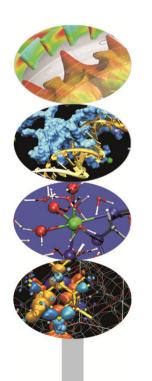


Advanced MPI



PARALLEL COMPUTING USING MPI AND OPENMP

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Pack



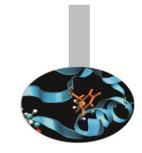
The MPI library enables packing different data in one buffer, that can be sent as a whole. Communication times can thus be reduced. To gather several data in a single buffer the function MPI_PACK may be used.

```
INTERFACE
SUBROUTINE MPI_PACK(inbuf,incount,datatype,outbuf,outsize,position,comm,ierr)
    INTEGER, INTENT(IN) :: INCOUNT, DATATYPE, OUTSIZE, COMM
    <type>, INTENT(IN) :: INBUF(:)
    <type>, INTENT(OUT) :: OUTBUF(:)
    INTEGER, INTENT(INOUT) :: POSITION
    INTEGER, INTENT(OUT) :: IERR
    END SUBROUTINE MPI_PACK
END INTERFACE
```

INCOUNT elements of type DATATYPE of the buffer INBUF are copied in the buffer OUTBUF from position POSITION (in byte). On exit POSITION has the value of the next free address.







Unpack

The function MPI_UNPACK is used by the receiving processes to extract data from the buffer INBUF.

```
INTERFACE
   SUBROUTINE MPI_UNPACK (inbuf, insize, position, outbuf, outcount, datatype,
        comm, ierr)
        INTEGER, INTENT(IN) :: INSIZE, DATATYPE, OUTCOUNT, COMM
        <type>, INTENT(IN) :: INBUF(:)
        <type>, INTENT(OUT) :: OUTBUF(:)
        INTEGER, INTENT(INOUT) :: POSITION
        INTEGER, INTENT(OUT) :: IERR
        END SUBROUTINE MPI_UNPACK
        END INTERFACE
```







Pack/Unpack

As an example, let's say the root (0) process shall send the following values to the other processes:

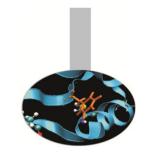
MPI_DOUBLE_PRECISION: SWV(2), Range

MPI_INTEGER: XYdots, Niter

1. root process packs data in the buffer pckd_data, 32 bytes long:







Pack/Unpack

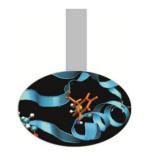
2. data in buffer is distributed:

```
CALL MPI_BCAST (pckd_data, 32, MPI_PACKED , 0, & MPI_COMM_WORLD, ierr)
```

3. receiving processes unpack data:







Derived data types

If the data to be communicated are structured it may be convenient to define a MPI derived data type. The basic MPI data types are:

```
MPI_INTEGER
MPI_REAL
MPI_DOUBLE_PRECISION
MPI_COMPLEX
MPI_DOUBLE_COMPLEX
MPI_LOGICAL
MPI_CHARACTER
MPI_BYTE
MPI_PACKED
```

```
MPI_CHAR
MPI_SHORT
MPI_INT
MPI_LONG
MPI_LONG
MPI_UNSIGNED_CHAR
MPI_UNSIGNED_SHORT
MPI_UNSIGNED
MPI_UNSIGNED
MPI_UNSIGNEDLONG
MPI_FLOAT
MPI_DOUBLE
MPI_LONG_DOUBLE
MPI_BYTE
MPI_PACKED
```

Derived data types are defined using basic data types and formerly defined derived data types.

Dtype = $[(typ_0 , pos_0), (typ_1 , pos_1), ..., (typ_n-1 , pos_n-1)]$







Derived data types

To define a derived data type it is required:

- To specify the structure of the new data type, on the basis of previously defined or basic data types.
- To register the new data type

The newly defined data type must be registered to MPI with the following function:

```
int MPI_Type_commit ( MPI_Datatype *mpi_mytype ) c/c++
```

Once committed the new data type becomes a recognized MPI data type.







Derived data types

Whenever a defined data type is of no use any more, the following function should be used:

```
int MPI_Type_free ( MPI_Datatype *mpi_mytype )
```

Pending operations will complete normally.

fortran

C/C++







A MPI derived data type is built from blocks of homogeneous elements. For example, if we are interested in communicating the following data structure:

4 blocks may be defined, one for each component of the structure:

Block #1: 2 doubles

Block #2: 1 double

Block #3: 1 integer

Block #4: 1 integer







The MPI representation of a generic data structure requires three arrays to be defined:

v_len_blk - actual length of each block (in elements)

v_head - starting postion of each block (in bytes)

v_el_typ - data type of the elements in each block

It should be noted that the values in v_head must be given in bytes because the elements of each block may be of different type with different byte extensions.

The data structure can then be described in MPI using the MPI_Type_struct function







The function mpi_type_struct has the following interface:







Example: the MPI description of the structure

MPI_DOUBLE_PRECISION: SWV(2), Range

MPI_INTEGER: XYdots, Niter

is defined assigning the values:

C language structures and Fortran derived data types may be easily mapped into MPI derived data types.

The programmer must anyhow be sure that the relative positions of the structure components are not modified by compiler optimizations. For this reason Fortran derived types should contain the SEQUENCE instruction







Contiguous elements

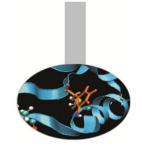
An array of contiguous and homogeneous elements is the simplest derived type to be defined. From element to element there must be no spaces.

```
interface
    subroutine mpi_type_contiguous (num_el, el_type, new_type, ierr)
        integer, intent(in) :: num_el ! How many elements in the array
        integer, intent(in) :: el_type ! Element type
        integer, intent(out) :: new_type ! New data type handler
        integer, intent(out) :: ierr ! Error code
    end subroutine mpi_type_contiguous
        fortran
end interface
```

This function defines the new data type starting from an array of num_el elements. All the elements must be of the same (derived) data type.







Contiguous elements

As an example, if

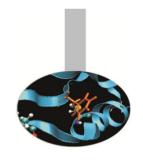
```
El_type = {(double, 0), (char, 8)}
```

is a 16 bytes data type and 3 elements of that type are filed in an array, then

Of course there is no point in *El_type* being a basic MPI type even if it may be as well.







Making things a bit more complicated, the following function is used to define arrays with useful data separated by fixed strides. i.e. arrays may be seen as sequences of identical blocks containing elements to be communicated and elements to be discarded

```
interface
    subroutine mpi_type_vector(num_blk,len_blk,blk_siz,el_typ,new_typ,errcode)
    integer, intent(in) :: num_blk ! How many blocks
    integer, intent(in) :: len_blk ! How many useful elements per block
    integer, intent(in) :: blk_siz ! Total number of elements per block
    integer, intent(in) :: el_typ ! Data type of the block elements
    integer, intent(out) :: new_typ ! New data type handler
    integer, intent(out) :: ierr ! Error code
    end subroutine mpi_type_vector
end interface
```







It can be noted that the size and the useful length of the blocks is given in number of elements. As an example if blk_size=10 and len_blk=7 and the elements are of type MPI_INTEGER, then the actual size of each block is $4 \times 10 = 40$ bytes. But only $4 \times 7 = 28$ elements are communicated and $4 \times (10-7) = 12$ bytes are never sent.

Example: block_array (Fortran and C)





The following function must be used to define arrays with blocks of different dimensions. Two vectors are needed to define the lengths because each block has its own number of useful and discarded elements.

Please note that instead of specifying the total length of each block, the starting position of the blocks have to be passed to the function.







As an example, if we have to describe data structured in three blocks, 3 elements parted each other and containing 5, 13 and 7 elements, the arrays v_len_blk and v_head must be defined as follow:

```
v_len_blk = (/ 5, 13, 7 /)
v_head = (/ 0, 8, 24 /)
```

The following function may be used to know the extension of a MPI (either basic or derived) data type:

```
int MPI_Type_extent( MPI_Datatype datatype, MPI_Aint *ext )
```







Useful functions

The function mpi_type_hvector is similar to mpi_type_vector, but blk_siz is given in bytes. The function mpi_type_hindexed is alike mpi_type_indexed, but v_head is measured in bytes.

The function mpi_address returns the starting address of an object. It is important for portability issues.

```
interface
    subroutine mpi_address (obj, address, ierr)
    integer, intent(in) :: obj     ! Input object or variable
    integer, intent(out) :: address    ! Starting address
    integer, intent(out) :: ierr     ! Error code
    end subroutine mpi_address
end interface
```







Groups of processes

In MPI terminology the process is the computing unit. MPI processes behave following the MIMD model. Each process is an indipendent unit and has its own memory space; it should be thought of as running on its own computing machine.

Every MPI process belongs to one or more MPI group and has its own identification number or rank. MPI ranks are always numbered starting from 0. The 0 process is often called the *master* and usually acts as the boss in master-slave programming model, but it is not mandatory. MPI groups may be generated and destroyed but they are otherwise static.





Groups of processes

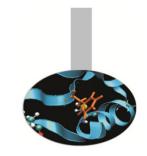
Each group has its own handle but is an opaque object: the programmer can not access its details. Proper functions must be used to manage group properties:

```
call mpi_group_size(group, size, ierr)
call mpi_group_rank(group, rank, ierr)
```

At the beginning all processes belong to the default group, the one associated to the default communicator MPI_COMM_WORLD. All other groups must be explicitly generated. MPI processes may belong to different groups.







Groups of processes

Given a communicator the following function returns the handle of the associated group:







The following function enables generating a new group on the basis of an existing group. The process with rank RANKS (I) in the old group is given rank I in the new group:

```
interface
    subroutine mpi_group_incl(group, n, ranks, newgroup, ierr)
    integer, intent(in) :: group, n, ranks
    integer, intent(out) :: newgroup, ierr
    end subroutine mpi_group_incl
end interface

fortran
```

```
int MPI_Group_incl(MPI_Group group, int n, int *ranks, MPI_Group *newgroup) c/c++
```







Example:

if GROUP contains 8 processes (numbered from 0 to 7) and the array has values RANKS (1:3) = (1,5,2), the instruction

```
call mpi_group_incl (group, 3, ranks, newgroup, ierr)
```

generates the new NEWGROUP with the three processes above numbered.

The following table shows correspondence between the two groups:

Group	Newgroup	
1	0	
5	1	
2	2	







On the contrary in the following function the array RANKS (I) specify the processes of GROUP to be eliminated for building NEWGROUP:

```
interface
    subroutine mpi_group_excl(group, n, ranks, newgroup, ierr)
    integer, intent(in) :: group, n, ranks
    integer, intent(out) :: newgroup, ierr
    end subroutine mpi_group_excl
end interface
```

int MPI_Group_excl(MPI_Group group, int n, int *ranks, MPI_Group *newgroup) c/c++

It is also possible to specify a range of indexes, like RANGES (1:N, 1:3). In the following functions the second dimension of the array specifies the first and the last index to be included and the stride.

```
call mpi_group_range_incl (group, n, ranges, newgroup, ierr)

call mpi_group_range_excl (group, n, ranges, newgroup, ierr)

call mpi_group_range_excl (group, n, ranges, newgroup, ierr)
```





Example:

If group contains 1000 processes and a new group is to be generated with half the number of the processes, taken from the odd positions, the array may be defined as RANGES (1,1)=2, RANGES (1,2)=1000, RANGES (1,3)=2 and the program should issue the following instruction:

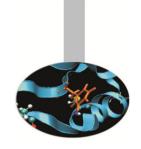
call mpi_group_range_excl (group, n, ranges, newgroup, ierr) fortran

The correspondence between the two groups would be:

Group	Newgroup	
1	0	
3	1	
5	2	







The operations to manage groups are local and do not involve communications.

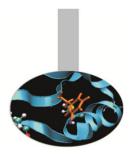
The following instruction may be used to know the relevant rank of the processes in two different groups.

RANKS1(:) are the known ranks of the processes in GROUP1; RANKS2(:) are the related ranks in GROUP2:

```
int MPI_Group_translate (group1, n, ranks1, group2, ranks2, ierr)
```







It is possible to check whenever two groups are similar:

```
interface
    subroutine mpi_group_compare(group1, group2, result, ierr)
    integer, intent(in) :: group1, group2
    integer, intent(out) :: result, ierr
    end subroutine mpi_group_compare
end interface
```

```
int MPI_Group_compare (group1, group2, result, ierr) c/c++
```

The returned values may be one out of the following:

- MPI_IDENT if the groups have the same processes with identical ranks
- MPI_SIMILAR if the groups have the same processes but unequal ranks
- MPI_UNEQUAL if the groups are different







Communicators

A communicator defines the processes that can communicate each other. Each communicator has its own handle, is an opaque object and can be managed by proper functions only.

The default communicator is named MPI_COMM_WORLD, but in a real program it is often useful to generate additional communicators, otherwise the program has to directly manage communications among process subsets with loss of performance and error prone code.

Communicator handles must always be specified in sending or receiving functions.





Managing communicators

The following function may be used to generate a new communicator connected to an existing group:

```
interface
    subroutine mpi_comm_create(comm, group, newcomm, ierr)
        integer, intent(in) :: comm, group
        integer, intent(out) :: newcomm, ierr
    end subroutine mpi_comm_create
end interface

fortran
```

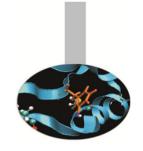
```
int MPI_Comm_create ( MPI_Comm comm, MPI_Group group, MPI_Comm *newcomm ) c/c++
```

- COMM is an existing communicator related to a wider process group; the function must be called by all processes in the COMM communicator
- GROUP is a sub-group of the process group related to COMM
- NEWCOMM is the handle of the newly generated communicator

Example: comm_create (Fortran and C)

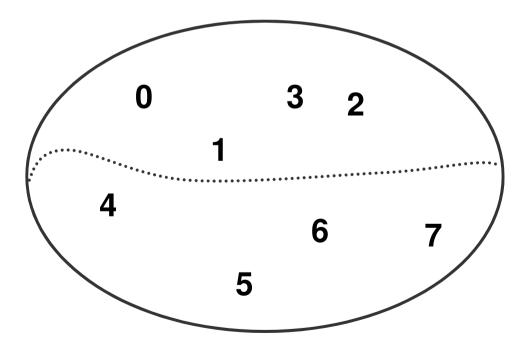






Managing communicators

Suppose there is a communicator connected to a group of 8 processes and 2 new communicators are required by dividing the communicator in two parts as follow:







Managing communicators

To accomplish this task all the processes of the existing communicator may issue the following instructions:

```
call mpi_comm_rank (comm, rank, ierr)
call mpi_comm_size (comm, size, ierr)
color = 2*rank/size
key = size - rank - 1
call mpi_comm_split (comm, color, key, newcomm, ierr)
fortran
```

Each process receives a new communicator handle and will have the rank:

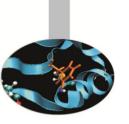
Communicator 1		Communicator 2	
Rank in new group	Rank in old group	Rank in new group	Rank in old group
0	3	0	7
1	2	1	6
2	1	2	5
3	0	3	4

If for some process COLOR=MPI_UNDEFINED, the function MPI_COMM_SPLIT returns NEWCOMM=MPI_COMM_NULL





Communications between groups



Once the processes have been separated in several groups it is possible to realize client-server connections by connecting disjoined groups.

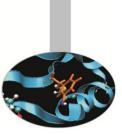
Communications between separated groups can only be of point-to-point type: no collective communications are available.

Whenever a new inter-communicator has been created, the sending process must specify the rank of the receiving process (relevant to the other group); the receiving process must specify the rank of the sender (relevant to the other group).

To enable this, while the functions mpi_comm_size, mpi_comm_rank, mpi_comm_group return informations relevant to the local communicator, the functions mpi_comm_remote_size, mpi_comm_remote_group instead return informations on the disjoined intercommunicator group.







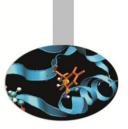
A communicator connecting disjoined groups is called an intercommunicator and can be generated by calling the function mpi_intercomm_create. This function requires:

- A leading process for each one of two disjoined groups
- An intra-communicator between the two leading processes
- A tag for safe communications between the two leading processes





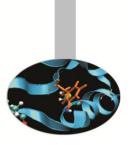
Communications between groups



The following function generates an inter-communicator NEWINTERCOMM between the processes LOCALLEADER and REMOTELEADER of the intra-communicator LOCALCOMM, using TAG and the point-to-point communicator PEERCOMM. It should be noted that REMOTELEADER and PEERCOMM are referred to the local process, while TAG must have the same value for both the processes:



Communications between groups



The intra-communicator NEWINTRACOMM may be generated from an intercommunicator INTERCOMM calling the function:

```
interface
    subroutine mpi_intercomm_merge(intercomm, high, newintracomm, ierr)
        integer, intent(in) :: intercomm, high
        integer, intent(out) :: newintracomm, ierr
    end subroutine mpi_intercomm_merge
end interface
```

int MPI_Intercomm_merge(MPI_Comm intercomm, int high, MPI_Comm *newintracomm) c/c++

This way two separated groups may be joined. The value of <code>HIGH</code> must be the same for all the processes belonging to the same group. If HIGH = .FALSE. for group 1 and HIGH = .TRUE. for group 2, in the new communicating group the processes are ordered starting from group 1; i.e. the processes in group 2 have a higher rank.

Example: two_groups (Fortran and C)







In many programs it may be important to arrange the processes in a given topology. MPI enables the definition of topologies, with an explicit support for cartesian topology. This topology may be defined by calling the function:







The MPI_CART_CREATE function returns the new communicator COMM_CART, connected to a grid with NDIMS dimensions. The extent of each dimension must be defined in LDIMS (1:NDIMS) and it is possible to specify periodicity for each dimension. The REORDER variable is used to allow reordering of the processes.

In cartesian topologies the processes are ordered by rows.

Functions dealing with informations and details about the topology associated to a communicator are available.







Given a communicator COMM, the function MPI_TOPO_TEST returns the associated topology:

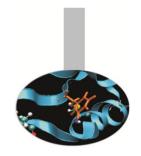
```
MPI_GRAPH: graph topology
MPI_CART: cartesian topology
MPI_UNDEFINED: no topology
```

```
interface
    subroutine mpi_topo_test(comm, topol, ierr)
        integer, intent(in) :: comm
        integer, intent(out) :: topol, ierr
    end subroutine mpi_topo_test
end interface
```

```
int MPI_Topo_test ( MPI_Comm comm, int *topol ) c/c++
```







Given a communicator COMM, with cartesian topology, the function MPI_CARTDIM_GET returns the number of dimensions

```
interface
    subroutine mpi_cartdim_get(comm, ndims, ierr)
        integer, intent(in) :: comm
        integer, intent(out) :: ndims, ierr
    end subroutine mpi_cartdim_get
end interface
```

```
int MPI_Cartdim_get ( MPI_Comm comm, int *ndims ) c/c++
```





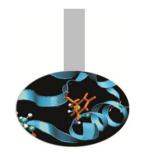


The function MPI_CART_GET, returns the number DIMS (:) of processes in each dimension, the periodicity for each dimension, the process coordinates.

```
interface
    subroutine mpi_cart_get(comm, maxdims, dims, periods, coords, ierr)
    integer, intent(in) :: comm, maxdims
    integer, intent(out) :: ierr
    integer, dimension(:), intent(out) :: dims, coords
    logical, dimension(:), intent(out) :: periods
    end subroutine mpi_cart_get
end interface
```







Given a communicator associated to a cartesian topology a the process coordinates, the following function returns the process rank:

```
int MPI_Cart_rank( MPI_Comm comm, int *coords, int *rank)
```







The following function returns the coordinates of a process in a cartesian topology:

```
interface
    subroutine mpi_cart_coords(comm, rank, maxdims, coords, ierr)
        integer, intent(in) :: comm, rank, maxdims
        integer, dimension(:), intent(out) :: coords
        integer, intent(out) :: ierr
    end subroutine mpi_cart_coords
end interface

fortran
```

```
int MPI_Cart_coords( MPI_Comm comm, int rank, int maxdims, int *coords) c/c++
```







Topologies may be useful to send messages along specific directions.

As an example, suppose that every process in a cartesian topology has to send data toward the DIM dimension to a DELTA distance. The following function returns the ranks of the processes SOURCE and DEST

int MPI_Cart_shift(MPI_Comm comm, int dim, int delta, int *source, int *dest) c/c++

to be passed to the function

```
CALL MPI SENDRECV(SENDBUF, SENDCOUNT, SENDTYPE, DEST, & SENDTAG, RECVBUF, RECVCOUNT, RECVTYPE, & SOURCE, RECVTAG, COMM, STATUS, IERROR)
```







Example: MPI_CART_SHIFT

```
C find process rank

CALL MPI_COMM_RANK(comm, rank, ierr))

C find cartesian coordinates

CALL MPI_CART_COORDS(comm, rank, maxdims, coords, ierr)

C compute shift source and destination

CALL MPI_CART_SHIFT(comm, 0, coords(2), source, dest, ierr)

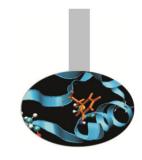
C skew array

CALL MPI_SENDRECV_REPLACE(A, 1, MPI_REAL, dest, 0, source, 0, comm, & status, ierr)
```

Example: cart_create (Fortran and C)







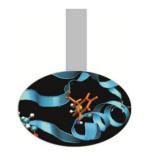
The following function generates new cartesian topologies by cutting a wider cartesian space along the given dimensions:

Example: if COMM is associated to a cartesian topology with extensions 2x3x4 and REMAIN_DIMS=(.T.,.T.,.F.), four new topologies are generated with extension 2x3.

Each process is returned one communicator handle; the former group is divided in 4 new groups with 6 processes each.







MPI+OpenMP

It is possible to develop parallel programs mixing MPI calls and OpenMP directives.

Intel compilers: mpixxx -openmp -O3 -o nomefile.exe nomefile.xxx

PGI compilers: mpixxx-mp -O3 -o nomefile.exe nomefile.xxx

GNU compilers: mpi*xxx* -fopenmp -O3 -o nomefile.exe nomefile.*xxx*

Execution:

export OMP_NUM_THREADS=threads

mpirun -np 2 -machinefile mc -x OMP_NUM_THREADS nomefile.exe

