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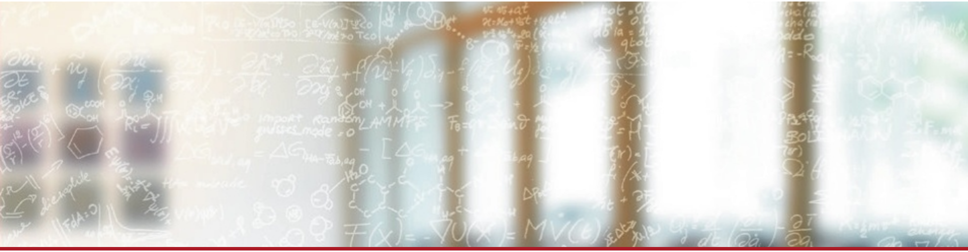


Message Passing Interface (MPI)

Summer School 2016 – Effective High Performance Computing

Maxime Martinasso, CSCS

July 20 – 21, 2016

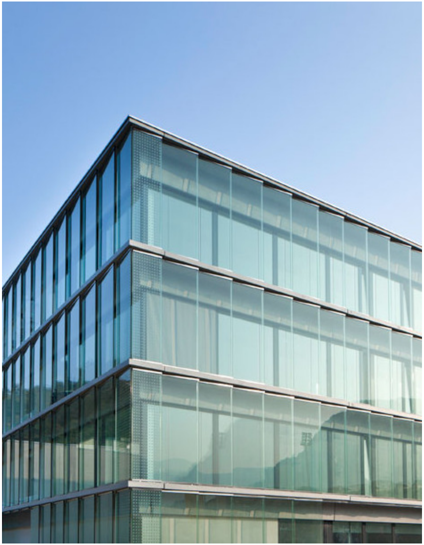
Previous course summary

- Point-to-point communication, Blocking and non-blocking
- Collective operations
- Derived datatypes

Course Objectives

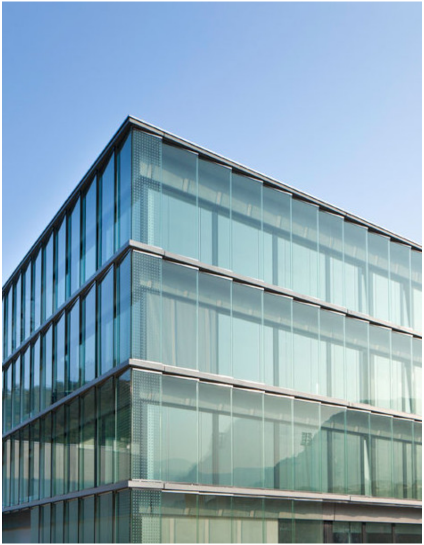
- The understanding of a topology and communicators
- How to build and use a topology

General Course Structure



- An introduction to MPI
- Point-to-point communications
- Collective communications
- Datatypes
- Topology

General Course Structure



- An introduction to MPI
- Point-to-point communications
- Collective communications
- Datatypes
- Topology
  - Groups and communicator
  - Topology with MPI
  - Domain decomposition
  - Cartesian topology
  - Graph topology

Topology

Groups and communicator

- A group is an ordered set of processes, each with a unique integer rank. In MPI, a group is represented within system memory as an object. It is accessible to the programmer only by a ”handle”. A group is always associated with a communicator object.
- A communicator encompasses a group of processes that may communicate with each other. All MPI messages must specify a communicator. Like groups, communicators are accessible to the programmer only by ”handles”. The handle for the communicator that comprises all processes is `MPI_COMM_WORLD`.

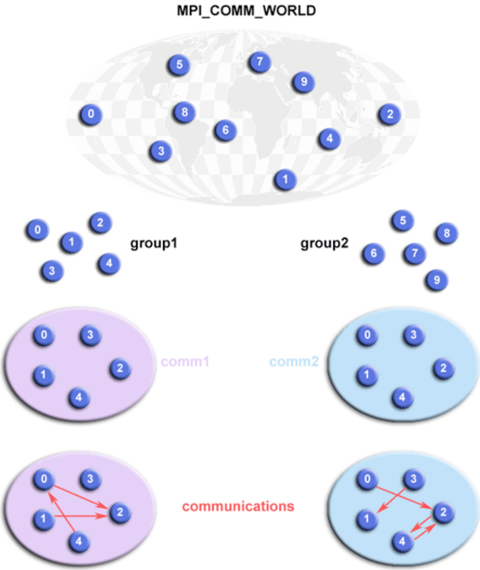
From the programmer’s perspective, a group and a communicator are one. The group routines are primarily used to specify which processes should be used to construct a communicator.

Groups and communicator

Goals:

- Allow you to organize tasks, based upon function, into task groups.
- Enable Collective Communications operations across a subset of related tasks.
- Provide basis for implementing user defined virtual topology.

Remarks: Groups/communicators can be created and destroyed during program execution. Processes may be in more than one group/communicator having a unique rank within each group/communicator.



Defining a new communicator: the simple approach

Fortran

```
MPI_group MPI_GROUP_WORLD
MPI_group first_row_group
MPI_Comm first_row_comm
Integer row_size
Parameter(row_size=2)
Integer process_ranks(row_size)

Do i = 1, row_size
   process_ranks(i) = i-1
Enddo

Call MPI_COMM_GROUP(MPI_COMM_WORLD, MPI_GROUP_WORLD, ierr)

Call MPI_GROUP_INCL(MPI_GROUP_WORLD, row_size,
                    process_ranks, first_row_group, ierr)

Call MPI_COMM_CREATE(MPI_COMM_WORLD, first_row_group,
    first_row_comm)
```

Defining a new communicator: the smart approach

Fortran
```fortran
MPI_COMM_SPLIT(comm, color, key, comm_out)
```

color (INTEGER) identifies the group

key (INTEGER) specifies a member of the group (rank)

6 ranks

P0	P1
P2	P3
P4	P5

row_comm

P0	P1
P2	P3
P4	P5

col_comm

P0	P1
P2	P3
P4	P5

myRank	0	1	2	3	4	5
iRow	0	0	1	1	2	2
jCol	0	1	0	1	0	1

Fortran
```fortran
! logical 2D topology with nrow=3 rows and mcol=2 columns
! 6 ranks, it is a collective operation
iRow = myRank/mcol          !! logical row number
jCol = mod(myRank, mcol) !! logical column number
comm2D = MPI_COMM_WORLD

CALL MPI_COMM_SPLIT(comm2D, iRow, jCol, row_comm, ierr)
CALL MPI_COMM_SPLIT(comm2D, jCol, iRow, col_comm, ierr)
```

Topology with MPI

- A virtual topology describes the ”connectivity” of MPI processes in a communicator.
- The two main types of topology are Cartesian and Graph.
- MPI topology are virtual - there may be no relation between the physical structure of the parallel machine and the process topology.
- Virtual topology are built upon MPI communicators and groups.

Cartesian topology

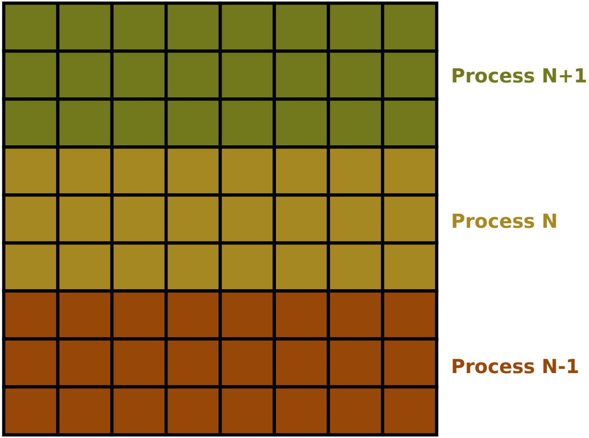
- Each process is connected to its neighbors in a virtual grid
- Boundaries can be cyclic
- Identified by (discrete) Cartesian coordinates (i, j, k)

Graph topology

- Graphs are used to describe communication patterns
- The most general description of communication patterns

Domain decomposition

Planar distribution: data are distributed linearly between processors. Default mapping when using `MPI_COMM_WORLD`.

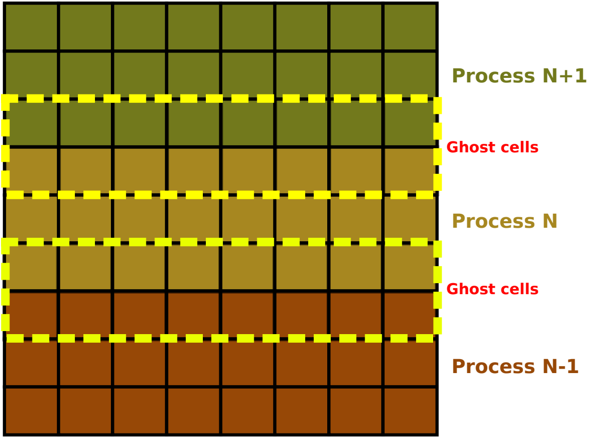


Domain decomposition

Planar distribution: data are distributed linearly between processors.

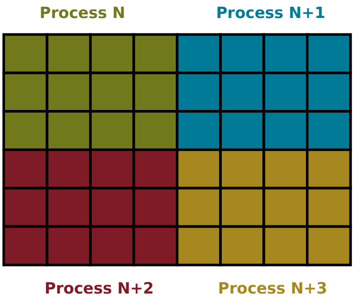
Default mapping when using `MPI_COMM_WORLD`.

Ghost cells are exchanged: processor N communicates with N-1 and N+1



Domain decomposition

Cartesian distribution: data are distributed linearly between processors.



This is in general a more effective way of distribute the domain, since:

- It is much more scalable
- Communicated data volume can be smaller (especially when a large number of processors is used)
- It can better map the geometry of the problem and of the algorithm

However, it is more difficult to handle: who are my neighbors?

Cartesian topology

Fortran
```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder,
    comm_cart)
```

comm_old	input communicator
ndims	number of dimensions of Cartesian grid
dims	specifies the number of processes in each dimension
periods	specifies whether the grid is periodic (true) or not (false) in each dimension
reorder	ranking may be reordered (true) or not (false)
comm_cart	communicator with new Cartesian topology

Row-major numbering:

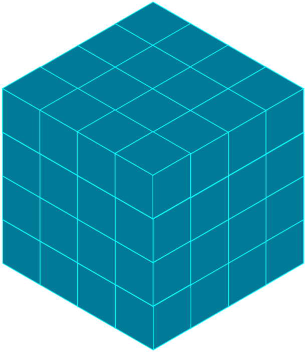
0 (0,0)	1 (0,1)	2 (0,2)	3 (0,3)
4 (1,0)	5 (1,1)	6 (1,2)	7 (1,3)
8 (2,0)	9 (2,1)	10 (2,2)	11 (2,3)
12 (3,0)	13 (3,1)	14 (3,2)	15 (3,3)

Cartesian topology example

Fortran
```fortran
INTEGER :: comm_cart
INTEGER :: ierr
INTEGER :: dims(3)
LOGICAL :: periods(3)

dims(1) = NprocX
dims(2) = NprocY
dims(3) = NprocZ
periods = .TRUE.

Call MPI_CART_CREATE (MPI_COMM_WORLD,
    3, dims, periods, .TRUE., comm_cart
    , ierr)
```



Periods and reorder

Periods: Define if the boundary of the grid are periodic or not.

periods = False					
-1	←0	1	2	3→	-1
periods = True					
3	←0	1	2	3→	0

Note: `MPI_PROC_NULL=-1`

Reorder: allows MPI processes reordered for efficiency, possibly so as to choose a good embedding of the virtual topology onto the physical machine.

Utility functions

Create dimensions:

Fortran
```
MPI_DIMS_CREATE(NNODES, NDIMS, DIMS, IERROR)
INTEGER NNODES, NDIMS, DIMS(*), IERROR
```

Retrieves Cartesian topology information associated with a communicator:

Fortran
```
MPI_CARTDIM_GET(COMM, NDIMS, IERROR)
INTEGER COMM, NDIMS, IERROR

MPI_CART_GET( COMM, NDIMS, DIMS, PERIODS, COORDS, IERROR)
INTEGER COMM, MAXDIMS, DIMS(*), COORDS(*), IERROR
LOGICAL PERIODS(*)
```

Coordinates to rank:

Fortran
```
MPI_CART_RANK(COMM, COORDS, RANK, IERROR)
INTEGER COMM, COORDS(*), RANK, IERROR
```

Rank to coordinates:

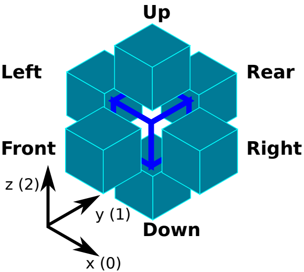
Fortran
```
MPI_CART_COORDS(COMM, RANK, MAXDIMS, COORDS, IERROR)
GER COMM, RANK, MAXDIMS, COORDS(*), IERROR
```

Finding neighbors: Shift

Fortran
```
MPI_CART_SHIFT(comm, direction, disp, rank1,
    rank2)
```

comm	communicator with Cartesian structure
direction	coordinate dimension of shift
disp	displacement
rank1	rank of nearby process
rank2	rank of nearby process

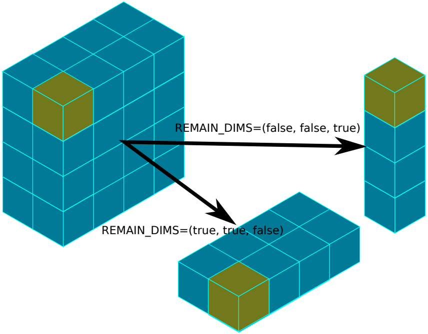
Fortran
```
Call MPI_CART_SHIFT(comm_cart, 0, 1, left,
    right, ierr)
Call MPI_CART_SHIFT(comm_cart, 1, 1, front,
    rear, ierr)
Call MPI_CART_SHIFT(comm_cart, 2, 1, down, up,
     ierr)
```



Sub-grids in Cartesian topology

Fortran
```
MPI_CART_SUB(comm, remain_dims,
    newcomm)
```

comm	communicator with Cartesian structure
remain_dims	the ith entry of remain_dims specifies whether the ith dimension is kept in the subgrid (true) or is dropped (false)
newcom	communicator containing the subgrid including the calling process



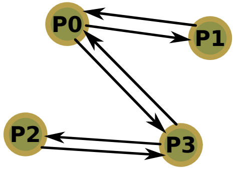
Graph topology

Fortran
```
MPI_GRAPH_CREATE(comm_old, nnodes, index, edges, reorder,
    comm_graph)
```

comm_old	input communicator
nnodes	number of nodes in graph
index	array of integers describing node degrees
edges	array of integers describing graph edges
reorder	ranking may be reordered (true) or not (false)
comm_graph	communicator with graph topology added

Process	Neighbors
0	1,3
1	0
2	3
3	0,2

nnodes = 4
index = 2, 3, 4, 6
edges = 1, 3, 0, 3, 0, 2



Other functions

- Manage communicators:

  `MPI_Comm_compare, MPI_Comm_dup` ...

- Manipulate groups:

  `MPI_Group_union, MPI_Group_intersection` ...

- Cartesian topology, map a process:

  `MPI_Cart_map`

- Graph topology:

  `MPI_Graph_map, MPI_Graph_get` ...

Practicals

Exercise: 05.MPI_Topo

1. Create a 1-dimension topology - a ring
2. Ghost cell exchanges using a topology

Thank you for your attention.