22nd Summer School on PARALLEL COMPUTING

MPI Virtual Topologies

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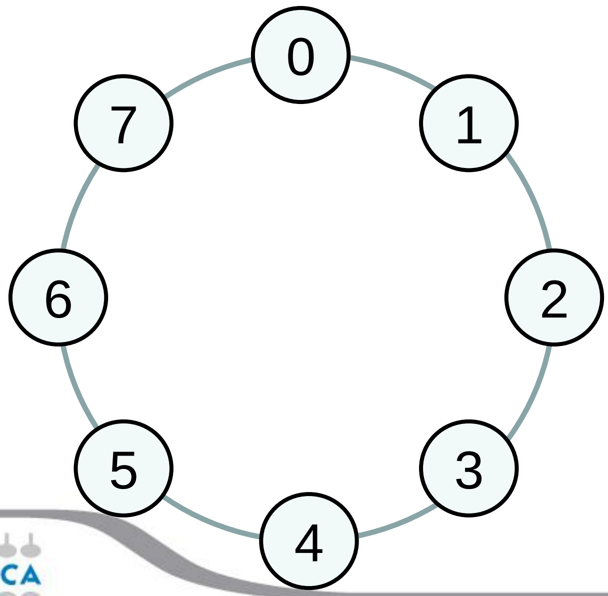
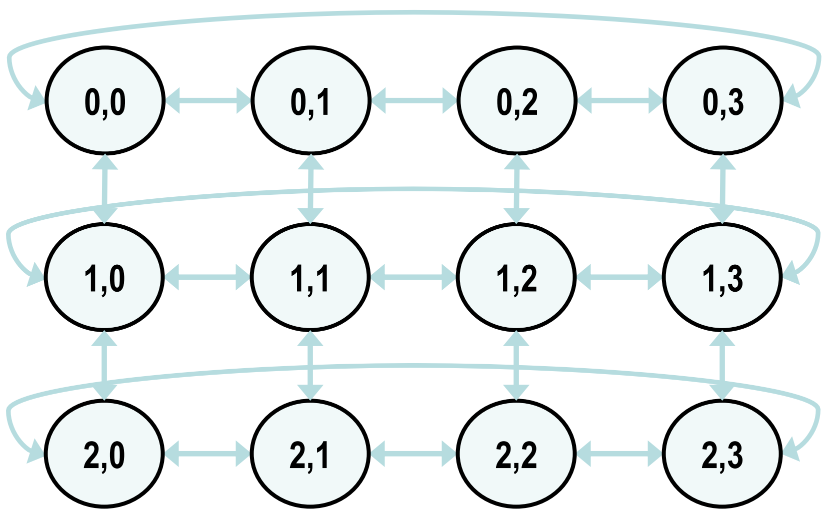
Outline

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

Virtual Topologies

- Many applications often support an intrinsic topology in the problem they are trying to address
- A topology is a geometric organization of connected elements
- MPI provides communicators to virtual topology attribute
  - describes a mapping/ordering of processes:
  - it's virtual in the sense that no assumptions are made on the distribution of processes on physical hardware





Virtual Topologies

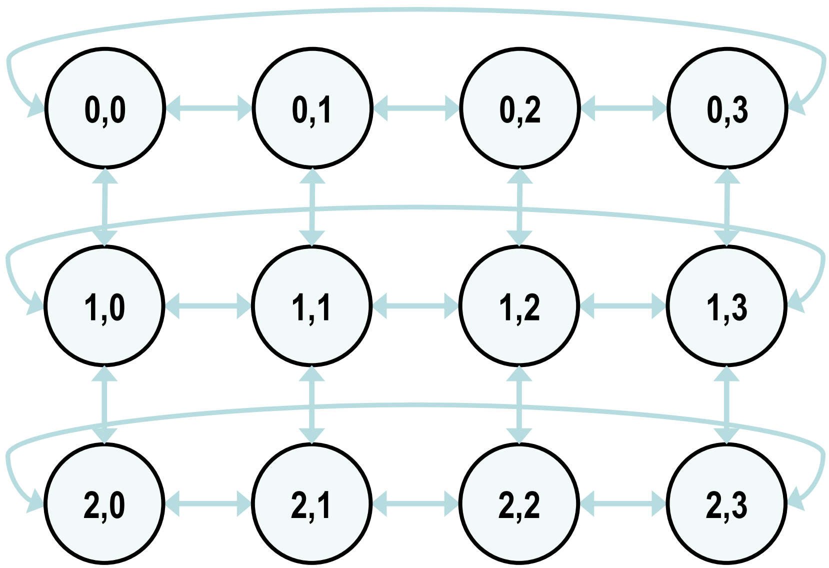
- Advantages:
  - simplify code and clarify programmer's intentions
  - ***may*** assist MPI runtime in mapping processes onto hardware (*implementation dependent*)

- MPI supported topologies:
  - **Cartesian**: n-dimensional grid of ordered processes
  - **Graphs:** very general graph connected processes

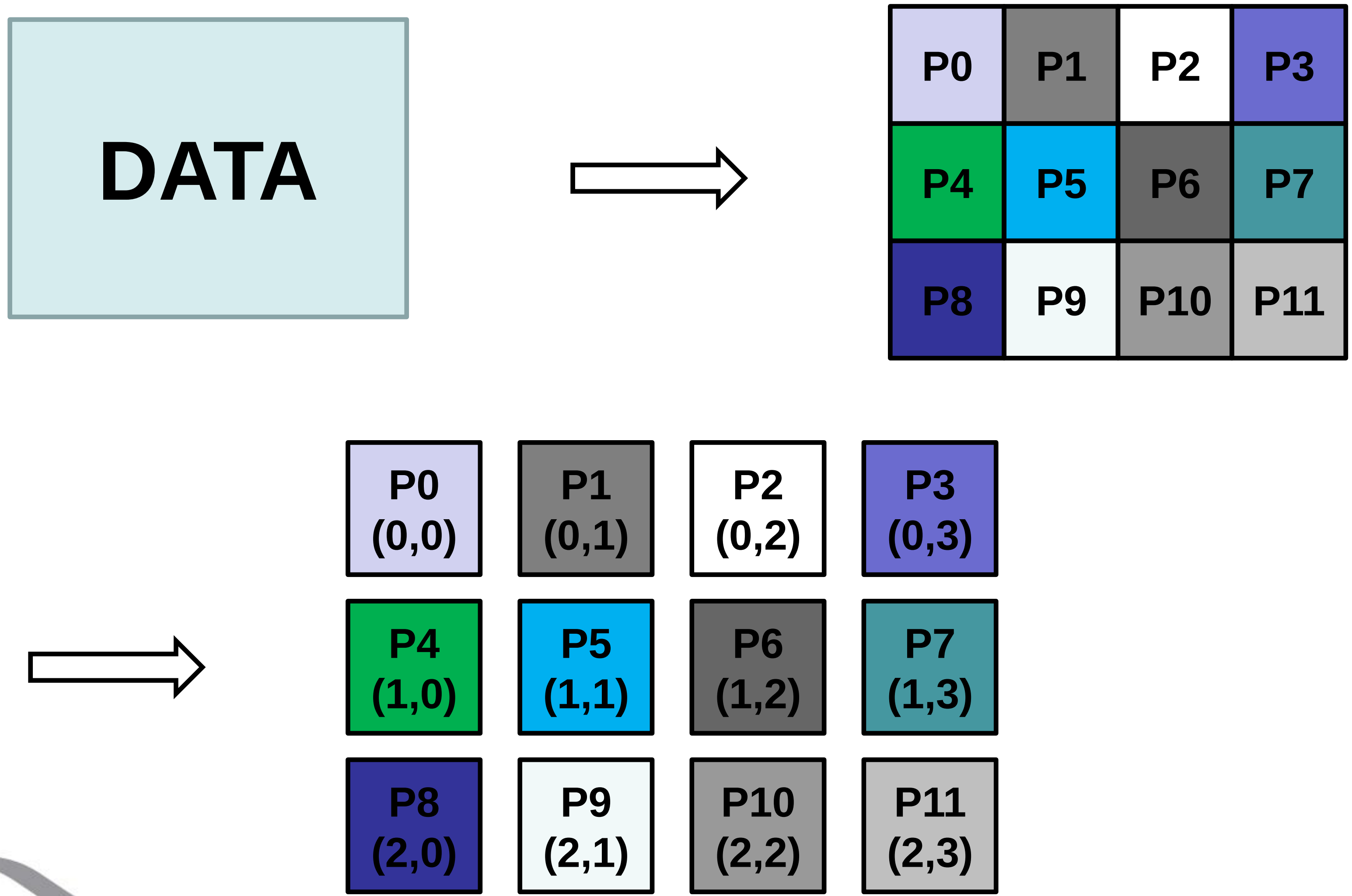
Cartesian Topology

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

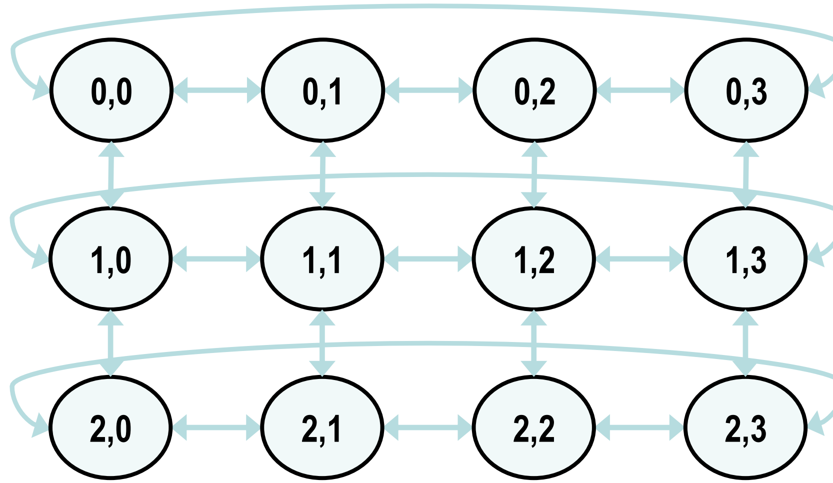

```
#include <mpi.h>

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

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```
// 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 sorting 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");
  }
}
```

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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

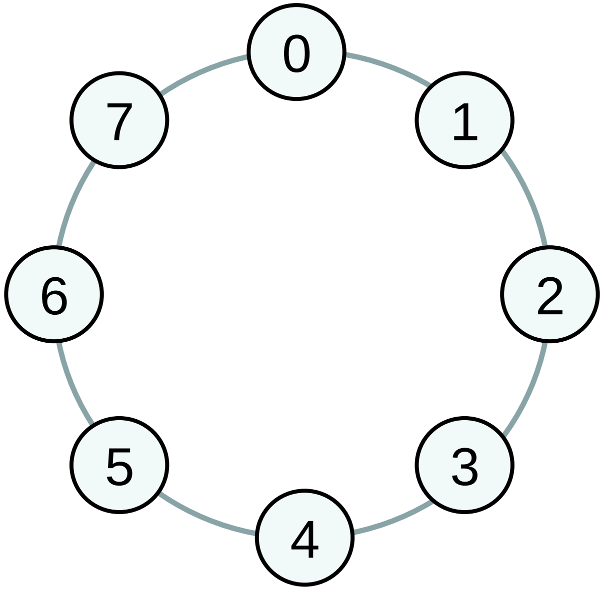

```
int cart_rank;
MPI_Comm_rank(cart_comm, &cart_rank);

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);
}
```

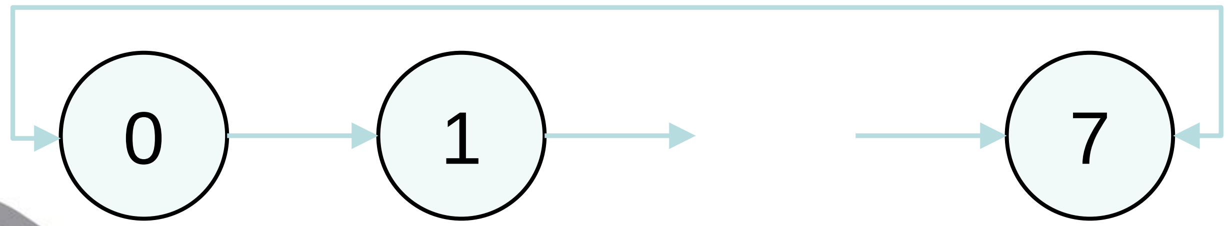
Circular Shift: a 1D Cartesian Topology

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



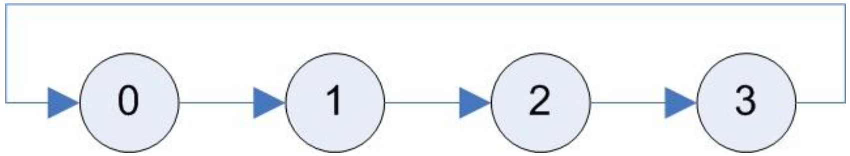


Sendrecv with Cartesian Topologies: MPI_Cart_shift


```
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
```

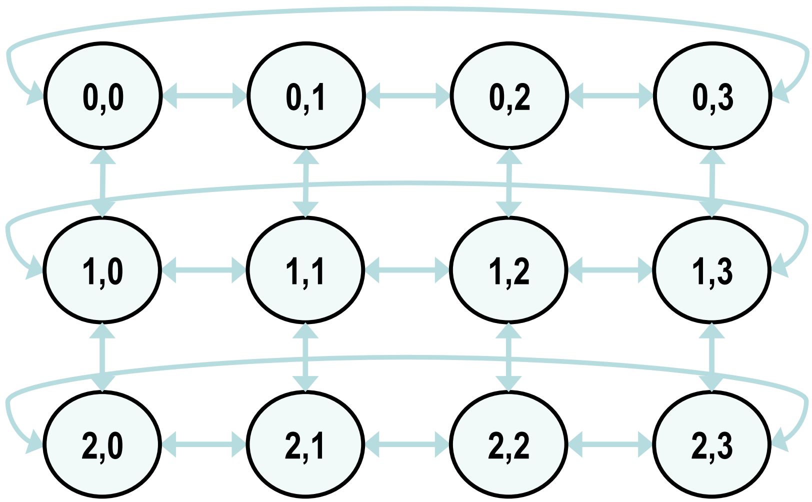
- Depending on the periodicity of the Cartesian group in the specified coordinate direction, MPI_CART_SHIFT provides the identifiers for a circular or an end-o shift.
- In the case of an end-o shift, the value **MPI_PROC_NULL** may be returned in rank_source or rank_dest, indicating that the source or 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 ???