{ACF}

Introduction to Message Passing Interface

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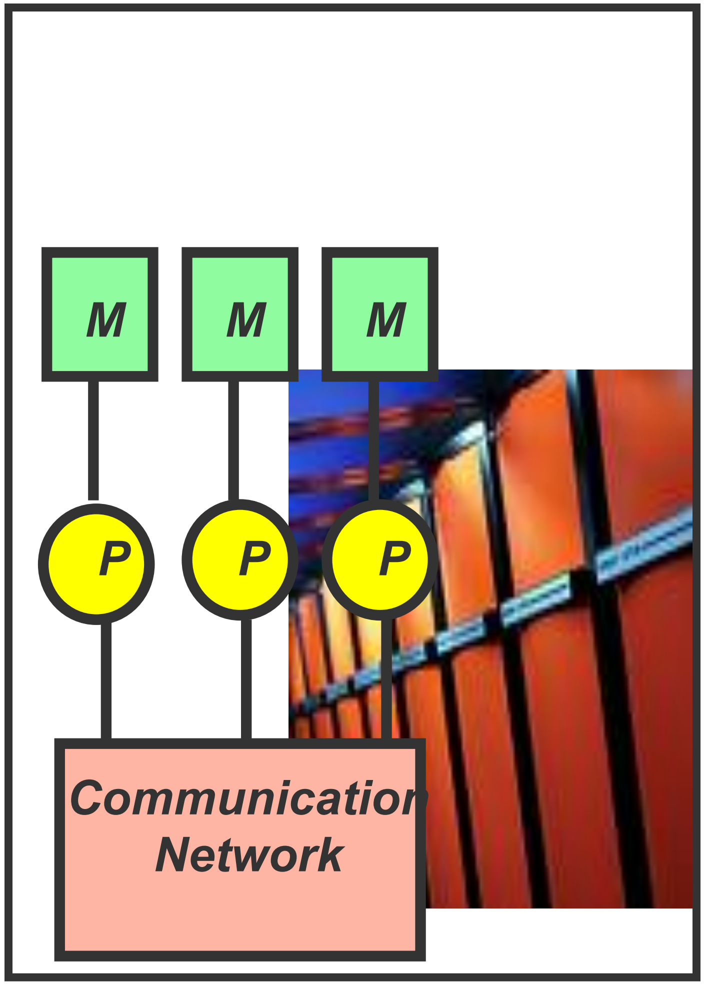
Message Passing Interface (MPI) Distributive Node level communication

Topics:

- Message Passing Interface
- Point to Point Communication
- Collective Communication
- Derived Datatype
- Parallel Code Development



Message Passing Interface (MPI)

- A first portable message passing communications standard defined by the MPI Forum which consists of hardware vendors, researchers, academics, software developers, and users, representing over forty different organizations
- MPI library (implementation) consists of a set of MPI function calls to facilitate transfer of data across processes
- The syntax of MPI call is standardized
- The functional behavior of MPI call is standardized
- About 20+ calls are in general needed!
- Vendors have tuned MPI calls to suit the underlying hardware (interconnect, arch) and software (OS)
- IBM MPI : IBM implementation for the SP, Cray MPT
- Intel MPI, MPICH, OpenMPI ..

Simple Hello World C Program

```
/* Simple serial Hello World C Example : hello.c */
#include <stdio.h>

int main (int argc, char *argv[])
{
     int rank, size;
     printf( "Hello World from process %d of %d\n", rank, size );
return 0;
}
```

```
/* Parallel Hello world C Example : hello.c */
#include <stdio.h>
#include <mpi.h>

int main (int argc, char *argv[])
{
     int rank, size;
     MPI_Init (&argc, &argv);    /* starts MPI */
     MPI_Comm_rank (MPI_COMM_WORLD, &rank);    /* get current process id */
     MPI_Comm_size (MPI_COMM_WORLD, &size);    /* get number of processes */
     printf( "Hello World from process %d of %d\n", rank, size );
     MPI_Finalize();
return 0;
}
```

To compile : > icc –o hexe ./hello.c
To run serial code : > ./hexe

To compile : > mpiicc –o hexe ./hello.c
To run in parallel : > mpirun –n 4 ./hexe

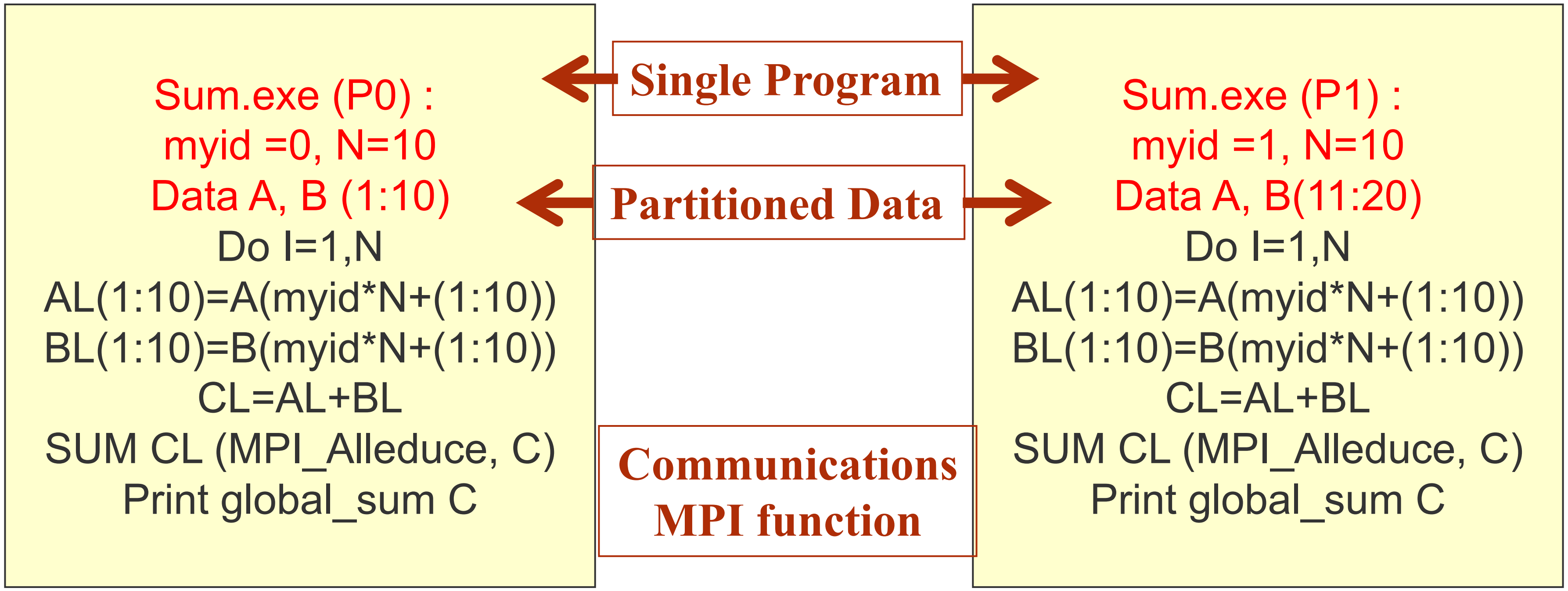
SPMD

- Single Program, Multiple Data Programming Paradigm
- Same program runs on all processors, however, each processor operates on different set of data
- The simplest parallel parallel paradigm
- Generally contains :

```
      if ( my_processor_id  .eq. designated_id ) then
              -------
      end if
```

Message Passing Programming

- Used primarily on distributed memory computing environment
- Since memory are local, any data stored in remote processor's memory must be explicitly requested by programmer.
- Each processor runs the SAME program using partitioned data set
- Written in sequential language (FORTRAN, C, C++) + MPI functions



```
Sum.exe (P0) :
myid =0, N=10
Data A, B (1:10)
Do I=1,N
AL(1:10)=A(myid*N+(1:10))
BL(1:10)=B(myid*N+(1:10))
CL=AL+BL
SUM CL (MPI_Alleduce, C)
Print global_sum C
```

```
Sum.exe (P1) :
myid =1, N=10
Data A, B(11:20)
Do I=1,N
AL(1:10)=A(myid*N+(1:10))
BL(1:10)=B(myid*N+(1:10))
CL=AL+BL
SUM CL (MPI_Alleduce, C)
Print global_sum C
```

MPI Message Components

- Envelope:
  - sending processor (processor_id)
  - source location (group_id, tag)
  - receiving processor (processor_id)
  - destination location (group_id, tag)
- Data (letter) :
  - data type (integer, float, complex, char….)
  - data length (buffer size, count, strides)

Typical Message Passing Subroutines

- Environment Identifiers
  - processor_id, group_id, initialization
- Point to Point Communications
  - blocking operations
  - non-blocking operations
- Collective Communications
  - barriers
  - broadcast
  - reduction operations

Essentials of MPI programs

- Header file:
  - C : #include<mpi.h>
  - Fortran : include ‘mpif.h’
- Initializing MPI :
  - C : int MPI_Init(int argc, char**argv)
  - Fortran : call MPI_INIT(IERROR)
- Exiting MPI :
  - C : int MPI_Finalize()
  - Fortran :call MPI_FINALIZE(IERROR)

MPI Function Format

- MPI
  - MPI_Xxxx(parameter, ………)
- C :
  - error = MPI_Xxxxx(parameter, ……….)
  - Case is IMPORTANT
- Fortran:
  - call MPI_XXXX(parameter,….., IERROR)
  - Case is NOT important

MPI Process Identifiers

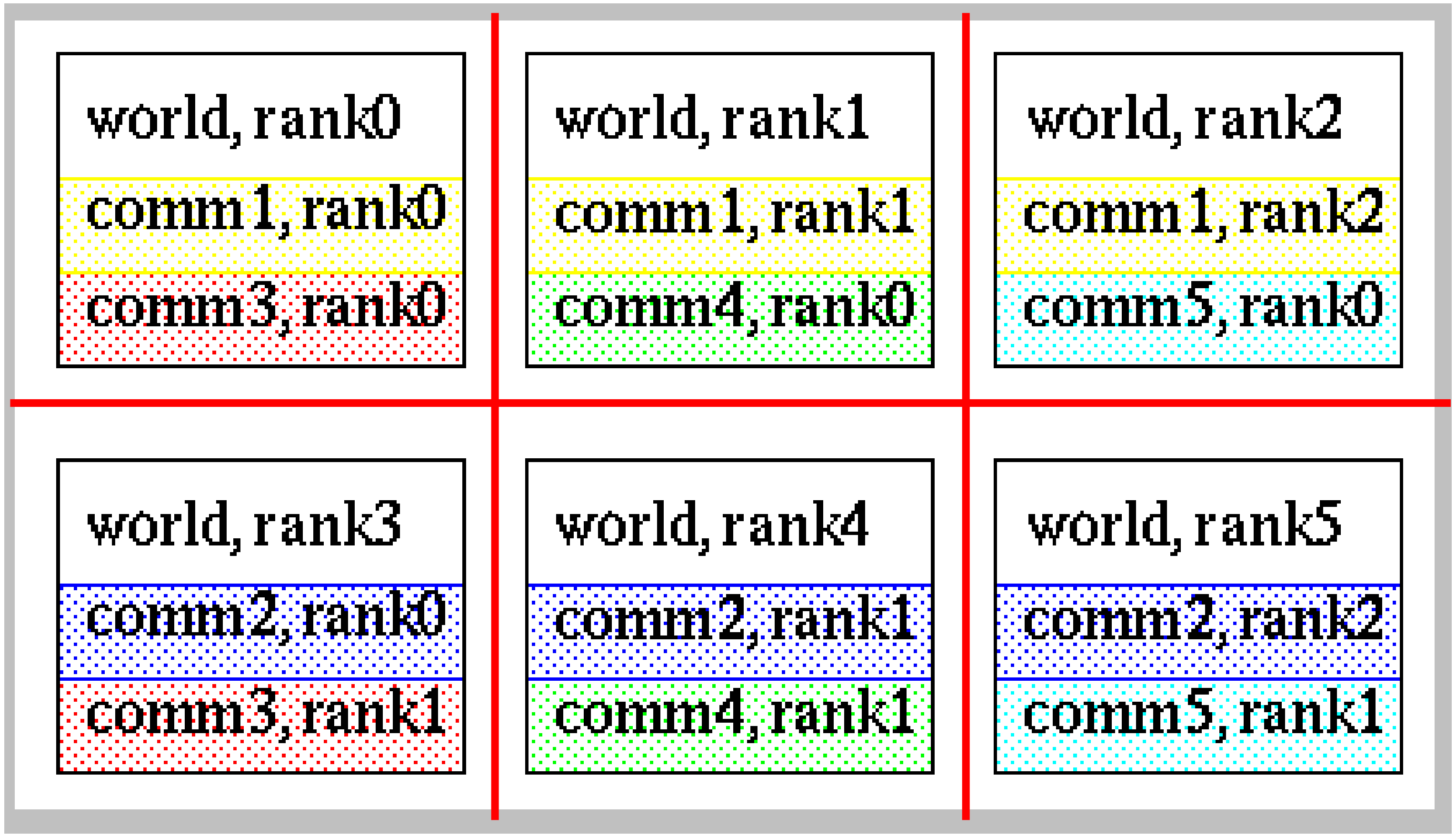
- MPI_COMM_RANK:
  - Gets a process’s rank (ID) within a process group
  - C : int MPI_Comm_rank(MPI_Comm comm, int *rank)
  - F : call MPI_COMM_RANK(mpi_comm,rank,ierror)
- MPI_COMM_SIZE:
  - Gets the number of processes within a process group
  - C : int MPI_Comm_size(MPI_Comm comm, int *size)
  - F : call MPI_COMM_SIZE(mpi_comm,size,ierror)
- MPI_Comm : Communicator

MPI Communicator

- A communicator is the communicating space among processes
- All MPI communication calls require a communicator argument and MPI processes can only communicate if they share a communicator.
- Every communicator contains a group of tasks with a *system supplied identifier* (for message context) as an extra match field.
- MPI _Init initializes all tasks with MPI_COMM_WORLD
- So, the base group is the group that contains all processes, which is associated with the MPI_COMM_WORLD communicator.
- Communicators are particularly important for user supplied libraries
- Communicators are used to create independent "message universe"

Communicating Group

ALL : MPI_COMM_WORKD (world)
ROW : comm1, comm2 ; COLUMN : comm3, comm4, comm5
Every process has three communicating groups and a distinct rank associated to it



Sample Program : Hello World

```
#include <stdio.h>
#include "mpi.h"
main(int argc, char** argv) {
  int my_PE_num;
  MPI_Init(&argc, &argv);
      MPI_Comm_rank(MPI_COMM_WORLD, &my_PE_num);
  printf("hello from %d. \n", my_PE_num);
  MPI_Finalize();
}
```

```
program Hello_World
include 'mpif.h'
integer my_PE_num, ierror
call MPI_INIT(ierror)
call MPI_COMM_RANK(MPI_COMM_WORLD,my_PE_num, ierror)
print *, 'Hello from', my_PE_num
call MPI_FINALIZE(ierror)
end
```

Compiling and Running MPI (MPICH PC Cluster)

- Compile :
  - mpicc -o fileexe filename.c
  - mpif77 -o fileexe filename.f
- Running :
  - mpirun -np <num_of_processes> fileexe
- Options :
  - -np : number of processes
  - -machinefile : list of machines to be used
  - -t : testing option
  - use “man mpirun” to see more details

```
%mpirun –np 3 –machinefile hostfile hello.exe
hello from 0
hello from 2
hello from 1
```

Compiling and Running – (ACF)

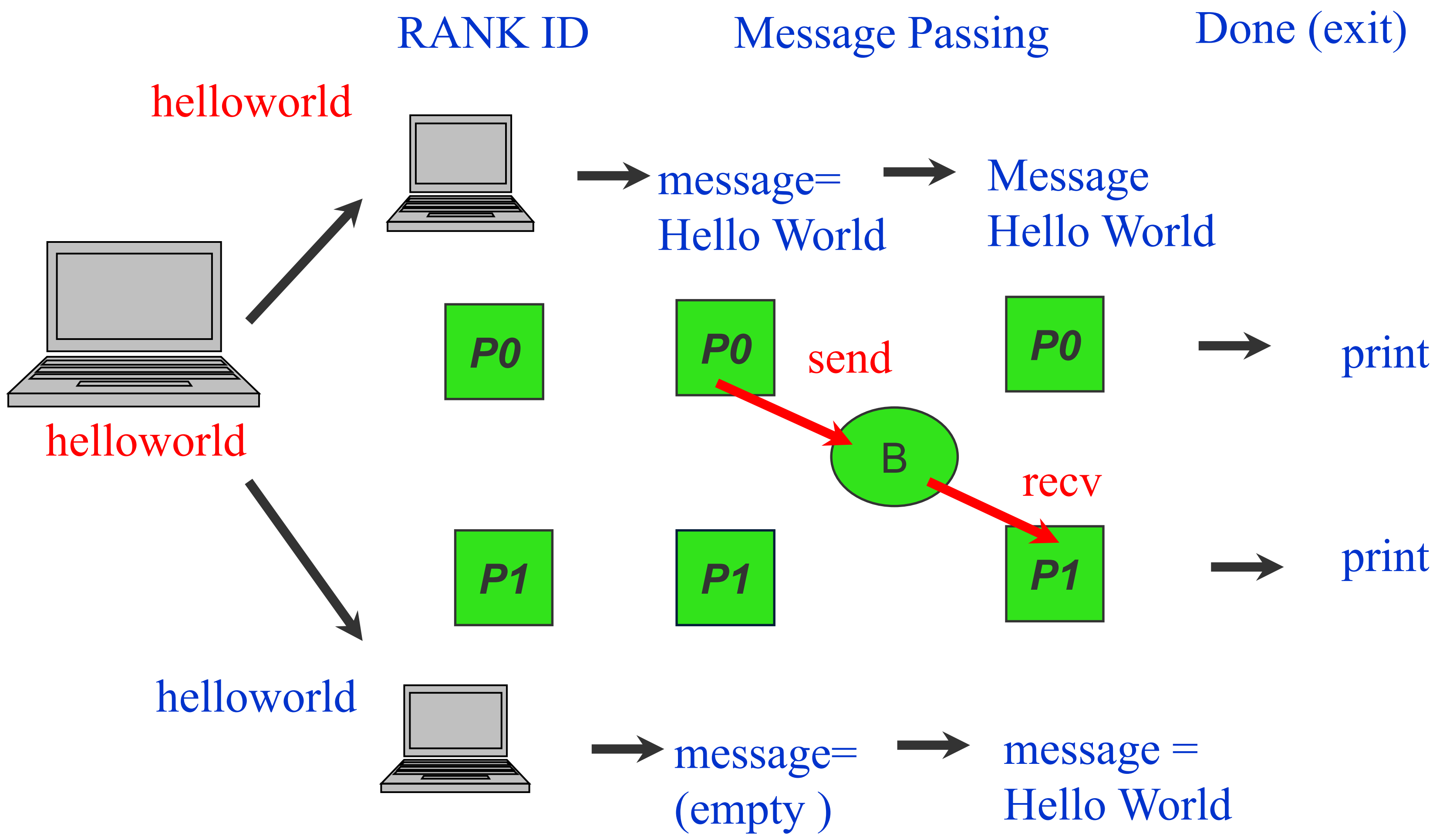
- Compile (PE-intel) : mpiicc -o hello hello.c or mpiifort -o hello hello.f
- Compile (PE-gnu) : mpicc -o hello hello.c or mpif90 -o hello hello.f
- PBS Batch Script, e.g. submit.pbs
- run : qsub submit.pbs

```
#!/bin/bash
#PBS -A your-project-id
#PBS -N test
#PBS -j oe
#PBS -l walltime=1:00:00,-l nodes=1:ppn=12
cd $PBS_O_WORKDIR
date
mpirun -np 4 ./hello
```

Hello World Again

```
program Hello_World
include ‘mpif.h’
integer me, ierror, ntag, status(MPI_STATUS_SIZE)
character(12) message
call MPI_INIT(ierror)
call MPI_COMM_RANK(MPI_COMM_WORLD, me, ierror)
ntag = 100
if ( me .eq . 0) then
    message = ‘Hello, World’
    call MPI_Send(message, 12, MPI_CHARACTER, 1, ntag,
     MPI_COMM_WORLD, ierror)
else
    call MPI_Recv(message, 12, MPI_CHARACTER, 0, ntag,
     MPI_COMM_WORLD, status, ierror)
    print *, ‘node’,me, ‘:’, message
endif
call MPI_FINALIZE(ierror)
end
```

Parallel Processing



Example: Passing a Message – Hello World Again!

```
program Hello_World
include 'mpif.h'
integer me, ierror, ntag, status(MPI_STATUS_SIZE)
character(12) message
call MPI_INIT(ierror)
call MPI_COMM_RANK(MPI_COMM_WORLD, me, ierror)
ntag = 100
if ( me .eq . 0) then
     message = 'Hello, World'
     call MPI_Send(message, 12, MPI_CHARACTER, 1, ntag,
  MPI_COMM_WORLD, ierror)
else if ( me .eq . 1) then
     call MPI_Recv(message, 12, MPI_CHARACTER, 0, ntag,
  MPI_COMM_WORLD, status, ierror)
     print *, 'Node',me, ':', message
endif
call MPI_FINALIZE(ierror)
end
```

Example: Passing a Message – Hello World Again!

```
#include "mpi.h"
#include <iostream>
#include <string>
int main(int argc, char ** argv)
  {
        int my_PE_num, ntag = 100;
        char message[13] = "Hello, world";
        MPI::Status status;
        MPI::Init(argc, argv);
        my_PE_num = MPI::COMM_WORLD.Get_rank();

        if ( my_PE_num == 0 )
          MPI::COMM_WORLD.Send(message,12,MPI::CHAR,1,ntag);
        else if ( my_PE_num == 1 ) {
          MPI::COMM_WORLD.Recv(message,12,MPI::CHAR,0,ntag, status);
          cout << "Node " << my_PE_num <<" : " << message << endl; }
        MPI::Finalize();
  }
```

MPI Point to Point Communications

- Communication between two processes
- Source process sends message to destination process
- Communication takes place within a communicator
- Blocking v.s non-blocking calls
- MPI defines four communication modes for blocking and non-blocking send : synchronous, buffered, ready, and standard
- The receive call does not specify communication mode-- it is simply blocking and non-blocking.
- Two messages sent from one process to another will arrive in that relative order.

Sending a Message

- C :: Standard send

  int MPI_Send(&buf, count, datatype, dest, tag, comm)
  - &buf : pointer of object to be sent
  - count : the number of items to be sent, e.g. 10
  - datatype : the type of object to be sent, e.g. MPI_INT
  - dest : destination of message (rank of receiver), e.g. 6
  - tag : message tag, e.g. 78
  - comm : communicator, e.g.(MPI_COMM_WORLD)
- Fortran ::

  call MPI_SEND(buf, count, datatype, dest, tag, comm, ierror)

Receiving a Message

- C :: Blocking receive

  int MPI_Recv(&buf, count, datatype, source, tag, comm, &status)

  – source : the node to receive from, e.g. 0

  – &status : a structure which contains three fields, the source, tag, and error code of the incoming message.

- Fortran ::

  call MPI_RECV(buf, count, datatype, source, tag, comm,
  status(MPI_STATUS_SIZE), ierror)

  – status : an array of integers of size MPI_STATUS_SIZE

MPI Basic Datatypes - C

MPI Datatypes	C Datatypes	MPI Datatypes	C Datatypes
MPI_CHAR	signed char	MPI_SHORT	signed short int
MPI_INT	signed int	MPI_UNSIGNED_CHAR	unsigned char
MPI_LONG	signed long int	MPI_UNSIGNED_SHORT	unsigned short int
MPI_FLOAT	float	MPI_UNSIGNED_LONG	unsigned long int
MPI_LONG_ DOUBLE	long double	MPI_UNSIGNED	unsigned int
MPI_BYTE	--------	MPI_PACKED	---------

MPI Basic Datatypes - Fortran

MPI Datatypes	Fortran Datatypes
MPI_INTEGER	INTEGER
MPI_REAL	REAL
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_COMPLEX	COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER(1)
MPI_BYTE	-------------
MPI_PACKED	-------------

Sample Program : Send and Receive

```
#include “mpi.h”

main(int argc, char ** argv) {

         int my_PE_num, numtorecv,  numtosend=42;

        MPI_Status status;

        MPI_Init(&argc, &argv);

        MPI_Comm_rank(MPI_COMM_WORLD, &my_PE_num);


        if ( my_PE_num == 0) {

           MPI_Recv(&numtorecv, 1, MPI_INT, MPI_ANY_SOURCE,
                        MPI_ANY_TAG, MPI_COMM_WORLD, &status);

           printf(“Number received is : %d\n”, numtorecv); }

        else MPI_Send ( &numtosend, 1, MPI_INT, 0, 10, MPI_COMM_WORLD) ;

        MPI_Finalize() ;

}
```

MPI Send

- MPI has 8 different types of Send
- The nonblocking send has an extra argument of request handle

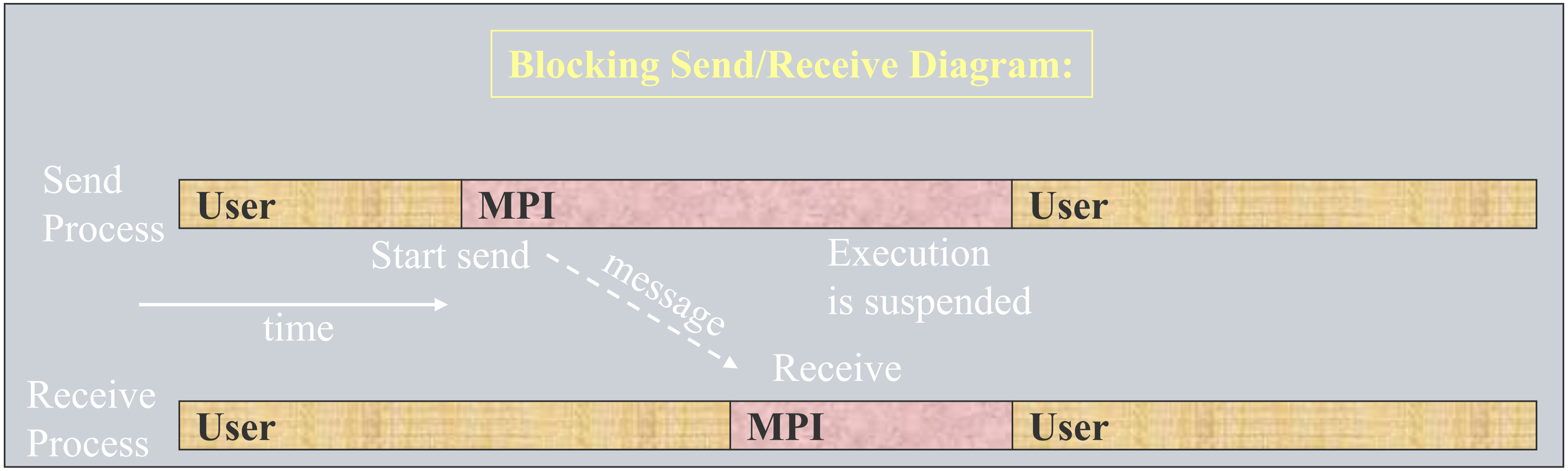
	blocking	nonblocking
standard	MPI_Send	MPI_Isend
synchronous	MPI_Ssend	MPI_ISsend
buffer	MPI_Bsend	MPI_Ibsend
ready	MPI_Rsend	MPI_Iresend

Blocking Calls

- A blocking send or receive call suspends execution of user's program until the message buffer being sent/received is safe to use.
- In case of a blocking send, this means the data to be sent have been copied out of the send buffer, but they have not necessarily been received in the receiving task. The contents of the send buffer can be modified without affecting the message that was sent
- The blocking receive implies that the data in the receive buffer are valid.

Blocking Send and Receive

- A blocking MPI call means that the program execution will be suspended until the message buffer is safe to use. The MPI standards specify that a blocking SEND or RECV does not return until the send buffer is safe to reuse (for MPI_SEND), or the receive buffer is ready to use (for MPI_RECV).

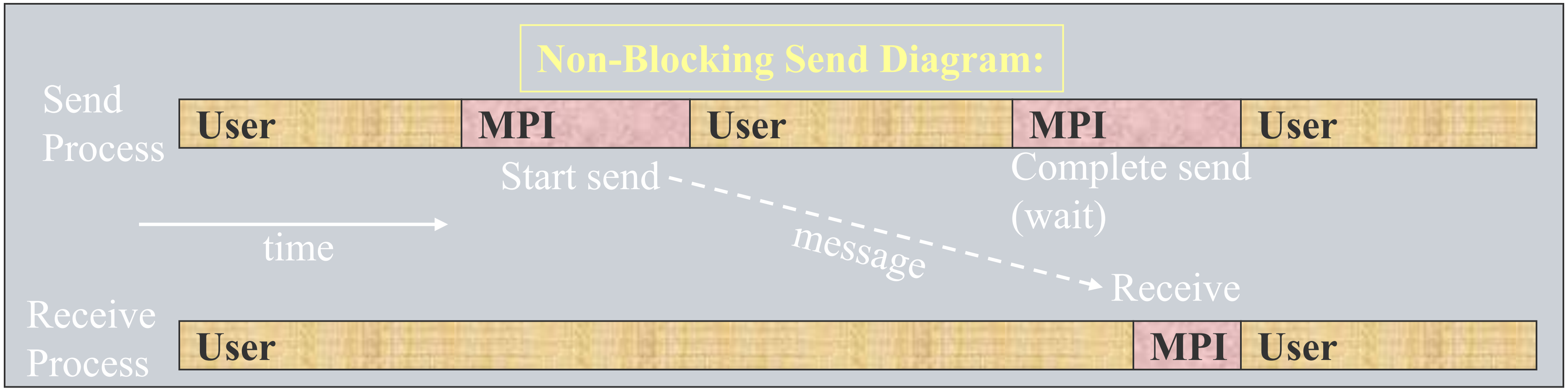


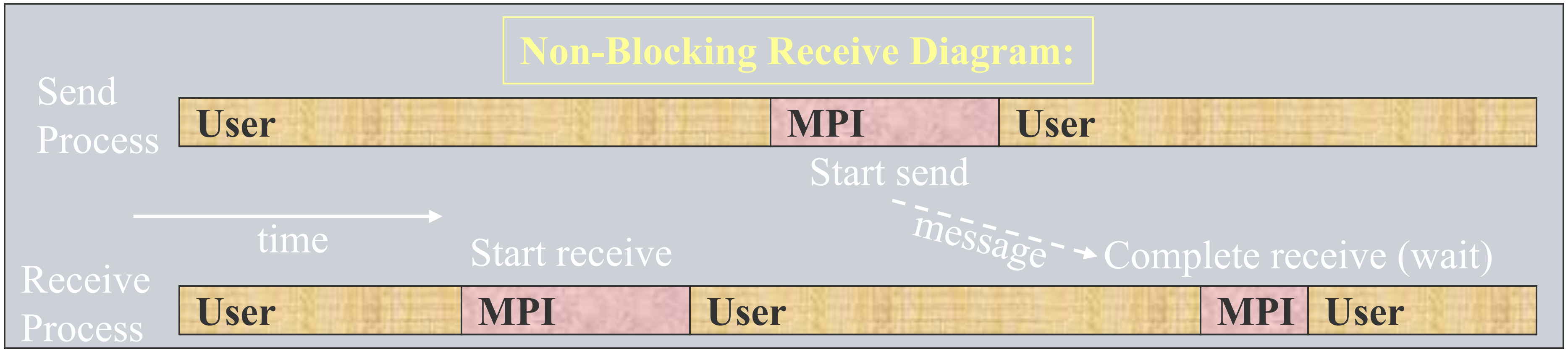
Non-Blocking Calls

- Non-blocking calls return immediately after initiating the communication.
- In order to reuse the send message buffer, the programmer must check for its status.
- The programmer can choose to block before the message buffer is used or test for the status of the message buffer.
- A blocking or non-blocking send can be paired to a blocking or non-blocking receive

Non-Blocking Send and Receive

- Separate Non-Blocking communication into three phases:
  - Initiate non-blocking communication.
  - Do some work (perhaps involving other communications?)
  - Wait for non-blocking communication to complete.





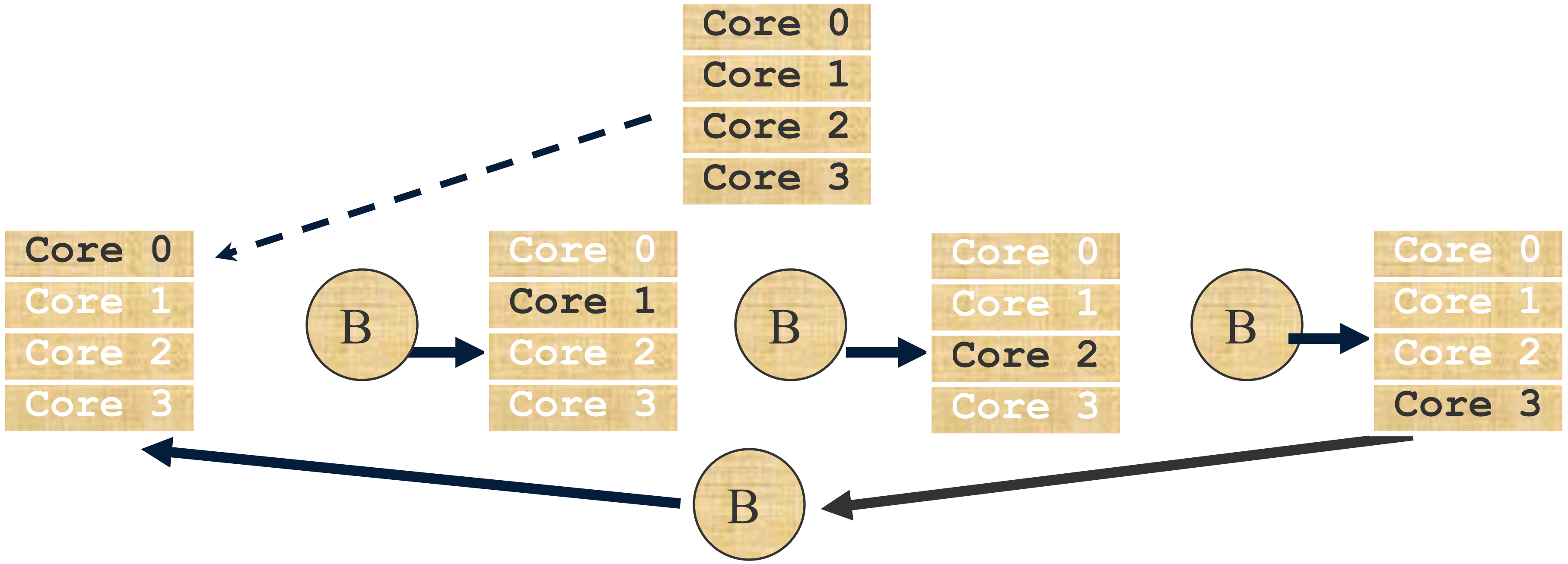
Deadlock

- all tasks are waiting for events that haven’t been initiated
- common to SPMD program with blocking communication, e.g every task sends, but none receives
- insufficient system buffer space is available
- remedies :
  - arrange one task to receive
  - use MPI_Ssendrecv
  - use non-blocking communication

Example - Ring

```
#include <stdio.h>
#include “mpi.h”
main(int argc, char *argv[])
{
  int myrank, nprocs, leftid, rightid, val, sum, tmp;
  MPI_Status recv_status;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  if((leftid=(myrank-1)) < 0) leftid = nprocs -1;
  if((rightid=(myrank+1) == nprocs) rightid = 0;
  val = myrank
  sum = 0;
 do {
   MPI_Send(&val,1,MPI_INT,rightid,99, MPI_COMM_WORLD);
   MPI_Recv(&tmp,1, MPI_INT, leftid, 99, MPI_COMM_WORLD, &recv_status);
   val = tmp;
   sum += val;
  } while (val != myrank);
  printf(“proc %d sum = %d \n”, myrank, sum);
  MPI_Finalize();
}
```

Example: Ring (Blocking Communication) – Schematic



```
myrank=0
size=4
leftid=3
rightid=1
Val=3,2,1,0
```

```
myrank=1
size=4
leftid=0
rightid=2
Val=0,3,2,1
```

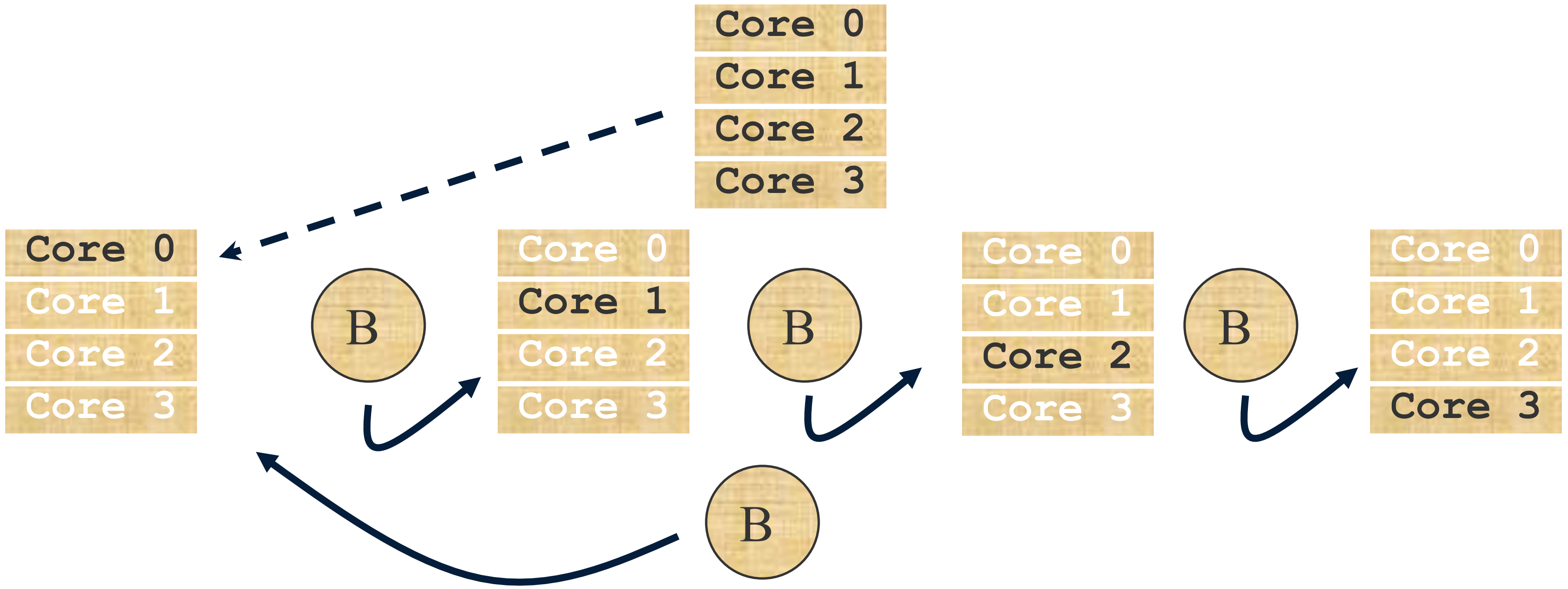
```
myrank=2
size=4
leftid=1
rightid=3
Val=1,0,3,2
```

```
myrank=3
size=4
leftid=2
rightid=0
Val=2,1,0,3
```

Example: Ring (Blocking Communication) – Fortran

```
      PROGRAM ring
      IMPLICIT NONE
      include "mpif.h"
      INTEGER ierror, val, my_rank, nprocs, rightid, leftid, tmp, sum, request
      INTEGER send_status(MPI_STATUS_SIZE), recv_status(MPI_STATUS_SIZE)
      CALL MPI_INIT(ierror)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, my_rank, ierror)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierror)
      rightid = my_rank + 1
      IF (rightid .EQ. nprocs) rightid = 0
      leftid = my_rank - 1
      IF (leftid .EQ. -1) leftid = nprocs-1
      sum = 0
      val = my_rank
 100  CONTINUE
      CALL MPI_SEND(val, 1, MPI_INTEGER, rightid, 99,
     $     MPI_COMM_WORLD, request, ierror)
      CALL MPI_RECV(tmp, 1, MPI_INTEGER, leftid, 99,
     $     MPI_COMM_WORLD, recv_status, ierror)
      sum = sum + tmp
      val = tmp
      IF(tmp  .NE. my_rank) GOTO 100
      PRINT *, 'Proc ', my_rank, ' Sum = ',sum
      CALL MPI_FINALIZE(ierror)
      STOP
      END
```

Example: Ring (Non-blocking Communication) – Schematic



```
myrank=0
size=4
leftid=3
rightid=1
```

```
myrank=1
size=4
leftid=0
rightid=2
```

```
myrank=2
size=4
leftid=1
rightid=3
```

```
myrank=3
size=4
leftid=2
rightid=0
```

Example: Ring (Non-blocking Communication) – C

```
#include <stdio.h>
#include "mpi.h"
main(int argc, char *argv[]) {
  int myrank, nprocs, leftid, rightid, val, sum, tmp;
  MPI_Status recv_status, send_status;
  MPI_request send_request;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  if((leftid=(myrank-1)) < 0) leftid = nprocs -1;
  if((rightid=(myrank+1) == nprocs) rightid = 0;
  val = myrank
  sum = 0;
 do {
   MPI_Issend(&val,1,MPI_INT,right,99, MPI_COMM_WORLD,&send_request);
   MPI_Recv(&tmp,1, MPI_INT, left, 99, MPI_COMM_WORLD, &recv_status);
   MPI_Wait(&send_request,&send_status);
   val = tmp;
   sum += val;
  } while (val != myrank);
  printf("proc %d sum = %d \n", myrank, sum);
  MPI_Finalize();              }
```

Example: Ring (Non-blocking Communication) – Fortran

```
      PROGRAM ring
      IMPLICIT NONE
      include "mpif.h‶
      INTEGER ierror, val, my_rank, nprocs, rightid, leftid, tmp, sum
      INTEGER send_status(MPI_STATUS_SIZE), recv_status(MPI_STATUS_SIZE)
      INTEGER request
      CALL MPI_INIT(ierror)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, my_rank, ierror)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierror)
      rightid = my_rank + 1
      IF (rightid .EQ. nprocs) rightid = 0
      leftid = my_rank – 1
      IF (leftid .EQ. -1) leftid = nprocs-1
      sum = 0
      val = my_rank
 100  CONTINUE
      CALL MPI_ISSEND(val, 1, MPI_INTEGER, rightid, 99,
     $     MPI_COMM_WORLD, request, ierror)
      CALL MPI_RECV(tmp, 1, MPI_INTEGER, leftid, 99,
     $     MPI_COMM_WORLD, recv_status, ierror)
      CALL MPI_WAIT(request, send_status, ierror)
      sum = sum + tmp
      val = tmp
      IF(tmp .NE. my_rank) GOTO 100
      PRINT *, 'Proc ', my_rank, ' Sum = ',sum
      CALL MPI_FINALIZE(ierror)
      STOP
      END
```

Example: MPI Communication Timing Test

- The objective of this exercise is to investigate the amount of time required for message passing between two processes, i.e. an MPI communication timing test is performed.
- In this exercise different size messages are sent back and forth between two processes a number of times. Timings are made for each message before it is sent and after it has been received. The difference is computed to obtain the actual communication time. Finally, the average communication time and the bandwidth are calculated and output to the screen.
- For example, one can run this code on two nodes (one process on each node) passing messages of length 1, 100, 10,000, and 1,000,000 and record the results in a table.

Sendrecv

- useful for executing a shift operation across a chain of processes
- system take care of possible deadlock due to blocking calls

MPI_Sendrecv(sbuf, scount, stype, dest, stag, rbuf, rcount, rtype, source, rtag, comm, status)

– sbuf (rbuf) :	initial address of send (receive)buffer
– scount (rcount) :	number of elements in send (receive) buffer
– stype (rtype) :	type of elements in send (receive) buffer
– stag (rtag) :	send (receive) tag
– dest :	rank of destination
– source :	rank of source
– comm :	communicator
– status :	status object

Non-blocking Communications

- The non-blocking calls have the same syntax as the blocking calls, with two exceptions:
  - Each call has an “I” immediately following the “_”
  - The last argument is a handle to an opaque request object that contains information about the message
- Non-blocking call returns immediately after initiating the communication
- The programmer can block or check for the status of the message buffer : MPI_Wait or MPI_Test.

Non-blocking Send and Receive

- **Fortran :**

```
call MPI_Isend(buf,count,datatype,dest,tag,comm,handle,ierr)
call MPI_Irecv(buff,count,datatype,src,tag,comm,handle,ierr)
call MPI_Test(handle, flag, status, ierr)
call MPI_Wait (handle, status, ierr)
```

- **C :**

```
MPI_Isend(&buf, count, datatype, dest, tag, comm, &handle)
MPI_Irecv(&buff, count, datatype, src, tag, comm, &handle)
MPI_Wait (&handle, &status)
MPI_Test(&handle, &flag, &status)
```

Testing Communications for Completion

- MPI_Wait (request, status)

  These routines block until the communication has completed. They are useful when the data from the communication buffer is about to be re-used

- MPI_Test (request, flag, status)

  This routine blocks until the communication specified by the handle *request* has completed. The *request* handle will have been returned by an earlier call to a non-blocking communication routine. The routine queries completion of the communication and the result (TRUE of FALSE) is returned in *flag*

Timer

- C

  double MPI_Wtime(void)

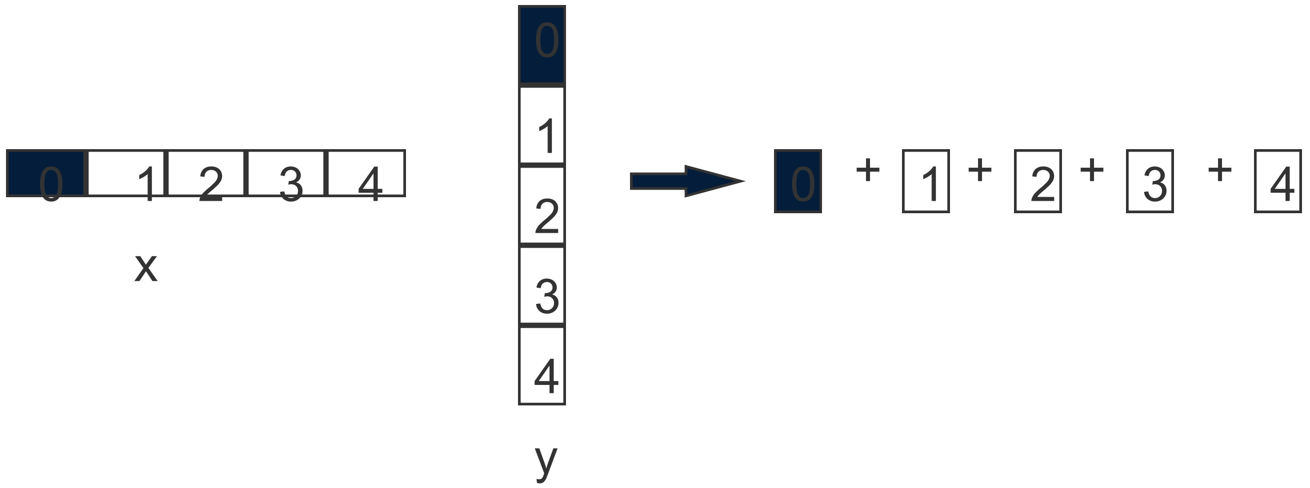
- Fortran :

  double precision MPI_Wtime()

- Time is measured in seconds.
- Time to perform a task is measured by consulting the timer before and after
- Modify your program to measure its execution time and print it out

Inner Product (Parallel)

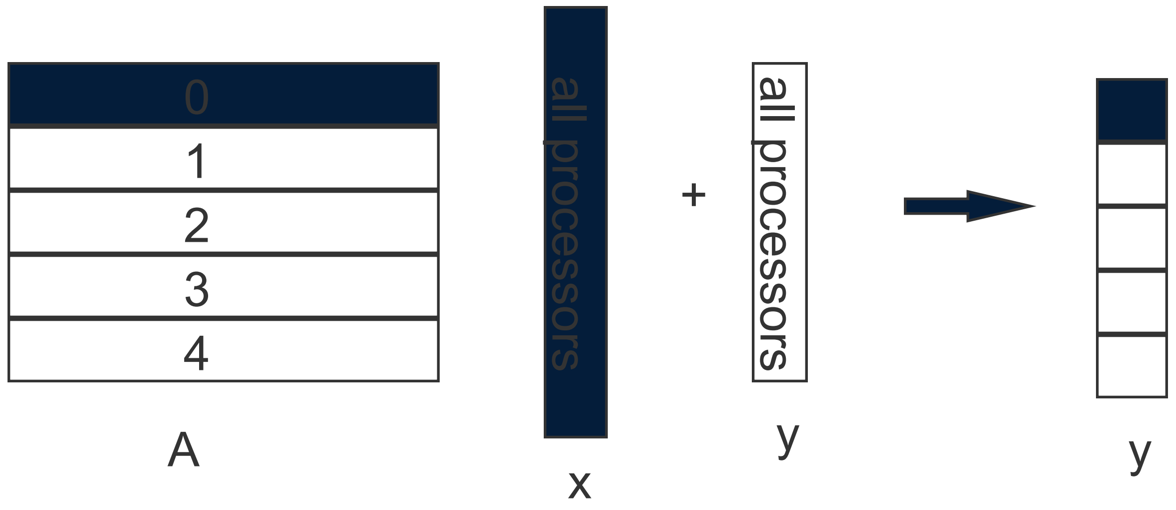
- **Compute the inner product of two vectors,** $sdot = \sum_{i=1}^{n} x^T y$



- Blockwise distribution of the vectors is used. Each processor computes a portion of the value of the inner product. The result is obtained by summing the partial values together.

Matrix - Vector Product

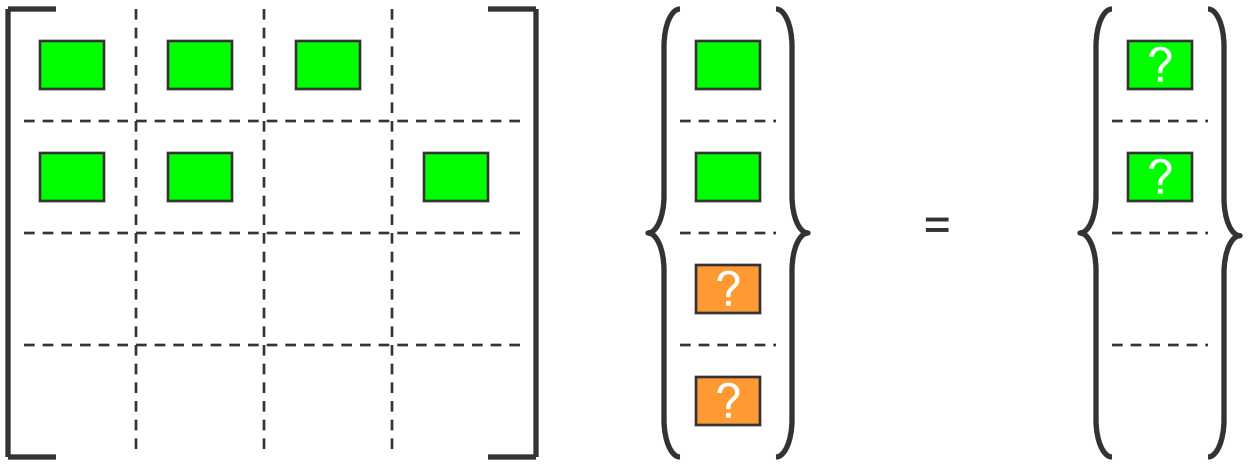
- **Compute the product of a matrix, A, and a vector, x, y=y+Ax**



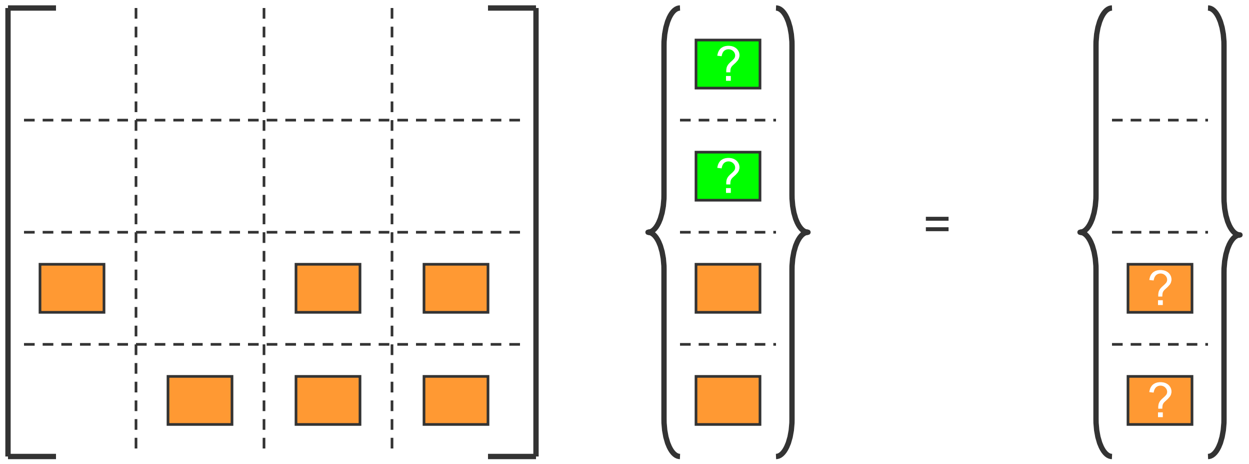
- Matrix A can be distributed to processors with a block-striped partition scheme or a block cyclic scheme. Entire vector x will be needed for calculation of y in every processor. Vector x may be distributed or duplicated among processors. Each processor compute the value of a portion of the matrix vector product The resultant y vector is obtained by summing the partial values.

Parallel M-V Multiplication

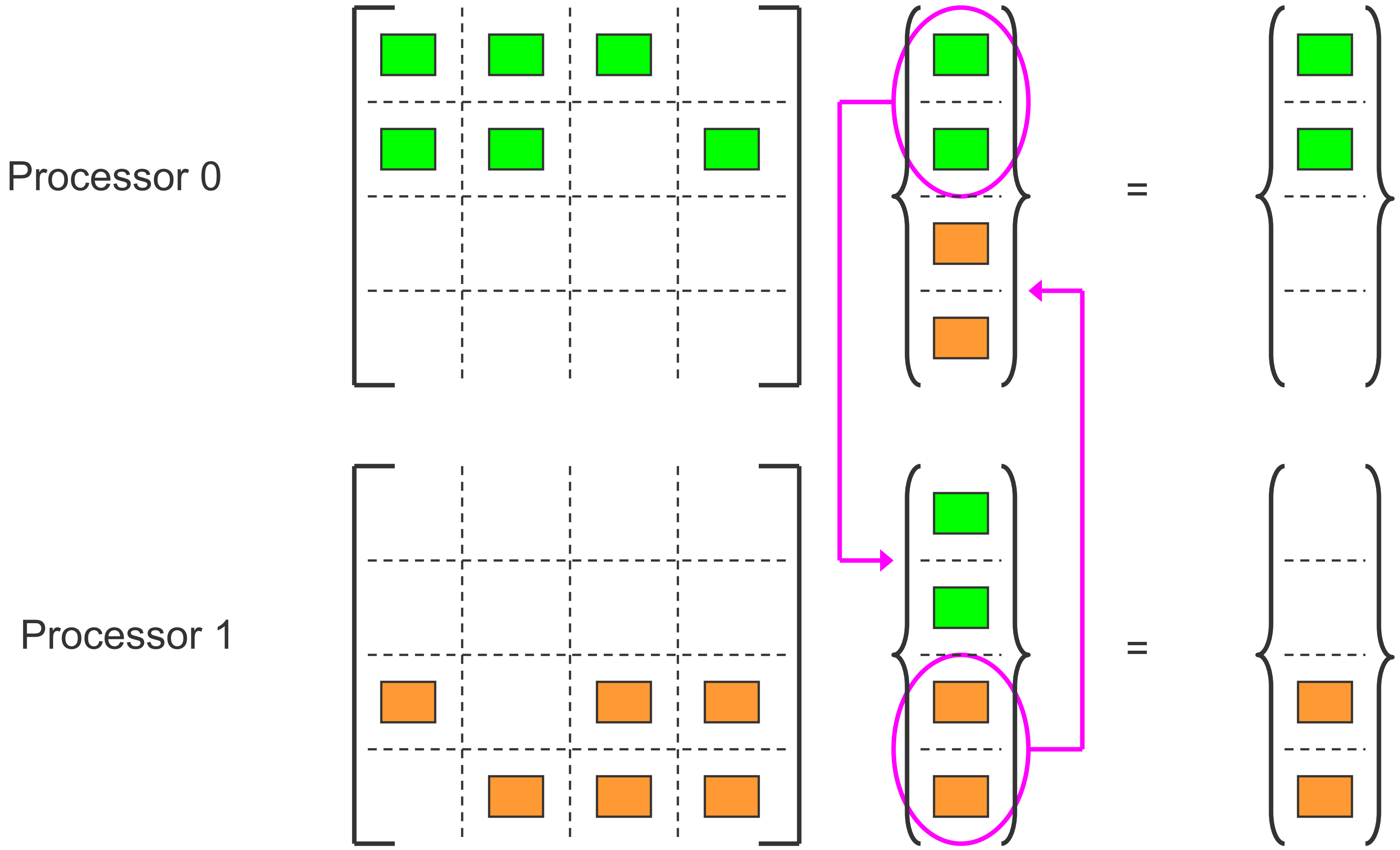
Processor 0



Processor 1

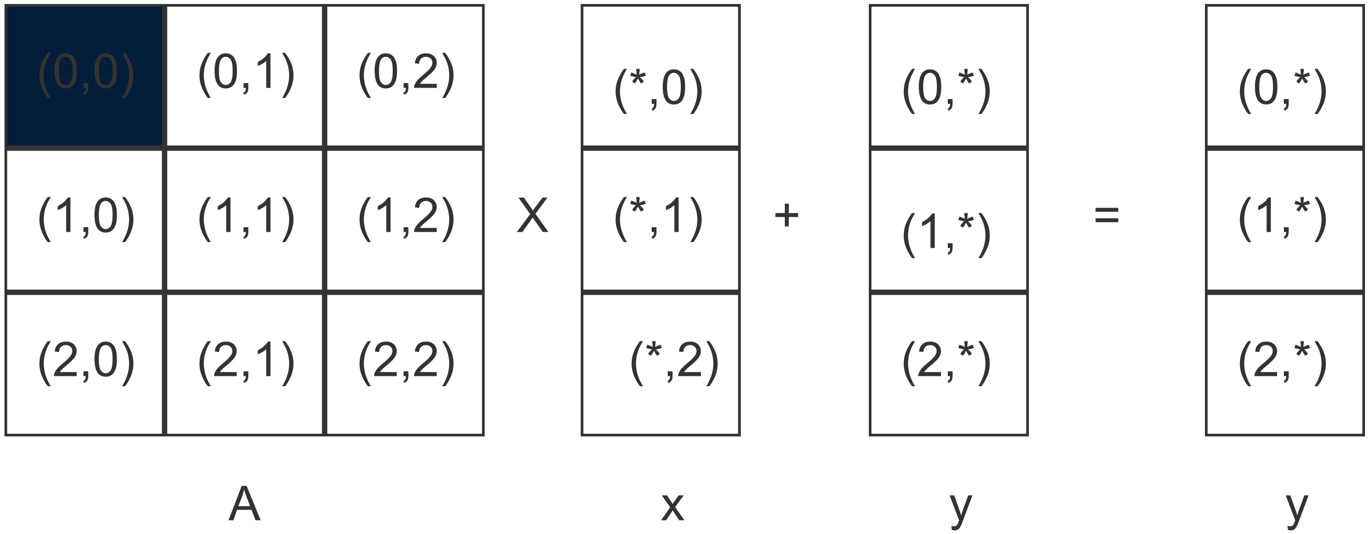


Parallel M-V Multiplication



Data Mapping Scheme

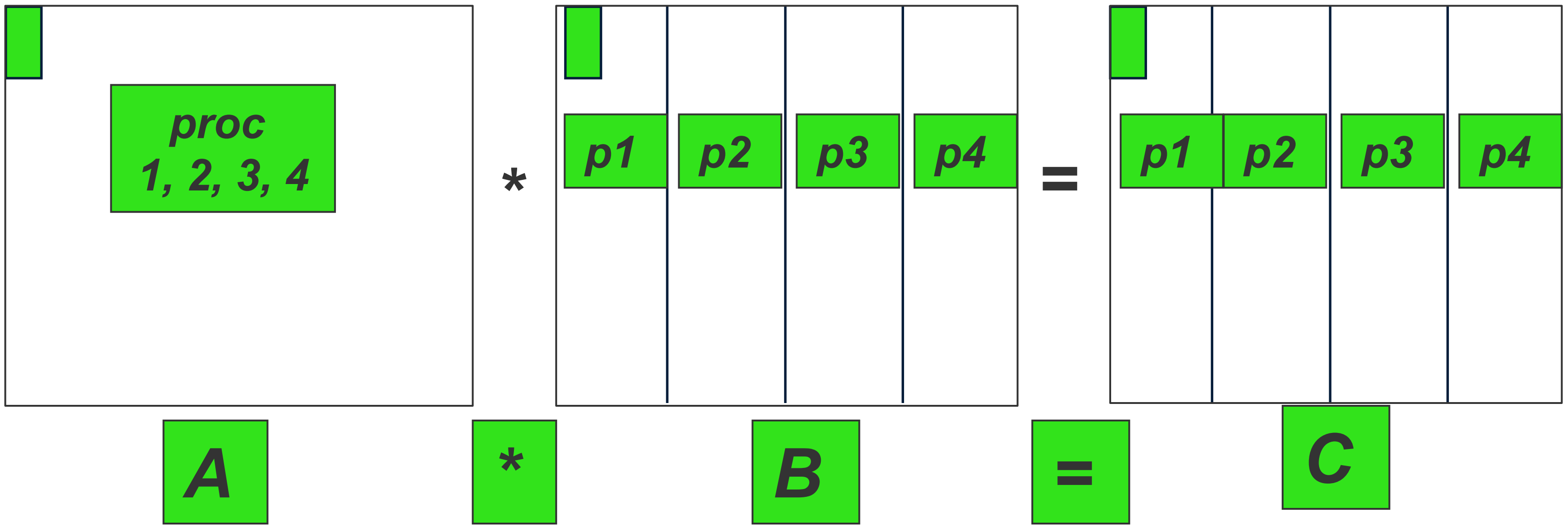
- **The matrix A can be distributed to processors in a** checkerboard partition**, a two dimensional block-block distribution.**



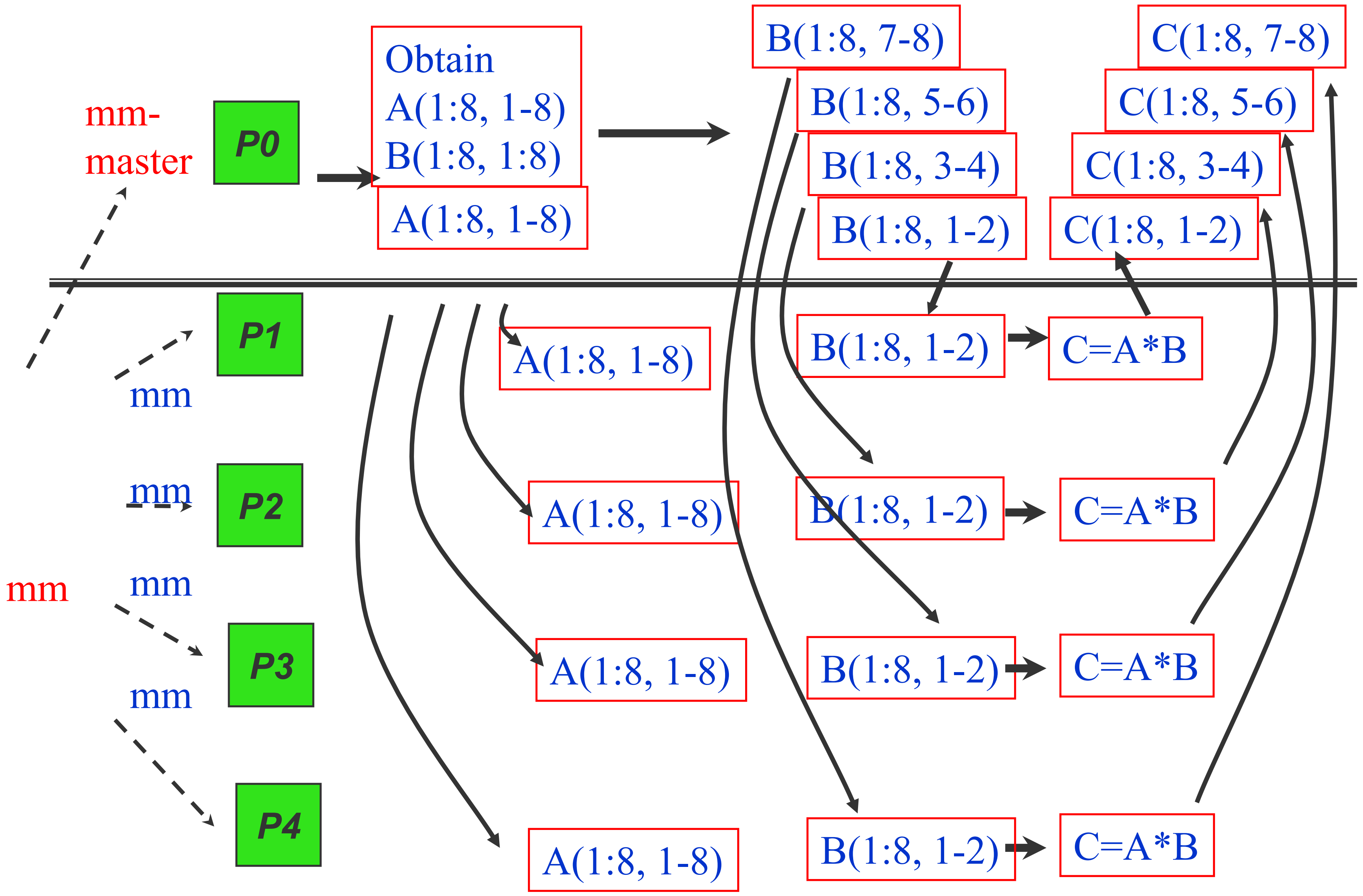
- For an nxn matrix, n^2 processors can be used. The vector x is distributed to the processors sharing the same column number. The partial products computed for each row are added together to obtain the resultant vector y.
- This mapping scheme scales more efficiently because a larger number of processors can be used, however, it requires additional amount of communication work.

Simple Matrix Multiplication Algorithm

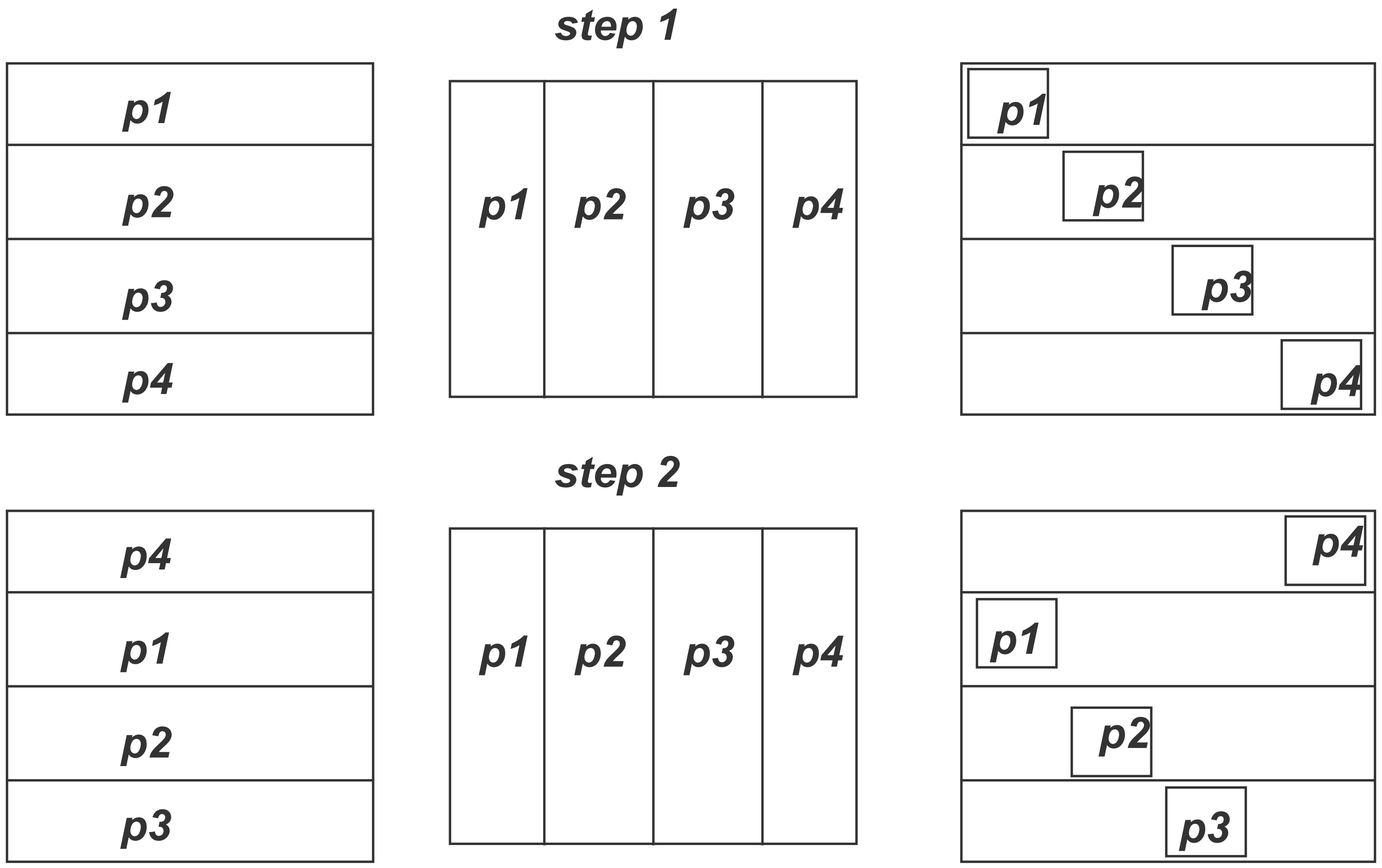
- Matrix A is copied to every processors (FORTRAN)
- Matrix B is divided into blocks and distributed to processors
- Perform matrix multiplication simultaneously
- Output solutions



Parallel Processing

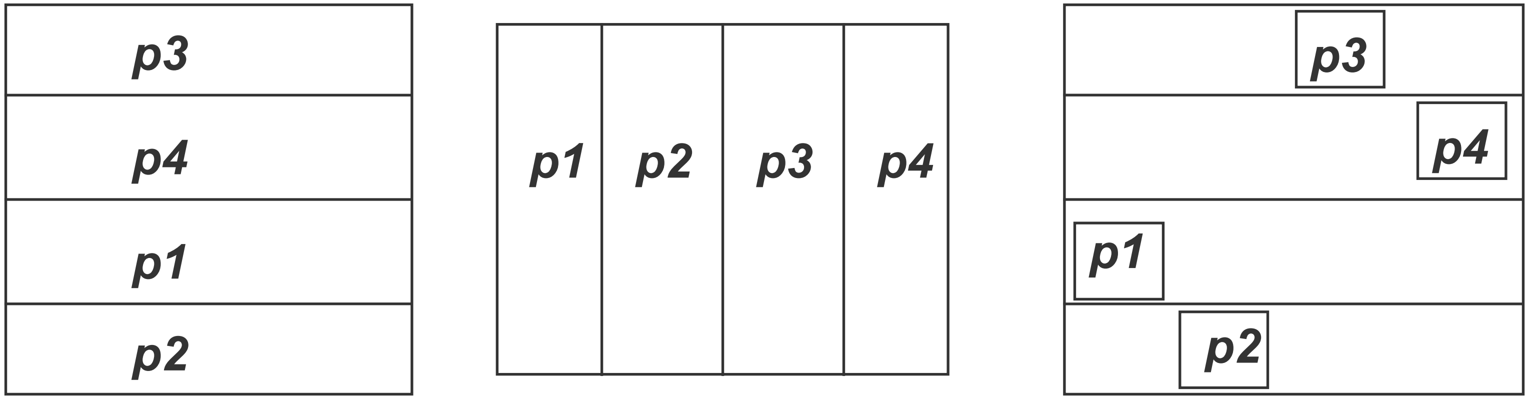


Matrix Multiplication

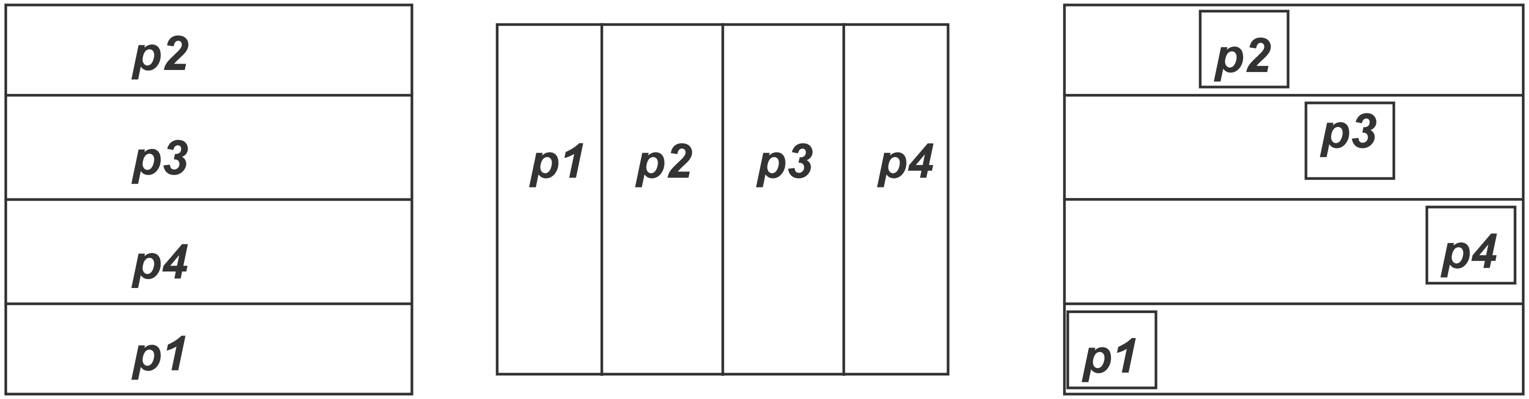


Matrix Multiplication (continued)

step 3

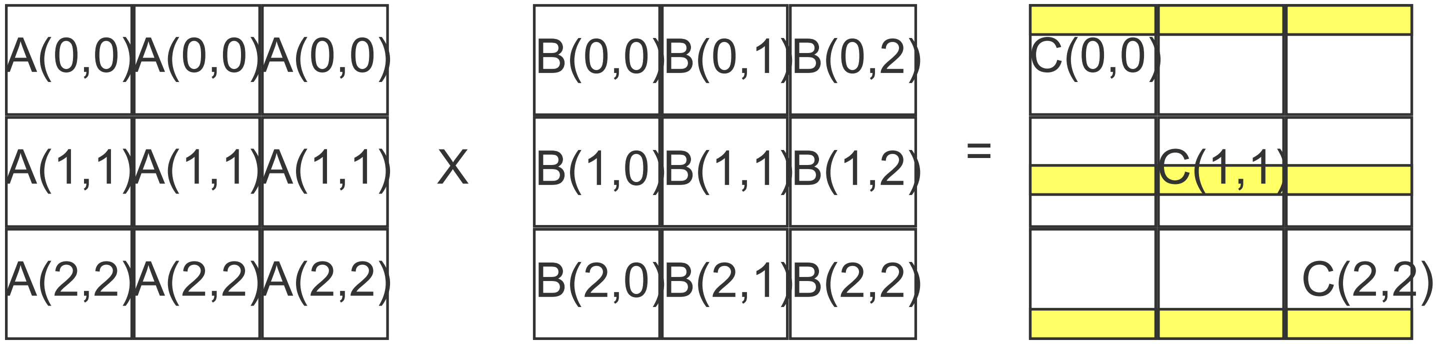


step 4



Fox's Algorithm (1)

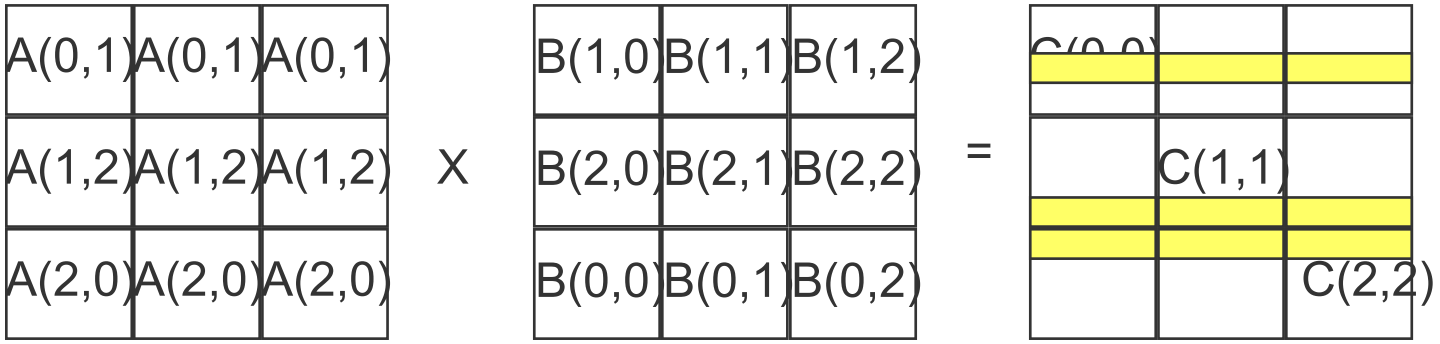
- **Broadcast the diagonal element of block A in rows, perform multiplication.**



- C(0,0) = A(0,0)*B(0,0) + A(0,1)*B(1,0) + A(0,2)*B(2,0)
- C(0,1) = A(0,0)*B(0,1) + A(0,1)*B(1,1) + A(0,2)*B(2,1)
- C(0,2) = A(0,0)*B(0,2) + A(0,1)*B(1,2) + A(0,2)*B(2,2)
- C(1,0) = A(1,0)*B(0,0) + A(1,1)*B(1,0) + A(1,2)*B(2,0)
- C(1,1) = A(1,0)*B(0,1) + A(1,1)*B(1,1) + A(1,2)*B(2,1)
- C(1,2) = A(1,0)*B(0,2) + A(1,1)*B(1,2) + A(1,2)*B(2,2)
- C(2,0) = A(2,0)*B(0,0) + A(2,1)*B(1,0) + A(2,2)*B(2,0)
- C(2,1) = A(2,0)*B(0,1) + A(2,1)*B(1,1) + A(2,2)*B(2,1)
- C(2,2) = A(2,0)*B(0,2) + A(2,1)*B(1,2) + A(2,2)*B(2,2)

Fox's Algorithm (2)

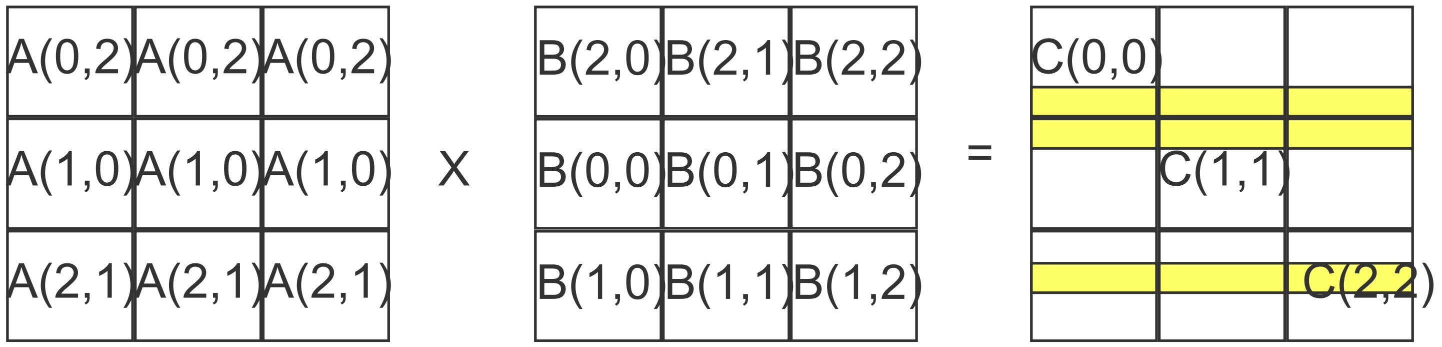
- **Broadcast next element of block A in rows, shift Bij in column, perform multiplication.**



- C(0,0) = A(0,0)*B(0,0) + A(0,1)*B(1,0) + A(0,2)*B(2,0)
- C(0,1) = A(0,0)*B(0,1) + A(0,1)*B(1,1) + A(0,2)*B(2,1)
- C(0,2) = A(0,0)*B(0,2) + A(0,1)*B(1,2) + A(0,2)*B(2,2)
- C(1,0) = A(1,0)*B(0,0) + A(1,1)*B(1,0) + A(1,2)*B(2,0)
- C(1,1) = A(1,0)*B(0,1) + A(1,1)*B(1,1) + A(1,2)*B(2,1)
- C(1,2) = A(1,0)*B(0,2) + A(1,1)*B(1,2) + A(1,2)*B(2,2)
- C(2,0) = A(2,0)*B(0,0) + A(2,1)*B(1,0) + A(2,2)*B(2,0)
- C(2,1) = A(2,0)*B(0,1) + A(2,1)*B(1,1) + A(2,2)*B(2,1)
- C(2,2) = A(2,0)*B(0,2) + A(2,1)*B(1,2) + A(2,2)*B(2,2)

Fox's Algorithm (3)

- Broadcast next element of block A in rows, shift Bij in column, perform multiplication.



- C(0,0) = A(0,0)*B(0,0) + A(0,1)*B(1,0) + A(0,2)*B(2,0)
- C(0,1) = A(0,0)*B(0,1) + A(0,1)*B(1,1) + A(0,2)*B(2,1)
- C(0,2) = A(0,0)*B(0,2) + A(0,1)*B(1,2) + A(0,2)*B(2,2)
- C(1,0) = A(1,0)*B(0,0) + A(1,1)*B(1,0) + A(1,2)*B(2,0)
- C(1,1) = A(1,0)*B(0,1) + A(1,1)*B(1,1) + A(1,2)*B(2,1)
- C(1,2) = A(1,0)*B(0,2) + A(1,1)*B(1,2) + A(1,2)*B(2,2)
- C(2,0) = A(2,0)*B(0,0) + A(2,1)*B(1,0) + A(2,2)*B(2,0)
- C(2,1) = A(2,0)*B(0,1) + A(2,1)*B(1,1) + A(2,2)*B(2,1)
- C(2,2) = A(2,0)*B(0,2) + A(2,1)*B(1,2) + A(2,2)*B(2,2)

Collective Communications

- Substitutes for a more complex sequence of p-p calls
- Involve all the processes in a process group
- Called by all processes in a communicator
- All routines block until they are locally complete
- Receive buffers must be exactly the right size
- No message tags are needed
- Divided into three subsets :
  - synchronization, data movement, and global computation

Barrier Synchronization Routines

- To synchronize all processes within a communicator
- A node calling it will be blocked until all nodes within the group have called it.
- C:

```
ierr = MPI_Barrier(comm)
```

- Fortran:

```
call MPI_Barrier(comm, ierr)
```

Broadcast

- one processor sends some data to all processors in a group
- C

  ```
  ierr = MPI_Bcast(buffer, count, datatype, root, comm)
  ```

- Fortran

  ```
  call MPI_Bcast(buffer,count,datatype, root, comm, ierr)
  ```

- The MPI_Bcast must be called by each node in a group, specifying the same communicator and root. The message is sent from the root process to all processes in the group, including the root process.

Scatter

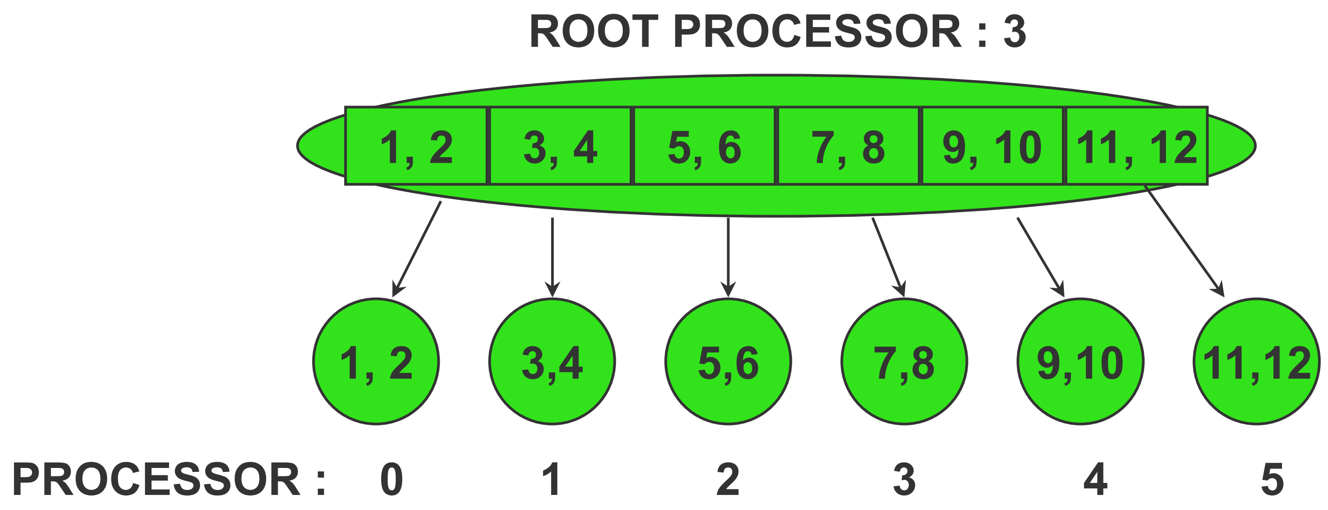
- Data are distributed into n equal segments, where the ith segment is sent to the ith process in the group which has n processes.
- C :

```
ierr = MPI_Scatter(&sbuff, scount, sdatatype, &rbuf, rcount,
    rdatatype, root, comm)
```

- Fortran :

```
call MPI_Scatter(sbuff, scount, sdatatype, rbuf, rcount,
    rdatatype, root , comm, ierr)
```

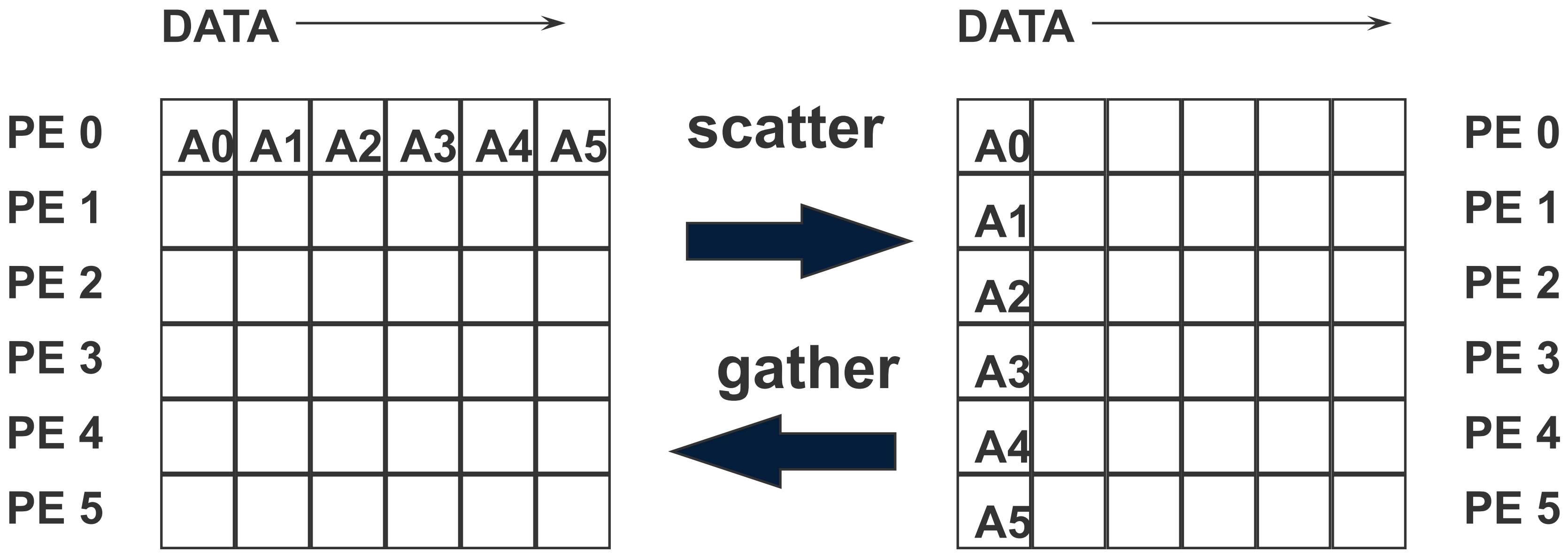
Example : Scatter



```
real sbuf(12), rbuf(2)

call MPI_Scatter(sbuf, 2, MPI_INT, rbuf, 2, MPI_INT, 3,
    MPI_COMM_WORLD, ierr)
```

Scatter and Gather



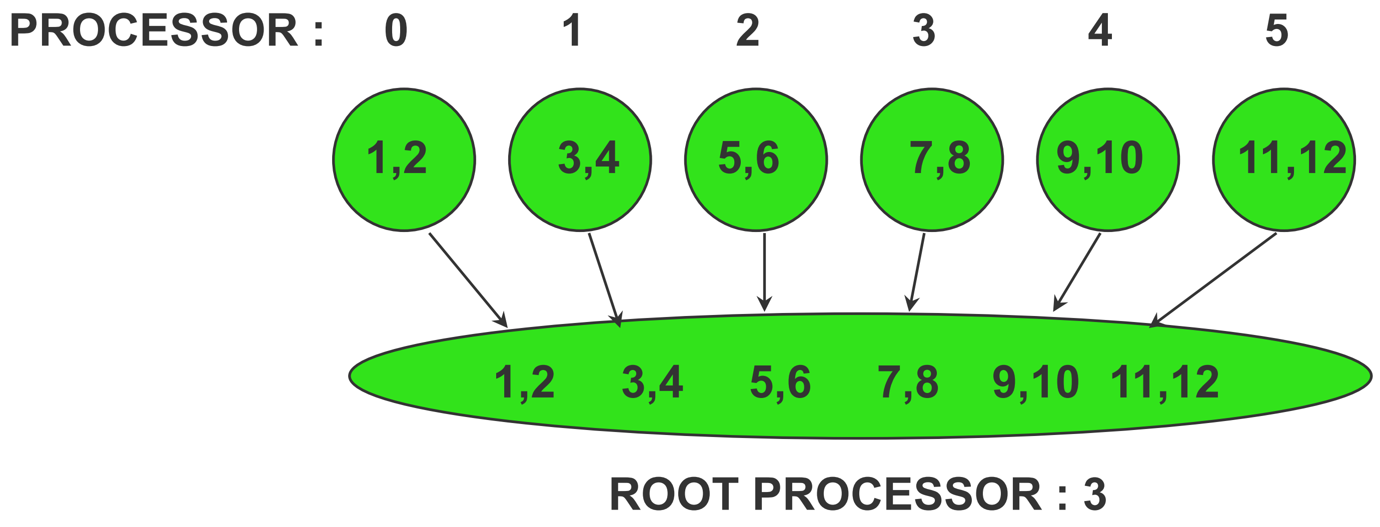
Gather

- Data are collected into a specified process in the order of process rank, reverse process of scatter.
- C :

  ierr = MPI_Gather(&sbuf, scount, sdtatatype, &rbuf, rcount, rdatatype, root, comm)
- Fortran :

  call MPI_Gather(sbuff, scount, sdatatype, rbuff, rcount, rdtatatype, root, comm, ierr)

Example : Gather



```
real sbuf(2),rbuf(12)

call MPI_Gather(sbuf,2,MPI_INT, rbuf, 2, MPI_INT, 3,
    MPI_COMM_WORLD, ierr)
```

Scatterv and Gatherv

- allow varying count of data and flexibility for data placement
- C :

  ```
  ierr = MPI_Scatterv( &sbuf, &scount, &displace, sdatatype,
      &rbuf, rcount, rdatatype, root, comm)
  ```

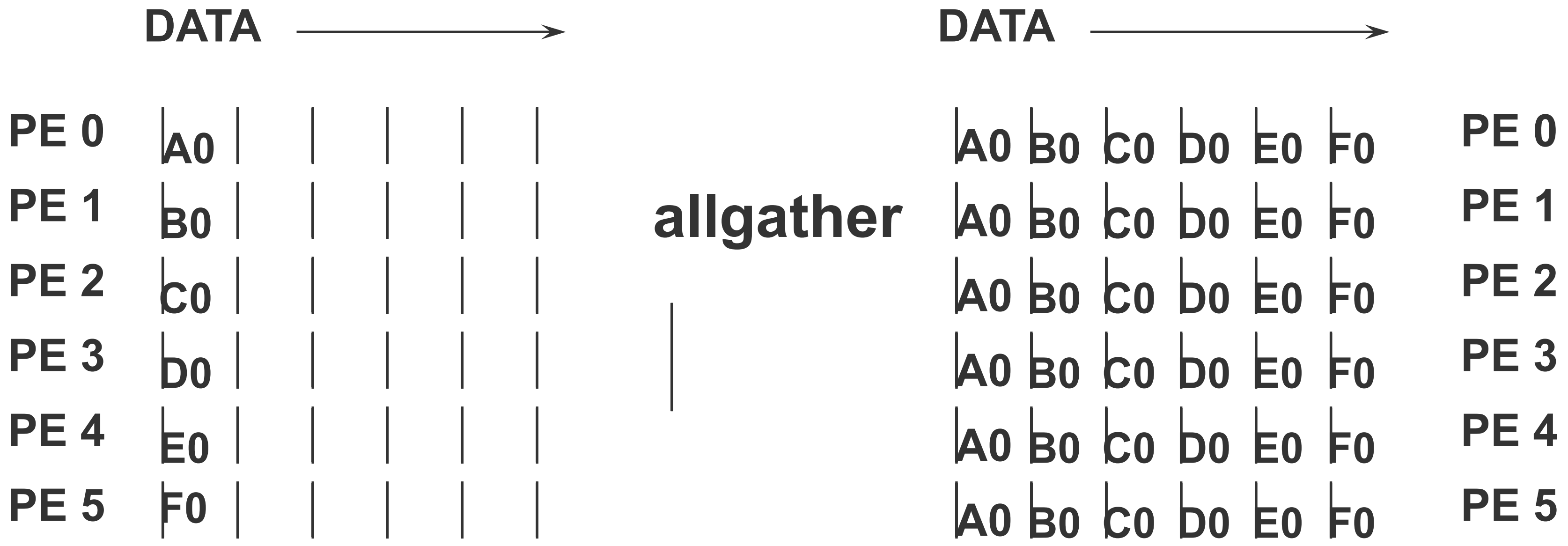
  ```
  ierr = MPI_Gatherv(&sbuf, scount, sdatatype, &rbuf, &rcount,
      &displace, rdatatype, root, comm)
  ```

- Fortran :

  ```
  call MPI_Scatterv(sbuf,scount,displace,sdatatype, rbuf, rcount,
      rdatatype, root, comm, ierr)
  ```

Allgather

ierr = MPI_Allgather(&sbuf, scount, stype,&rbuf, rcount, rtype, comm)

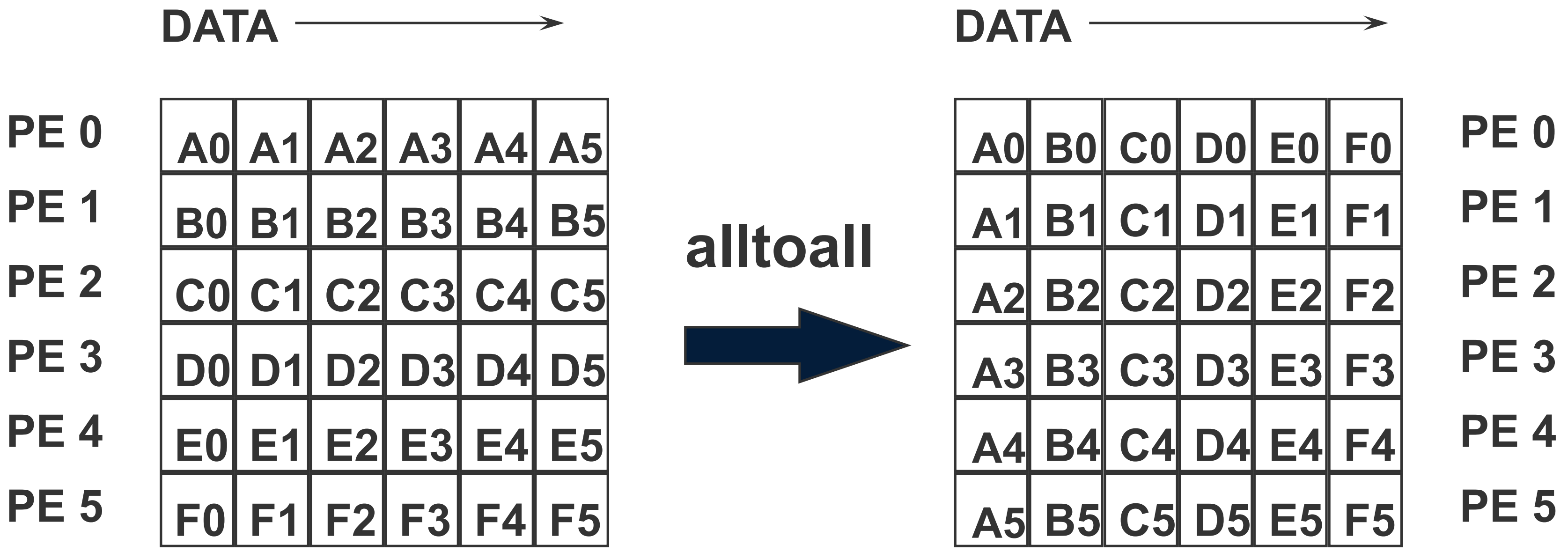


All to All

MPI_Alltoall(sbuf, scount, stype, rbuf, rcount, rtype, comm)

sbuf :	starting address of send buffer (*)
scount :	number of elements sent to each process
stype :	data type of send buffer
rbuff :	address of receive buffer (*)
rcount :	number of elements received from any process
rtype :	data type of receive buffer elements
comm :	communicator

All to All


DATA
PE 0
PE 1
PE 2
PE 3
PE 4
PE 5
A0 A1 A2 A3 A4 A5
B0 B1 B2 B3 B4 B5
C0 C1 C2 C3 C4 C5
D0 D1 D2 D3 D4 D5
E0 E1 E2 E3 E4 E5
F0 F1 F2 F3 F4 F5
alltoall
DATA
A0 B0 C0 D0 E0 F0
A1 B1 C1 D1 E1 F1
A2 B2 C2 D2 E2 F2
A3 B3 C3 D3 E3 F3
A4 B4 C4 D4 E4 F4
A5 B5 C5 D5 E5 F5
PE 0
PE 1
PE 2
PE 3
PE 4
PE 5

Global Reduction Routines

- The partial result in each process in the group is combined together using some desired function.
- The operation function passed to a global computation routine is either a predefined MPI function or a user supplied function
- Examples :
  - global sum or product
  - global maximum or minimum
  - global user-defined operation

Reduce and Allreduce

- **MPI_Reduce(sbuf, rbuf, count, stype, op, root, comm)**
- **MPI_Allreduce(sbuf, rbuf, count, stype, op, comm)**

sbuf :	address of send buffer
rbuf :	address of receive buffer
count :	the number of elements in the send buffer
stype :	the datatype of elements of send buffer
op :	the reduce operation function, predefined or user-defined
root :	the rank of the root process
comm :	communicator

-- mpi_reduce returns results to single process

-- mpi_allreduce returns results to all processes in the group

Predefined Reduce Operations

MPI NAME	FUNCTION	MPI NAME	FUNCTION
MPI_MAX	Maximum	MPI_LOR	Logical OR
MPI_MIN	Minimum	MPI_BOR	Bitwise OR
MPI_SUM	Sum	MPI_LXOR	Logical exclusive OR
MPI_PROD	Product	MPI_BXOR	Bitwise exclusive OR
MPI_LAND	Logical AND	MPI_MAXLOC	Maximum and location
MPI_LOR	Bitwise AND	MPI_MINLOC	Minimum and location

Example of Reduce w/Sum

```
c     A routines that computes the dot product of two vectors that are distributed
c   across a group of processses and returns the answer to node zero
      subroutine PAR_BLAS1( m , a , b , c , comm)
      real a(m) , b(m) , sum , c
      integer m , comm , I , ierr

      sum = 0.0
      do I = 1 , m
         sum = sum + a( I ) * b ( I )
      end do

      call MPI_Reduce( sum , c , 1 , MPI_REAL , MPI_SUM,0, comm , ierr )
      return
```

Derived Datatypes

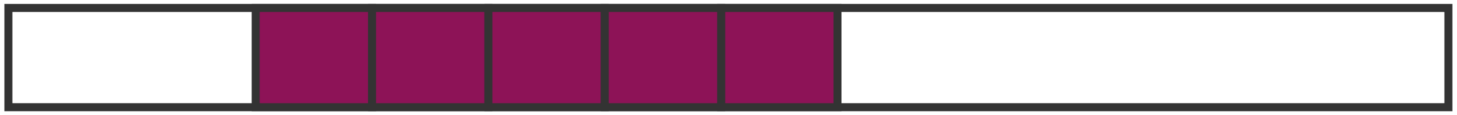
- To provide a portable and efficient way of communicating non-contiguous or mixed types in a message
- datatypes that are built from the basic MPI datatypes.
- MPI datatypes are created at run-time through calls to MPI library
- Steps required
  - construct the datatype : define shapes and handle
  - allocate the datatype : commit types
  - use the datatype : use constructors
  - deallocate the datatype : free types

Datatypes

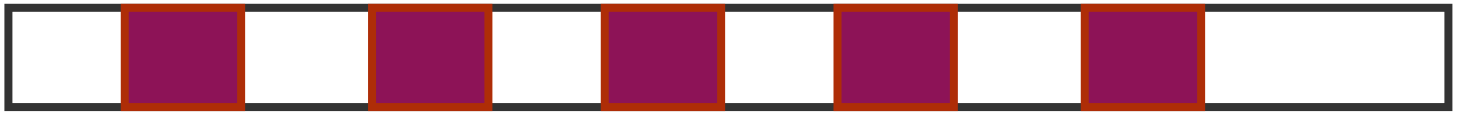
- Basic datatypes :
  - MPI_INT, MPI_REAL, MPI_DOUBLE, MPI_COMPLEX,
  - MPI_LOGICAL, MPI_CHARACTER, MPI_BYTE ….
- MPI also supports array sections and structures through general datatypes. A general datatypes is a sequence of basic datatypes and integer byte displacements. These displacements are taken to be relative to the buffer that the basic datatype is describing. ==> *typemap*
  - Datatype = { (type0, disp0) , (type1, disp1) , ….., (typeN, dispN)}

Defining Datatypes

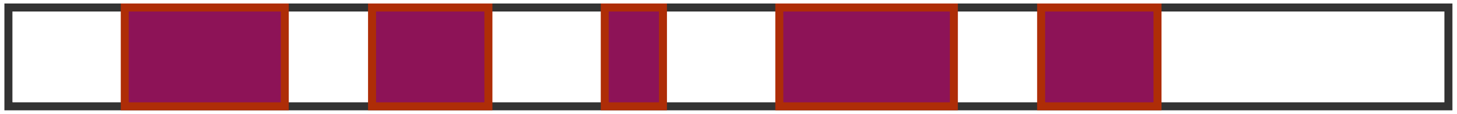
MPI_Type_contiguous(count,oldtype,newtype,ierr)
- ‘count’ copies of ‘oldtype’ are concatenated



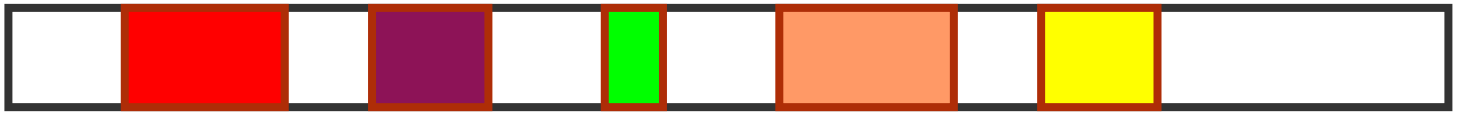
MPI_Type_vector(count, buffer, strides, oldtype,newtype,ierr)
- ‘count’ blocks with ‘blen’ elements of ‘oldtype’ spaced by ‘stride’



MPI_Type_indexed(count, buffer, strides, oldtype,newtype,ierr)
- Extension of vector: varying ‘blens’ and ‘strides’



MPI_Type_struct(count, buffer, strides, oldtype,newtype,ierr)
-extension of indexed: varying data types allowed

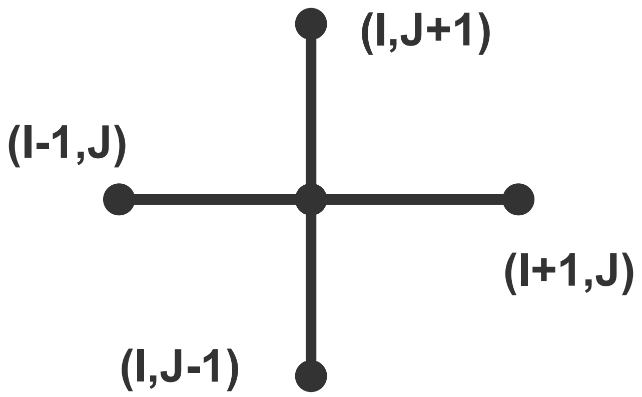


Parallel Code Development

Example : Laplace Equation

$$\nabla^2 T = \frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} = 0$$

5- POINT FD STENCIL



POINT JACOBI ITERATION

```
T( I , J ) =  0.25 * { Told( I -1 , J  )
                       +( Told( I+1 , J )
                       +( Told( I , J  -1 )
                       +( Told( I , J + 1) }
```

Codes

Initial guess : T = 0 ,

Boundaries : T = 100 ,

Grid : 1000x1000

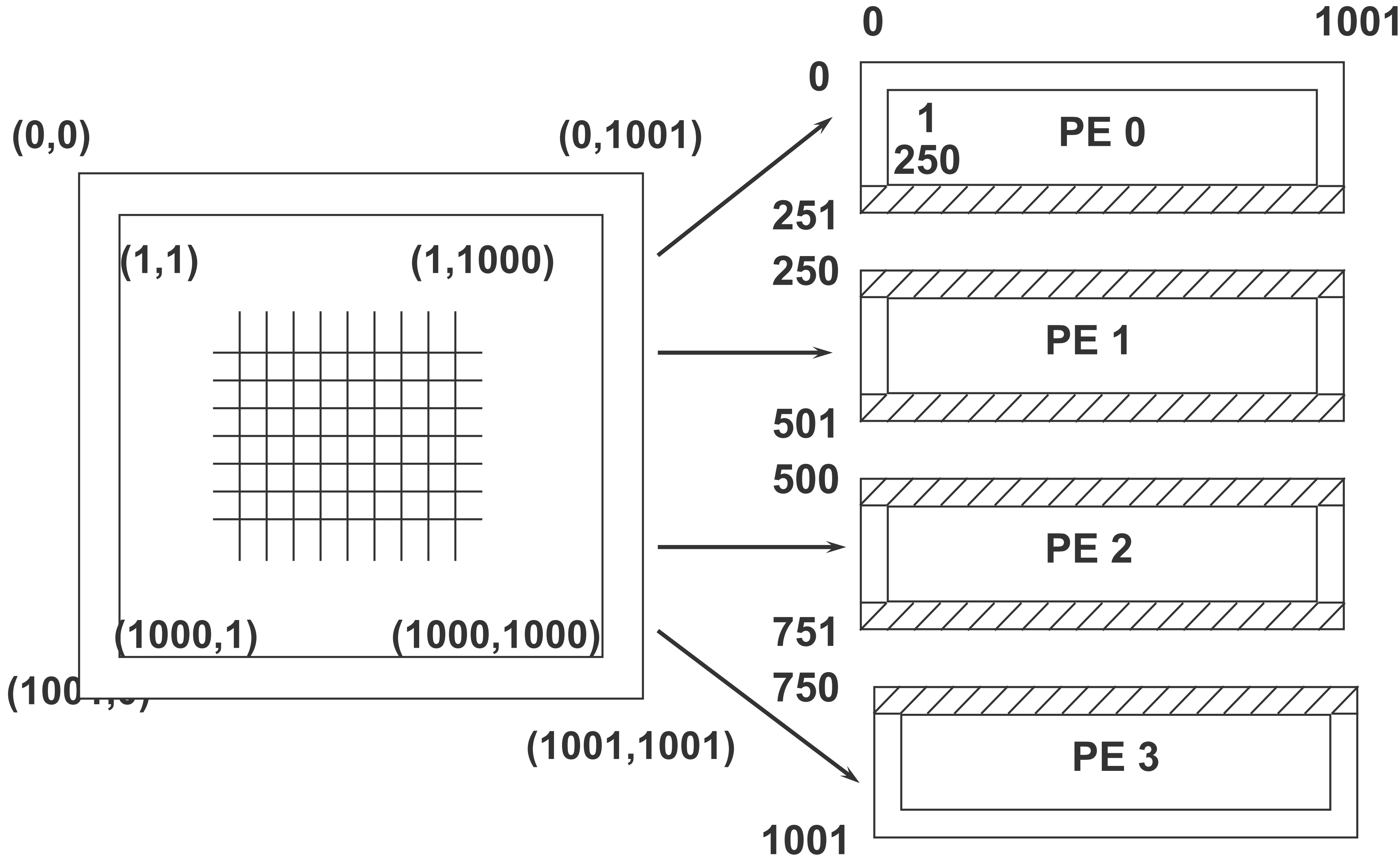
Fortran :

```
Do J = 1 , NC
  Do I = 1 , NR
  T ( I , J ) = 0.25 * (Told ( I -1 ,J ) + Told ( I + 1 ,J) + Told( I , J-1 ) + Told(I, J+1) )
  end do
end do
```

C :

```
for  ( I=1 ;  I <=NR ;  I++)
  for (j=1 ; j <= NC ; j++ )
  T[I][j] = 0.25*( Told[I+1][j]  + Told[I-1][j] + Told[I][j+1] + Told[I][j-1] );
```

Domain Decomposition



Program formulation

- Include file
- Initialization
- processor information
- Iteration : {
  - do averaging
  - copy T into Told
  - send values down
  - send values up
  - receive values from above
  - receive values from below
  - find the max change
  - synchronize }

Processor Information

- **Header:**

  #include <mpi.h> or include ‘mpif.h’

- **Initialization :**

  call MPI_Init(ierr)

  ierr = MPI_Init(& argc, & argv)

- **Number of processors:**

  call MPI_Comm_size(MPI_COMM_WORLD, npes, ierr)

  ierr = MPI_Comm_size(MPI_COMM_WORLD, &npes)

- **Processor number :**

  call MPI_Comm_rank(MPI_COMM_WORLD, mype, ierr)

  ierr= MPI_Comm_rank(MPI_COMM_WORLD, &mype)

Initialization

Serial (interior)

```
for (I = 0 ; I <= NR + 1 ; I ++)
      for ( J = 0 ; <= NC +1 ; J++)
                T[I][J] = 0. 0;


do I = 0 , NR +1
      do J =0 , NC + 1
                T( I, J ) = 0.0
      enddo
enddo
```

Parallel (boundaries)

```
/* Left and right boundaries */
for (I = 0; I <= NRL + 1; I++) {
        T[I][0] = 100.0;
        T[I][NCL+1] =100.0; }


/*Top and Bottom Boundaries*/
if (MYPE == 0)
        for (J = 0; J <=NCL+1; j++)
                T[0][J] = 100.0;
if (MYPE == NPES - 1)
        for (J = 0 ; J <= NCL +1 ; J++)
                T[NRL+1][J] = 100.0
```

Do Averaging

NRL : NR / NPES

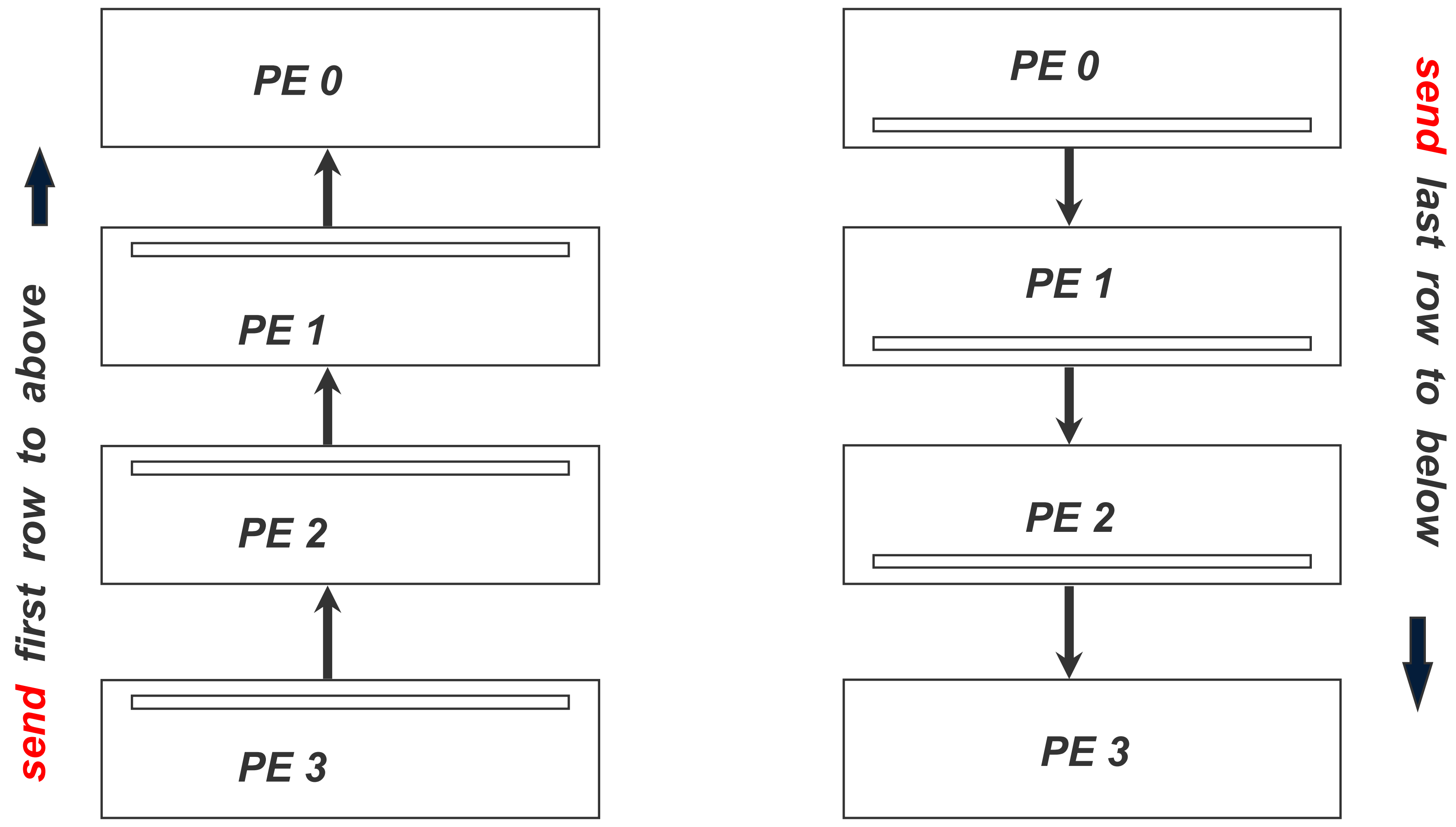
Fortran :

```
          Do J = 1 , NC
            Do I = 1 , NRL
            T ( I , J ) = 0.25 * (Told ( I -1 ,J ) + Told ( I + 1 ,J) + Told( I , J-1
)                   + Told(I, J+1) )
            end do
          end do
```

C :

```
          for  ( I=1 ;  I <=NRL ;  I++)
            for (j=1 ; j <= NC ; j++ )
            T[I][j] = 0.25*( Told[I+1][j]  + Told[I-1][j] + Told[I][j+1] +
                    Told[I][j-1] );
```

Parallel Send



Updating T Values at Domain Boundaries (Send)

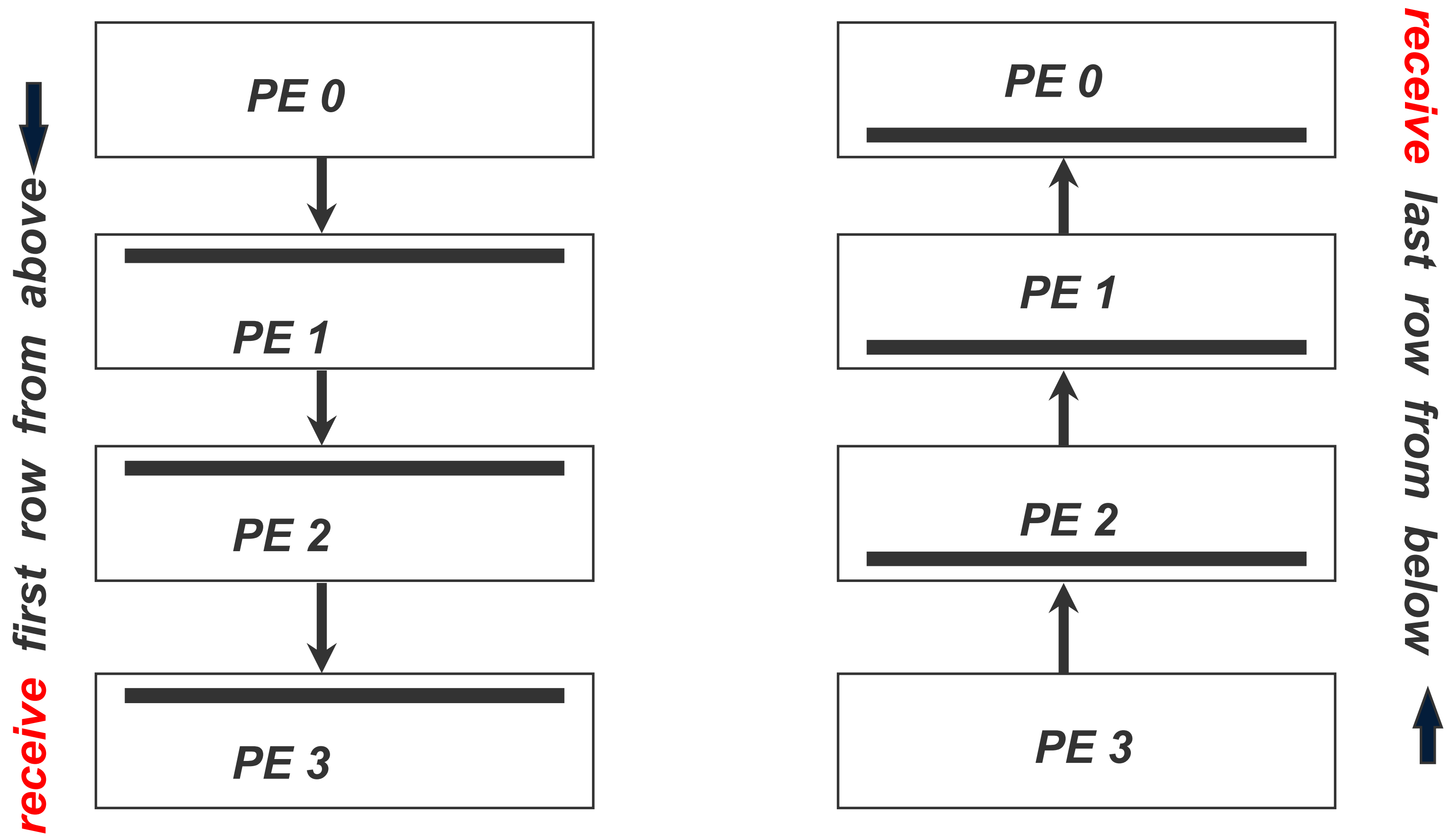
Sending up :

```
If (mype != 0 )    MPI_Send( &t[1][1], NC, MPI_FLOAT, mype-1, UP,
              MPI_COMM_WORLD )
```

Sending down :

```
If (mype < npes-1 )    MPI_Send( &t[NRL][1], NC, MPI_FLOAT, mype+1, UP,
     MPI_COMM_WORLD)
```

Parallel Template : Receive



Updating Values at Domain Boundaries (Receive)

Receiving from up :

```
If (mype != 0 )    MPI_Recv( &t[0][1], NC, MPI_FLOAT,
     MPI_ANY_SOURCE, DOWN, &status, MPI_COMM_WORLD )
```

Receiving from down :

```
If (mype  != npes-1 )    MPI_Recv( &t[NRL+1][1], NC, MPI_FLOAT,
     MPI_ANY_SOURCE, UP, &status, MPI_COMM_WORLD)
```

Find Maximum Change

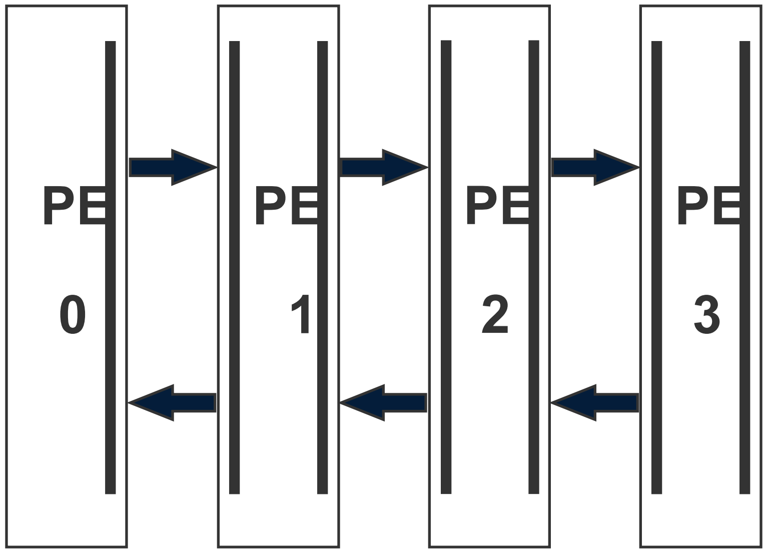
- each processor finds its own maximum change, *dt*
- find the global change using reduce, *dtg*

```
MPI_Reduce (&dt, &dtg, 1, MPI_FLOAT, MPI_MAX, PE0, comm)
call MPI_Reduce( dt, dtg, 1, MPI_FIOAT, MPI_MAX, PE0, comm, ierr)
```

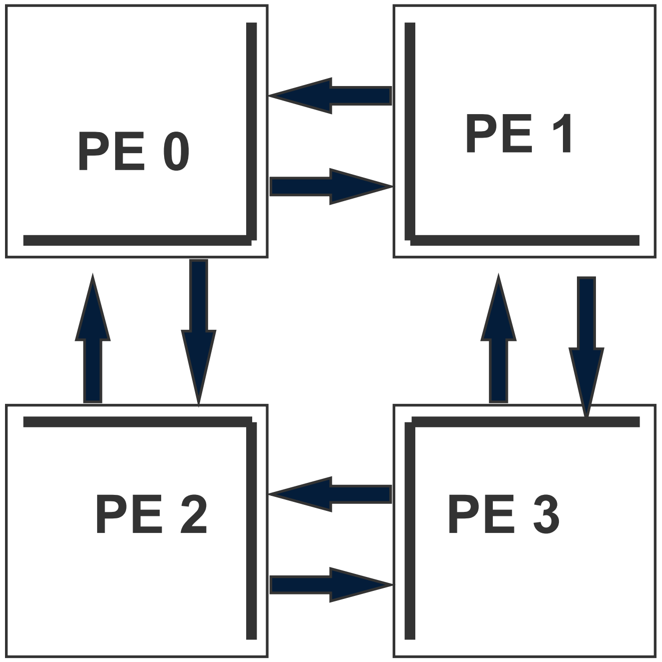
- synchronization :

```
MPI_Barrier(MPI_COMM_WORLD)
call MPI_Barrier(MPI_COMM_WORLD, ierr)
```

Data Distribution



Columnwise domain decomposition with grid overlap (FORTRAN)



X-Y 2Ddomain decomposition with grid overlap

Performance Evaluation of Codes

- Profiling of codes
  - Use profiling tools, e.g. prof, to identify segment of code that requires intensively computing
  - craypat on the XT5
- Timing codes
  - timers depend on machines platform
  - $ time *executable* ---> cpu time, elapsed time
  - etime, dtime, ctime, itime
  - should provide good timing resolution for section of codes
- MPI timer
  - MPI_Wtime() ---> return seconds of elapse wall-clock time
  - MPI_Wtick() ----> return value of seconds between successive clock ticks

Communication Issues

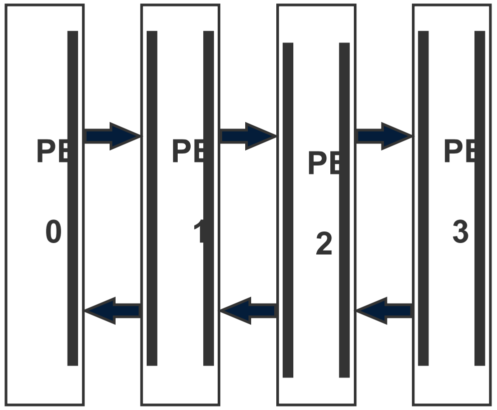
- Contentions, or traffic jams
  - Have good distribution of messages. Circular or round-robin methods in one or two dimensions are fairly efficient for certain problems.
  - Avoid as much as possible the use of indirect addressing.
  - Use threads on multicore
- Ready mode in MPI or post receive before send
  - use MPI_Rsend when you are *sure* that a matching receive (MPI_Recv) has been posted appropriately
  - this allows faster transfer protocols
  - -HOWEVER! behavior is undefined if receive was not posted in time!
  - Post receive before send on Cray
- Mask communication with computation
  - Use asynchronous mode,
  - Avoid barrier

I/O and Parallel I/O

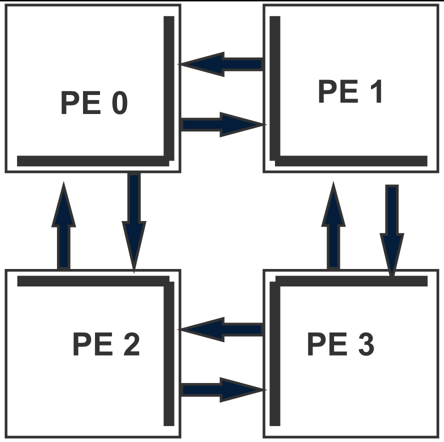
- I/O can be a serious bottleneck for certain applications. The time to read/write data to disks could be an issue. But sometimes the shear size of the data file is a problem.
- Parallel I/O systems allow (in theory) the efficient manipulation of huge files
- Unfortunately, parallel I/O is only available on some architectures, and software is not always good. (MPI-2 has parallel MPI-IO on ROMIO implementation)
- They are restricted to few (around 4 or so) parallel disk drives, through designated I/O nodes.
- On the IBM with GPFS
- Lustre on the CRAY XT5
- One single files vs file/process
- Using local /tmp for input output
- Progress is still needed in this area!

Mapping Problem

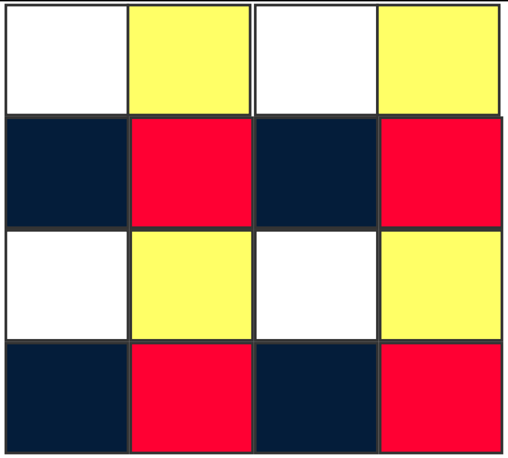
- Each processor should have a similar amount of work
- Expensive communications should be minimized.
- Communications should be:
  - eliminated where feasible
  - localized otherwise (i.e. communicate between close CPU neighbors) (not crucial anymore)
- Concurrency should be maximized
- NOTE: finding the best mapping is an NP-complete problem!   :-(



1D Decomposition



2D Decomposition


2D Block Cyclic

The End

Quote: “I think there is a world market for maybe five computers”
Thomas Watson, chairman of IBM, 1943