COMS4040A & COMS7045A: High Performance Computing & Scientific Data Management Introduction to MPI III

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MPI Derived Datatypes

Example 1

```
double x[1000];

comparison of the following is more efficient than using the for loop*/
if (my_rank == 0)
    MPI_Recv(&x[i], 1, MPI_DOUBLE, 0, 0, comm, &status);
}
/+the following is more efficient than using the for loop*/
if (my_rank == 0)
    MPI_Send(&x[0], 1000, MPI_DOUBLE, 1, 0, comm);
else
MPI_Recv(&x[0], 1000, MPI_DOUBLE, 0, 0, comm, &status);
```

In distributed-memory systems, communication can be much more expensive than local computation. Thus, if we can reduce the number of communications, we are likely to improve the performance of our programs.

MPI Built-in Datatypes

- The MPI standard defines many built in datatypes, mostly mirroring standard C/C++ or FORTRAN datatypes
- These are sufficient when sending single instances of each type
- They are also usually sufficient when sending contiguous blocks of a single type
- Sometimes, however, we want to send non-contiguous data or data that is comprised of multiple types
- MPI provides a mechanism to create derived datatypes that are built from simple datatypes



MPI Derived Datatypes cont.

- In MPI, a derived datatype can be used to represent any collection of data items in memory by storing both the types of the items and their relative locations in memory.
- Why use derived datatypes?
 - Primitive datatypes are contiguous;
 - Derived datatypes allow you to specify non-contiguous data in a convenient manner and treat it as though it is contiguous;
 - Useful to
 - Make code more readable
 - Reduce number of messages and increase their size (faster since less latency);
 - Make code more efficient if messages of the same size are repeatedly used.



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Typemap

Formally, a derived datatype in MPI is described by a typemap consists of a sequence of basic MPI datatypes together with a displacement for each of the datatypes. That is,

- a sequence of basic datatypes: {type₀, ..., type_{n-1}}
- a sequence of integer displacements: $\{displ_0, ..., displ_{n-1}\}$.
- Typemap = $\{(type_0, disp_0), \cdots, (type_{n-1}, disp_{n-1})\}$

For example, a typemap might consist of (double,0),(char,8) indicating the type has two elements:

- a double precision floating point value starting at displacement 0,
- and a single character starting at displacement 8.



Typemap cont.

- Types also have extent, which indicates how much space is required for the type
- The extent of a type may be more than the sum of the bytes required for each component
- For example, on a machine that requires double-precision numbers to start on an 8-byte boundary, the type (double,0),(char,8) will have an extent of 16 even though it only requires 9 bytes



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Creating and Using a New Datatype

Three steps are necessary to create and use a new datatype in MPI:

- Create the type using one of MPI's type construction functions
- Commit the type using MPI_Type_commit().
- Release the datatype using MPI_Type_free() when it is not needed any more.



MPI Derived Datatypes cont.

MPI provides several methods for constructing derived datatypes to handle a wide variety of situations.

- Contiguous
- Vector
- Indexed
- Struct



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Contiguous Type

Contiguous: The contiguous datatype allows for a single type to refer to contiguous multiple elements of an existing datatype.



To define the new datatype in this example and release it after finished using it:

```
MPI_Datatype rowtype;
MPI_Type_contiguous(4, MPI_DOUBLE,
    &rowtype);
MPI_Type_commit(&rowtype);
.....
MPI_Type_free(&rowtype);
```



Contiguous Type cont.

To define a new datatype:

- Declare the new datatype as MPI_Datatype.
- Construct the new datatype.
- Before we can use a derived datatype in a communication function, we must first commit it with a call to

```
int MPI_Type_commit(MPI_Datatype* datatype);
```

Commits new datatype to the system. Required for all derived datatypes.

 When we finish using the new datatype, we can free any additional storage used with a call to

```
int MPI_Type_free(MPI_Datatype* datatype)
```



Contiguous Type cont.

The new datatype is essentially an array of count elements having type oldtype. For example, the following two code fragments are equivalent:

```
MPI_Send (a,n,MPI_DOUBLE,dest,tag,MPI_COMM_WORLD);
```

and

```
MPI_Datatype rowtype;
MPI_Type_contiguous(n, MPI_DOUBLE, &rowtype);
MPI_Type_commit(&rowtype);
MPI_Send(a, 1, rowtype, dest, tag, MPI_COMM_WORLD);
```



Example 2

```
#define SIZE 4
         float a[SIZE][SIZE] =
           {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};
         float b[SIZE];
        MPI Status stat:
        MPI Datatype rowtype:
        MPI_Init(&argc,&argv);
        MPI Comm rank (MPI COMM WORLD, &rank);
        MPI Comm size (MPI COMM WORLD, &numtasks);
        MPI Type contiguous (SIZE, MPI_FLOAT, &rowtype);
        MPI_Type_commit (&rowtype);
         if (numtasks == SIZE) {
           if(rank == 0)
14
             for (i=0; i<numtasks; i++)</pre>
16
               MPI_Send(&a[i][0], 1, rowtype, i, tag, MPI_COMM_WORLD);
          MPI_Recv(b, SIZE, MPI_FLOAT, source, tag, MPI_COMM_WORLD, &stat);
18
          printf("rank= %d b= %3.1f %3.1f %3.1f %3.1f\n",
             rank,b[0],b[1],b[2],b[3]);
20
21
        MPI_Type_free (&rowtype);
        MPI Finalize():
```



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Vector Type

Vector: The vector datatype is similar to the contiguous datatype but allows for a constant non-unit stride between elements.

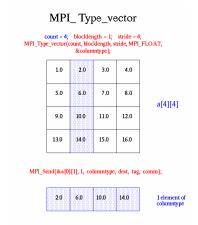
```
int MPI_Type_vector(
    int count,
    int blocklength,
    int stride,
    MPI_Datatype oldtype,
    MPI_Datatype *newtype )
```

Input parameters

- count: number of blocks (nonnegative integer)
- blocklength: number of elements in each block (integer)
- stride: number of elements between each block (integer)
- oldtype: old datatype

Vector Type cont.

- Output parameter
 - newtype: new datatype





Vector Type cont.

For example, the following two types can be used to communicate a single row and a single column of a matrix $(ny \times nx)$:

```
MPI_Datatype rowType, colType;
MPI_Type_vector(nx, 1, 1, MPI_DOUBLE, &rowType);
MPI_Type_vector(ny, 1, nx, MPI_DOUBLE, &colType);
MPI_Type_commit(&rowType);
MPI_Type_commit(&colType);
```



Example 3

```
#define SIZE 4
         float a[SIZE][SIZE] =
           \{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};
         float b[SIZE];
         MPI Status stat;
         MPI Datatype coltype;
         MPI Init (&argc, &argv);
8
         MPI Comm rank (MPI COMM WORLD, &rank);
9
         MPI Comm size (MPI COMM WORLD, &numtasks);
10
         MPI Type vector(SIZE, 1, SIZE, MPI FLOAT, &coltype);
         MPI_Type_commit(&coltype);
         if (numtasks == SIZE) {
           if (rank == 0) {
14
             for (i=0; i<numtasks; i++)</pre>
15
16
               MPI_Send(&a[i][0], 1, coltype, i, tag, MPI_COMM_WORLD);
18
           MPI Recv (b, SIZE, MPI FLOAT, source, tag, MPI COMM WORLD, &stat);
19
20
         MPI Type free (&coltype);
21
         MPI Finalize();
```



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Indexed Type

Indexed: The indexed datatype provides for varying strides between elements.

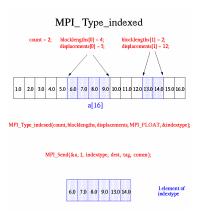
```
int MPI_Type_indexed(
    int count,
    int blocklens[],
    int indices[],
    MPI_Datatype oldtype,
    MPI_Datatype *newtype )
```

Input parameters

- count: number of blocks also number of entries in indices and blocklens
- blocklens: number of elements in each block (array of nonnegative integers)
- indices: displacement of each block in multiples of oldtype (array of integers)
- oldtype: old datatype

Indexed Type cont.

- Output parameters
 - newtype: new datatype





Indexed Type cont.

Indexed type generalizes the vector type; instead of a constant stride, blocks can be of varying length and displacements.



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Struct Type

Struct: The most general constructor allows for the creation of types representing general C/C++ structs/classes.

 We can use MPI_Type_create_struct to build a derived datatype that consists of individual elements that have different basic types:

```
int MPI_Type_create_struct(
  int count, //number of elements in the datatype
  int array_of_blocklengths[], //length of each element
  MPI_Aint array_of_displacements[], //displacements in bytes
  MPI_Datatype array_of_types[],
  MPI_Datatype* new_type_p)
```



Struct Type cont.

- count: number of blocks, also number of entries in arrays
 array_of_types, array_of_displacements and array_of_blocklengths
- array_of_blocklengths: number of elements in each block
- array_of_displacements: byte displacement of each block
- array_of_types: type of elements in each block
- Output Parameters: newtype: new datatype



Struct Type Cont.

To find the displacements, we can use the function

```
MPI_Get_address:
   int MPI_Get_address(
      void* location_p,
      MPI_Aint* address_p);
```

- It returns the address of the memory location referenced by location_p.
- MPI_Aint is an integer type that is big enough to store an address on the system.



Example 4 (Moving particles between processes)

In N-body problems, the force between particles become less with growing distance. At great enough distance, the influence of a particle on others is negligible. A number of algorithms for N-body simulation take advantage of this fact. These algorithms organize the particles in groups based on their locations using tree structures such quad-tree. One important step in the implementation of these algorithms is that of transferring particles from one process to another as they move. Here, we only discuss a way in which movement of particles can be done in MPI.

Assume a particle is defined by

```
typedef struct {
    int x,y,z;
    double mass;
}Particle;
```



 To send a particle from one process to another, or broadcast the particle, it makes sense in MPI to create a datatype instead of sending the elements in the struct individually.

Example 4 cont.



Struct Type cont.

Example 4 cont.

```
void Build_mpi_type( int* x_p, int* y_p, int* z_p, double* mass_p,
          MPI_Datatype* particletype_p) {
        int array of blocklengths[4] = {1, 1, 1, 1};
        MPI_Datatype array_of_types[4] = {MPI_INT, MPI_INT, MPI_INT,
            MPI DOUBLE };
        MPI Aint array of displacements[4] = {0};
        MPI Get address(x p, &array of displacements[0]);
        MPI Get address(v p. &arrav of displacements[1]);
        MPI Get address(z p. &arrav of displacements[2]);
        MPI Get address (mass p. &array of displacements[3]);
        for (int i=3; i<=0; i++)
9
          array_of_displacements[i] -= array_of_displacements[0];
        MPI_Type_create_struct(4, array_of_blocklengths,
        array of displacements, array of types,
        particletype p);
        MPI Type commit (particletype p);
14
         /* Build mpi type */
15
```



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Some Important MPI Features

- Groups
- Contexts
- Communicators



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Groups

- A group is an ordered set of processes.
- A group is used within a communicator to describe the participants in a communication "universe" and to rank such participants.
- Special predefined group: MPI_GROUP_EMPTY a group with no members.
- Predefined constant: MPI_GROUP_NULL a value used for invalid group handles. For example, MPI_GROUP_NULL is returned when a group is freed.
- MPI_GROUP_EMPTY is a valid group handles. MPI_GROUP_NULL is invalid group handles.



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Contexts

- A context is the communication environment.
- A context is a property of communicators that allows partitioning of the communication space.
- A message sent in one context cannot be received in another context. Separate contexts are entirely independent.
- Contexts are not explicit MPI objects; they appear only as part of the realization of communicators.
- A context is essentially a system-managed tag (or tags) needed to make a communicator safe for point-to-point and MPI-defined collective communication.



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Communicators

- Communicators bring together the concepts of group and context.
- MPI communication operations reference communicators to determine the scope and the "communication universe" in which a point-to-point or collective operation is to operate.
- Each communicator contains a group of valid participants.
- For collective communication, the intra communicator specifies the set of processes that participate in the collective operation.
 - Intracommunicator: Refers to the regular communicators of communication within a group.
 - Intercommunicator: Communicators target group-to-group communication



Communicators cont.

- Predefined intracommunicator MPI_COMM_WORLD of all processes the local process can communicate with after initialization is defined once MPI Init has been called.
- Predefined MPI_COMM_NULL is the value for invalid communicator handle. Used as an error result from some functions.
- Predefined MPI_COMM_SELF includes only the process itself.
- Avoid using two communicators that overlap.
- You always start with an existing communicator and subdivide it to make one or more new ones.



Why go beyond MPI_COMM_WORLD

- To use collective communication on only some processes
- Need to do a task on only some processes
- Want to do several tasks in parallel



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Example 5 (Monte Carlo Computation of Π)

- If the radius of a circle is 1, then the area is π , and the area of the square around the circle, with the same center point as the circle, is 4.
- The ratio r of the area of the circle to that of the square is $\frac{\pi}{4}$.
- Compute r by generating random points (x, y) in the square and counting how many of them turn out to be in the circle $(x^2 + y^2 < 1)$.



Example 5 cont.

- Use only one process (called server) to generate the random numbers, and distribute these to the other processes.
- We want the processes other then the server to compute the ratio
 need to use collective communication.
- We need to have two communicators.

```
MPI_Comm world=MPI_COM_WORLD, workers;

MPI_Group world_group, worker_group;

int ranks[1];

MPI_Init(&argc, &argv);

MPI_Comm_size(world, &numprocs);

MPI_Comm_rank(world, &myid);

server = numprocs - 1; // the last process

MPI_Comm_group(world, $world_group); //exatract the group

ranks[0] = server;

MPI_Group_excl(world_group, 1, ranks, &worker_group);

MPI_Comm_create(world, worker_group, &workers);

MPI_Group_free(&worker_group);

MPI_Group_free(&world_group);
```

Example 5 cont.

The program may continue in the following way:

- The server process receives requests from workers for chunks of random numbers, generate these numbers, and then sends a unique chunk of random numbers to each worker who sent their requests.
- A worker process sends a request for random numbers to the server, receives the numbers, proceeds to test whether a pair of points fall in the circle or not, and accumulate the number of points fall in the circle, and those fall outside the circle, respectively.
- After computing a chunk of random numbers, the workers do a collective communication MPI_Allreduce in this case, to compute an estimation of number π . If the estimation is not good enough, a worker needs to send another round of request to the server for a new chunk of random numbers.
- The stopping criteria is the error of estimated number π is less than a threshold, or a total number of random points to beWITS inspected.

Example 5 cont.

• Complete Example 5 as an exercise.



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Group Management

Group Accessors

- int MPI_Group_size(MPI_Group group, int *size)
 Returns the number of processes in the group.
- int MPI_Group_rank (MPI_Group group, int *rank)
 Returns the rank of calling process in the group



 Group Constructors: Construct new groups from existing groups using various set operations.

Creates a group newgroup that consists of the n processes in group with ranks ranks [0], ..., ranks [n-1]. If n = 0, then newgroup = MPI_GROUP_EMPTY.

• int MPI_Comm_group (MPI_Comm comm, MPI_Group *group)

Returns in group a handle to the group of comm.



Group Constructors

This function creates a group of processes newgroup that is obtained by deleting from group those processes with ranks

```
ranks[0], . . ., ranks[n-1].
```



More group constructing functions:

```
int MPI_Group_union(
    MPI_Group group1,
    MPI_Group group2,
    MPI_Group* newgroup)
int MPI_Group_intersection(
    MPI Group group1,
    MPI Group group2,
    MPI_Group* newgroup)
int MPI Group difference (
    MPI Group group1,
    MPI Group group2,
    MPI Group* newgroup)
```



Set operations in group construction

- Union: Returns in newgroup a group consisting of all processes in group1 followed by all processes in group2, with no duplication
- Intersection: Returns in newgroup all processes that are in both groups, ordered as in group1
- Difference: Returns in newgroup all processes in group1 that are not in group2, ordered as in group1



Group Destructors

```
int MPI_Group_free(MPI_Group *group)
```



Communicator Constructors

Communicator constructors

- Collective routine within the communicator comm
- Creates a new communicator which is associated with group
- MPI_COMM_NULL is returned to processes not in group
- All group arguments must be the same on all calling processes
- group must be a subset of the group associated with comm.



MPI_Comm_create() Example

Consider dividing the processes in the MPI_COMM_WORLD into two groups and create a new communicator for each group.



MPI_Comm_create() Example

```
#define NPROCS 8
    int rank, new_rank, sendbuf, recvbuf, comm_sz;
    int ranks1[4]=\{0,1,2,3\}, ranks2[4]=\{4,5,6,7\};
4
    MPI Group orig group, new group;
    MPI_Comm new_comm;
6
    MPI Init (&argc, &argv);
8
    MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
    MPI Comm rank (MPI COMM WORLD, &rank);
    sendbuf = rank:
12
13
    /* Extract the original group handle */
    MPI_Comm_group (MPI_COMM_WORLD, &orig_group);
```



MPI_Comm_create() Example

```
/* Divide tasks into two distinct groups based upon rank */
    if (rank < NPROCS/2)</pre>
      MPI Group incl(orig group, NPROCS/2, ranks1, &new group);
    else
      MPI_Group_incl(orig_group, NPROCS/2, ranks2, &new_group);
    /* Create new communicator and then perform collective communications
7
8
    MPI_Comm_create(MPI_COMM_WORLD, new_group, &new_comm);
    MPI Allreduce (&sendbuf, &recvbuf, 1, MPI INT, MPI SUM, new comm);
9
   MPI_Group_rank(new_group, &new rank);
11
12
    printf("rank = %d new_rank = %d recvbuf = %d\n", rank, new_rank,
        recvbuf);
```



MPI_Comm_free()

Communicator Destructor

```
int MPI_Comm_free(MPI_Comm *comm)
```

When you have finished using a communicator, free (delete/destroy) it.



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Communicator Management

- Communicator accessors
 - int MPI_Comm_size(MPI_Comm comm, int *size)
 - int MPI_Comm_rank(MPI_Comm comm, int *rank)



Communicator Constructors

```
MPI_Comm_dup(
     MPI_Comm oldcomm,
     MPI_Comm *newcomm)
```

Creates a new communicator that is an exact replica of an existing communicator.



MPI_Comm_split()

Communicator constructors

- Partitions the group associated with the given communicator into disjoint subgroups.
- color controls the subset assignment,
- key controls the rank assignment.



MPI_Comm_split() cont..

- A collective operation.
- All the processes that pass in the same value of color will be placed in the same communicator, and that communicator will be the one returned to them.
- The key argument is used to assign ranks to the processes in the new communicator.
 - If all processes passing the same color value also pass the same key value, the order of the ranks in the new communicator will be the same as in the old one. Note that color ≥ 0.
 - If they pass in different values for key, then these values are used to determine their order in the new communicator.
 - For simplicity, key = 0 you don't care about the order.
 - MPI_UNDEFINED is used as the color for processes not to be included in any of the new groups.



MPI_Comm_split() cont..

 MPI_Comm_split creates several new communicators but each process is given access only to one of the new communicators.

| Rank | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---------|---|---|---|---|---|---|---|---|---|---|----|----|
| Process | а | b | С | d | е | f | g | h | i | j | k | 1 |
| Color | U | 3 | 1 | 1 | 3 | 2 | 3 | 3 | 1 | 2 | U | 2 |
| Key | 0 | 1 | 2 | 3 | 1 | 9 | 3 | 8 | 1 | 0 | 0 | 0 |

Both process a and k are returned MPI_COMM_NULL. 3 new groups are created: $\{b, e, g, h\}, \{c, d, i\}, \{f, j, 1\}.$



MPI_Comm_split() Example.

Example 6

Suppose we create NROW \times NCOL number of processes. We want to form a communicator for the processes in each row, and do some computation using each communicator. How? Similarly, we can also formulate a communicator for the processes in each column.



Example 6 cont.

```
1 #define NROW 3
2 #define NCOL 4
4 int irow, icol, color, key, rank_in_world;
5 MPI Comm row comm, col comm;
6 MPI_Init(&argc, &argv);
7 MPI Comm rank (MPI COMM WORLD, &rank in world);
9 irow = rank in world%NROW;
10 icol = rank in world/NROW;
11 // Build row communicators
12 color = irow;
13 key = rank in world;
14 MPI_Comm_split(MPI_COMM_WORLD, color, key, &row_comm);
15 // Build column communicators
16 color = icol;
17 MPI_Comm_split(MPI_COMM_WORLD, color, key, &col_comm);
```



Example 6 cont.

```
int row_procs[NCOL], col_procs[NROW];
int max_rank_row, max_rank_col, my_max;

my_max = rank_in_world;

MPI_Allgather(&my_max,1,MPI_INT,row_procs,1,MPI_INT,row_comm);

MPI_Allgather(&my_max,1,MPI_INT,col_procs,1,MPI_INT,col_comm);

max_rank_row = row_procs[0];

for(int i = 1; i < NCOL; i++)

if(row_procs[i] > max_rank_row) max_rank_row = row_procs[i];

max_rank_col = col_procs[0];

for(int i = 1; i < NROW; i++)

if(col_procs[i] > max_rank_col) max_rank_col = col_procs[i];
```



Creating a Communicator

- For example, in matrix-vector or matrix-matrix multiplications, we can take tiled matrix decomposition approach.
- In such a case, we want to create a virtual mesh of processes a Cartesian topology.
- Function MPI_Dims_create returns an array of integers specifying the number of nodes in each dimension of the grid.
- Its syntax:

- nodes: input specifies the number of nodes in the grid;
- dims: input specifies the number of dimensions in the grid;
- size: both input and output for the size of each dimension; input: if size[i]=0 (i=0, 1, ..., dims-1), the function is free to decide the sizes of the grid dimensions; if size[i]>0, then the size of the dimension is determined by the value of size[i]. output: after the function call returns, size contains the size grid dimensions.

For example,

```
int p = 16;
int size[2];
.....
size[0]=size[1]=0;
MPI_Dims_create(p,2,size);
```



- After determining the process grid size, we can create a communicator with this topology using function MPI_Cart_create;
- Its syntax:

- old comm: the old communicator
- dims: the number of grid dimensions
- *size: an array of sizes for each grid dimension
- *periodic: an array of size dims. periodic[j] is 1 if dimension j is periodic and 0 otherwise. Periodic communication wraps around the edges of the grid.
- reorder: it is a flag parameter. If 0, the rank order of processes in the new communicator is the same as in the old communicator. If 0, the rank order of processes in the new communicator.

```
MPI_Comm cart_comm;
int p;
int size[2], periodic[2];
...
size[0] = size[1] = 0;
MPI_Dims_create(p,2,size);
periodic[0] = periodic[1] = 0;
MPI_Cart_create(MPI_COMM_WORLD, 2, size, periodic, 1, &cart_comm)
```



- In a Cartesian topology grid communicator, we need to know the ranks of the processes according to their Cartesian coordinates.
- Function

when called, returns the rank of a process with coord in the Cartesian communicator comm.



For example, suppose the Cartesian grid has r rows, the data matrix has m rows, and Row i of input matrix is mapped to the Row k of the process grid. Then we can find out the rank of a process according to its coordinate in the virtual grid.

```
int dest coords[2];
    int dest_id, grid_id, i;
    for (i=0; i<m; i++) {
      k = BLOCK OWNER(i,r,m);
      dest coord[0] = k;
      dest coord[1] = 0;
      MPI Cart rank (Cart comm, dest coord, &dest id);
      if (grid id == 0) {
        /* Read matrix row 'i' */
        /* Send matrix row 'i' to process 'dest id' */
       } else if (grid id == dest id) {
14
         /* Receive matrix row 'i' from process 0 */
15
16
18
```

- Similarly, a process can determine its coordinate in the virtual grid using its rank.
- Function

- comm: Cartesian communicator being examined;
- rank: the rank of the process whose coordinate we seek;
- dims: the number of dimensions in the virtual process grid;
- coords: holds the returned coordinate of the process.



References

- Using MPI-1: Portable Parallel Programming with the Message Passing Interface, William Gropp, Ewing Lusk, and Anthony Skjellum. MIT Press Cambridge, London, England.
- A. Grama, A. Gupta, G. Karypis and V. Kumar, Introduction to Parallel Computing, 2nd Edition, Chapter 6.
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- Parallel Programming in C with MPI and OpenMP, Michael J. Quinn, McGraw-Hill Education Group, 2003.

