as one big new datatype */
MPI File write(fh, local array, 1, memtype, &status);



Efficient non-contiguous IO with collective operations



- In general, accessing non-contiguous chunk of data from each process to storage resutls in very expensive operation and poor performance
 - many access requests can really knock out file systems servers
 - although MPI fileview ease the way of accessing to a file, if the fileview is not-contiguos, also accesses will be not-contiguos
- MPI-IO provides collective operation to gather fragmented accesses into fewer contiguous access operations, improving performance



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

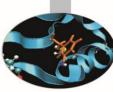
Performance are often better than for individual functions

 Even if each processor reads a non-contiguous segment, in total the read is contiguous





Simple Benchmark

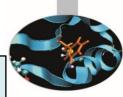


n columns					*		
m rows	P0 P1 (0,0) (0,1) P3 P4 (1,0) (1,1)		0,1) P4	P2 (0,2) P5 (1,2)	 Traditional I/O: master process gathers data and perform I/O MPI-IO: use MPI_Type_create_subarray to define the view for each process a perform a collective call local grid (per process): 10000x10000 double-precision 		rform I/O subarray to each process and call ss):
processi			1	2	8	16	32
filesize (Mb)		763	1526	6103	12207	24414	
Traditional-IO (s)		8	22	86	1738	3570	
MPI-IO (s)		2	4	18	33	48	

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



Collective, blocking IO



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

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

- With collective IO ALL the processors defined in a communicator execute the IO operation
- 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

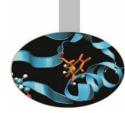
MPI_Wait must be used for synchronization.

Can be used to overlap IO with computation





Collective, nonblocking IO



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

```
MPI_File_read_all_begin( MPI_File mpi_fh, void *buf, int count, MPI_Datatype datatype )
...computation...
```

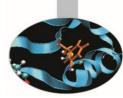
MPI_File_read_all_end(MPI_File mpi_fh, void *buf, MPI_Status *status);

- 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





Consistency



- No consistency problems rise when there are no overlapping regions (bytes) accessed by any two processes
- MPI does *not* guarantee that data will automatically read correctly, when accesses of any two processes overlap in the file

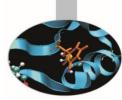
MPI_File_open(MPI_COMM_WORLD, "file",, &fh1)
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ...)
MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ...)

MPI_File_open(MPI_COMM_WORLD, ``file",, &fh2)
MPI_File_write_at(fh2, 100, buf, 100, MPI_BYTE, ...)
MPI_File_read_at (fh2, 0, buf, 100, MPI_BYTE, ...)

- The user must take care of consistency. There are three choices:
 - using *atomic* accesses
 - close and reopen the file
 - ensure that no "write sequence" on any process is concurrent with "any sequence (read/write)" on another process







Change file-access mode to atomic before the write on each process

Computing Applications and Innovation

• MPI guarantees that written data can be read immediately by another process

```
MPI_File_open(MPI_COMM_WORLD, "file", ...., &fh1) MPI_File_open(MPI_COMM_WORLD, "file", ...., &fh2)
MPI_File_set_atomicity(fh1, 1) MPI_File_set_atomicity(fh2, 1)
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ...) MPI_File_write_at(fh2, 100, buf, 100, MPI_BYTE, ...)
MPI_Barrier(MPI_COMM_WORLD) MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ...)
```

 note: the *barrier* after the writes to ensure each process has completed its write before the read is issued from the other process



Close/Open file for Consistency



• Close the file and reopen just after write operations if other processes need data just written by other processes

MPI_File_open(MPI_COMM_WORLD, "file",, &fh1) M
MPI_File_write_at(fh1, 0, buf, 100, MPI_BYTE, ...) M
MPI_File_close(&fh1) M
MPI_File_open(MPI_COMM_WORLD, "file",, &fh1) M
MPI_File_read_at(fh1, 100, buf, 100, MPI_BYTE, ...) M

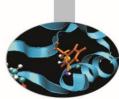
MPI_File_open(MPI_COMM_WORLD, "file",, &fh2)
MPI_File_write_at(fh2, 100, buf, 100, MPI_BYTE, ...)
MPI File close(&fh2)

- MPI_File_open(MPI_COMM_WORLD, "file",, &fh2)
- MPI_File_read_at (fh2, 0, buf, 100, MPI_BYTE, ...)

 note: each file open operation will create a different MPI context context will be cleared after each close operation



Understanding IO Sequences

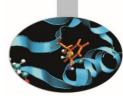


- An IO sequence is defined as a set of file operations bracketed by any pair of the functions MPI_File_open, MPI_File_close, MPI_File_sync
- A sequence is a "write sequence" if contains write operations
- MPI guarantees that the data written by a process can be read by another process if the "write sequence" is not concurrent (in time) with any sequence on any other process

```
MPI File open (MPI COMM WORLD, "file", ...., &fh1)
                                                        MPI File open (MPI_COMM_WORLD, "file", ...., &fh2)
MPI File write at(fh1, 0, buf, 100, MPI BYTE, ...)
MPI File sync(&fh1)
                                                        MPI File sync(&fh2)
MPI Barrier (MPI COMM WORLD)
                                                        MPI_Barrier(MPI_COMM_WORLD)
MPI File sync(&fh1)
                                                        MPI File sync(&fh21)
                                                        MPI File write at(fh12, 0, buf, 100, MPI BYTE, ... )
                                                        MPI File sync(&fh2)
MPI_File_sync(&fh1)
MPI_Barrier(MPI_COMM_WORLD)
                                                        MPI Barrier (MPI COMM WORLD)
MPI File sync(&fh1)
                                                        MPI File sync(&fh2)
MPI File read at(fh1, 100, buf, 100, MPI_BYTE, ...)
                                                        MPI File read at(fh2, 0, buf, 100, MPI BYTE, ... )
MPI File close(&fh1)
                                                        MPI File close(&fh2)
```



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

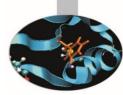
2. The file contains a list of tasks, each task requires a different amount of computing time

- Solution: MPI_FILE_READ_SHARED
 - Non-collective with a shared file pointer
 - Same view on all processes (mandatory)





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

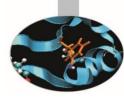
- Collective with individual file pointers
- Different views: filetype with MPI_TYPE_CREATE_SUBARRAY

Internally: both may be implemented in the same way.





Use cases



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

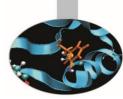
Solution: MPI_FILE_READ_ALL_BEGIN/END

- 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, think I/O carefully!
 - 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





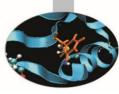
Useful links



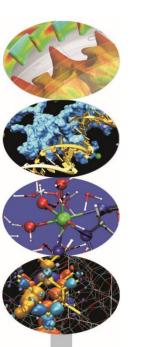
- MPI The Complete Reference vol.2, The MPI Extensions (W.Gropp, E.Lusk et al. 1998 MIT Press)
- Using MPI-2: Advanced Features of the Message-Passing Interface (W.Gropp, E.Lusk, R.Thakur 1999 MIT Press)
- Standard MPI-3.x (http://www.mpi-forum.org/docs)
- Users Guide for ROMIO (Thakur, Ross, Lusk, Gropp, Latham)
- ... a bit of advertising: corsi@cineca.it (http://www.hpc.cineca.it)
- ... practice practice practice







QUESTIONS ???



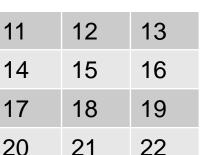


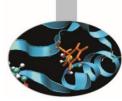
 Write a program which decomposes an integer matrix (m x n) using a 2D MPI Cartesian grid

- Handle the remainders for non multiple sizes
- Fill the matrix with the row-linearized indexes

 $A_{ii} = m \cdot i + j$

- Reconstruct the absolute indexes from the local ones
- Remember that in C the indexes of arrays start from 0
- Writes to file the matrix using MPI-I/O collective write and using MPI data-types
 - Which data-type do you have to use?

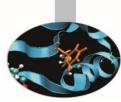




SuperComputing Applications and Innova Hands-on 2: MPI-I/O & subarrays



Hands-on 2: MPI-I/O & subarrays



- Check the results using:
 - Shell Command

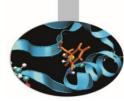
```
od -i output.dat
```

- Parallel MPI-I/O read functions (similar to write structure)
- Serial standard C and Fortran check
 - only rank=0 performs check
 - read row-by-row in C and column-by-column in Fortran and check each element of the row/columns
 - use binary files and fread in C
 - use unformatted and access='stream' in Fortran
- Which one is the most scrupoulous check?
 - is the Parallel MPI-I/O check sufficient?





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