MPI Lab

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Introduction to Parallel Computing
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MPI Lab

- Parallelization (Calculating π in parallel)
  - How to split a problem across multiple processors
  - Broadcasting input to other nodes
  - Using MPI_Reduce to accumulate partial sums
- Sharing Data Across Processors (Updating ghost cells)
  - How Ghosts Cells are used in Finite Difference problems
  - How to use SendRecv for deadlock-free transfers involving simultaneous Sends and Receives on a node.

Getting Started

- Login to tg-login.ranger.tacc.teragrid.org
- Untar the lab source code

```
login3% cd $HOME
login3% tar xf ~train00/mpi_lab.tar
```

- Part 1: Calculating PI

```
cd $HOME/mpi_lab/pi
```

- Part 2: Ghost Cell Update

```
cd $HOME/mpi_lab/ghosts
```

Part 1: Calculating π – Basic Course of Action

- Objective: parallelize serial π calculation, starting with serial code (serial_pi.c or serial_pi.f90).

```
for (i = 1; i <= n; i++) {
  x   = h * ( (double)(i) - 0.5e0 );
  sum = sum + f(x); }
```

```
do i = 1, n
  x = h * (dble(i) - 0.5_KR8)
  sum = sum + f(x)
end do
```

- Each processor will perform partial sum: for $x_i, x_{i+N}, x_{i+2N}, x_{i+3N}$,… where N is the processor count, and i is the rank.

```
for(i = myid+1; i <= n; i = i + numprocs) {
  x = h * ( (double)(i) - 0.5e0 );
  sum = sum + f(x); }
```

```
do i = myid+1, n, numprocs
  x = h * (dble(i) - 0.5_KR8)
  sum = sum + f(x)
end do
```

- Accumulate and add partial sums on processor 0.

```
ierr = MPI_Reduce(&part_pi,&pi,1,MPI_DOUBLE,          MPI_SUM,0,MPI_COMM_WORLD     )
call   MPI_Reduce(mypi,     pi,1,MPI_DOUBLE_PRECISION,MPI_SUM,0,MPI_COMM_WORLD,ierr)
```

Calculating π – MPI_Init and Finalize

- Modify the serial_pi.f or serial_pi.c file.
  - `cp serial_pi.f90 pi.f90` or `cp serial_pi.c pi.c`
  - Include MPI startup and finalization routines at the beginning and end of pi.c/f90. Also include declaration statements for the rank and number of processors (myid and numprocs, respectively)

```
C: #include "mpi.h“  or  F90:  include “mpif.h”
 …MPI_Init(…)
 …MPI_Comm_rank(MPI_COMM_WORLD...)
 …MPI_Comm_size(MPI_COMM_WORLD…)
…

 …MPI_Finalize(…)
```

Top of Code

Serial Code

End of Code

Don't forget: (declare myid, numprocs and ierr as ints in C and integers in fortran
Use “call” and an error argument in FORTRAN; and use error return in C code.
use myid and numprocs for the rank and processor count)

Calculating π – Read & Form Partial Sums

- Have rank 0 processor read n, the total # elements to integrate
  - Make the read statement conditional, only on root, with:
    if (myid == 0) read…
  - Broadcast n to the other nodes
    MPI_Bcast(n,1,<datatype>,0,MPI_COMM_WORLD…)
    Use MPI_INTEGER and MPI_INT for Fortran and C datatypes, respectively. (Use &n address for C).
- Specify integral elements for each processor
  - F90: do i = 1,n → do i = myid+1, n, numprocs
  - C: for(i=1; i<=n; i++) →for(i=myid+1; i<=n; i=i+numprocs)

Calculating π – MPI_reduce partial sums

- Assign the sum from each rank to a partial sum
  - declare part_pi as a double [real(KR8) in F90]
  - after the loop, replace “pi = h * sum” with :
    part_pi = h * sum; followed by
- Sum the partial sums with an MPI_Reduce call

  …MPI_Reduce(part_pi,pi,1,<type>,MPI_SUM,0,
                                                MPI_COMM_WORLD…)

  where <type> is MPI_DOUBLE or MPI_DOUBLE_PRECISION for C and F90, respectively; use addresses &part_pi and &pi in C code
- Write out π & calc. pi, from rank 0 proc (use if)
  - if (myid == 0) print…

Calculating π

- Compile code:

```
mpif90 –O3 pi.f90
mpicc  –O3 pi.c
```

- Prepare job (edit ‘job’ in current directory)

  Modify the processor count:

  Keep the # of processors per node set to 16 (keep the “16way)

  The last argument, divided by 16, is the number of nodes.

  Add a line to identify your account:

  ```
  #$ -A 20090528HPC
  ```

  – create a file called “input” and include the total number of elements (n) on the first line

  ```
  echo 2000 >input
  ```

- Submit job

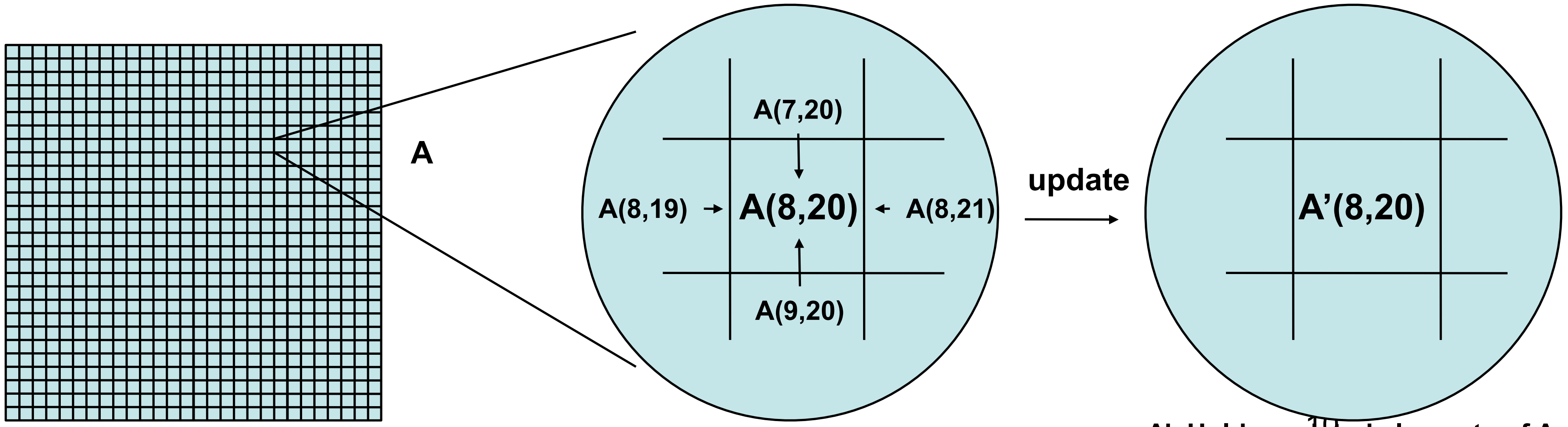
```
qsub  job
```

- See parallel_pi.c (.f90) for finished parallel versions.

Part 2: Sharing Data Across Processors

Overview

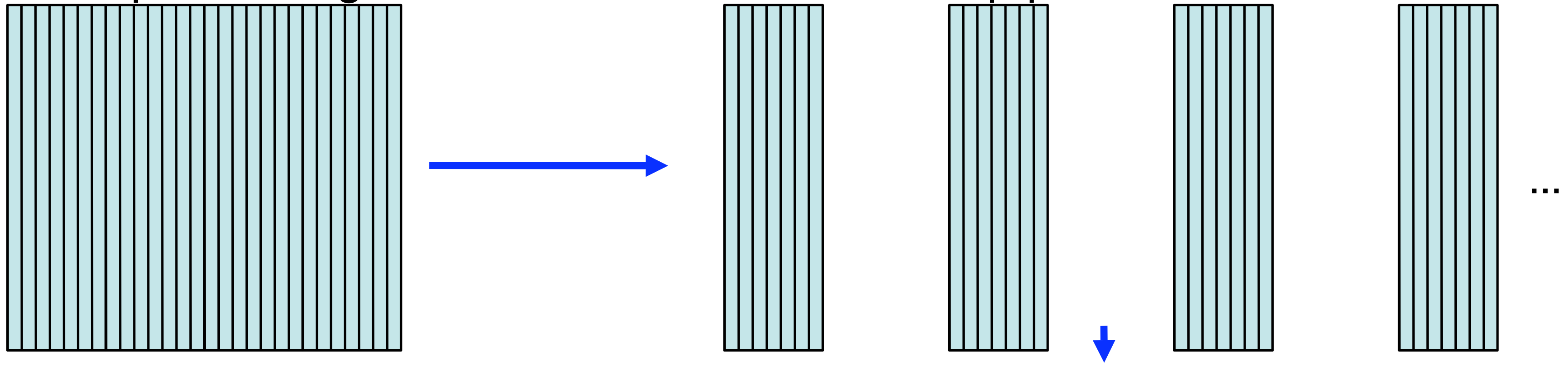
Solve 2-D partial differential equation (finite difference)
- Represent x-y domain as 2-D grid of points*
- Solution Matrix=A(x,y)
- Initialize grid elements with guess.
- Iteratively update Solution Matrix (A) until converged.
- Each iteration uses “neighbor” elements to update A.



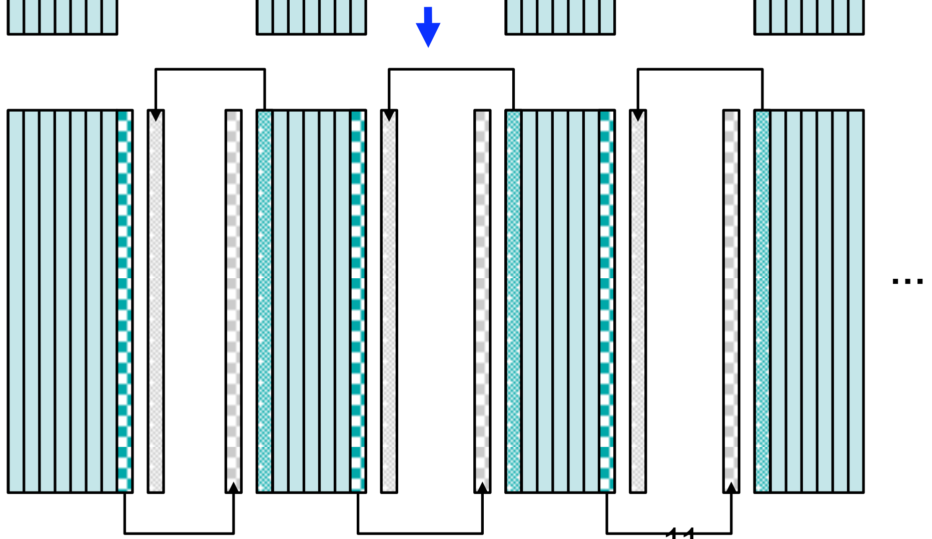
A’, Holds updated elements of A

Domain Decomposition

Decompose 2-D grid into column blocks across p processors



Need to duplicate edge columns on neighbor processors & send updated values after each iteration. That is, create ghost columns (gray) from real (patterned) column on neighbor processor.



Sharing Data Across Processors – Serial to //

From a simple serial code, decompose a domain (matrix) into column slices for each processor, include ghost cells, and create a subroutine for transferring real (calculated) columns to ghost column on the neighbor processor. Extend the A matrix to hold the neighbors: A(N,N)→A(N,N+2).

Instructions

```
cd $HOME/mpi_lab/ghosts
cp serial.c myghost.c     (for C programmers)
cp serial.f90 myghost.f90 (for F90 programmers)
```

(ghost_1d.c/f90 are example, completed codes)

Sharing Data Across Processors – Outline: Serial To Parallel

serial code (serial) → parallel code (myghost)

```
main program
  matrix A



loop
  jacob_update(A)

end loop



end main
jacob_update
```

```
main program
  matrix A  {include ghosts in A}

initialize MPI, get rank size

loop
  jacob_update(A)
  ghost_exchange(A)
end loop

finalize MPI

end main
jacob_update modify for ghost
routine  ghost_exchange
```

Domain Decomposition

- Look over the serial.c or serial.f90 code.
  - The code loops over a jacob_update routine which simply increases all values in a matrix (to emulate a stencil update in a Finite Difference code).

Fortran

```
real*8 :: A(n,n)
..

do iter = 1,LOOPS
  call jacob_update(a,n,iter)
end do
…
subroutine jacob_update()
   A(i,j) = iter
```

C

```
#define A(i,j)  a( (i-1) + (j-1)*n )
double a[n*n];

for(iter=1; iter<=LOOPS; iter++){
   jacob_update(a,n,iter)
}
…
Void jacob_update(){
   A(i,j) = (double) (iter);
```

Domain Decomposition

Matrix Layout – Serial Code

columns

$$\begin{array}{c|cccc|}
\text{rows} & 1 & 2 & 3 & 4 \; j \\ \hline
1 & 1 & 5 & 9 & 13 \\
2 & 2 & 6 & 10 & 14 \\
3 & 3 & 7 & 11 & 15 \\
4 \; i & 4 & 8 & 12 & 16 \\ \hline
\end{array}$$

Fortran

```
indexing: { i = 1,n; j=1,n }

real*8 :: A(n,n);

A(i,j)…
```

C

```
indexing: { i = 1,n; j=1,n }

#define A(i,j)  a( (i-1) + (j-1)*n )
double  a[ n*n ];

A(i,j)...
```

Domain Decomposition

Matrix Layout with Ghost Cells

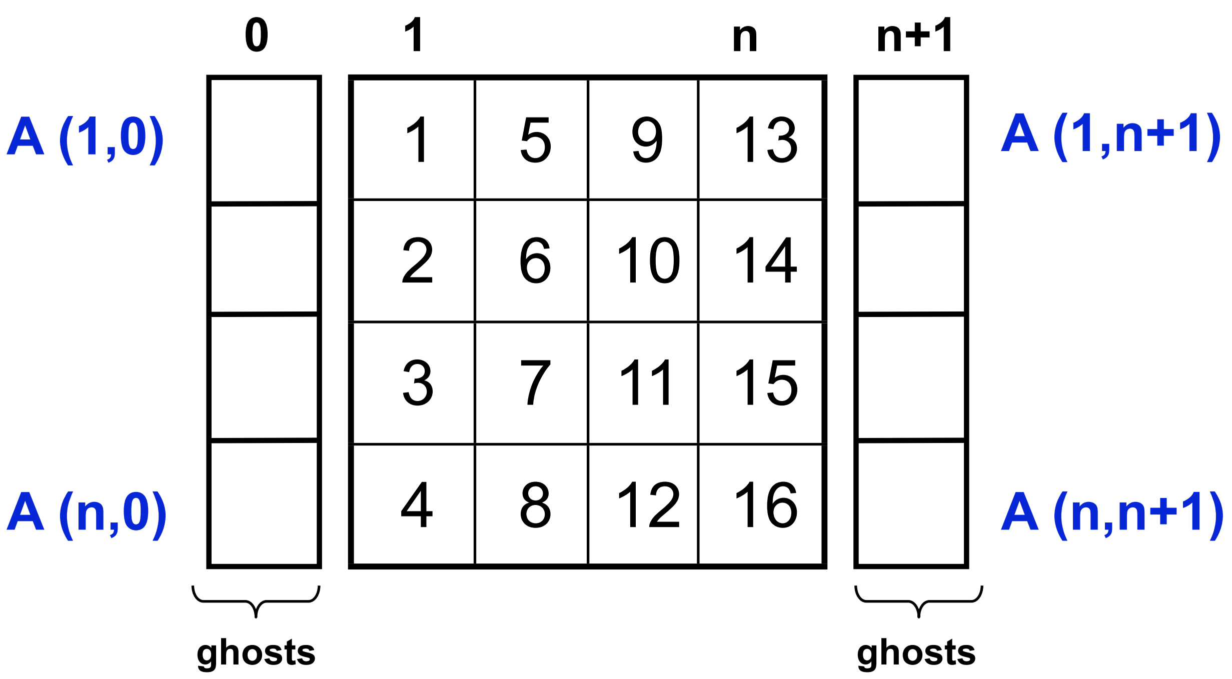
Redefine Array for easy ghost access

```
real*8 :: A(n, 0:n+1)
```

Fortran

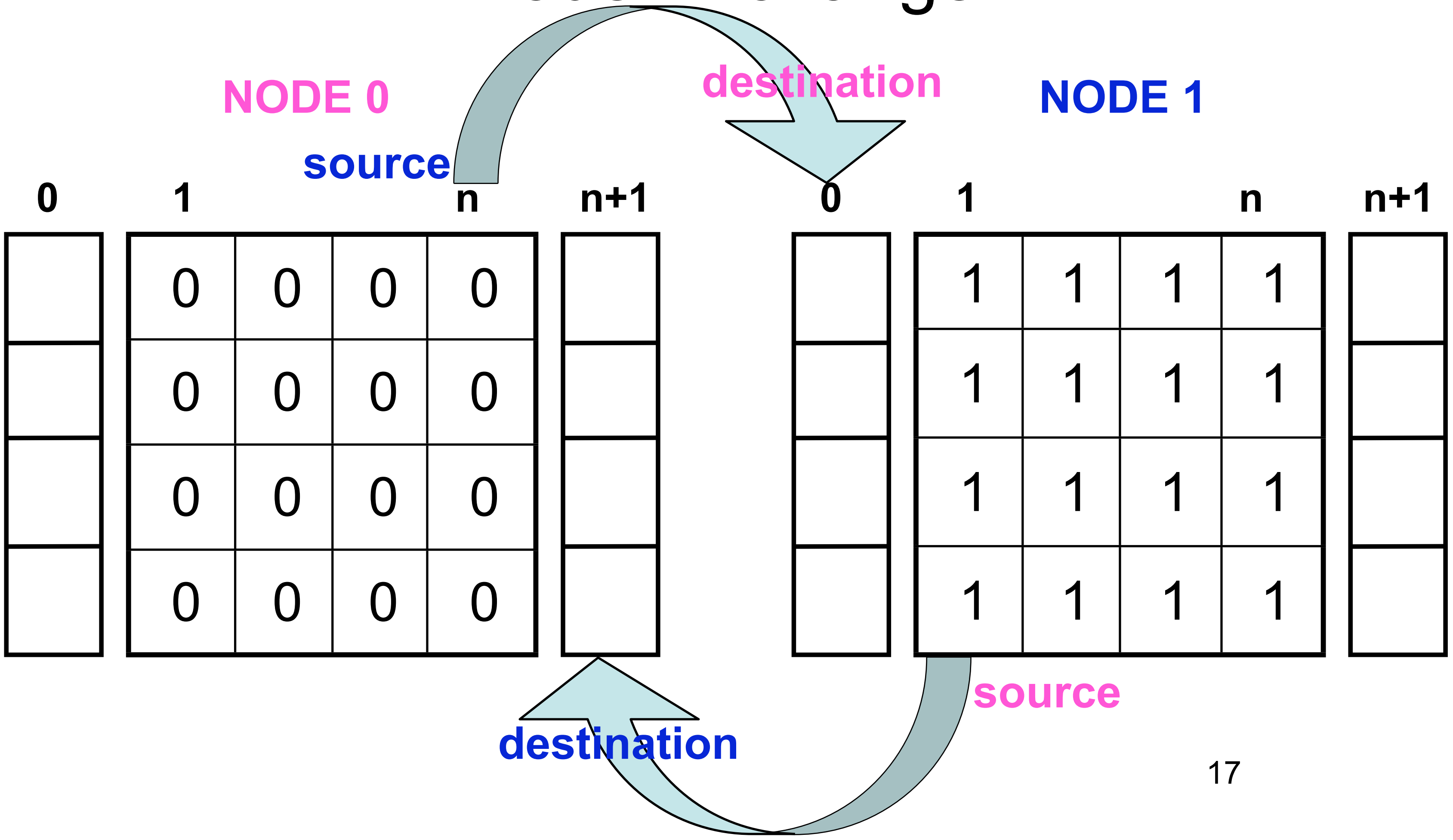
```
#define A(i,j)  a( (i-1) + (j)*n )
double a[n*(n+2)];
```

C



Domain Decomposition

Node Exchange



Domain Decomposition

- Include the usual MPI_Init & MPI_Finalize statements:

```
define ierr, irank, nranks as integers

…MPI_Init(…);
…MPI_Comm_rank(MPI_COMM_WORLD, irank*,...);
…MPI_Comm_size(MPI_COMM_WORLD, nranks*…);
…
…MPI_Finalize(…);
```

(Don't forget to include mpif.h or mpi.h.)
(Don't forget to declare irank and nranks.)
*** &irank and &nranks for C code**

Domain Decomposition

- Create a subroutine for the exchange:
  ghost_exchange(a,n,iter,irank,nranks)
- Create destination and source numbers for the exchange

```
idest = irank +  1;
isrc  = irank -  1;
if(idest == nranks) idest = MPI_PROC_NULL;
if(isrc  ==     -1) isrc  = MPI_PROC_NULL;
```

C prototype: void ghost_exchange(double *a, int n, int iter, int irank, int nranks);
include type statements for idest, isrc (integers)

Domain Decomposition

- Send right data column to right, into the left ghost column.

```
MPI_Sendrecv(A(1, n), n, <type>, idest, 8,
                        A(1, 0), n, <type>, isrc ,  8,  MPI_COMM_WORLD, status,…);
```

See top arrow(s) of slide 17.   Use   &A(1,n), &A(1,0), &status for C.

- Send left data columns to left, into the right ghost column.

```
MPI_Sendrecv(A(1,    1), n, <type>, isrc,   9,
                        A(1,n+1), n, <type>, idest , 9,  MPI_COMM_WORLD, status,…);
```

See bottom arrow(s) of slide 17.   Use &A(1,1), &A(1,n+1), &status for C.

C declaration: MPI_Status status   F90: integer status(MPI_STATUS_SIZE)

Domain Decomposition jabobi_update modifications

- Ghost column 0 & n+1 accommodated by C define:

```
#define A(i,j)  a( (i-1) + (j-1)*n )   ──→   #define A(i,j)  a( (i-1) + (j)*n )
double  a[N*N];                               double  a[N*(N+2)];
```

```
for(i=1; i<=n; i++){            no        for(i=1; i<=n; i++){
  for(j=1; j<=n; j++){          change      for(j=1; j<=n; j++){
    A(i,j) = (double) (iter);   ──→           A(i,j) = (double) (iter);
} }                                       } }
```

- Ghost column 0 & n+1 accommodated by F90 array declaration:

```
                          no
                          change
A(1:N, 1:N) = iter;       ──→             A(1:N, 1:N) = iter;
```

Because new indexing in declaration accommodates ghost vectors:

```
real*8  :: A(1:n, 1:n)    ──→             real*8 :: A(n, 0:n+1)
```

Domain Decomposition

- Compile code:

```
mpif90 –O3 myghost.f90
mpicc  –O3 myghost.c
```

- Prepare job

  Modify the processor count:

  Keep the # of precessors per node set to 16 (keep the “16way)

  The last argument, divided by 16, is the number of nodes.

  `#$ -pe  16way 16`   → change 16 to 32, 48, 64, etc.

  Add a line to identify your account:

  `#$ -A 20090528HPC`

- Submit job

```
qsub  job
```

- See ghost_1d.c (.f90) for finished parallel version.