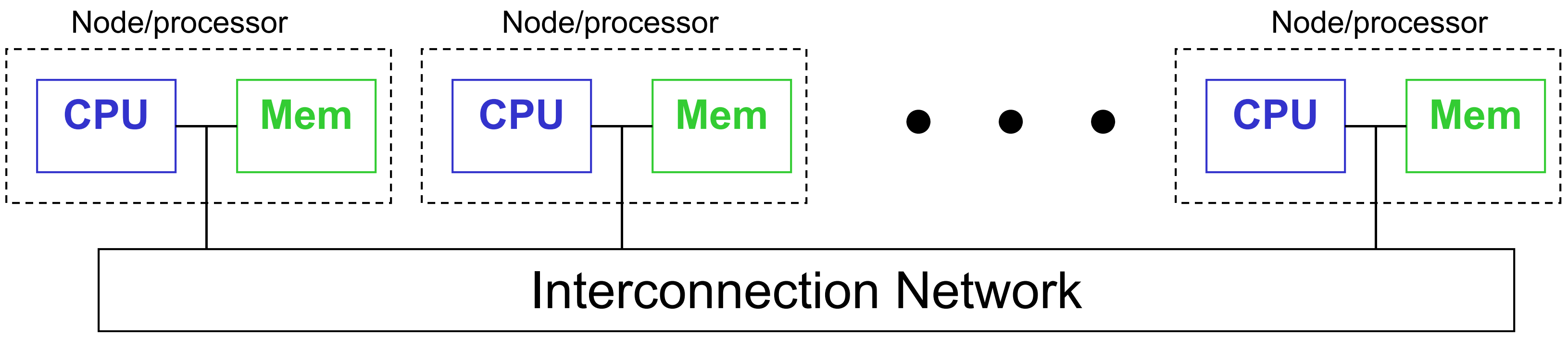
Lecture 6 – Introduction to MPI

- Some simple codes in Fortran and C
- Initialization and simple communicators
- Point to point communication
- Collective communication
- Derived datatypes
- Communicators and topology
- Examples

Message Passing Programming



- Each processor has its own private memory and address space
- The processors communicate with one another through the network
- Ideally, each node is directly connected to every other node → too expensive to build
- A compromise is to use crossbar switches connecting the processors
- Use simple topology: e.g. linear array, ring, mesh, hypercube
- Communication time is the bottleneck of message passing programming

Message Passing Programs

- **Separate processors**
- **Separate address spaces**
- **Processors execute independently and concurrently**
- **Processors transfer data cooperatively**
- **Single Program Multiple Data (SPMD)**
  - All processors are executing the same program, but act on different data
- **Multiple Program Multiple Data (MPMD)**
  - Each processor may be executing a different program
  - Ex: multi-disciplinary where some processors are running fluid, others heat conduction, others structures, etc.
- **Common software tools: PVM, MPI**

What is MPI?

- **Message-passing library specification (IEEE Standard)**
  - Message-passing model
  - Not a compiler specification
  - Not a specific product
- **For parallel computers, clusters, and heterogeneous networks**
- **Designed to permit the development of parallel software libraries**
- **Designed to provide access to advanced parallel hardware for**
  - End users
  - Library writers
  - Tool developers

Who Designed MPI?

- **Broad group of participants**
- **Vendors:**
  - IBM, Intel, TMC, Meiko, Cray, Convex, nCube
- **Library developers:**
  - PVM, p4, Zipcode, TCGMSG, Chameleon, Express, Linda
- **Application specialists and consultants**
  - Companies: ARCO, KAI, NAG, Parasoft, Shell,…
  - Labs: ANL, LANL, LLNL, ORNL, SNL,…
  - Universities: almost 20

Why Use MPI?

- **Standardization:**
  - The only message passing library which can be considered a standard
- **Portability:**
  - There is no need to modify the source when porting codes from one platform to another
- **Performance:**
  - Vendor implementations should be able to exploit native hardware to optimize performance
- **Availability:**
  - A variety of implementations are available, both vendor and public domain, e.g. MPICH implementation by ANL, OpenMP by openmp.org
- **Functionality:**
  - It provides around 200 subroutine/function calls

Features of MPI

- **General:**
  - Communicators combine context and group for message security
  - Thread safety
- **Point to point communication:**
  - Structured buffers and derived datatypes, heterogeneity
  - Modes: standard, synchronous, ready (to allow access to fast protocols), buffered
- **Collective communication:**
  - Both built-in and user defined collective operations
  - Large number of data movement routines
  - Sub-group defined directly or by topology

Is MPI Large or Small?

- **MPI is large – around 200 functions**
  - Extensive functionality requires many functions/subroutines
- **MPI is small – 6 basic functions**
  - MPI_Init: Initialize MPI
  - MPI_Comm_size: Find out how many processes there are
  - MPI_Comm_rank: Find out which process I am
  - MPI_Send: Send a message
  - MPI_Recv: Receive a message
  - MPI_Finalize: Terminate MPI
- **MPI is just right**
  - One can use its flexibility when it is required
  - One need not master all parts of MPI to use it

Example: Hello, World! C-Code

- #include “mpi.h” provides basic MPI definitions and types
- MPI_Init starts MPI
- MPI_Finalize exists MPI
- Note that all non-MPI routines are local; thus printf runs on each process.

```
#include “mpi.h”
#include <stdio.h>

int main(argc, argv)
int argc;
char **argv;
{
   MPI_Init(&argc, &argv);
   printf(“Hello, world!\n”);
   MPI_Finalize();
   return 0;
}
```

Example: “Advanced” Hello, World! C-Code

- **MPI_Comm_rank determines the proc id (0 to nproc-1)**
- **MPI_Comm_size determines the # of procs**
- **Note: for some parallel systems, only a few designated procs can do I/O. MPI-2 Standard defines API for parallel I/O**
- **What does the output look like?**

```
#include “mpi.h”
#include <stdio.h>

int main(argc, argv)
int argc;
char **argv;
{
    int rank, size;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    printf(“Hello, world! I am %d of %d\n”, rank, size);
    MPI_Finalize();
    return 0;
}
```

Example: Hello, World ! Fortran Code

```
program hello

   implicit real(kind=8) (a-h, o-z), integer(kind=4) (i-n)
   include "mpif.h"
   character*80 foo

   call MPI_Init(ierror)
   if(ierror/=0) then
     print*,'Problems initializing MPI'
     stop
   endif
   call MPI_Comm_Rank(MPI_COMM_WORLD,myid,ierror)
   if(ierror/=0) then
     print*,'Problem identifying myid',myid
     stop
   endif
   call MPI_Comm_Size(MPI_COMM_WORLD,nprocs,ierror)
   if(ierror/=0) then
     print*,'Problem identifying number of processors',nprocs
     stop
   endif
```

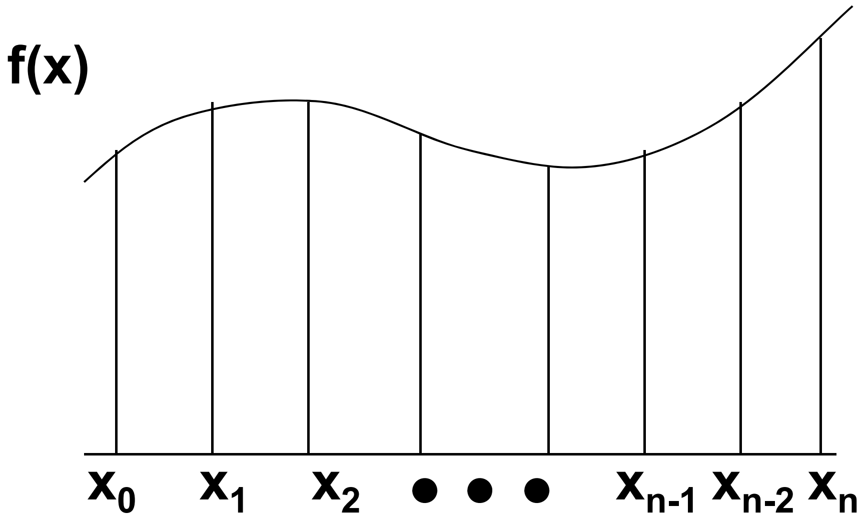
Example: Hello, World ! Fortran Code (cont)

```
if(myid==0) then
   open(unit=11,file='hellothere.txt',iostat=ierror)
   read(11,'(a80)') foo
endif

call MPI_Bcast(foo,80,MPI_CHARACTER,0,MPI_COMM_WORLD,ierror)

write(6,*) trim(foo), myid

call MPI_FINALIZE(ierror)

end program hello
```

Code is on smartsite: Codes/hello

Another Example: Calculate π

- **Well-known formula:** $$\int_0^1 \frac{4}{1+x^2}\,dx = \pi$$
- **Numerical integration (trapezoidal rule):**



$$\int_a^b f(x)\,dx \approx h\left[\frac{1}{2}f(x_0)+f(x_1)+\cdots f(x_{n-1})+\frac{1}{2}f(x_n)\right]$$

$$x_i = a + i\,h,\quad h = \frac{(b-a)}{n},\quad n = \#\text{ of intervals}$$

Calculate π Serial C-Code

- **A sequential function Trap(a,b,n) approximates the integral from a to b of f(x) using the trapizoidal rule with n sub-intervals:**

```
 int n;
double a,b,integral,pi;
a = 0.0;  /*DEFINE INTERVAL START*/
b = 1.0;  /*DEFINE INTERVAL STOP */
/*READ THE NUMBER OF SUB-INTERVALS */
printf("INPUT THE NUMBER OF SUB-INTERVALS");
scanf("%i",&n);
  integral = trapc(a,b,n)
  printf("PI = %d",integral)
return 0
```

```
double Trap(a,b,n) {
    f = 4./(1.+x*x);
    h = (b-a)/n;
    integral = (f(a)+f(b))/2;
    for (i=1; i<=n-1; i++) {
        x = a+i*h;
        integral = integral + f(x);
    }
    integral = h*integral;
    return integral;
}
```

Code is on smartsite: Codes/calcpi

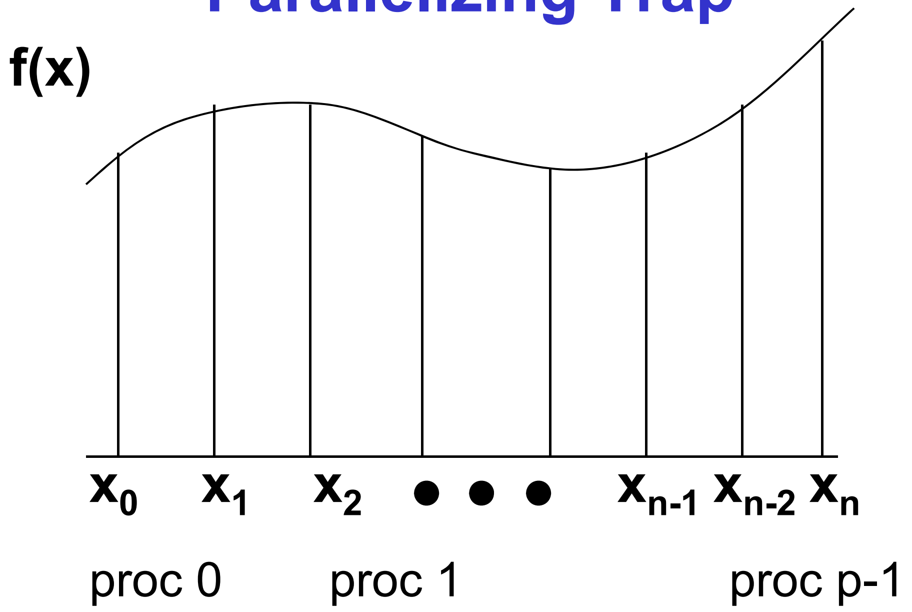
Calculate π Serial Fortran-Code

```
PROGRAM CALCPI
IMPLICIT NONE
REAL(kind=8) :: A,B,PI
INTEGER :: N
A = 0.0d0   !DEFINE INTERVAL START
B = 1.0d0   !DEFINE INTERVAL STOP
!READ THE NUMBER OF SUB-INTERVALS
PRINT *,'INPUT THE NUMBER OF SUB-INTERVALS'
READ(*,*) N
CALL TRAP(A,B,N,PI)
PRINT *,'PI = ',PI
STOP
END
```

```
 SUBROUTINE TRAP(A,B,N,INTEGRAL)
!CALCULATE INTEGRAL OF FUNCTION WITH &
 EVEN INTERVAL
IMPLICIT NONE
REAL(kind=8)  :: A,B,F,H,INTEGRAL,X
INTEGER :: N,I
F(X) = 4.0d0/(1.d0+X**2)             !FUNCTION
 DEFINITION
H(A,B,N) = (B-A)/REAL(N)     !INTERVAL DEFINITION
INTEGRAL = 0.5d0*(F(A)+F(B)) !INITIALIZE INTEGRAL
DO I = 1,N-1
  X = A + REAL(I)*H(A,B,N)
  INTEGRAL = INTEGRAL + F(X)
END DO
INTEGRAL = H(A,B,N)*INTEGRAL
RETURN
END
```

Code is on web: Codes/calcpi

Parallelizing Trap



- **Divide the interval [a,b] into p equal sub-intervals**
- **Each processor calculates the local approximate integral using the Trap routine simultaneously**
- **Finally, combine the local values to obtain the total integral.**

Calculate π Parallel Fortran Code

```
PROGRAM CALCPIP
IMPLICIT NONE

include "mpif.h"
REAL(kind=8)  :: A,AK,B,BK,H,PI,SUBPI
INTEGER :: K,MYID,N,NK,NPROCS
INTEGER :: IERROR,TAG,STATUS

! INITIALIZE MPI
CALL MPI_Init(IERROR)

! DETERMINE MY PROCESSOR ID
! ARGUMENTS: COMM, MYID, IERROR
CALL MPI_Comm_rank(MPI_COMM_WORLD,MYID,IERROR)

! FIND OUT HOW MANY PROCESSORS ARE USED
! ARGUMENTS: COMM, NPROCS, IERROR
CALL MPI_Comm_size(MPI_COMM_WORLD,NPROCS,IERROR)

IF(MYID == 0) THEN
  !READ THE NUMBER OF SUB-INTERVALS
  PRINT *,'INPUT THE NUMBER OF SUB-INTERVALS'
  READ(*,*) N
  IF(N < NPROCS) GO TO 1000
END IF
```

Calculate π Parallel Fortran Code

```
! BROADCAST THE NUMBER OF SUB-INTERVALS
! ARGUEMENTS: BUFFER, COUNT, DATATYPE, ROOT, COMM, IERROR
CALL MPI_Bcast(N,1,MPI_INTEGER,0,MPI_COMM_WORLD,IERROR)

A = 0.0d0   !DEFINE INTERVAL START
B = 1.0d0   !DEFINE INTERVAL STOP
H  = (B-A)/REAL(N)
! N INTERVALS MUST BE EVENLY DIVISIBLE BY NPROCS
NK = N/NPROCS
AK = A + REAL(MYID)*REAL(NK)*H
BK = AK + REAL(NK)*H

! COMPUTE LOCAL INTEGRAL
CALL TRAP(AK,BK,NK,SUBPI)

! SET UP A MASTER-SLAVE RELATIONSHIP WHERE THE MASTER
! IS RESPONSIBLE FOR ACCUMULATING THE SUB-INTEGRALS
! AND WRITING OUT THE ANSWER
```

Calculate π Parallel Fortran Code

```
   IF(MYID == 0) THEN
    ! SUM UP THE INTEGRALS FROM THE OTHER PROCESSORS
    PI = SUBPI
    ! ADD THE SUBPI'S FROM THE OTHER PROCESSORS
    ! ARGUMENTS: BUFFER, COUNT, DATATYPE, SOURCE, TAG,
    !                    COMM, STATUS, IERROR
    DO K = 1,NPROCS-1
       CALL MPI_Recv(SUBPI,1,MPI_DOUBLE_PRECISION,K,TAG,
  &                      MPI_COMM_WORLD,STATUS,IERROR)
       PI = PI + SUBPI
    END DO
    PRINT *,'PI = ',PI
   ELSE
    ! SEND THE INTEGRAL TO THE MASTER
    ! ARGUMENTS: BUFFER, COUNT, DATATYPE, DEST, TAG,
    !                    COMM, IERROR
    CALL MPI_Send(SUBPI,1,MPI_DOUBLE_PRECISION,0,TAG,
  &                    MPI_COMM_WORLD,IERROR)
   END IF

      ! TERMINATE MPI
1000 CALL MPI_Finalize(IERROR)
      STOP
      END
```

Code on web:
Codes/calcpi

Calculate π Parallel Fortran Code

- **We could replace the MPI_Send, MPI_Recv and the subsequent sum with another MPI routine that gather/adds the sub-pi's: MPI_Reduce**
- **The last slide then can be replaced with:**

```
      ! GATHER/ADD THE SUB-PI'S
      ! ARGUMENTS: SENDBUF, RECVBUF, COUNT, DATATYPE, OP,ROOT, COMM, ERR
      CALL MPI_Reduce(PI,SUBPI,1,MPI_DOUBLE_PRECISION,MPI_SUM,0,
   &                          MPI_COMM_WORLD,IERROR)
      ! TERMINATE MPI
 1000 CALL MPI_Finalize(IERROR)
      STOP
      END
```

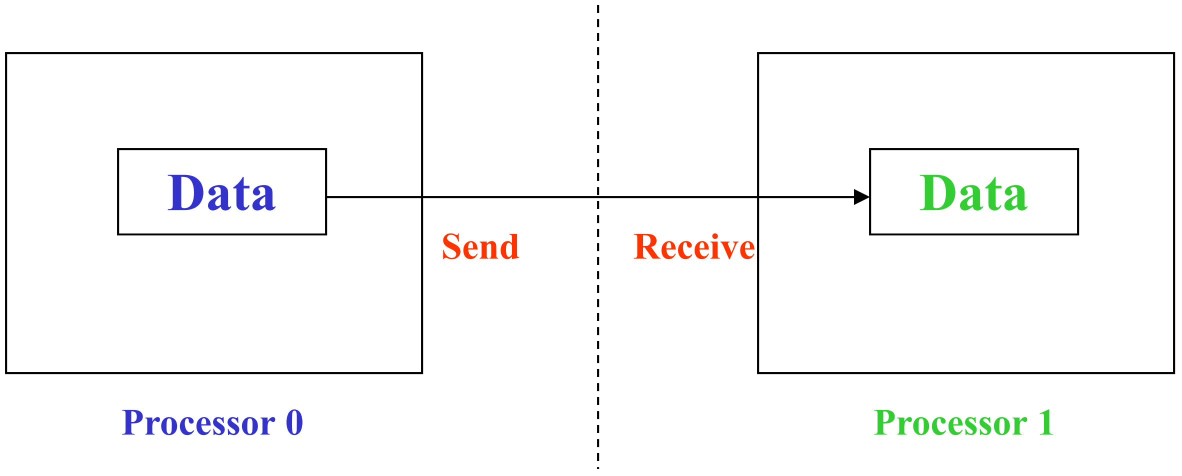
- **Embarrassingly parallel – no communication needed during the computations of the local integrals**

Timing

- **MPI_Wtime() returns the wall-clock time**

```
double start, finish, time;

MPI_Barrier(MPI_COMM_WORLD);
start = MPI_Wtime();
.
.
.
MPI_Barrier(MPI_COMM_WORLD);
finish = MPI_Wtime();
time = finish – start;
```

Send and Receive



- Cooperative data transfer
- To (from) whom is data sent (received)?
- What is sent?
- How does the receiver identify it?

Message Passing: Send

MPI_Send(address, count, datatype, dest, tag, comm)

- **(address, count) = a contiguous area in memory containing the message to be sent**
- **datatype = Type of data, e.g. integer, double precision (note that MPI had standard datatypes)**
- **dest = integer identifier representing the processor to send the message to**
- **tag = non-negative integer that the destination can use to selectively screen messages**
- **comm = communicator = group of processors**

Message Passing: Receive

MPI_Recv(address, count, datatype, source, tag, comm,
status)

- (address, count) = a contiguous area in message reserved for the message to be received
- datatype = Type of data, e.g. integer, double precision (note that MPI had standard datatypes)
- source = integer identifier representing the processor that sent the message
- tag = non-negative integer that the destination can use to selectively screen messages
- comm = communicator = group of processors
- status = information about the message that is received

Single Program Multiple Data (SPMD)

- **Proc 0 and Proc 1 are actually performing different operations**
- **However, not necessary to write separate programs for each processor**
- **Typically, use conditional statement and proc id to define the job of each processor:**

```
integer :: a(10)

if(my_id == 0) then
   MPI_Send(a,10,MPI_INT,1,0,MPI_COMM_WORLD)
else if(my_id == 1) then
   MPI_Recv(a,10,MPI_INT,0,0,MPI_COMM_WORLD)
end if
```

Different Types of Sends and Receives

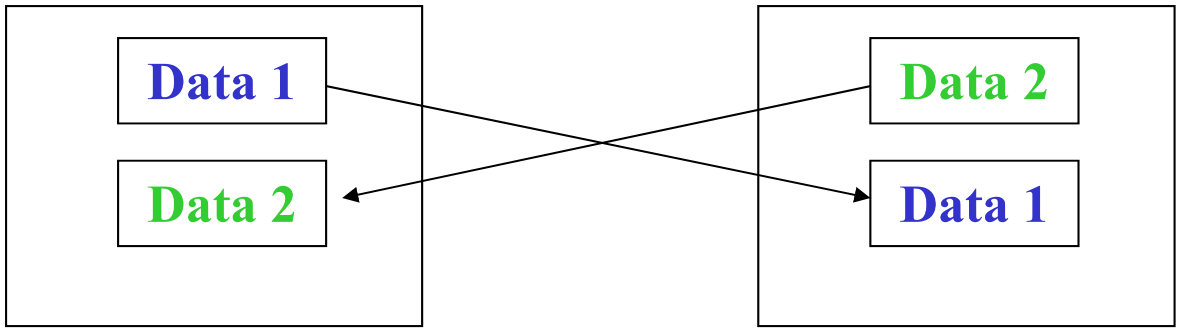
- **There are 4 types of Sends and Receives:**
  - Standard (blocking)
  - Synchronous
  - Buffered
  - Ready
- **Each of these types can be performed in:**
  - Blocking mode
  - Non-blocking mode
- **The code programmer must make the choice of which type and mode to use depending on the circumstance**

Send/Receive Types

- Standard: similar to Blocking except receive will not allow processor to continue only until its buffer can be reused.
- Blocking: receive will not allow processor to continue until it has received its message. Receive acts as a Barrier to that processor.
- Synchronous: send (or receive) does not start until a matching receive (or send) is posted indicating it is ready. Send acts as "blocking" until matching receive occurs. In this case, send acts as a Barrier for those processors.
- Buffered: either a system or user-defined buffer is made available for send/receive so that communication can proceed.

Deadlock

- Example: exchange data between 2 procs:



Processor 0	Processor 1
MPI_Send	MPI_Send
MPI_Recv	MPI_Recv

- MPI_Send is a synchronous operation. If no system buffering is used, it keeps waiting until a matching receive is posted.

Deadlock

- Both processors are waiting for each other →deadlock
- However, OK if system buffering exists →unsafe programming, however
- Note: MPI_Recv is blocking and non-buffered
- Another real deadlock:

Proc 0	Proc 1
MPI_Recv	MPI_Recv
MPI_Send	MPI_Send

- Fix by reordering communication

Proc 0	Proc 1
MPI_Send	MPI_Recv
MPI_Recv	MPI_Send

Buffered/Nonbuffered Communications

- **No-buffering (phone calls)**
  - Proc 0 initiates the send request and rings Proc 1. It waits until Proc 1 is ready to receive. The transmission starts.
  - Synchronous communication – completed only when the message was received by the receiving proc
- **Buffering (beeper)**
  - The message to be sent (by Proc 0) is copied to a system-controlled block of memory (buffer)
  - Proc 0 can continue executing the rest of its program
  - When Proc 1 is ready to receive the message, the system copies the buffered message to Proc 1
  - Asynchronous communication – may be completed even though the receiving proc has not received the message

Buffered Communication

- **Buffering requires system resources, e.g. memory, and can be slower if the receiving proc is ready at the time of requesting the send**
- **Application buffer: address space that holds the data in the user's computer program**
- **System buffer: system space for storing messages. In buffered communication, data in application buffer is copied to/from system buffer**
- **MPI allows communication in buffered mode:**

  MPI_Bsend, MPI_Ibsend
- **User allocates the buffer by:**

  MPI_Buffer_attach(buffer, buffer_size)
- **Free the buffer by MPI_Buffer_detach**
- **An alternate to MPI_Buffer commands is to allocate memory for buffer with standard allocate statement**

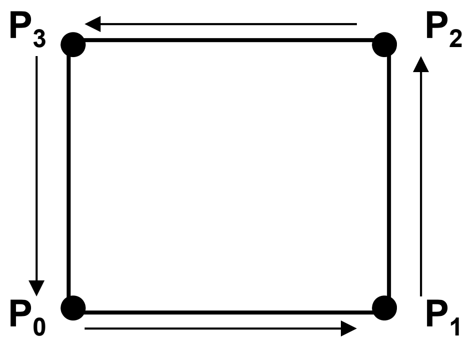
Blocking / Non-blocking Communication

- **Blocking Communication (McDonald’s)**
  - The receiving proc has to wait if the message is not ready and has not received initial signal from sending proc
  - Different from synchronous communication (where sending proc will not begin sending until it has received explicit permission from receiving proc)
  - Proc 0 may have already buffered the message to system and Proc 1 is ready, but the interconnection network is busy
- **Non-blocking Communication (In & Out)**
  - Proc 1 checks with the system if the message has arrived yet. If not, it continues doing other stuff. Otherwise, get the message from the system.
- **Useful when computation and communication can be performed at the same time**
- **MPI allows both non-blocking send and receive**

MPI_Isend and MPI_Irecv

- **In non-blocking send, program identifies an area in memory to serve as a send buffer. Processing continues immediately without waiting for message to be copied out from the application buffer**
- **The user's program *should not* modify the application buffer until the non-blocking send has completed**
- **Non-blocking communication can be combined with non-buffering: MPI_Issend, or buffering: MPI_Ibsend**
- **Use MPI_Wait or MPI_Test to determine if the non-blocking send or receive has completed**

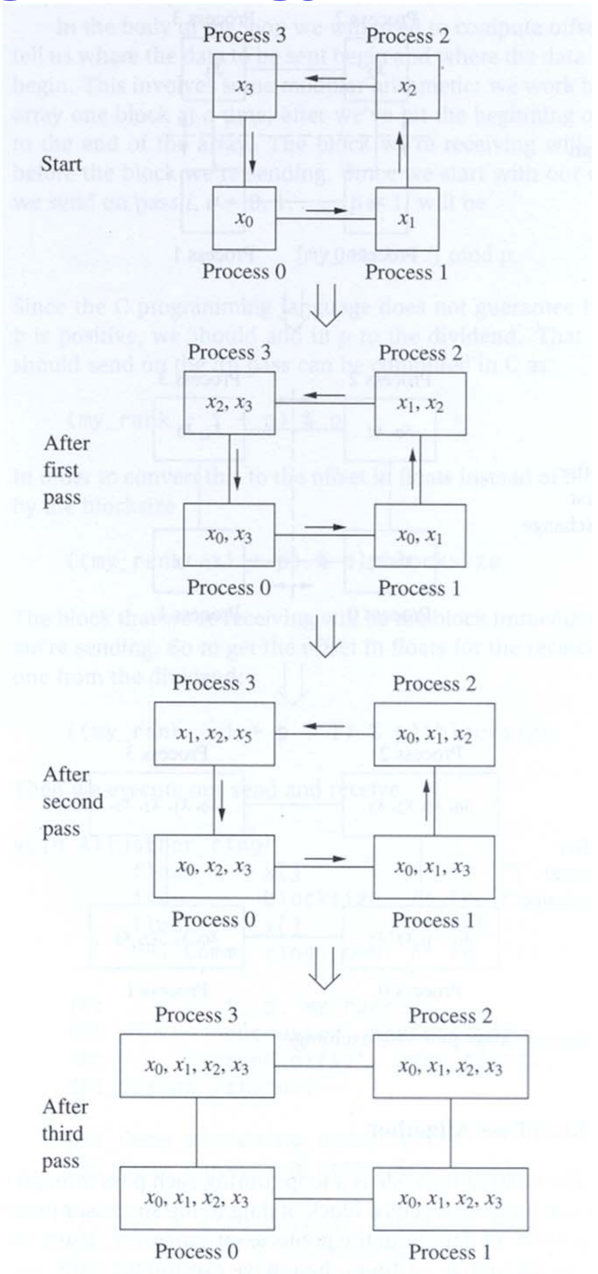
Example: Data Exchange in a Ring Topology



Analogous to
MPI_Allgather

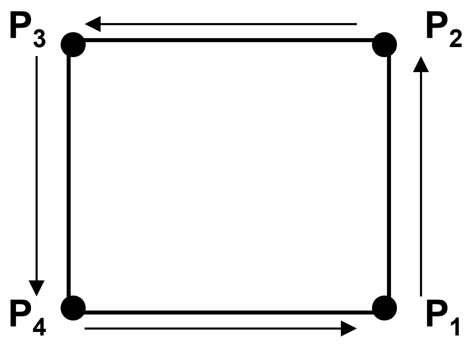
- **Blocking version:**

```
for (i=0; i<p; i++) {
     send_offset = ((my_id-i+p)%p)*blksize;
     recv_offset  = ((my_id-i-1+p)%p)*blksize;
     MPI_Send(y+send_offset,blksize,MPI_FLOAT,
                        my_id+1,0,ring_com);
     MPI_Recv(y+recv_offset,blksize,MPI_FLOAT,
                        my_id-1,0,ring_com,&status);
}
```



From Pacheco

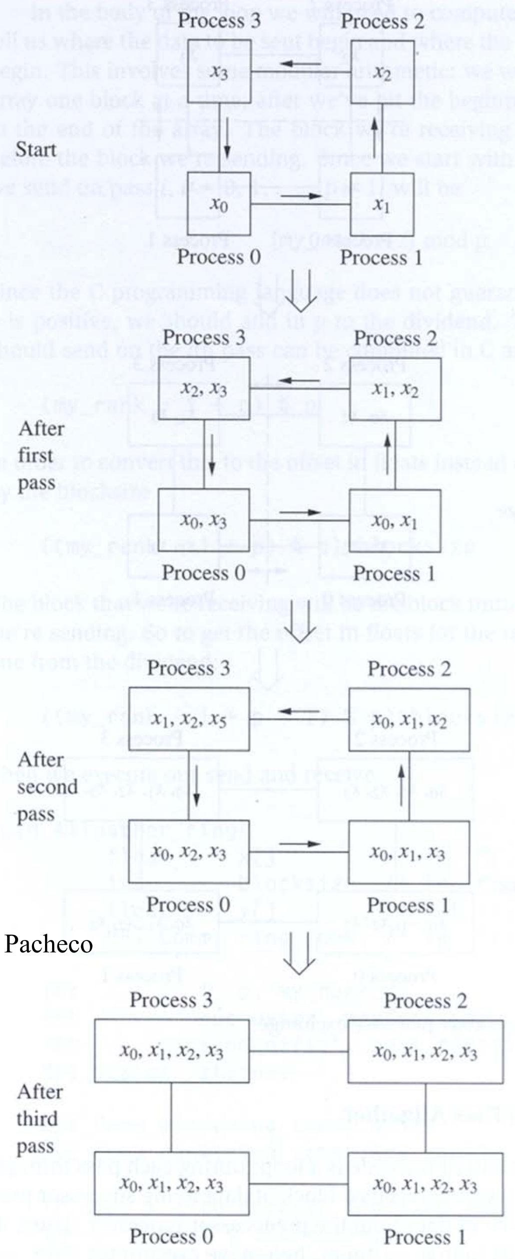
Example: Data Exchange in a Ring Topology



- **Non-Blocking version:**

```
send_offset = my_id*blksize;
recv_offset  = (my_id-1+p)*blksize;
for (i=0; i<p; i++) {
     MPI_Isend(y+send_offset,blksize,MPI_FLOAT,
                         my_id+1,0,ring_com,&send_request);
     MPI_Irecv(y+recv_offset,blksize,MPI_FLOAT,
                        my_id-1,0,ring_com,&recv_request);
     send_offset = ((my_id-i-1+p)%p)*blksize;
     recv_offset  = ((my_id-i-2+p)%p)*blksize;
     MPI_Wait(&send_request,&status);
     MPI_Wait(&recv_request,&status);
}
```

- **The communication and computations of next offsets are overlapped.**



From Pacheco

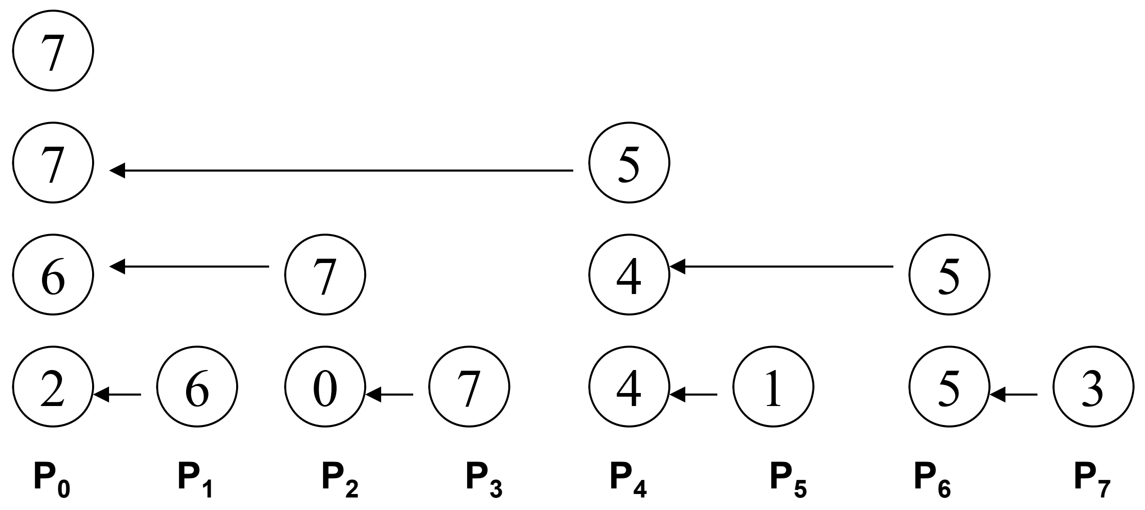
Summary of Communication Modes

- **4 communication modes in MPI: standard (blocking), buffered, synchronous, ready. They can be either blocking or non-blocking**
- **In standard (blocking) modes (MPI_Send, MPI_Recv,…), it is up to the system to decide whether messages should be buffered. Note there is a limited, finite amount of memory for system buffers.**
- **In synchronous mode, a send will not complete until a matching receive has been posted which has begun reception of the data**
  - MPI_Ssend (blocking), MPI_ISsend (non-blocking)
  - No system buffering
- **In buffered mode, the completion of a send does not depend on the existence of a matching receive**
  - MPI_Bsend (blocking), MPI_IBsend (non-blocking)
  - System buffering by MPI_Buffer_attach and MPI_Buffer_detach
- **Ready mode not discussed**

Collective Communications

- **Communication pattern involving all the procs; usually more than 2**
- **MPI_Barrier: synchronize all processors**
- **Broadcast (MPI_Bcast)**
  - A single proc sends the same data to every other proc
- **Reduction (gather/add) (MPI_Reduce)**
  - All the procs contribute data that is combined using a binary operation
  - Example: max, min, sum, etc.
  - One proc obtains the final answer
- **Allreduce (MPI_Allreduce)**
  - Same as MPI_Reduce but every proc contains the final answer
  - Effectively as MPI_Reduce + MPI_Bcast, but more efficient

An Implementation of the “Max” Function

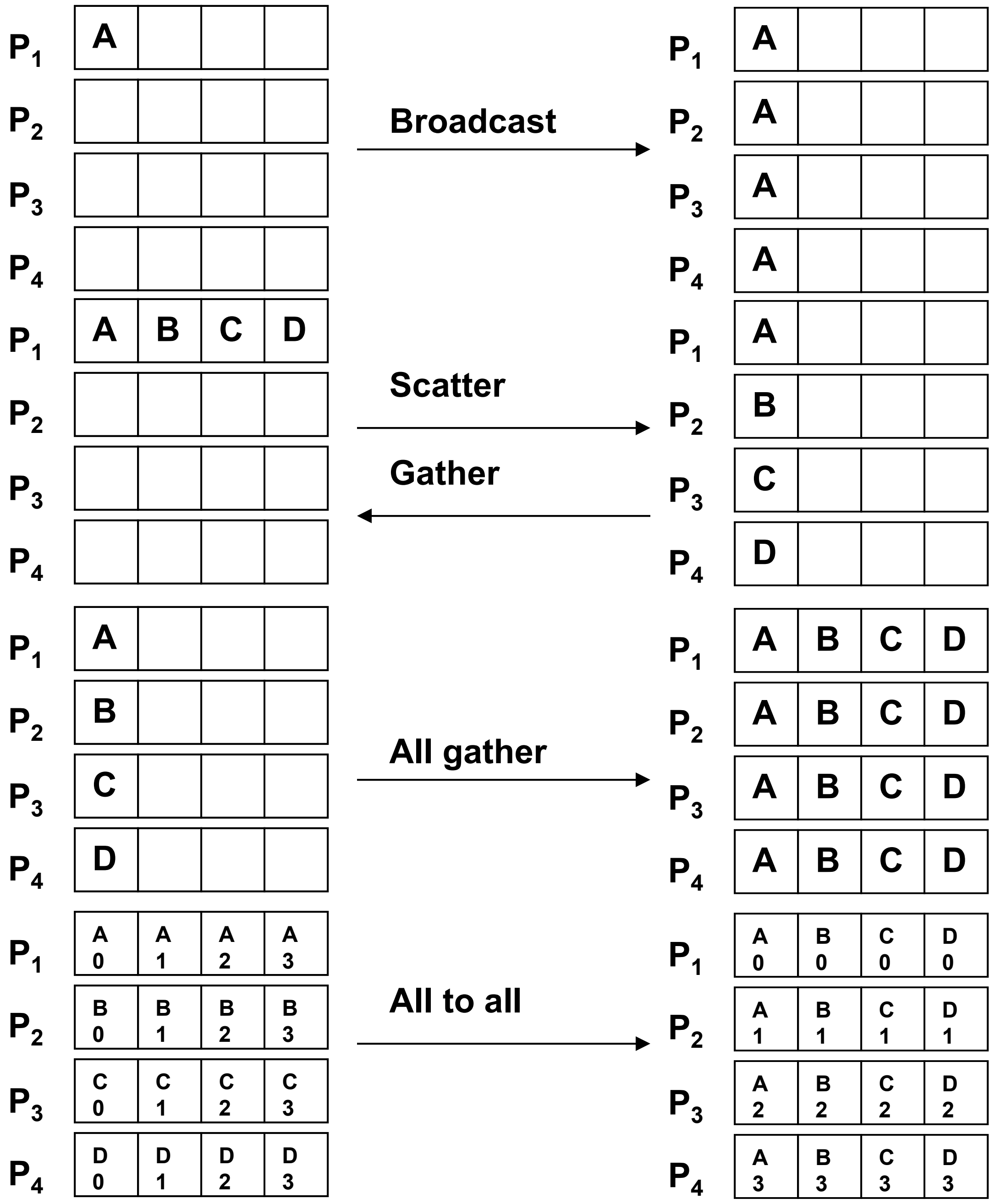


- **Tree-structured communication: (find the maximum among procs)**
- **Only needs $\log_2 p$ stages of communication**
- **Not necessarily optimum on a particular architecture**

Other Collective Communicators

- **Scatter (MPI_Scatter)**
  - Split the data on the root processor into p segments
  - The 1st segment is sent to proc 0, the 2nd to proc 1, etc.
  - Similar to but more general than MPI_Bcast
- **Gather (MPI_Gather)**
  - Collect the data from each processor and store the data on root processor
  - Similar to but more general than MPI_Reduce
- **Can collect and store the data on all procs using MPI_Allgather**

Comparison of Collective Communicators



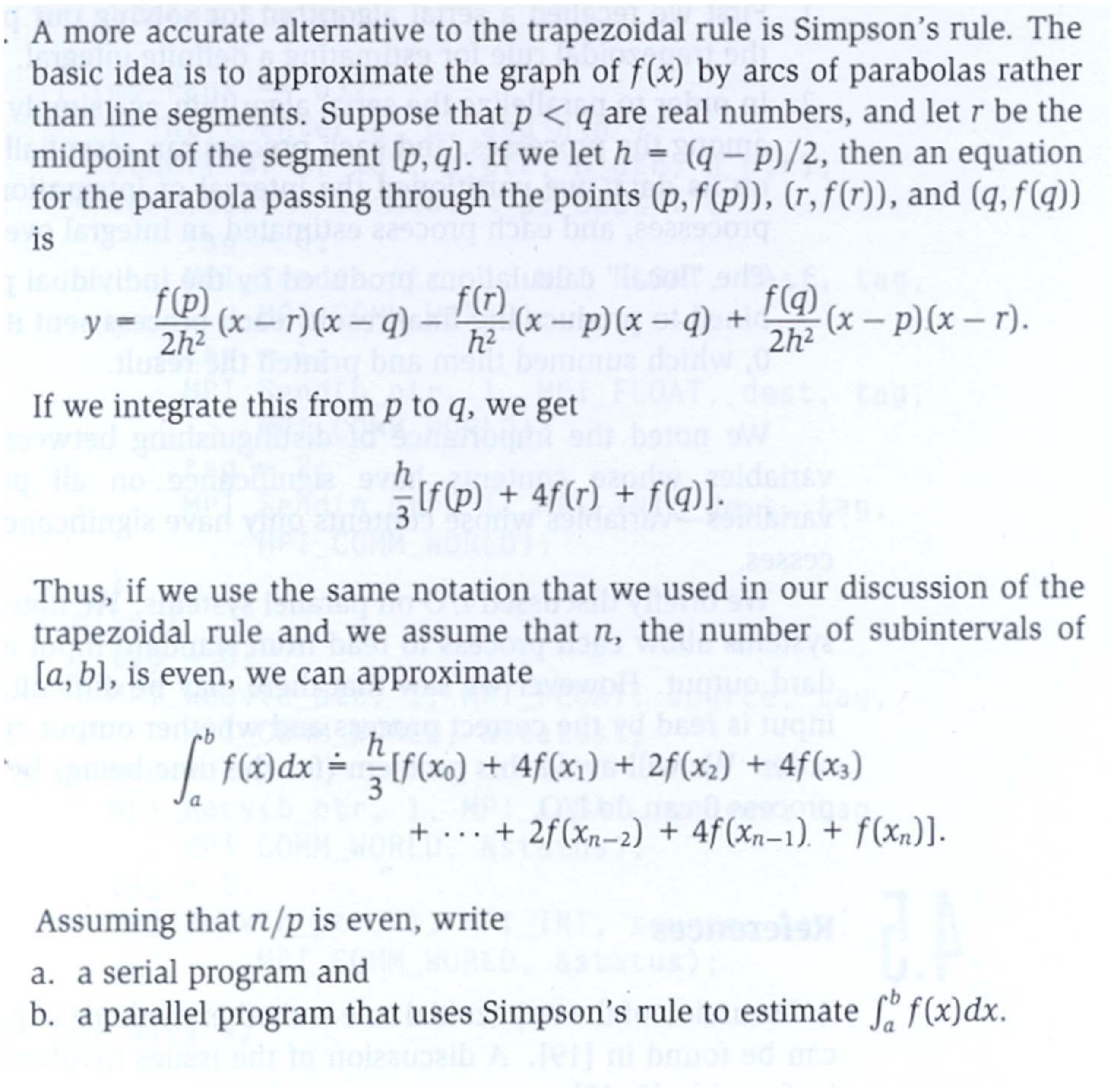
Homework 3

- **Finish reading Chap. 1-3 of <u>Using MPI</u> by Gropp et al.**

- **Look at the parallel routine to compute π (calcpip) in the Codes directory**

- **Due Thursday Oct. 22: Modify the calcpip.f routine to do a more accurate integration (Simpson's Rule) described in the next slide**
  - Provide a listing of all subroutines and test this algorithm for different numbers of processors using parallel run.qsub batch submit procedure on wopr
  - Provide the CPU time as a function of the number of processors (up to 8) and the answer

Homework 3



A more accurate alternative to the trapezoidal rule is Simpson's rule. The basic idea is to approximate the graph of $f(x)$ by arcs of parabolas rather than line segments. Suppose that $p < q$ are real numbers, and let r be the midpoint of the segment $[p, q]$. If we let $h = (q - p)/2$, then an equation for the parabola passing through the points $(p, f(p))$, $(r, f(r))$, and $(q, f(q))$ is

$$y = \frac{f(p)}{2h^2}(x-r)(x-q) - \frac{f(r)}{h^2}(x-p)(x-q) + \frac{f(q)}{2h^2}(x-p)(x-r).$$

If we integrate this from p to q, we get

$$\frac{h}{3}[f(p) + 4f(r) + f(q)].$$

Thus, if we use the same notation that we used in our discussion of the trapezoidal rule and we assume that n, the number of subintervals of $[a, b]$, is even, we can approximate

$$\int_a^b f(x)dx \doteq \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)].$$

Assuming that n/p is even, write

a. a serial program and
b. a parallel program that uses Simpson's rule to estimate $\int_a^b f(x)dx$.

From Parallel Programming with MPI by Pacheco