Parallel Programming Using MPI

Short Course on HPC

15th February 2019

Aditya Krishna Swamy

adityaks@iisc.ac.in

SERC, Indian Institute of Science

When Parallel Computing Helps?

- Want to speed up your calculation
- Your problem size is too large for a single node
- Current trend - multicore processors, accelerators (GPGPU).
- Solution:
  - Split the work between several processor cores so that they can work in parallel
  - Exchange data between them when needed
- How? Popular tools in Scientific Computing
  - OpenMP directives on shared memory node
  - Message Passing Interface (MPI) on distributed memory systems
  - and others (CUDA/OpenCL, ...)

What is MPI?

- MPI stands for Message Passing Interface
- It is a message-passing specification, a standard for the vendors to implement
- In practice, MPI is a library consisting of C functions and Fortran subroutines (Fortran) used for exchanging data between processes
- An MPI library exists on **ALL** parallel computers so it is **highly portable**
- The scalability of MPI is not limited by the number of processors/cores on one computation node, as opposed to shared memory parallel models
- Also available for Python (mpi4py.scipy.org), R (Rmpi)

MPI

Context: Distributed memory parallel computers

- Each processor has its own memory and cannot access the memory of other processors
- A copy of the same executable runs on each MPI process (processor core)
- Any data to be shared must be explicitly transmitted from one to another

Most message passing programs use the *single program multiple data* (SPMD) model

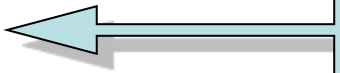
- Each processor executes the same set of instructions
- Parallelization is achieved by letting each processor operate on a different piece of data
- Not to be confused with SIMD: Single Instruction Multiple Data *a.k.a vector computing*

A sample MPI program in Fortran 90

```
Program mpi_code
  ! Load MPI definitions
    use mpi (or include mpif.h)

  ! Initialize MPI
    call MPI_Init(ierr)
  ! Get the number of processes
    call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
  ! Get my process number (rank)
    call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

    Do work and make message passing calls…

  ! Finalize
    call MPI_Finalize(ierr)

end program mpi_code
```

Header file

```
Program mpi_code
  ! Load MPI definitions
    use mpi

  ! Initialize MPI
    call MPI_Init(ierr)
  ! Get the number of processes
    call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
  ! Get my process number (rank)
    call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

    Do work and make message passing calls…

  ! Finalize
    call MPI_Finalize(ierr)

end program mpi_code
```

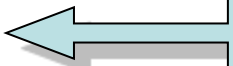


- Defines MPI-related parameters and functions
- Must be included in all routines calling MPI functions
- Can also use include file:

  include mpif.h

Initialization

```
Program mpi_code
  ! Load MPI definitions
    use mpi

  ! Initialize MPI
    call MPI_Init(ierr)
  ! Get the number of processes
    call MPI_Comm_size(MPI_COMM_WO
  ! Get my process number (rank)
    call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

    Do work and make message passing calls…

  ! Finalize
    call MPI_Finalize(ierr)

end program mpi_code
```



- Must be called at the beginning of the code before any other calls to MPI functions
- Sets up the communication channels between the processes and gives each one a rank.

How many processes do we have?

- Returns the number of processes available under MPI_COMM_WORLD communicator
- This is the number used on the mpiexec (or mpirun) command:

  mpiexec –n nproc a.out

```
      call MPI_Init(ierr)
    ! Get the number of processes
      call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
    ! Get my process number (rank)
      call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

      Do work and make message passing calls…

    ! Finalize
      call MPI_Finalize(ierr)

  end program mpi_code
```

What is my rank?

```
Program mpi_code
  ! Load MPI definitions
    call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
  ! Get my process number (rank)
    call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

    Do work and make message passing calls…

  ! Finalize
    call MPI_Finalize(ierr)

end program mpi_code
```

- Get my rank among all of the nproc processes under MPI_COMM_WORLD
- This is a unique number that can be used to distinguish this process from the others

Termination

```
Program mpi_code
  ! Load MPI definitions
    use mpi (or include mpif.h)

  ! Initialize MPI
    call MPI_Init(ierr)
  ! Get the number of processes
    call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
  ! Get my process number (rank)
    call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

    Do work and make message passing calls…

  ! Finalize
    call MPI_Finalize(ierr)

end program mpi_code
```

- Must be called at the end of the properly close all communication channels
- No more MPI calls after finalize

A sample MPI program in C

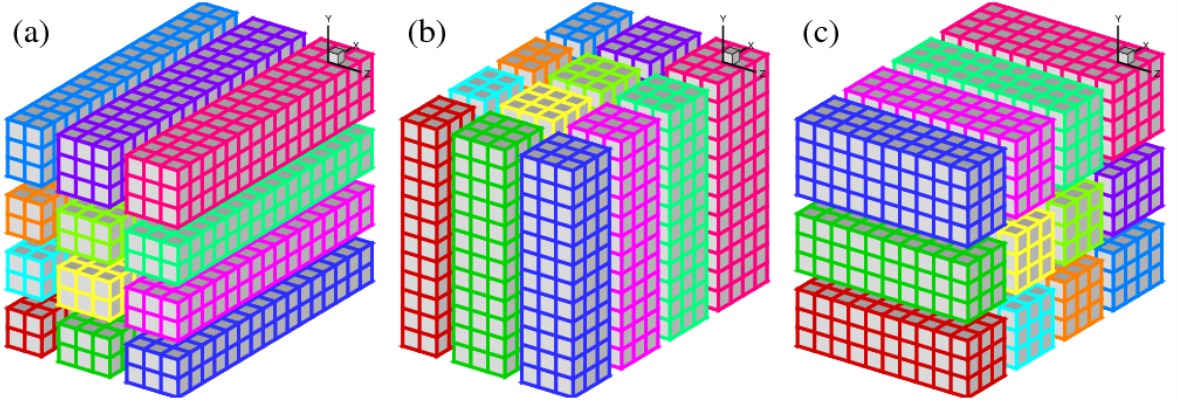
```
#include "mpi.h"
int main( int argc, char *argv[] )
{
  int nproc, myrank;
  /* Initialize MPI */
    MPI_Init(&argc,&argv);
  /* Get the number of processes */
    MPI_Comm_size(MPI_COMM_WORLD,&nproc);
  /* Get my process number (rank) */
    MPI_Comm_rank(MPI_COMM_WORLD,&myrank);

    Do work and make message passing calls…

  /* Finalize */
    MPI_Finalize();
 return 0;
}
```

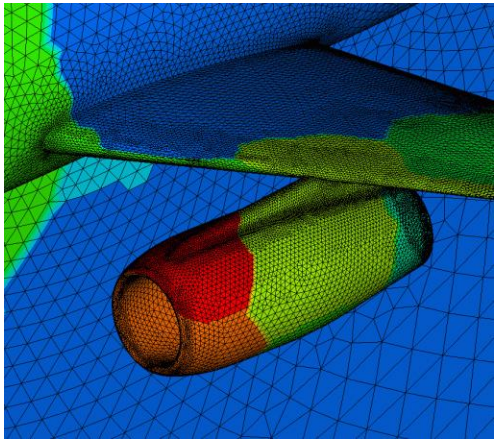
How much do I need to know?

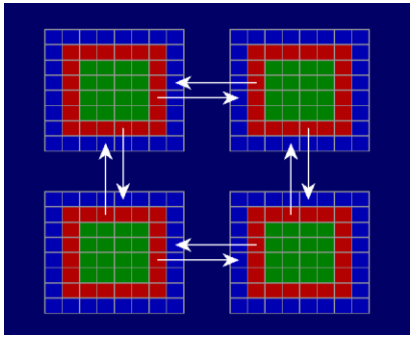
- MPI-1 has over 125 functions/subroutines
- Can actually do everything with about 6 of them
- Collective functions are EXTREMELY useful since they simplify the coding and vendors optimize them for their interconnect hardware
- One can access flexibility when it is required.
- One need not master all parts of MPI to use it.

How to split the work between ranks?
Domain Decomposition

- Most widely used method for grid-based calculations

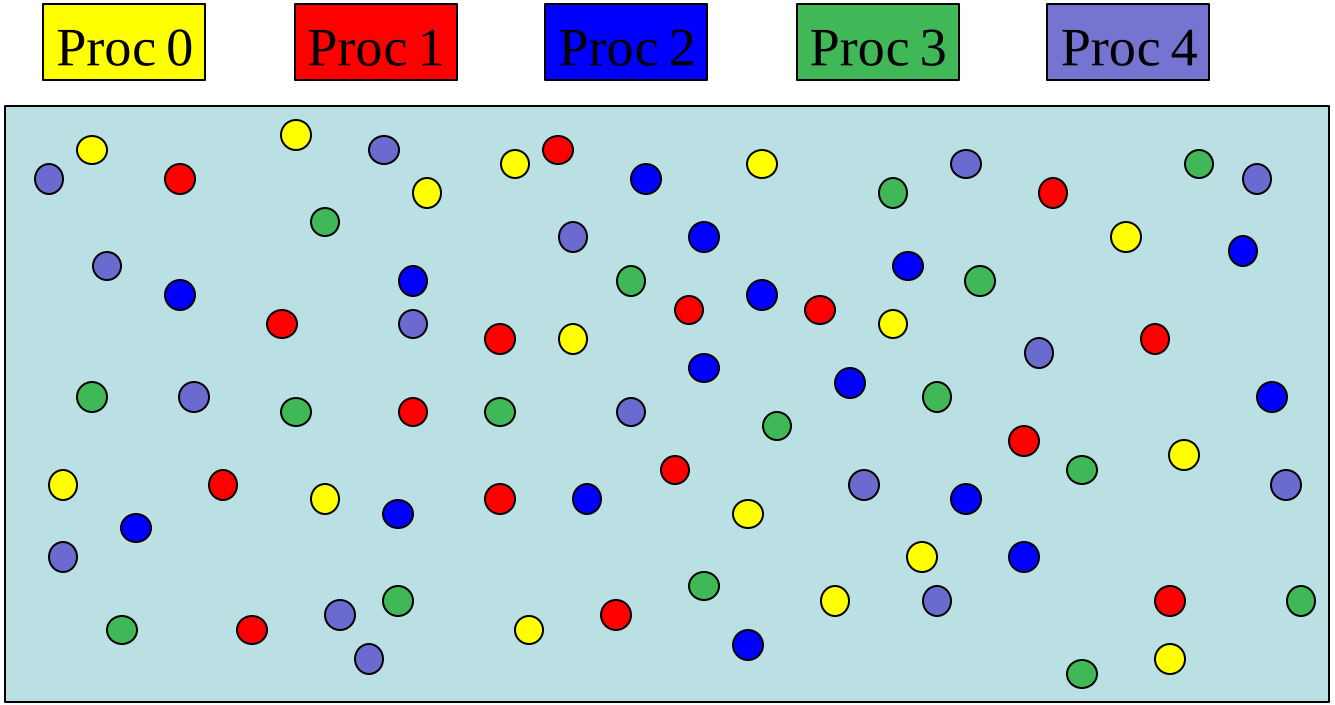






How to split the work between ranks?
"Coloring"

- Useful for particle simulations



MPI Communicators

- A communicator is an identifier associated with a group of processes
  - Each process has a unique rank within a specific communicator (the rank starts from 0 and has a maximum value of (nprocesses-1)).
  - Internal mapping of processes to processing units
  - Always required when initiating a communication by calling an MPI function or routine.
- Default communicator MPI_COMM_WORLD, which contains all available processes.
- Several communicators can coexist
  - A process can belong to different communicators at the same time, but has a unique rank in each communicator

Basic MPI calls to exchange data

- Point-to-Point communications
  - Only 2 processes exchange data
  - It is the basic operation of all MPI calls
- Collective communications
  - A single call handles the communication between all the processes in a communicator
  - There are 3 types of collective communications
    - Data movement (e.g. MPI_Bcast)
    - Reduction (e.g. MPI_Reduce)
    - Synchronization: MPI_Barrier

Point-to-point communication

Point to point: 2 processes at a time

```
MPI_Send(buf,count,datatype,dest,tag,comm,ierr)

MPI_Recv(buf,count,datatype,source,tag,comm,status,ierr)
```

```
MPI_Sendrecv(sendbuf,sendcount,sendtype,dest,sendtag,
    recvbuf,recvcount,recvtype,source,recvtag,comm,status,ierr)
```

where the datatypes are:

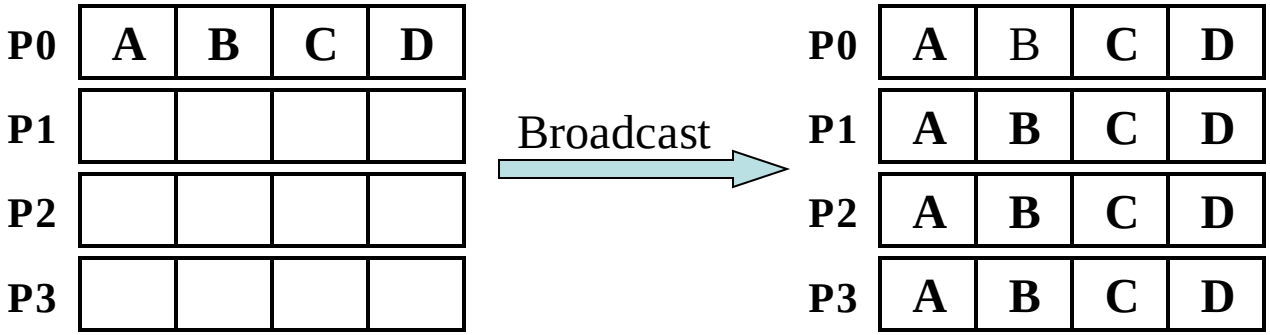
FORTRAN: MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_COMPLEX,MPI_CHARACTER, MPI_LOGICAL, etc…

C : MPI_INT, MPI_LONG, MPI_SHORT, MPI_FLOAT, MPI_DOUBLE, etc…

Predefined Communicator: MPI_COMM_WORLD

Collective communication: Broadcast

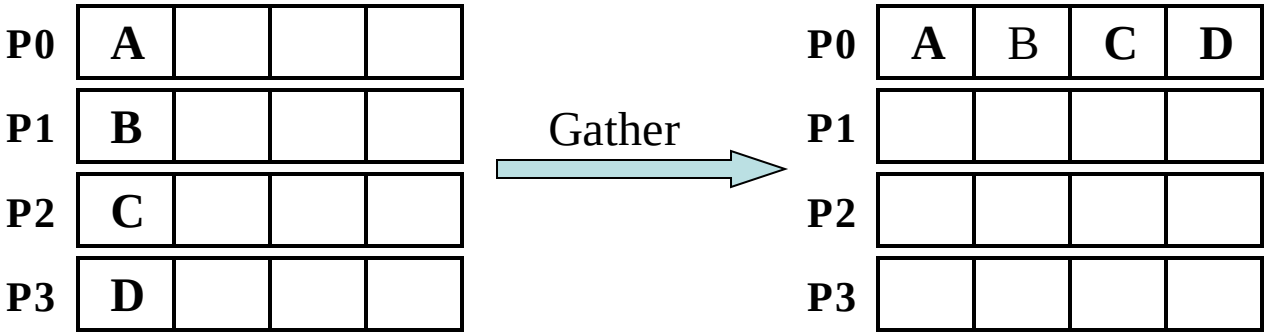
```
MPI_Bcast(buffer,count,datatype,root,comm,ierr)
```



- One process (called "root") sends data to all the other processes in the same communicator
- Must be called by ALL processes with the same arguments

Collective communication: Gather

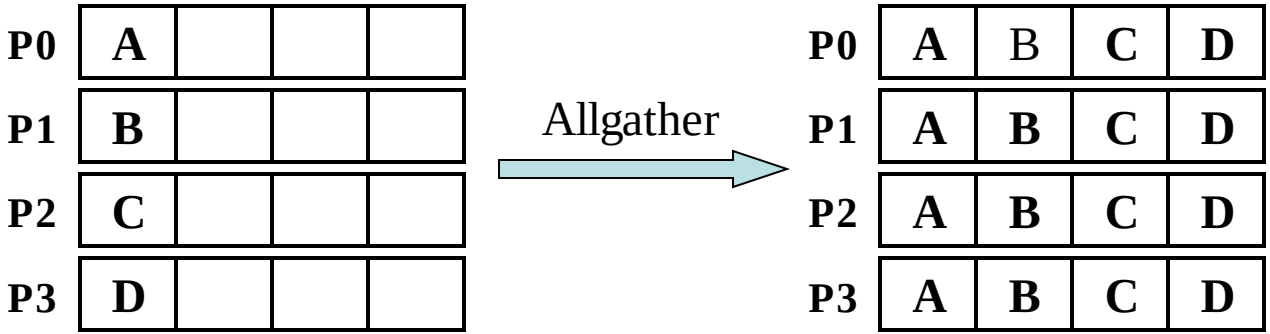
```
MPI_Gather(sendbuf,sendcount,sendtype,recvbuf,recvcount,
           recvtype,root,comm,ierr)
```



- One root process collects data from all the other processes in the same communicator
- Must be called by all the processes in the communicator with the same arguments
- "sendcount" is the number of basic datatypes sent, not received (example above would be sendcount = 1)
- Make sure that you have enough space in your receiving buffer!

Collective communication: Gather to All

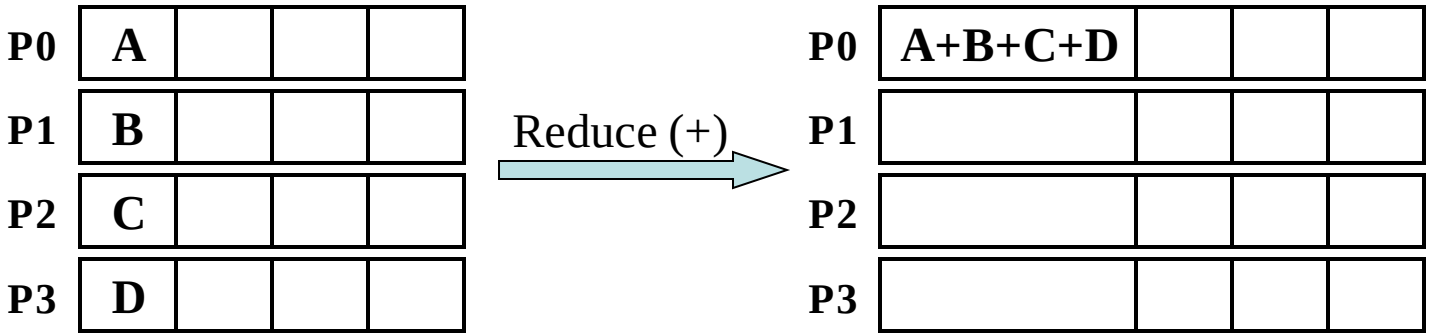
```
MPI_Allgather(sendbuf,sendcount,sendtype,recvbuf,recvcount,
              recvtype,comm,info)
```



- All processes within a communicator collect data from each other and end up with the same information
- Must be called by all the processes in the communicator with the same arguments
- Again, sendcount is the number of elements sent

Collective communication: Reduction

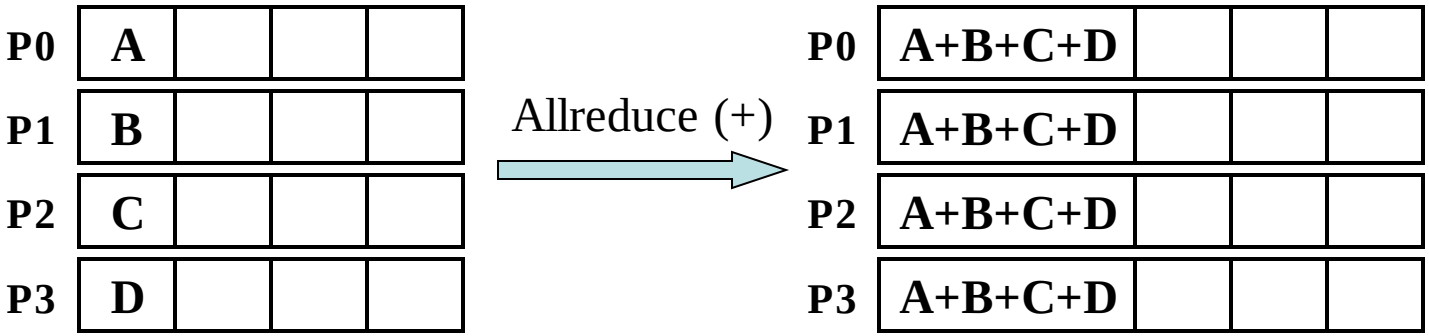
```
MPI_Reduce(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```



- One root process collects data from all the other processes in the same communicator and performs an operation on the received data
- Called by all the processes with the same arguments
- Operations are: MPI_SUM, MPI_MIN, MPI_MAX, MPI_PROD, logical AND, OR, XOR, and a few more
- User can define own operation with MPI_Op_create()

Collective communication: Reduction to All

```
MPI_Allreduce(sendbuf,recvbuf,count,datatype,op,comm,ierr)
```



- All processes within a communicator collect data from all the other processes and performs an operation on the received data
- Called by all the processes with the same arguments
- Operations are the same as for MPI_Reduce

More MPI collective calls

One "root" process send a different piece of the data to each one of the other Processes (inverse of gather)

```
MPI_Scatter(sendbuf,sendcnt,sendtype,recvbuf,recvcnt,
            recvtype,root,comm,ierr)
```

Each process performs a scatter operation, sending a distinct message to all the processes in the group in order by index.

```
MPI_Alltoall(sendbuf,sendcount,sendtype,recvbuf,recvcnt,
             recvtype,comm,ierr)
```

Synchronization: When necessary, all the processes within a communicator can be forced to wait for each other although this operation can be expensive

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

How to time your MPI code

- Several possibilities but MPI provides an easy to use function called "MPI_Wtime()". It returns the number of seconds since an arbitrary point of time in the past.

```
FORTRAN: double precision MPI_WTIME()
      C: double MPI_Wtime()

starttime=MPI_WTIME()
   ... program body ...
endtime=MPI_WTIME()
elapsetime=endtime-starttime
```

Debugging tips

Use "unbuffered" writes to do "printf-debugging" and always write out the process id:

```
C:        fprintf(stderr,"%d: …",myid,…);
Fortran:  write(0,*)myid,': …'
```

If the code detects an error and needs to terminate, use MPI_ABORT. The errorcode is returned to the calling environment so it can be any number.

```
C:        MPI_Abort(MPI_Comm comm, int errorcode);
Fortran:  call MPI_ABORT(comm, errorcode, ierr)
```

To detect a "NaN" (not a number):

```
C:        if (isnan(var))
Fortran:  if (var /= var)
```

Use a parallel debugger such as Totalview or DDT

References

- Keywords for google “mpi”, or “mpi standard”, or “mpi tutorial”…
- http://www.mpi-forum.org (location of the MPI standard)
- http://www.llnl.gov/computing/tutorials/mpi/
- http://www.nersc.gov/nusers/help/tutorials/mpi/intro/

- MPI on Linux clusters:
  - MPICH (http://www-unix.mcs.anl.gov/mpi/mpich/)
  - Open MPI (http://www.open-mpi.org/)

Example: calculating π using numerical integration

```
#include <stdio.h>
#include <math.h>
int main( int argc, char *argv[] )
{
    int n, myid, numprocs, i;
    double PI25DT = 3.14159265358979323846264643;
    double mypi, pi, h, sum, x;
    FILE *ifp;

    ifp = fopen("ex4.in","r");
    fscanf(ifp,"%d",&n);
    fclose(ifp);
    printf("number of intervals = %d\n",n);

    h   = 1.0 / (double) n;
    sum = 0.0;
    for (i = 1; i <= n; i++) {
        x = h * ((double)i - 0.5);
        sum += (4.0 / (1.0 + x*x));
    }
    mypi = h * sum;

    pi = mypi;
    printf("pi is approximately %.16f, Error is %.16f\n",
           pi, fabs(pi - PI25DT));
    return 0;
}
```

C version

Root reads input and broadcast to all

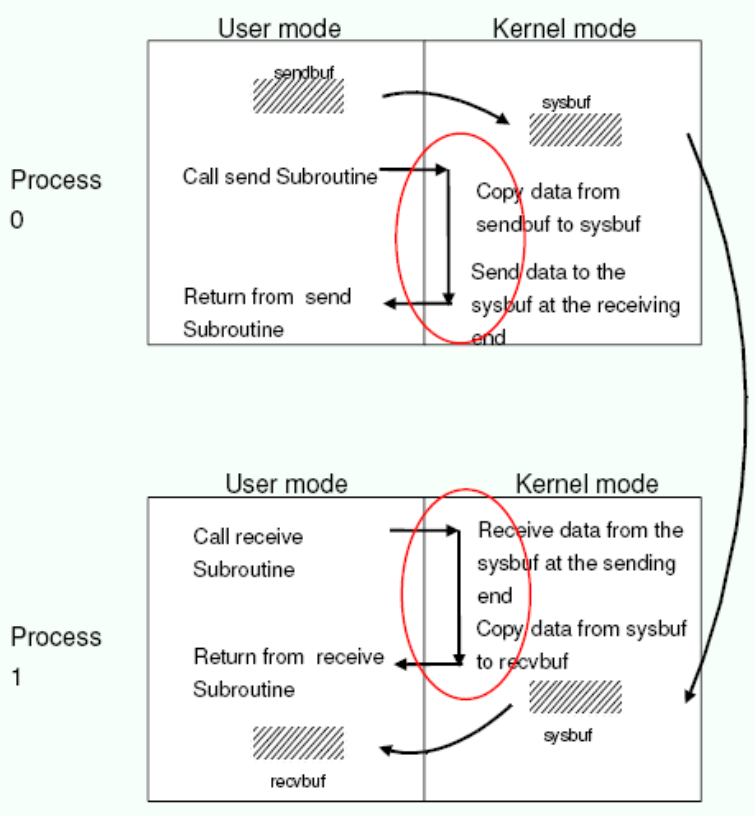
```
#include "mpi.h"
#include <stdio.h>
#include <math.h>
int main( int argc, char *argv[] )
{
    int n, myid, numprocs, i, j, tag, my_n;
    double PI25DT = 3.14159265358979323846264643;
    double mypi,pi,h,sum,x,pi_frac,tt0,tt1,ttf;
    FILE *ifp;
    MPI_Status  Stat;
    MPI_Request request;

    n = 1;
    tag = 1;
    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD,&myid);

    tt0 = MPI_Wtime();
    if (myid == 0) {
       ifp = fopen("ex4.in","r");
       fscanf(ifp,"%d",&n);
       fclose(ifp);
       //printf("number of intervals = %d\n",n);
    }
 /* Global communication. Process 0 "broadcasts" n to all other processes */
    MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
```

Each process calculates its section of the integral and adds up results with MPI_Reduce

```
…
    h   = 1.0 / (double) n;
    sum = 0.0;
    for (i = myid*n/numprocs+1; i <= (myid+1)*n/numprocs; i++) {
        x = h * ((double)i - 0.5);
        sum += (4.0 / (1.0 + x*x));
    }
    mypi = h * sum;

    pi = 0.;  /* It is not necessary to set pi = 0 */

 /* Global reduction. All processes send their value of mypi to process 0
    and process 0 adds them up (MPI_SUM) */
    MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);

    ttf = MPI_Wtime();
    printf("myid=%d  pi is approximately %.16f, Error is %.16f  time = %10f\n",
              myid, pi, fabs(pi - PI25DT), (ttf-tt0));

    MPI_Finalize();
    return 0;
}
```

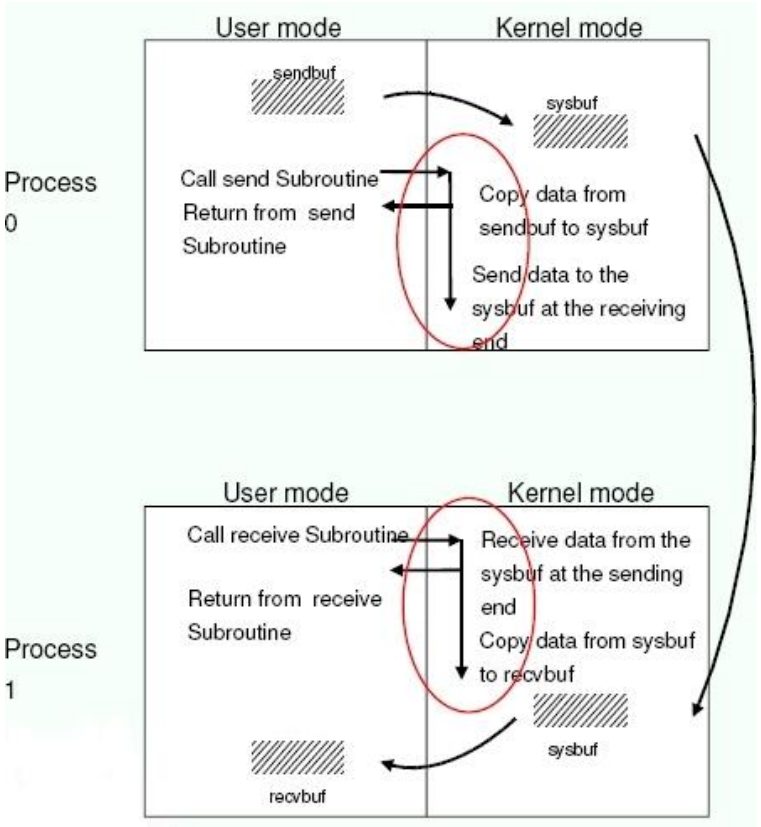
Thank you...

Blocking communications



- The call waits until the data transfer is done
  - The sending process waits until all data are transferred to the system buffer (differences for *eager vs rendezvous* protocols...)
  - The receiving process waits until all data are transferred from the system buffer to the receive buffer
- All collective communications are blocking

Non-blocking



- Returns immediately after the data transferred is initiated
- Allows to overlap computation with communication
- Need to be careful though
  - When send and receive buffers are updated before the transfer is over, the result will be wrong

Non-blocking send and receive

Point to point:

```
MPI_Isend(buf,count,datatype,dest,tag,comm,request,ierr)

MPI_Irecv(buf,count,datatype,source,tag,comm,request,ierr)
```

The functions MPI_Wait and MPI_Test are used to complete a nonblocking communication

```
MPI_Wait(request,status,ierr)

MPI_Test(request,flag,status,ierr)
```

MPI_Wait returns when the operation identified by "request" is complete. This is a non-local operation.

MPI_Test returns "flag = true" if the operation identified by "request" is complete. Otherwise it returns "flag = false". This is a local operation.

MPI-3 standard introduces "non-blocking collective calls"