Intermediate MPI:Domain Decomposition

A Tutorial with Exercises

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This tutorial was adapted from the class with exercises of the same name taught to NCCS computer users on May 2001. It constitutes a second course on MPI after "INTRODUCTION TO MPI: A Tutorial with Exercises". (You might want to start with the introductory tutorial if you are new to MPI programming, or if you would like a quick review of the proper use of basic MPI routines).

As you follow this tutorial, you will explore the basic steps and concepts involved in using domain decomposition to run your model or simulation in parallel. You will also get acquainted with and use MPI_CART routines, the set of MPI routines designed to manage domain decomposition in your MPI parallel program.

Exercises (and their solutions) are provided for you to practice each new concept. While you can review the pages of the tutorial relatively quickly, you will derive the most benefit from it if you solve the exercises on your own before reviewing their solutions. Finally, although the examples and exercises are presented using Fortran programming, C versions are also available, courtesy of Dr. Hamid Oloso. They are stored both in jsimpson and an anonymous ftp site on UniTree under the sub-directory "C".

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- Why use Domain Decomposition?
- Parallelization by Domain Decomposition.
- Steps and requirements of Domain Decomposition
- Using MPI_CART routines for Domain Decomposition
- Examples and Exercises.

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Domain Decomposition

Domain Decomposition

Question:

How do I code my model in parallel using MPI?

One Answer:

If your code lends itself to it, divide the work among the processes through domain decomposition.

What is Domain Decomposition?

- A parallelization method
- Domain portions are assigned to individual processes

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A Typical Example - a

A Typical Example

I have a finite difference model on a 64x64x64 cell domain.

It updates the arrays:

- rho(1:64,1:64,1:64)
- vel(1:64,1:64,1:64)

I want to run it on a parallel machine on 8 processors.

===> Assign a portion of the domain to each process.

......(8 blocks, 1 block to each processor)



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A Typical Example - b

A Typical Example -- cont.

There are many ways to break up the 3D domain into blocks, not just "cubes". You should choose the way that best suits your code.

e.g. 8 columns of 3D data. One column to each processor*...



*This partitioning works well with many codes that have a lot of 1D computation along the z axis -- thus requiring no communication with neighboring columns.

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A Typical Example - c

A Typical Example -- cont.

Another way to break up the 3D domain into blocks: "slices"

e.g. 8 slices of 3D data. One slice to each processor...



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D. Decomposition: Steps

Domain Decomposition

Steps:

- 1. Break up the domain into blocks.
- 2. Assign blocks to MPI-processes one-to-one.
- **3.** Write or modify your code so it only updates a single block.
- 4. Provide a "map" of neighbors to each process.
- 5. Insert communication subroutine calls where needed.
- 6. Adjust the boundary conditions code.
- 7. Can your code use "guard cells"?

Note: For ease of illustration, we will use mostly 1D and 2D examples. The concepts and techniques extend naturally to 3D, the most common type of parallel application.

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First Step:Break up the Domain

e.g. 4 blocks (2D):



In the code:

rho(nx,ny) -----> rho(nx_block,ny_block)

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Step 2: Distribute Blocks

Second Step:Distribute Blocks

e.g. 4 processes: Assign one block to each of the 4 processes



Step 3: Code for 1 Block

Third Step:Code for 1 Block

REMEMBER: Each process will run the same code to update its block! Thus,

• Adjust array dimensions to block size. e.g.:

```
rho(nx,ny) --> rho(nx_block,ny_block)
```

• Code explicitly for specific blocks (i.e. processes) where necessary. e.g.

```
if (my_rank == 0) then
    {assign initial data for block [0,0]..}
else if (my_rank == 1) then
    {assign initial data for block [0,1]..}
else if (my_rank == 2) then
    ...
end if
```

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Step 4: Map of Neighbors

Fourth Step:"Map" of Neighbors

I am block [i,j] and I need data from my neighbors.

WHO are my neighbors?

=====> "map" of neighboring processes to each process

	Block in Process #26	
	·	
Block in Process #12	Block [i,j] my_neigh_left=12 my_neigh_right=16 my_neigh_bottom=10 my_neigh_top =26 my_neigh_bot_left=8 etc.	Block in Process #16
Block in Process #8	Block in Process #10	

Fourth Step:"Map" of Neighbors - cont.

1D Example (internal block):

```
.
do i=1,nx_block
rho(i)= ( v(i) - v(i-1) ) *dt/dx
end do
```

- \bigcirc Need "v(0)" to update rho(1).
- \circ v(0) corresponds to v(nx_block) at my neighboring block.
- \bigcirc Fetch v(0) from my neighbor.
- ..but first find out which process holds my neighbor!



===> my_neigh_left=12

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Step 5: Communication Calls

Fifth Step:Communication Calls

- Examine the code/algorithm.
- Does this process need data from its neighbor(s)?
- Yes? ==> Insert communication calls where needed.

• There are two types of MPI communications routines:

○ MPI collective routines (e.g. global average).

○ MPI Point to Point routines (see the example below).

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Step 5: 1D Example

Fifth Step:Communication Calls

Example (internal block):

```
.
do i=1,nx_block
rho(i)= ( v(i) - v(i-1) ) *dt/dx
end do
```

- \bigcirc Need "v(0)" to update rho(1).
- \circ v(0) corresponds to v(nx_block) at my neighboring block.
- Fetch v(0) from my neighbor.



Pseudocode:

```
if (my_rank==12) call mpi_send( v(nx-block),...,13...
if (my_rank==13) then
   call mpi_recv( v(0),...,12,...)
   do i=1,nx_block
    rho(i)=....
```

. end do end if

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1D Example Pseudocode

Pseudocode:

The very simplified advection code of our example may proceed as follows:

- 1. Identify my neighbor's process (my_neighbor_left)
- 2. Post an mpi_receive of v(0) from my_neighbor_left:
- 3. My_neighbor_left posts a corresponding mpi_send to me of v(nx_block)
- 4. Update rho(1:nx_block)

do i=1,nx_block
rho(i)=(v(i) - v(i-1)) *dt/dx
end do

- 5. Update v(1:nx_block)
- 6. Repeat for next time step -- Return to step 2.

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Coordinate Update of all Blocks:

All blocks send v(nx_block) to the right, and receive v(0) from the left.



call mpi_sendrecv(v(nx_block),1,...my_neighbor_right,... v(0), 1,....my_neighbor_left,...)

Note:

- The choice of dimensioning v(0:nx_block) is arbitrary, a special case of: v(start_block : start_block+nx_block)
- with start_block=0

....what if my block is at a physical boundary?

Step 6:Domain Boundaries

Domain Boundaries

What if my block is at a physical boundary?

In addition to "knowing" who its neighbors are, each process needs to "know" whether any of its boundaries is in fact a physical boundary.

Why?

- 1. To avoid programming errors.
- 2. To apply boundary conditions correctly.

We will discuss the two cases:

- Periodic Boundary Conditions
- Non-Periodic Boundary Conditions

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Periodic Bdry. Cond.

Domain Boundaries:

Periodic Boundary Conditions:

The ''map'' of neighbors should reflect the periodic boundary conditions.



Under periodic boundary conditions, the blocks at the ends are treated as any other "internal" block by just defining the correct map of neighbors:

- For process 12, my_neighbor_right=0
- For process 0, my_neighbor_left=12

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Non-Periodic Bdry. Cond.

Domain Boundaries:

Non-Periodic Boundaries

On a physical boundary you should:

- 1. Avoid sending or receiving data from a non-existent block.
- 2. Apply boundary conditions.

A simple way to accomplish both tasks is by using the MPI constant handle:

MPI_PROC_NULL.

Let us illustrate with an example:

e.g. suppose process 12 corresponds to a right boundary block:

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1. Avoid sending (or receiving) data from a bdry.

2. Boundary conditions.... e.g. (Pseudocode)

```
if (my_neighbor_right == MPI_PROC_NULL) &
      [ APPLY APPROPRIATE BOUNDARY CONDITIONS ]
```

* When mpi_send is called with MPI_PROC_NULL as a ''destination'' argument, the mpi_send routine does nothing.

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Step 7: Guard Cells

Guard Cells:

- What are "Guard Cells"?
 - Guard cells are variables, arrays, or array sections that are defined with the sole purpose of storing data from a neighboring block.

How are guard cells used? They avoid repeated "fetching" of data from a

neighboring block, when that data is needed more than once before it is updated by the neighbor.

• They allow for more "tidy" coding, as in our simple 1D advection example:

In our ID advection example:

do i=1,nx_block
rho(i)=(v(i) - v(i-1)) *dt/dx
end do



v(0) is a guard cell.

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MPI_CART Routines

MPI_CART Routines

In principle, you are ready to write your code in parallel using domain decomposition. You now know the basic issues to consider when writing a parallel code using domain decomposition. Together with basic MPI communication routines (e.g. mpi_send mpi_recv, etc) you have all the tools you need to write your parallel code.

If you ask:

Do I have to design a ''map'' of neighbors for each process/block?

The answer is: *Not Necessarily*.

You can use MPI_CART routines to manage domain decomposition for you.

Minimal set of routines:

- MPI_CART_CREATE
- MPI_CART_GET
- MPI_CART_RANK

Very Useful MPI_CART routines:

MPI_CART_SHIFTMPI_CART_COORDS

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MPI_CART Routines - 2

MPI_CART Routines - 2

How does it work?

- 1. MPI_CART_CREATE creates a new communicator with Cartesian topology according to the programmer's specifications.
 - (All processes in an existing communicator make an identical call to MPI_CART_CREATE)
 - The new communicator (e.g. comm_cart) "stores" all the necessary information about the "grid" --- size, shape, map of processes to blocks, etc. -- in each process.
- 2. Each process can then access grid information about comm_cart by calling an assortment of local MPI_CART routines, e.g.
 - MPI_CART_GET

MPI_CART_RANK MPI_CART_SHIFT MPI_CART_COORDS

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MPI_CART Routines - 3

MPI_CART Routines - 3

In other words...

- I start with an existing communicator (MPI_COMM_WORLD) with n processes.
- I call MPI_CART_CREATE and:
 - It logically arranges the n processes on an ndims-dimensional Cartesian grid of dimensions: dims(1:ndims)
 - Each process knows the position of all of the processes in this Cartesian grid.
 - To access this and other Cartesian grid information, a process needs to call the "inquiring" MPI_CART routines.

MPI_CART Routines - 4

MPI_CART Routines -- 4

- 1. Information available through comm_cart on each process, includes:
 - Coordinate parameters* of each process.
 - Type of boundaries (periodic or non-periodic).
 - Topological dimension of the grid.
 - How many processes in each dimension.
 - etc.
- 2. Information can be accessed by calling:
 - MPI_CART_GET
 - MPI_CART_RANK
 - MPI_CART_SHIFT
 - MPI_CART_COORDS

*Note that the coordinate parameters are the coordinates of each process on the grid of processes. Not to be confused with the *physical* coordinates of the cells or grid points in the model or simulation.

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MPI_CART_CREATE

MPI_CART_CREATE(comm_old,ndims,dims,periods,reo

comm_cart,ierror)

comm_old =input communicator (handle)

ndims = # of dimensions of Cartesian grid (integer)

dims(ndims) = # of processes in each dimension (int. array)

periods = are boundaries periodic? (logical)

reorder = ranks may be reordered (true) or not (false)
 (logical)

comm_cart =communicator with new Cartesian
topology(handle)

■ ierror =return error code (integer)

NOTE: The only return argument -- other than ierror -- is the handle to the new Cartesian communicator (comm_cart)!

MPI_CART_CREATE: An Example

MPI_CART_CREATE: An Example

In order to obtain the Cartesian topology for domain decomposition of our example (4 blocks):



ndims=2 dims(1:ndims)=2 periods(1:ndims)=.true.

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Other MPI_CART Routines

Other MPI_CART Routines

MPI_CART_CREATE returns a handle (comm_cart). Each process can use comm_cart to inquire:

What are my coords in the grid? ==> MPI_CART_GET(comm_cart.... MPI_CART_COORDS(comm_cart....

What are the coords of any other process in the grid? MPI_CART_COORDS(comm_cart....

Who are my neighbors? ==> MPI_CART_SHIFT(comm_cart.... MPI_CART_RANK(comm_cart....

Number of dimensions of the grid (1D,2D,3D..)? ==> MPI_CARTDIM_GET(comm_cart....

What are the dimensions of the grid? ==> MPI_CART_GET(comm_cart.... etc.

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MPI_CART_COORDS

Inquiring MPI_CART Routines: MPI_CART_COORDS

Q:Which block was assigned to process with rank=*some_rank*? A:Call MPI_CART_COORDS and get the block's coordinate parameters.

MPI_CART_COORDS(comm_cart,rank,m: coords,ierror)

- comm_cart =Cartesian communicator (handle)
- rank = rank of process we are inquiring about(integer)
- maxdims = length of vector coords in the calling program

(integer)

coords(1:maxdims) = coordinate parameters of the the specified

process (integer)

■ ierror =return error code (integer)

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MPI_CART_COORDS:Illustration

MPI_CART_COORDS: Illustration

In our example of a 2D nx x ny domain decomposed into 4 blocks:



call MPI_CART_COORDS(comm_cart,....rank=0,..) ==> coords(1:2) = 0,0

call MPI_CART_COORDS(comm_cart,....rank=1,..) ==> coords(1:2) = 0,1

call MPI_CART_COORDS(comm_cart,....rank=2,..) ==> coords(1:2) = 1,0

call MPI_CART_COORDS(comm_cart,....rank=3,..) ==> coords(1:2) = 1,1

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MPI_CART_COORDS:Example 1

MPI_CART_COORDS: Example 1

Create a 2x2 2D Cartesian communicator (COMM_CART)

Print out the coordinate parameters of each process in COMM_CART.

call MPI_CART_COORDS(COMM_CART,my_rank,2,coords,: write(*,*)'The coords of process ',my_rank,' are

- The code above is an excerpt from example1.f90.
- The full program can be copied from jsimpson at: /scr/mpi-class2/example1.f90.
- It can also be downloaded by anonymous ftp to UniTree.

(In this example, each process finds and prints its own coordinate parameters. Keep in mind that any single process could have printed all the coordinate parameters -- see exercise 1)

```
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```

MPI_CART_COORDS:Exercise I

MPI_CART_COORDS: Exercise 1

 a. Copy and run example1.f90
 You can find it in jsimpson at /scr/mpi-class2, or It can also be downloaded by anonymous ftp to UniTree.

Note that each process "produces" its own coordinate parameters in the Cartesian group.

Output (if running 4 MPI processes):

```
jsimpson% mpirun -np 4 example1
The coords of process 1 are: 0, 1
```

The coords of process 0 are: 2*0 The coords of process 3 are: 2*1 The coords of process 2 are: 1, 0

Note that processes might be assigned different coordinate parameters on different computers.

 b. Modify example1.f90 so that process 0 "finds" and prints the Cartesian parameters of each of the processes in the Cartesian grid. (Find a solution in exercise1.f90 at /scr/mpi-class2, or download it by anonymous ftp to UniTree.

```
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```

Data Decomposition

Defining and Assigning Data to Arrays after Domain Decomposition

■ Suppose you have a 2D domain of 4x4 cells.

You want to initialize the array A(4,4) as some function of the physical coordinates:

```
x(4,4)
y(4,4)
```

```
e.g. A(i,j)=x(i,j)**2 + y(i,j)**2
```

After domain decomposition (e.g. into 4 blocks), you will need to define local arrays on each block:

x(2,2) y(2,2) A(2,2)

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Data Decomposition: Example 2

Defining and Assigning Data to Arrays after Domain Decomposition: Example 2

Given a 4x4 regular domain of cells, we will do domain decomposition into 4 processes.

Before decomposition:



The coordinate arrays are: x(1:4,j)= (0.1, 0.3, 0.5, 0.7) y(i,1:4)= (0.1, 0.3, 0.5, 0.7)

■ The cell size is dx=dy=0.2

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Example2 - 1.cont.

Defining and Assigning Data to Arrays after Domain Decomposition: Example 2-cont.

We choose to decompose the 4x4 domain into 4 blocks as shown in the figure below:



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Example2 - 2.cont.

Defining and Assigning Data to Arrays after Domain Decomposition: Example 2 cont.

After decomposition:



■ The coordinate arrays become x(1:2,1:2), y(1:2,1:2)

x(1:2,1:2), y(1:2,1:2) are different on each block:
 Block [0,0]:

■ Block [A 1].	x(1:2,j)=(0.1, 0.3) y(i,1:2)=(0.1, 0.3)				
– DIOCK [0,1].	x(1:2,j)=(0.1, 0.3) y(i,1:2)=(0.5, 0.7)				
■ etc.					

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- 1. Using example1.f90 as a template, have each process compute its own physical coordinate* arrays [x(1:2,1:2), y(1:2,1:2)].
- 2. Have each process print its process #, its Cartesian coordinate parameters, and its x and y arrays.
- **3.** Verify your results. Do they correspond to the previous figure?

HINT: Define the physical coordinates of the left-bottom corner of each process first.

```
! --The physical coordinates of the left-bottom cornel
x_corner= float( nx/dims(1) * coords(1) ) * d:
y_corner= float( ny/dims(2) * coords(2) ) * d;
```

- nx=number of cells along x on the whole domain
- ny=number of cells along y on the whole domain
- dims(1)=number of blocks along x
- dims(2)=number of blocks along y
- coords(1:2)=coord. parameters of this block.

SUGGESTION: Use the following output statements:

```
write(*,"('my rank.=',i2,', my coords=[',2i2,']
& x= ',4f4.1)"
& my_rank, coords, x
write(*,"('my rank.=',i2,', my coords=[',2i2,']
& y= ',4f4.1)"
& my_rank, coords, y
```

*Do not confuse the physical coordinate arrays (x,y), with the coordinate parameters of each block. The coordinate parameters are a pair of integers that "locate" the block within the Cartesian grid of blocks. The physical coordinate arrays (x,y) are the coordinates of the cells or points where physical data is defined.

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Output from Exercise 2

Output from Exercise 2.

mpirun -np 4 exercise2 my rank.= 0, my coords=[0 0] 0.1 0.3 0.1 0.3 $\mathbf{x}=$ my rank.= 0, my coords=[0 0] 0.1 0.1 0.3 0.3 y= , my rank.= 2, my coords=[1 0] x= 0.5 0.7 0.5 0.7 my rank.= 2, my coords=[1 0.1 0.1 0.3 0.3 0] v= my rank.= 1, my coords=[0 11 0.1 0.3 0.1 0.3 x= my rank.= 1, my coords=[0 1] 0.5 0.5 0.7 0.7 y= my rank.= 3, my coords=[1 1] 0.5 0.7 0.5 0.7 $\mathbf{x} =$ my rank.= 3, my coords=[1 1] , y= 0.5 0.5 0.7 0.7



Solution to Exercise 2

Excerpt from exercise2.f90

Note that this "solution" is not unique!

```
call MPI CART COORDS(COMM_CART, my_rank, 2, coords, &
                         & ierror)
!--The physical coordinates of my left-bottom corner:
      dx=0.2
      dy=0.2
      x_corner= float( nx/dims(1) * coords(1)
                                                 ) * d:
      y_corner= float( ny/dims(2) * coords(2) ) * dy
!--Use my corner coordinates to compute the cell
 coordinates in my block
!
      do i=1,2
       x(i,:)=x corner+(float(i)-0.5)*dx
      end do
      do j=1,2
       y(:,j)=y_corner+(float(j)-0.5)*dy
      end do
```

(See the full program at /scr/mpi-class2/exercise2.f90 in jsimpson, or use anonymous ftp to UniTree to retrieve exercise2.f90)

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More Decomposition Exercises

Exercises 2a-d

Below is a list of the next four exercises you will be working through. In all of them, cell sizes are dx=dy(=dz)=0.2. To begin (and get some hints), please go to the next page .

- 2a. Modify exercise2.f90 so it decomposes an 8x8 grid into 4 blocks (*along x and y*).
- 2b. Modify exercise2.f90 so it decomposes an 8x8 grid into 16 blocks (*along x and y*).
- 2c. Modify exercise2.f90 to do 3D decomposition of a 4x4x4 grid into 8 blocks (*along x, y, and z*).
- 2d. Modify exercise2.f90 to do 2D decomposition of a 4x4x4 grid into 4 blocks (*along x and y*).

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Exercise 2a

Exercise2a.f90

2a. Modify exercise2.f90 so it decomposes an 8x8 grid into 4 blocks (along x and y).



HINT: The grid of blocks is identical as that on exercise 2 (2x2). Only the data on each block will change.

- Array dimension and values of x and y.
- Values of nx and ny
- do loop parameters
- (output format...)

You can check your output against the next page --- note that the line order of output coming from different processes is bound to be different.

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Output from Exercise 2a

Output from exercise2a.f90

```
mpirun -np 4 exercise2a
my rank.= 3, my coords=[ 1 1] , x= 0.9 1.1 1.3 1.5 0
 1.5 0.9 1.1 1.3 1.5 0.9 1.1 1.3 1.5
my rank.= 2, my coords=[ 1 0] , x= 0.9 1.1 1.3 1.5 0
 1.5 0.9 1.1 1.3 1.5 0.9 1.1 1.3 1.5
my rank.= 3, my coords=[ 1 1] , y= 0.9 0.9 0.9 0.9 1
 1.1 1.3 1.3 1.3 1.3 1.5 1.5 1.5 1.5
my rank.= 1, my coords=[ 0 1] , x= 0.1 0.3 0.5 0.7 0
 0.7 0.1 0.3 0.5 0.7 0.1 0.3 0.5 0.7
                                    0.1 0.3 0.5 0.7 0
my rank.= 0, my coords=[0 0], x=
 0.7 0.1 0.3 0.5 0.7 0.1 0.3 0.5 0.7
my rank.= 2, my coords=[ 1 0] , y= 0.1 0.1 0.1 0.1 0
 0.3 0.5 0.5 0.5 0.5 0.7 0.7 0.7 0.7
my rank.= 1, my coords=[ 0 1] , y=
                                    0.9 0.9 0.9 0.9 1
 1.1 1.3 1.3 1.3 1.3 1.5 1.5 1.5 1.5
my rank.= 0, my coords=[ 0 0] , y= 0.1 0.1 0.1 0.1 0
 0.3 0.5 0.5 0.5 0.5 0.7 0.7 0.7 0.7
 STOP (PE 1)
               executed at line 89 in Fortran routine
              executed at line 89 in Fortran routine
 STOP (PE 0)
              executed at line 89 in Fortran routine
 STOP (PE 2)
 STOP (PE 3) executed at line 89 in Fortran routine
jsimpson%
```

Solution to Exercise 2a

Solution of exercise2a.f90

A solution code is available at jsimpson in: /scr/mpi-class2/exercise2a.f90, or by fetching exercise2a.f90 through anonymous ftp to UniTree

Only modifications pertaining to the data in each block are necessary:

```
jsimpson% diff exercise2.f90 exercise2a.f90
22c22
< real x(2,2),y(2,2),dx,dy
---</pre>
```

real x(4,4), y(4,4), dx, dy> 36,37c36,37 < nx=4< ny=4 _ _ _ nx=8> ny=8 > 67c67 do i=1,2 < _ _ _ do i=1,4 > 71c71 do j=1,2 < _ _ _ do j=1,4 > 78c78 & x= ',4f4.1)") & < _ _ _ & x= ',16f4.1)") & > 82c82 & y= ',4f4.1)") & < & y= ',16f4.1)") & > jsimpson%

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Exercise 2b

Exercise2b

2b. Modify exercise2.f90 so it decomposes an 8x8 grid into 16 blocks (along x and y).



HINT: The grid of blocks is larger than that on exercise 2 (4x4). The size of the x and y arrays in each block are the same as in exercise2. The variables and arrays that change are:

- Values of x and y. -- although you won't need to make modifications
- Values of nx and ny
- Values of array dims

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Output from exercise2b.f90

Output from exercise2b.f90

jsimpson% mpirun -np 16 exercise2b

my	<pre>rank.=12,</pre>	my	coords=[3	0]	,	\mathbf{x} =	1.3	1.5	1.3	1.5
my	<pre>rank.=12,</pre>	my	coords=[3	0]	,	y =	0.1	0.1	0.3	0.3
my	<pre>rank.= 5,</pre>	my	coords=[1	1]	,	\mathbf{x} =	0.5	0.7	0.5	0.7
my	<pre>rank.= 5,</pre>	my	coords=[1	1]	,	y =	0.5	0.5	0.7	0.7
my	rank.= 8,	my	coords=[2	0]	,	\mathbf{x} =	0.9	1.1	0.9	1.1
my	rank.= 8,	my	coords=[2	0]	,	y =	0.1	0.1	0.3	0.3
my	<pre>rank.= 6,</pre>	my	coords=[1	2]	,	\mathbf{x} =	0.5	0.7	0.5	0.7
my	<pre>rank.= 6,</pre>	my	coords=[1	2]	,	y =	0.9	0.9	1.1	1.1
my	rank.= 3,	my	coords=[0	3]	,	\mathbf{x} =	0.1	0.3	0.1	0.3
my	rank.= 3,	my	coords=[0	3]	,	y =	1.3	1.3	1.5	1.5
my	rank.=15,	my	coords=[3	3]	,	\mathbf{x} =	1.3	1.5	1.3	1.5
my	rank.=15,	my	coords=[3	3]	,	y =	1.3	1.3	1.5	1.5
my	<pre>rank.=13,</pre>	my	coords=[3	1]	,	\mathbf{x} =	1.3	1.5	1.3	1.5
my	<pre>rank.=13,</pre>	my	coords=[3	1]	,	y =	0.5	0.5	0.7	0.7
my	<pre>rank.=10,</pre>	my	coords=[2	2]	,	\mathbf{x} =	0.9	1.1	0.9	1.1
my	<pre>rank.=10,</pre>	my	coords=[2	2]	,	y =	0.9	0.9	1.1	1.1
my	rank.=0,	my	coords=[0	0]	,	\mathbf{x} =	0.1	0.3	0.1	0.3
my	rank.=0,	my	coords=[0	0]	,	y =	0.1	0.1	0.3	0.3
my	<pre>rank.=14,</pre>	my	coords=[3	2]	,	\mathbf{x} =	1.3	1.5	1.3	1.5
my	<pre>rank.=14,</pre>	my	coords=[3	2]	,	y =	0.9	0.9	1.1	1.1
my	<pre>rank.=11,</pre>	my	coords=[2	3]	,	\mathbf{x} =	0.9	1.1	0.9	1.1
my	<pre>rank.= 2,</pre>	my	coords=[0	2]	,	\mathbf{x} =	0.1	0.3	0.1	0.3
my	<pre>rank.=11,</pre>	my	coords=[2	3]	,	y =	1.3	1.3	1.5	1.5
my	<pre>rank.= 2,</pre>	my	coords=[0	2]	,	y =	0.9	0.9	1.1	1.1
my	<pre>rank.= 4,</pre>	my	coords=[1	0]	,	\mathbf{x} =	0.5	0.7	0.5	0.7
my	<pre>rank.= 4,</pre>	my	coords=[1	0]	,	y =	0.1	0.1	0.3	0.3
my	<pre>rank.= 1,</pre>	my	coords=[0	1]	,	\mathbf{x} =	0.1	0.3	0.1	0.3
my	rank.=7,	my	coords=[1	3]	,	x=	0.5	0.7	0.5	0.7
my	<pre>rank.= 9,</pre>	my	coords=[2	1]	,	x=	0.9	1.1	0.9	1.1
my	<pre>rank.= 1,</pre>	my	coords=[0	1]	,	y=	0.5	0.5	0.7	0.7
my	<pre>rank.= 7,</pre>	my	coords=[1	3]	,	y=	1.3	1.3	1.5	1.5
my	<pre>rank.= 9,</pre>	my	coords=[2	1]	,	y=	0.5	0.5	0.7	0.7
•											

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Solution to Exercise 2b

Solution of exercise2b

A solution code is available at jsimpson in: /scr/mpi-class2/exercise2b.f90 or by fetching exercise2b.f90 through anonymous ftp to UniTree

Only parameters nx,ny, and dims need to be modified:

```
jsimpson% diff exercise2.f90 exercise2b.f90
        integer, parameter :: dims_x=2, dims_y=2
<
                                                     !sai
_ _ _
        integer, parameter :: dims_x=4, dims_y=4
                                                     !sai
>
36,37c36,37
          nx=4
<
<
          ny=4
_ _ _
          nx=8
>
>
          ny=8
39a40
         dims(1:ndims)=(dims x,dims y)
                                            ! 2x2 grid (
>
     I
52a54
>
jsimpson%
```

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Exercise 2c

Exercise 2c

2c. Modify exercise2.f90 to do 3D decomposition of a 4x4x4 grid into 8 blocks (along x, y, and z).

HINTS:

Modify the calling parameters for MPI_CART_CREATE to correspond to a 3D decomposition.

■ Make the x and y arrays 3 dimensionsal.

■ Define a third array: z=third coordinate.

- Compute z following the steps for x and y.
- You will have a 2x2x2 topology of blocks
- Each block (process) will hold 2x2x2 arrays.



Output from Exercise 2c

Output from exercise2c.f90

A solution to exercise2c can be found at /scr/mpi-class2/exercise2c.f90 It can also be downloaded through anonymous ftp to UniTree

jsimpson% mpirun -np 8 exercise2c my rank.= 5, my coords=[1 0 1] , x= 0.5 0.7 0.5 0.7 0.5 0.7 my rank.= 5, my coords=[1 0 1] , y= 0.1 0.1 0.3 0.3 0.3 0.3 my rank.= 5, my coords=[1 0 1] , z= 0.5 0.5 0.5 0.5 0.7 0.7 my rank.= 0, my coords=[0 0 0] , x= 0.1 0.3 0.1 0.3

0.1 0.3 my rank.= 0, my coords=[0 0 0] , y= 0.1 0.1 0.3 0.3 0.3 0.3 my rank.= 0, my coords=[0 0 0] , z= 0.1 0.1 0.1 0.1 0.3 0.3 my rank.= 2, my coords=[0 1 0] , x= 0.1 0.3 0.1 0.3 0.1 0.3 0.5 0.7 0.5 0.7 my rank.= 6, my coords=[110], x= 0.5 0.7 my rank.= 2, my coords=[0 1 0] , y= 0.5 0.5 0.7 0.7 0.7 0.7 my rank.= 6, my coords=[1 1 0] , y= 0.5 0.5 0.7 0.7 0.7 0.7 my rank.= 2, my coords= $[0\ 1\ 0]$, z= 0.1 0.1 0.1 0.1 0.3 0.3 my rank.= 3, my coords=[0 1 1] , x= 0.1 0.3 0.1 0.3 0.1 0.3 my rank.= 7, my coords=[111], x= 0.5 0.7 0.5 0.7 0.5 0.7 my rank.= 6, my coords=[110], z= 0.1 0.1 0.1 0.1 0.3 0.3 my rank.= 1, my coords=[0 0 1] , x= 0.1 0.3 0.1 0.3 0.1 0.3 my rank.= 3, my coords=[011], y= 0.5 0.5 0.7 0.7 0.7 0.7 my rank.= 4, my coords=[1 0 0], x= 0.5 0.7 0.5 0.7 0.5 0.7 my rank.= 7, my coords=[111], y= 0.5 0.5 0.7 0.7 0.7 0.7 my rank.= 1, my coords=[0 0 1] , y= 0.1 0.1 0.3 0.3 0.3 0.3 my rank.= 3, my coords=[011], z= 0.5 0.5 0.5 0.5 0.7 0.7 my rank.= 4, my coords=[1 0 0], y= 0.1 0.1 0.3 0.3 0.3 0.3 my rank.= 7, my coords=[1 1 1] , z= 0.5 0.5 0.5 0.5 0.7 0.7 my rank.= 1, my coords=[0 0 1], z= 0.5 0.5 0.5 0.5 0.7 0.7 my rank.= 4, my coords=[1 0 0] , z= 0.1 0.1 0.1 0.1 0.3 0.3

Exercise 2d

Exercise 2d

2d. Modify exercise2.f90 to do 2D decomposition of a 4x4x4 grid into 4 blocks (along x and y).

HINTS:

- The calling parameters for MPI_CART_CREATE should be the same.
- Make the x and y arrays 3-dimensional -- each (2x2x4).
- Define a third array: z=third coordinate.
- Compute z following the steps for x and y.
- You will have a 2x2 topology of blocks
- Each block (process) will hold 2x2x4 arrays.



Output from exercise2d.f90

A solution to exercise2d can be found at /scr/mpi-class2/exercise2d.f90 It can also be downloaded through anonymous ftp to UniTree.

jsimpson% !!						
mpirun -np 4	exercise2d					
my rank.= 2, 0.7×10^{-10}	my coords=[1 0], x= 0.5	0.7	0.5	0.7	0
my rank.= 2,	my coords=[1 0], y= 0.1	0.1	0.3	0.3	0
0.3 0.1 0.1	0.3 0.3 0.1	0.1 0.3 0.3				
my rank.= 2,	my coords=[1 0], z= 0.1	0.1	0.1	0.1	0
0.3 0.5 0.5	0.5 0.5 0.7	0.7 0.7 0.7				
my rank.= 3,	my coords=[1 1], x= 0.5	0.7	0.5	0.7	0
0.7 0.5 0.7	0.5 0.7 0.5	0.7 0.5 0.7				
my rank.= 1,	my coords=[0 1], x = 0.1	0.3	0.1	0.3	0
0.3 0.1 0.3	0.1 0.3 0.1	0.3 0.1 0.3				
my rank.= 3,	my coords=[1 11, $y = 0.5$	0.5	0.7	0.7	0
0.7 0.5 0.5	0.7 0.7 0.5	0.5 0.7 0.7				-
mv rank = 0.	my coords=[$0 \ 01 \ x = 0.1$	0.3	0.1	0.3	0
0.3 0.1 0.3	$0.1 \ 0.3 \ 0.1$	0.30.10.3		••-		Ĩ
mv rank = 1	my coords=[$0.11 \cdot v = 0.5$	0.5	0.7	0.7	0
0.7 0.5 0.5	0.70.70.5	0.50.70.7	0.5	•••	•••	Ŭ
mv rank = 3		1 11 = 0 1	0 1	0 1	0 1	Λ
	$m_y = coords = [$	$ \begin{array}{c} 1 \\ 2 \\ 0 \\ 7 \\ 0 \\ 0 \\ 7 \\ 0 \\ 7 \\ 0 \\ 7 \\ 0 \\ 7 \\ 0 \\ 7 \\ $	0.1	0.1	0.1	U
0.5 0.5 0.5		0.70.70.7	0 1	0 2	0 2	Δ
$\begin{array}{c} \text{my rank 0,} \\ 0 & 2 & 0 & 1 & 0 \\ \end{array}$		0 0], y = 0.1	0.1	0.5	0.5	U
0.5 0.1 0.1		0.1 0.3 0.3	0 1	0 1	0 1	^
my rank = 1,			0.1	0.1	0.1	U
0.3 0.5 0.5	0.5 0.5 0.7	0.70.70.7	0 1	0 1	0 1	~
my rank.= 0 ,	my cooras=[0 0], z = 0.1	0.1	0.1	0.1	0
0.3 0.5 0.5	0.5 0.5 0.7	0.7 0.7 0.7				
STOP (PE 3)	executed a	at line 100 in H	ortr	ran r	routi	.ne
STOP (PE 0)	executed a	at line 100 in H	fortr	ran r	routi	ne
STOP (PE 1)	executed a	at line 100 in H	fortr	an r	outi	ne
STOP (PE 2)	executed a	at line 100 in H	fortr	an r	outi	ne

Communication

Communication within the Cartesian ''Grid''

Regroup:

- You know how to decompose your data into a Cartesian grid of blocks.
- If you have an embarrassingly parallel program -where processes contain all the data they need in local memory -- you are done.
- Otherwise, you will need to do inter-block communication.

Most programs require inter-block communications.

When a process needs to send or receive data from a neighboring process, the first thing needed is to find that neighbor's rank...

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Finding a Neighbor's Rank

Finding a Neighbor's Rank

■ I am a process of rank=my_rank

■ I need to send/receive data to/from a neighbor.

• One way to do it:

- Figure out my coordinates using:
 MPI_CART_GET, or
 MPI_CART_COORDS
- 2. Figure out the coordinates of the neighbor process e.g. If my coords are [i,j], my RHS neighbor is [i+1,j]
- 3. Use those coordinates to obtain the rank (e.g. n_rank) of the neighbor.
 - MPI_CART_RANK

(described on the next page)

4. Send/receive the data to/from process with rank n_rank.

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MPI_CART_RANK

Inquiring MPI_CART Routines:

MPI_CART_RANK

Q:What is the rank of the process with coordinates parameters=coords? A:Call MPI_CART_RANK and get the process's rank.

MPI_CART_RANK(comm_cart,coords,ran

comm_cart = Cartesian communicator (handle)

coords = coords of process we are inquiring about(integer array)

rank = rank of the process with the specified coords (integer)

■ ierror =return error code (integer)

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MPI_CART_RANK:Example 2

MPI_CART_RANK: Example 2

On a 2D Cartesian Grid of 4 Processes, each process finds the rank of its RHS neighbor (along x).

Excerpts from example2.f90 located at jsimpson in: /scr/mpi-class2/example2.f90

```
! --Given my rank (my_rank), find what my coords are.
call MPI_CART_COORDS(COMM_CART,my_rank,ndims, {
    &coords,ierror)
.
```

```
!--Who is my RHS neighbor?
! Well... Since my coords. are [coords(1),coords(2)]
! my RHS neighbor's coords are:
```

```
r_coords(1)=coords(1)+1
r_coords(2)=coords(2)
```

```
!--Get its rank (r_rank):
    call MPI_CART_RANK(COMM_CART,r_coords, &
    & r_rank,ierror)
```

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Output from Example 2

Output from Example 2

```
jsimpson% mpirun -np 4 example2
my_rank= 2 my coordinates, coords, are 1, 0
my_rank= 2 my RHS neighbor is: 0
my_rank= 1 my coordinates, coords, are 0, 1
my_rank= 1 my RHS neighbor is: 3
my_rank= 3 my coordinates, coords, are 2*1
```

```
my rank= 0
            my coordinates, coords, are
                                         2*0
my rank= 3 my RHS neighbor is:
                                  1
my_rank= 0 my RHS neighbor is:
                                  2
              executed at line 80 in Fortran routine
STOP (PE 0)
              executed at line 80 in Fortran routine
STOP (PE 3)
STOP (PE 2)
              executed at line 80 in Fortran routine
STOP (PE 1)
              executed at line 80 in Fortran routine
jsimpson%
```

```
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```

MPI_CART_RANK:Exercises 3

MPI_CART_RANK: Exercise 3

Copy and modify example2.f90 to:

■ **3a.Find the nearest neighbor along** y+ **of each process.**

Verify your answers. Do they make sense? Note the value of periods in the code.

- 3b.Change the value of periods(2) to .false. and rerun exercise 3a. (The code will break -- do you know why?)
- 3c.Find the nearest neighbor diagonally along the (x+,y+) direction (use periods=.true.).
 Verify your answers.

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Soln. and output:exercise 3a

Solution of exercise 3a

Modify the r_coords array:

- **r_coords**(1)=coords(1)
- **r_coords**(2)=coords(2)+1

Output from Exercise 3a

jsimpson ⁹	k mp	irun -	np 4 d	exer	cise	3a				
my_rank	= 0	my co	ordina	ates	, coo	ords	5, a	are	2*0	
my_rank:	= 0	my TO	P neig	ghbo	or is:	: 1	_			
my_rank:	= 1	my co	ordina	ates	, coc	ords	3, a	are	Ο,	1
my_rank:	= 1	my TO	P neig	ghbo	or is:	: 0)			
my_rank:	= 3	my co	ordina	ates	, coc	ords	3, a	are	2*1	
my_rank	= 3	my TO	P neig	ghbo	or is:	: 2	2			
my_rank:	= 2	my co	ordina	ates	, coc	ords	3, a	are	1,	0
my_rank:	= 2	my TO	P neig	ghbo	or is:	: 3	3			
STOP (P	E 2)	exe	cuted	at	line	80	in	For	tran	routine
STOP (P	E 3)	exe	cuted	at	line	80	in	For	tran	routine
STOP (P	E O)	exe	cuted	at	line	80	in	For	tran	routine
STOP (P	31)	exe	cuted	at	line	80	in	For	tran	routine
jsimpson ^g	6									

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Soln. and output: exercise 3c

Solution to Exercise 3c

Modify the r_coords array:

- **r_coords**(1)=coords(1)+1
- **r_coords**(2)=coords(2)+1

Output from Exercise 3c

```
jsimpson% f90 -o exercise3c exercise3c.f90
jsimpson% mpirun -np 4 exercise3c
my_rank= 2 my coordinates, coords, are
                                          1,
                                              0
my_rank= 2
            my TOP-RIGHT neighbor is:
                                         1
my rank= 0 my coordinates, coords, are
                                          2*0
my rank= 0
            my TOP-RIGHT neighbor is:
                                         3
my rank= 1
            my coordinates, coords, are
                                          0,
                                              1
my rank= 3
            my coordinates, coords, are
                                          2*1
my rank= 1
            my TOP-RIGHT neighbor is:
                                        2
            my TOP-RIGHT neighbor is:
my rank= 3
                                        0
               executed at line 80 in Fortran routine
 STOP (PE 1)
 STOP (PE 2)
               executed at line 80 in Fortran routine
               executed at line 80 in Fortran routine
 STOP (PE 0)
               executed at line 80 in Fortran routine
 STOP (PE 3)
jsimpson%
```

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Send-Receive along a Coordinate

Send-Receive along a Coordinate Direction

On a 1D domain decomposition*, all processes (blocks) will be sending v(nx_block) to their neighbor to the right [x+], and receiving v(0) from their neighbor to the left [x-].



Each process needs the dest (*my_neighbor_right*) and source (*my_neighbor_left*) arguments for mpi_sendrecv. How can it get them?

- Option 1: Use MPI_COORDS and MPI_RANK as explained before.
 - (somewhat cumbersome), or

• Option 2: Use MPI_SHIFT:

get source and dest arguments along a coordinate direction with a single subroutine call!

*In a 2D decomposition, a similar sendrecv exchange would take place along the y coordinate as well [e.g. v(:,ny_block) --> v(:,0)].

Inquiring MPI_CART Routines: MPI_CART_SHIFT

Send-Receive Communication along a Cartesian Coordinate Use the MPI_SHIFT routine to obtain the source (e.g. my_neighbor_left), and the dest (e.g. my_neighbor_right) argument for the MPI_SENDRECV call.

MPI_CART_SHIFT(comm_cart,direction,d rank_source,rank_dest,ierror)

- comm_cart =Cartesian communicator (handle)
- direction = coordinate dimension of shift (integer)
 - $\blacksquare direction=0 \dashrightarrow shift along "x"$
 - direction=1 --> shift along ''y''
 - etc.
- disp = displacement (>0: Up shift, <0: Down shift)
 (Integer)</pre>
 - disp=1 --> dest=nearest neighbor to the ''right'' (source=nearest neighbor to the ''left'')
 - disp=-1 --> dest=nearest neighbor to the ''left'' (source=nearest neighbor at ''right'')
 - disp=2 --> dest=second nearest neighbor to the "right"

etc.

rank_source = rank of source process (integer)

rank_dest = rank of destination process (integer)

■ ierror =return error code (integer)

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MPI_CART_SHIFT:Example 4

MPI_CART_SHIFT: Example 4

On a 1D Cartesian grid of 4 blocks. Each block stores 2 cells, and 1 guard cell.

Update guard cell data (v0) for array vel(0:2)

Excerpt from example4.f90:

parameter (ndims=1)	
dims(1:ndims)=4	
Find the coordinates of call MPI_CART_COORDS(co &nc	f this block omm_cart,my_rank, dims,coords,ierror)
!Assign some values to v do i=0,2 vel(i)=float(i+100* end do	vel(0:2) *coords(1))
<pre>!Find rank of neighbors direction=0 disp=1</pre>	along x !(along x) !immediate neighbors

Output from Example 4

Output from Example 4

Copy example4 from /scr/mpi_class2/example4.f90 in jsimpson and run it on 4 processes.

You can also get example4.f90 through anonymous ftp to UniTree.

The output should look like this:

```
jsimpson% f90 -o example4 example4.f90
jsimpson% mpirun -np 4 example4
         3
               4
                   is alive
Process
            of
         2 of 4
                   is alive
Process
         0 of
                4
                   is alive
Process
Process 1 of
              4
                   is alive
my rank= 0 source= 3 dest= 1
my_rank= 2 source= 1 dest= 3
my rank= 3 source= 2 dest= 0
my_rank= 1
                      dest = 2
            source= 0
```

```
MPI PROC NULL= -1
                      v0= 202.
my coords are:
                 3
my coords are:
                 2
                      v0=
                           102.
                           302.
my coords are:
                 0
                      v0=
my coords are:
                 1
                      v0=
                           2.
             executed at line 84 in Fortran routine
 STOP (PE 1)
 STOP (PE 0)
               executed at line 84 in Fortran routine
               executed at line 84 in Fortran routine
 STOP (PE 2)
             executed at line 84 in Fortran routine
 STOP (PE 3)
jsimpson%
```

Exercise 4

Exercise 4

Modify example4.f90 to update RHS guard cells.

Hints:

- Get "v3" from RHS neighbor.
- Modify "disp" in MPI_CART_SHIFT

Output from Exercise4:

```
jsimpson% f90 -o exercise4 exercise4.f90
jsimpson% mpirun -np 4 exercise4
                   is alive
Process
         3
            of
                4
            of
                4
                   is alive
Process
         0
         2 of
                4
                   is alive
Process
Process 1 of
                4
                   is alive
my rank= 3 source= 0
                       dest= 2
my rank= 0 source= 1
                       dest = 3
```

```
my rank= 2
            source= 3
                       dest = 1
my rank= 1
            source= 2 dest= 0
my coords are:
                3
                     v3=
                          1.
                          301.
my coords are:
                2
                     v3=
                     v3=
my coords are:
                          101.
                0
my coords are:
                          201.
                1
                     v3=
STOP (PE 1) executed at line 81 in Fortran routine
STOP (PE 2) executed at line 81 in Fortran routine
STOP (PE 3) executed at line 81 in Fortran routine
STOP (PE 0)
              executed at line 81 in Fortran routine
jsimpson%
```

Solution to Exercise 4

Solution to Exercise 4

Excerpt from exercise4.f90*:

```
disp=-1 !MODIFIED!
call MPI_CART_SHIFT(comm_cart,direction,disp,son
& dest,ierror)
.
.
!--Send vel(1) to the block to my left and receive v:
! my right -->Modified
sendtag=1
recvtag=1
call MPI_SENDRECV(vel(1),1,MPI_REAL,dest,sendtag, &
v3,1,MPI_REAL,source,recvtag, &
comm_cart,status,ierror)
!--Print out the updated v3
write(*,*)'my coords are: ',coords,' v3=',v3
```

*The full code of exercise4.f90 can be found in jsimpson at /scr/mpi-class2/exercise4.f90, or through anonymous ftp to UniTree

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Exercise 4a

Exercise 4a

Make the following change in example4.f90:

periods=.false.

And run the program.

- Compare the output you get for v0 to the periodic case of example4.
- Note how MPI_PROC_NULL is output by MPI_CART_SHIFT
- Note the effect of having

```
source=MPI_PROC_NULL
```

and

```
dest=MPI_PROC_NULL
```

on the physical boundary blocks.

Output from Exercise 4a

Output from Exercise 4a

Output....

```
dest=MPI PROC NULL at proc
                           3
                    v0=
                         3.
my coords are:
               2
source=MPI_PROC_NULL at proc
                             0
my coords are: 3
                    v0=
                         4.
my coords are:
               0
                    v0=
                         0.E+0
my coords are: 1
                    v0=
                         2.
```

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"Echo" MPI_CART Routines

"Echo" MPI_CART Routines

"Echo" routines inquire about the definition parameters of a Cartesian communicator, such as:

- ndims: Is the topology 1D,2D, ...?,
- periods(ndims): periodic?
- dims(ndims): Dimensions along each coordinate direction

There are two "echo" routines: MPI_CARTDIM_GET and MPI_CART_GET.

1.What is the Number of Dimensions in the Cartesian communicator comm_cart?

MPI_CARTDIM_GET(comm_cart, ndims,ierror)

comm_cart =communicator with Cartesian
topology(handle)

■ ndims = # of dimensions of Cartesian grid (integer)

■ ierror =return error code (integer)

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MPI_CART_GET

MPI_CART_GET

2.Number of processes and periodicity along each Cartesian direction. Also, coordinate parameters of the calling process.

MPI_CART_GET(comm_cart,maxdims, dims,

periods, coords, ierror)

- comm_cart =communicator with Cartesian
 topology(handle)
- maxdims = length of vectors dims, periods, coords (integer)
- dims = # of processes in each dimension (int. array)
- periods = are boundaries periodic? (logical array)
- coords =coords of calling process (int. array)
- ierror =return error code (integer)

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CONCLUSIONS

CONCLUSIONS

We covered the essentials of Domain Decomposition Using MPI_CART routines:

What is Domain Decomposition?

- **Basics of a Domain Decomposition Code.**
- Using MPI_CART Routines for Managing Domain Decomposition.
- **Explained the various MPI_CART routines available.**
- Examples and Exercises of Domain Decomposition into 1D, 2D, 3D Cartesian Topologies of "blocks".
- 2D Decomposition of a 3D Domain.

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REFERENCES

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- Argonne Natl. Lab MPI web-site
- Compendium of MPI tutorials' web-sites at NCCS User Pages