22nd Summer School on PARALLEL COMPUTING

MPI Virtual Topologies

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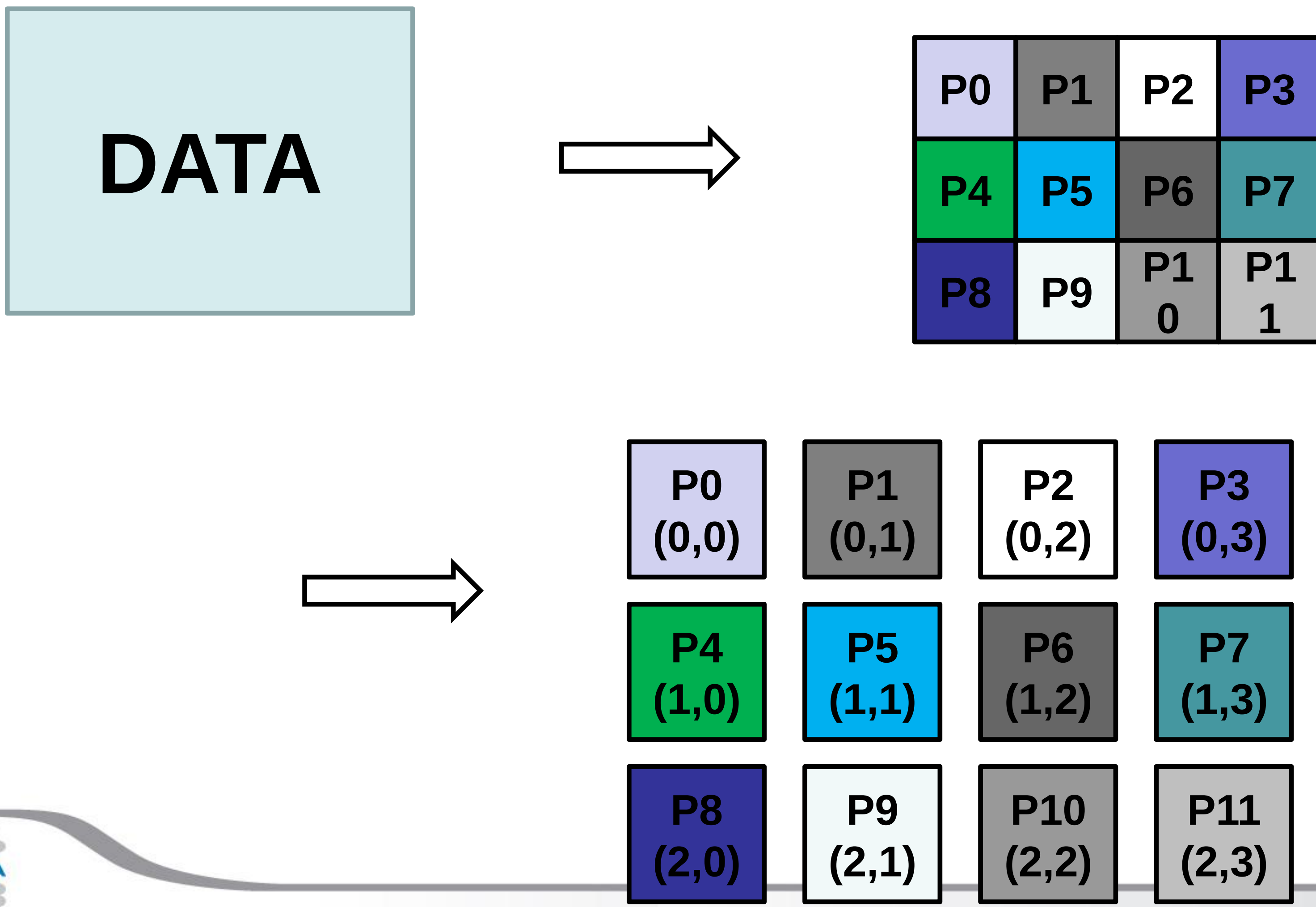
Outline

- Virtual topology: definition
- MPI supported topologies:
  - Cartesian
    - How to create
    - Cartesian mapping function
    - Cartesian partitioning
  - Graph

Example: 2D Domain decomposition



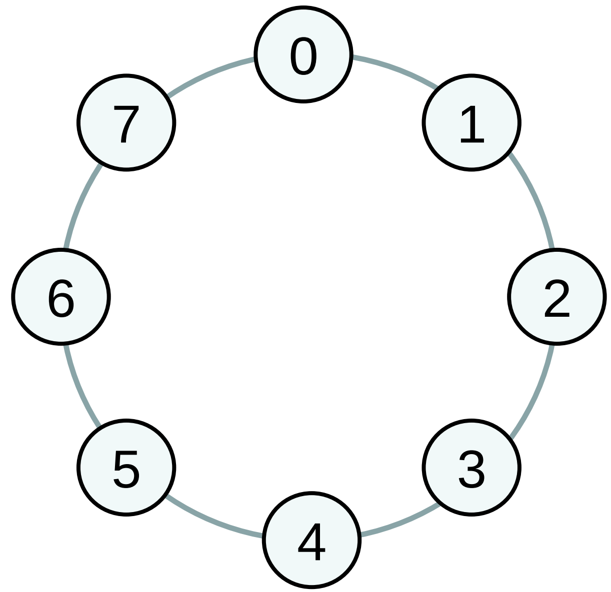
Virtual Topology

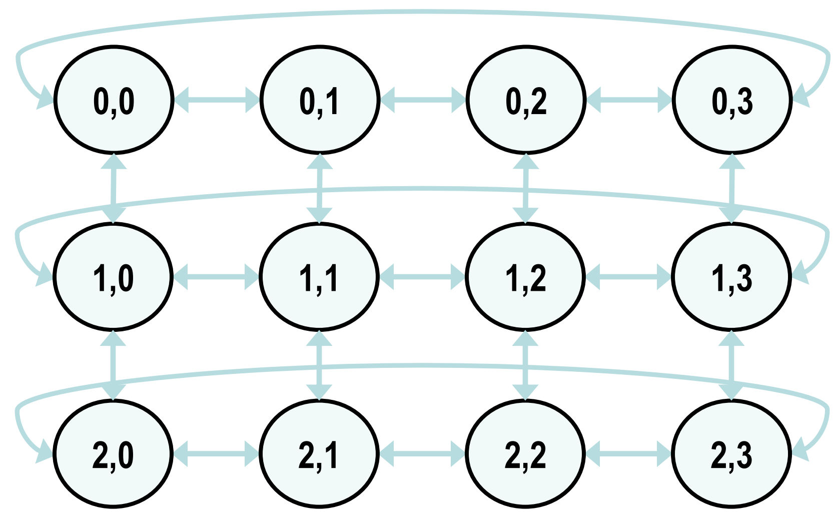
- **Topology:**
  - extra, optional attribute that can be given to an intra-communicator; topologies cannot be added to inter-communicators.
  - can provide a convenient naming mechanism for the processes of a group (within a communicator), and additionally, may assist the runtime system in mapping the processes onto hardware.
- **A process group in MPI is a collection of n processes:**
  - each process in the group is assigned a rank between 0 and n-1.
  - in many parallel applications a linear ranking of processes does not adequately reflect the logical communication pattern of the processes (which is usually determined by the underlying problem geometry and the numerical algorithm used).

Virtual Topology

- **Virtual topology:**
  - logical process arrangement in topological patterns such as 2D or 3D grid; more generally, the logical process arrangement is described by a graph.
- **Virtual process topology .vs. topology of the underlying, physical hardware:**
  - virtual topology can be exploited by the system in the assignment of processes to physical processors, if this helps to improve the communication performance on a given machine.
  - the description of the virtual topology depends only on the application, and is machine-independent.

Virtual Topology - Example





RING

2D-GRID WITH PERIODIC BOUNDARY CONDITION

MPI Supported Topologies

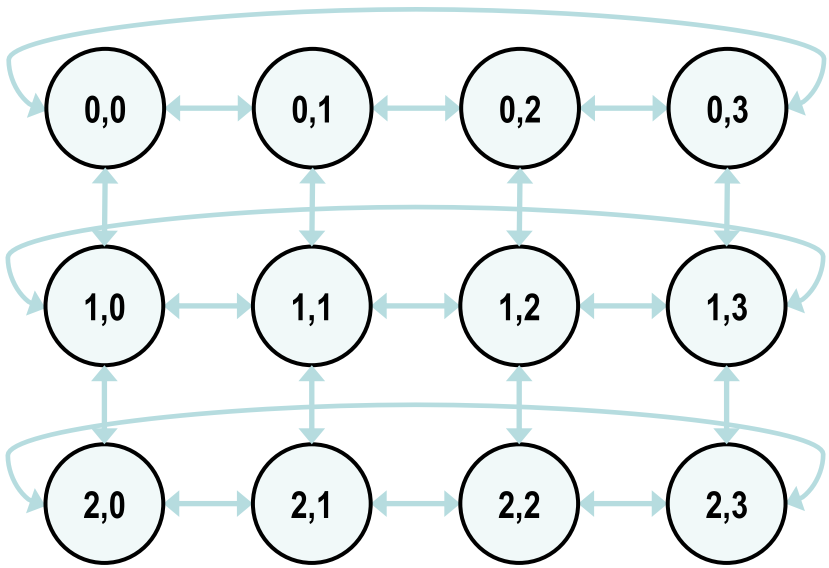
- Cartesian
- Graph
- Distributed graph

Note: Topology information is associated with communicators

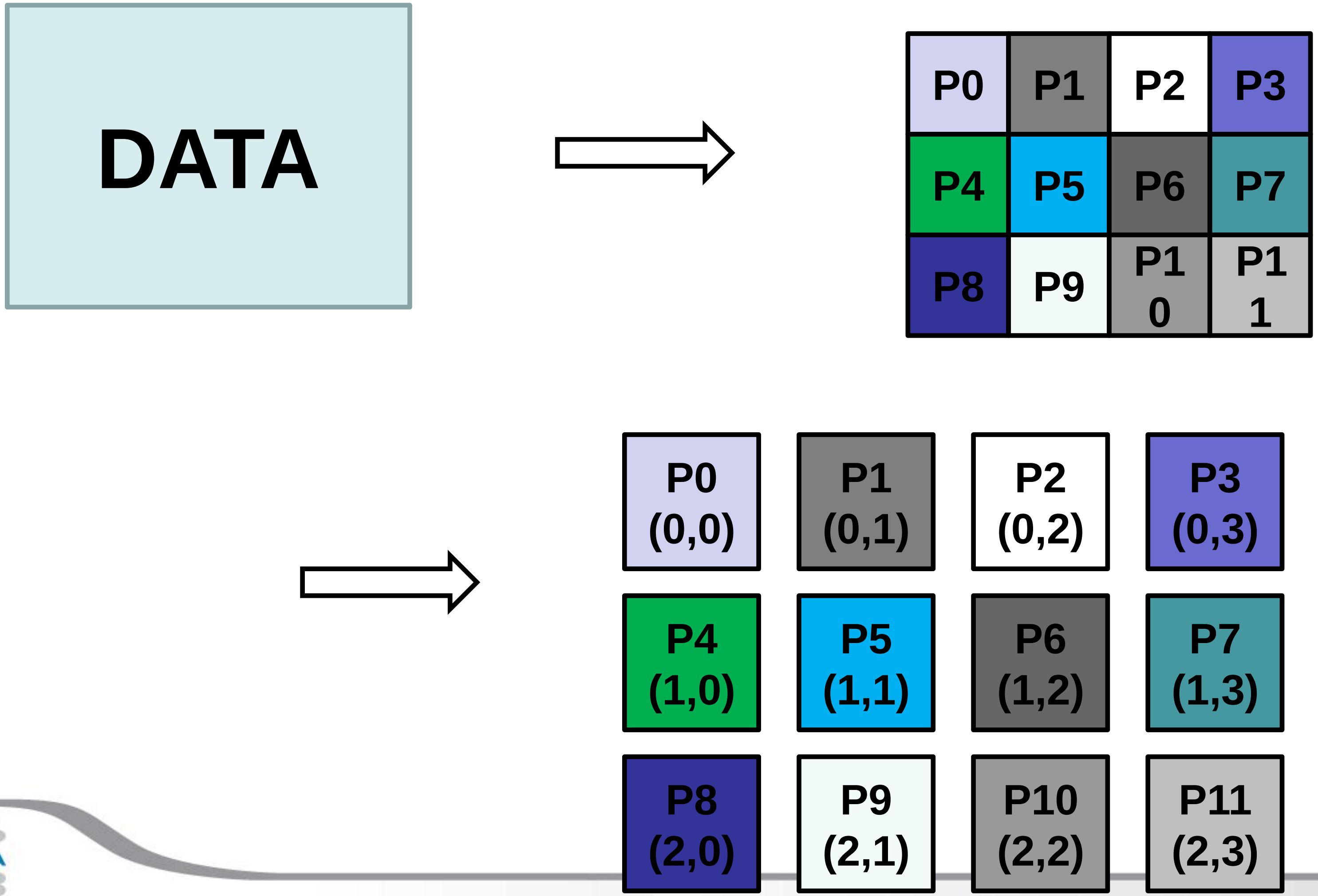
Cartesian Topology

A grid of processes is easily described with a cartesian topology:

- each process can be identified by cartesian coordinates
- periodicity can be selected for each direction
- communications are performed along grid dimensions only



Example: 2D Domain decomposition



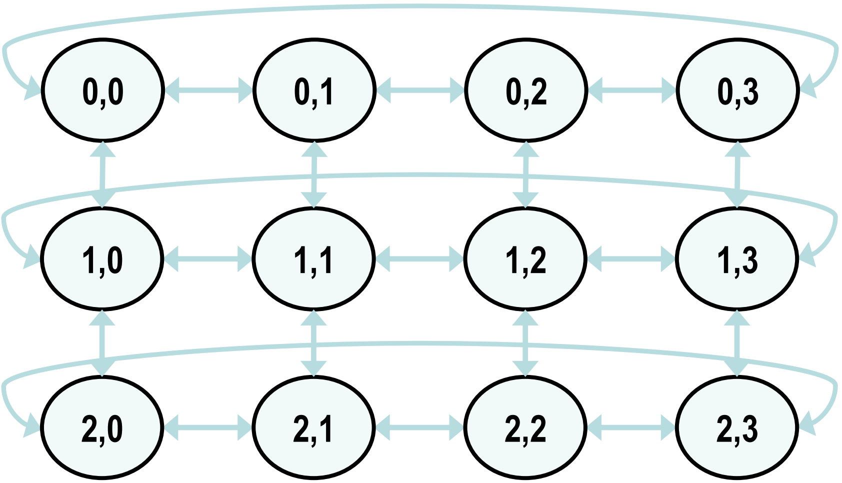
Cartesian Constructor

```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder,
comm_cart)
   IN comm_old: input communicator (handle)
   IN ndims: number of dimensions of Cartesian grid (integer)
   IN dims: integer array of size ndims specifying the number of
        processes in each dimension
   IN periods: logical array of size ndims specifying whether the
        grid is periodic (true) or not (false) in each dimension
   IN reorder: ranking may be reordered (true) or not (false)
   OUT comm_cart: communicator with new Cartesian topology (handle)
```

- Returns a handle to a new communicator to which the Cartesian topology information is attached.
- Reorder:
  - false: the rank of each process in the new group is identical to its reank in the old group.
  - True: the processes may be reordered, possibly so as to choose a good embedding of the virtual topology onto physical machine.
- If cart has less processes than starting communicator, left over processes have MPI_COMM_NULL as return

How to create a Cartesian Topology

```
#include <mpi.h>

int main(int argc, char *argv[])
{

  MPI_Comm cart_comm;
  int dim[] = {4, 3};
  int period[] = {1, 0};
  int reorder = 0;

  MPI_Init(&argc, &argv);

  MPI_Cart_create(MPI_COMM_WORLD, 2, dim, period, reorder,
   &cart_comm);
  ...
}
```



Cartesian Topology Utilities

- MPI_Dims_Create:
  - compute optimal balanced distribution of processes per coordinate direction with respect to:
    - a given dimensionality
    - the number of processes in a group
    - optional constraints
- MPI_Cart_coords:
  - given a rank, returns process's coordinates
- MPI_Cart_rank:
  - given process's coordinates, returns the rank
- MPI_Cart_shift:
  - get source and destination rank ids in SendRecv operations

Binding of MPI_Dims_create

```
MPI_DIMS_CREATE(nnodes, ndims, dims)
    IN nnodes: number of nodes in a grid (integer)
    IN ndims: number of Cartesian dimensions (integer)
    IN/OUT dims: integer array of size ndims specifying the number of
    nodes in each dimension
```

- Help user to select a balanced distribution of processes per coordinate direction, depending on the number of processes in the group to be balanced and optional constraints that can be specified by the user
- if `dims[i]` is set to a positive number, the routine will not modify the number of nodes in that i dimension
- negative value of `dims[i]` are erroneous

IN / OUT of "dims"

```
MPI_DIMS_CREATE(nnodes, ndims, dims)
    IN nnodes: number of nodes in a grid (integer)
    IN ndims: number of Cartesian dimensions (integer)
    IN/OUT dims: integer array of size ndims specifying the number of
    nodes in each dimension
```

dims before call	Function call	dims on return
(0, 0)	MPI_DIMS_CREATE(6, 2, dims)	(3, 2)
(0, 0)	MPI_DIMS_CREATE(7, 2, dims)	(7, 1)
(0, 3, 0)	MPI_DIMS_CREATE(6, 3, dims)	(2, 3, 1)
(0, 3, 0)	MPI_DIMS_CREATE(7, 2, dims)	erroneous call

Using MPI_Dims_create

```
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

int dim[3];
dim[0] = 0; // let MPI arrange
dim[1] = 0; // let MPI arrange
dim[2] = 3; // I want exactly 3 planes

MPI_Dims_create(nprocs, 3, dim);

if (dim[0]*dim[1]*dim[2] < nprocs) {
  fprintf(stderr, "WARNING: some processes are not in use!\n"
}

int period[] = {1, 1, 0};
int reorder = 0;

MPI_Cart_create(MPI_COMM_WORLD, 3, dim, period, reorder, &cube_comm);

   ...
```

Coordinate -> Rank: `MPI_Cart_rank`

```
MPI_CART_RANK(comm, coords, rank)
    IN comm: communicator with Cartesian structure
    IN coords: integer array (of size ndims) specifying the Cartesian
    coordinates of a process
    OUT rank: rank of specified process
```

- translation of the logical process coordinates to process ranks as they are used by the point-to-point routines
- if `dimension i` is periodic, when i-th coordinate is out of range, it is shifted back to the interval `0<coords(i)<dims(i)` automatically
- out-of-range coordinates are erroneous for non-periodic dimensions

Mapping: old and new ranks

```
// buffer to collect MPI_COMM_WORLD rank ids in new cartesian rank sorting
int *world_ranks = (int *) malloc (nprocs, sizeof(int));

int oldrank;
MPI_Comm_rank(MPI_COMM_WORLD, &oldrank);

MPI_Cart_create(MPI_COMM_WORLD, 2, dim, period, 1, &cart_comm);

// indexing dorting is now performed on rank id of comm_cart communicator
MPI_Gather(&oldrank, 1, MPI_INT, world_ranks, 1, MPI_INT, 0, comm_cart);

if (oldrank == 0) {
  for (int i=0; i<dim[0]; i++) {
    for (int j=0; j<dim[1]; j++) {
     int new_rank;
     int coords[2]; coords[0]=i; coords[1]=j;
     MPI_Cart_rank(cart_comm, coords, &new_rank);

     printf("([%d, %d]) ", new_rank, world_ranks[new_rank]);
    }; printf("\n");
  }
}
```

Rank -> Coordinate: MPI_Cart_coords

```
MPI_CART_COORDS(comm, rank, maxdim, coords)
   IN comm: communicator with Cartesian structure
   IN rank: rank of a process within group of comm
   IN maxdims: length of vector coords in the calling program
   OUT coords: integer array (of size ndims) containing the
   Cartesain coordinates of specified process
```

- For each MPI process in Cartesian communicator, the coordinate whitin the cartesian topology are returned

Usage of MPI_Cart_coords

```
. . .
ndim = (int*)calloc(dim,sizeof(int));
ndim[0] = row; ndim[1] = col;

period = (int*)calloc(dim,sizeof(int));
period[0] = period[1] = 0;

reorder = 0;

// 2D grid creation
MPI_Cart_Create(MPI_COMM_WORLD,dim,ndim,period,reorder, &comm_grid);
MPI_Comm_rank(comm_grid,&menum_grid);

// Coordinate of each mpi rank within the cartesian communicator
MPI_Cart_coords(comm_grid,menum,dim,coordinate);

printf("Procs %d coordinates in 2D grid (%d,%d)
    \n",menum,*coordinate,*(coordinate+1));
. . .
}
```

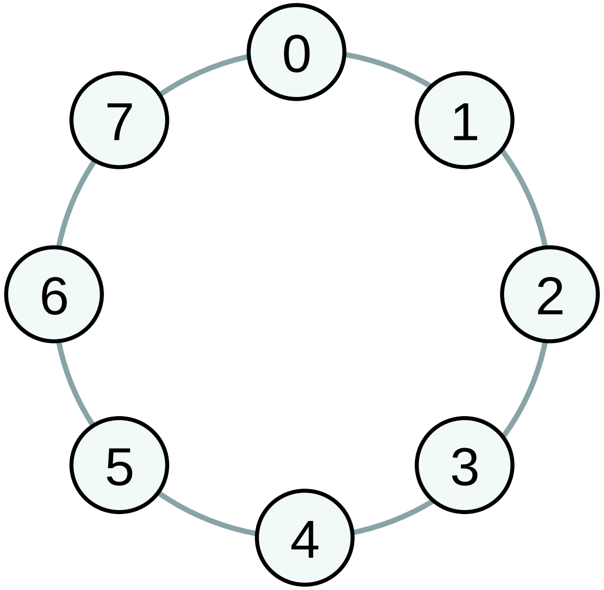
Mapping of Coordinates

```
int cart_rank;
MPI_Comm_rank(cart_comm, &cart_rank);

int coords[2];
MPI_Cart_coord(cart_comm, 2, cart_rank, coords);

// set linear boundary values on bottom/left-hand domain
if (coords[0] == 0 || coords[1] == 0) {
  SetBoundary( linear(min, max), domain);
}

// set sinusoidal boundary values along upper domain
if (coords[0] == dim[0]) {
  SetBoundary( sinusoid(), domain);
}

// set polynomial boundary values along right-hand of domain
if (coords[1] == dim[1]) {
  SetBoundary( polynomial(order, params), domain);
}
```

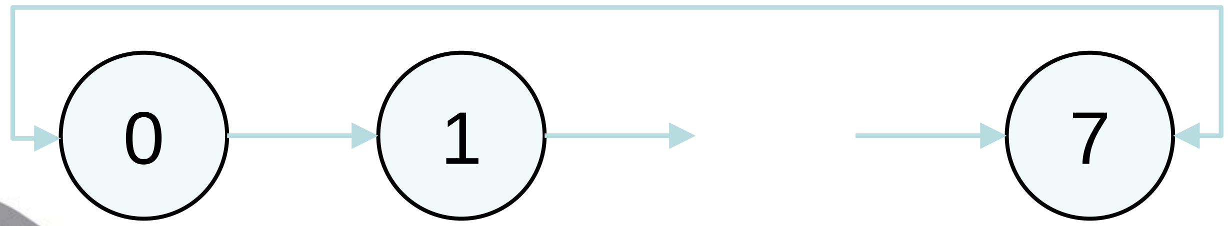
Circular Shift: a 1D Cartesian Topology

Circular shift is another tipical MPI communication pattern:

- each process communicate only with its neighbors along one direction
- periodic boundary conditions can be set for letting first and last processes partecipate in the communication



such a pattern is nothing more than a 1D cartesian grid topology with optional periodicity

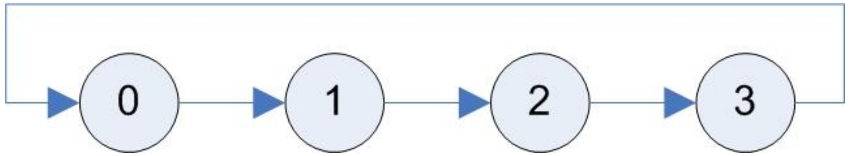


Sendrecv with Cartesian Topologies: MPI_Cart_shift

```
MPI_CART_SHIFT(comm, direction, disp, rank_source, rank_dest)
   IN comm: communicator with Cartesian structure
   IN direction: coordinate dimension of shift
   IN disp: displacement (>0: upwards shift; <0: downwards shift
   OUT rank_source: rank of source process
   OUT rank_dest: rank of destination process
```

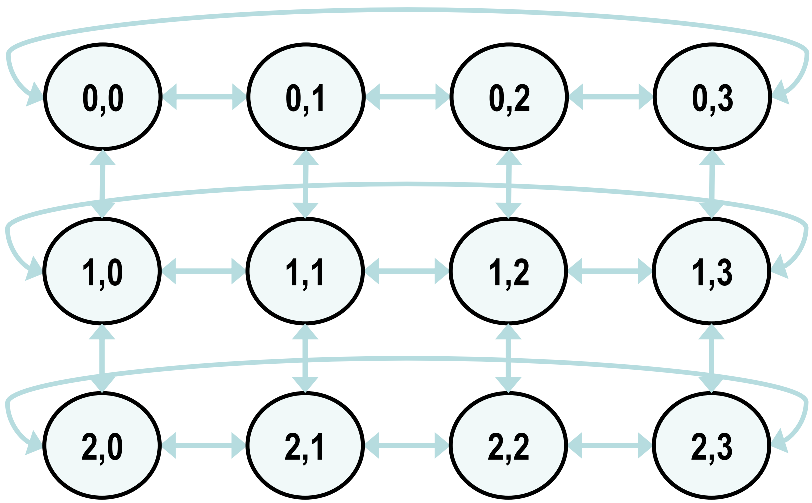
- Depending on the periodicity of the Cartesian group in the specied coordinate direction, MPI_CART_SHIFT provides the identiers for a circular or an end-o shift.
- In the case of an end-o shift, the value **MPI_PROC_NULL** may be returned in rank_source or rank_dest, indicating that the source or the destination for the shift is out of range.
- provides the calling process the ranks of source and destination processes for an MPI_SENDRECV with respect to a specified coordinate direction and step size of the shift

Sendrecv with 1D Cartesian Topologies




```
...

int dim[1] = nprocs;
int period[1] = 1;
MPI_Comm ring_comm;

MPI_Cart_create(MPI_COMM_WORLD, 1, dim, period, 0, &ring_comm);

int source, dest;
MPI_Cart_shift(ring_comm, 0, 1, &source, &dest);

MPI_Sendrecv(right_bounday, n, MPI_INT, dest, rtag,
             left_boundary, n, MPI_INT, source, ltag,
             ring_comm, &status);
...
```

Sendrecv with 2D Cartesian Topologies




```
...

int dim[] = {4, 3};
int period[] = {1, 0};
MPI_Comm grid_comm;

MPI_Cart_create(MPI_COMM_WORLD, 2,
   dim, period, 0, &grid_comm);

int source, dest;
for (int dimension = 0; dimension < 2; dimension++) {
  for (int versus = -1; versus < 2; versus+=2;) {
    MPI_Cart_shift(ring_comm, dimension, versus, &source, &dest);
    MPI_Sendrecv(buffer, n, MPI_INT, source, stag,
                 buffer, n, MPI_INT, dest, dtag,
                 grid_comm, &status);
  }
}
```

Partitioning of Cartesian Structures

- It is often useful to partition a cartesian communicator into subgroups that form lower dimensional cartesian subgrids
  - new communicators are derived
  - lower dimensional communicators cannot communicate among them
    - unless inter-communicator are used

Binding of MPI_Cart_sub

```
MPI_CART_SUB(comm, remain_dims, newcomm)
    IN comm: communicator with Cartesian structure
    IN remain_dims: the i-th entry of remain_dims specifies whether
        the i-th dimension is kept in the subgrid (true) or is
        dropped (false) (logical vector)
    OUT newcomm: communicator containing the subgrid that includes
        the calling process
```

```
int dim[] = {2, 3, 4};

int remain_dims[] = {1, 0, 1}; // 3 comm with 2x4 processes 2D
   grid
...
int remain_dims[] = {0, 0, 1}; // 6 comm with 4 processes 1D
   topology
```

News from MPI-3.x

MPI-3.0 introduces more functionalities for topologies:

- neighbor collective communications
  - enables optimizations in the MPI library because the communication pattern is known statically
  - the implementation can compute optimized message schedules during creation of the topology

  MPI_NEIGHBOR_ALL(GATHER[V] | TOALL[V])

- non-blocking collective communications:
  - semantic similar to non-blocking point-to-point

  MPI_INEIGHBOR_ALL(GATHER[V] | TOALL[V])

QUESTIONS ???