Introduction to MPI (Message-Passing Interface)
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Basic MPI Concepts

- **Messages and buffers.** *Sending* and *receiving* messages are the two fundamental operations. Messages can be typed with a *tag* integer. Allows message buffers to be more complex than a simple buffer and address combination by giving options to the user to create their own data types.
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- **Separating Families of Messages.** MPI programs can use the notion of *contexts* to separate messages in different parts of the code. Useful for writing libraries. The context are allocated at run time by the system in response to user (or library) requests.
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- Separating Families of Messages. MPI programs can use the notion of *contexts* to separate messages in different parts of the code. Useful for writing libraries. The context are allocated at run time by the system in response to user (or library) requests.

- Process Groups. Processes belong to *groups*. Each process is ranked in its group with a linear numbering. Initially, all processes belong to one default group.
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The *destination* or *source* specified in send or receive operation always refers to the rank of the process in the group identified by a communicator. For example, consider the following blocking send and blocking receive operations in MPI.

```c
MPI_Send(address, count, datatype, destination, tag, comm)
MPI_Recv(address, maxcount, datatype, source, tag, comm, status)
```

The status object in the receive holds information about the actual message size, source and tag.
Collective Communications. MPI provides two types of collective operations, performed by all the processes in the computation.

- **Data movement**: Broadcast, scattering, gathering and others.
- **Collective computation**: Reduction operations like minimum, maximum, sum, logical OR etc as well as user-defined operations.
Other MPI Features

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  - *Data movement:* Broadcast, scattering, gathering and others.
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- **Groups:** Operations of creating and managing groups in a scalable manner. These can be used to control the scope of the above collective operations.
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- **Groups:** Operations of creating and managing groups in a scalable manner. These can be used to control the scope of the above collective operations.

- **Virtual Topologies.** Allows processes to be conceptualized in an application-oriented topology. Grids and general graphs are supported.
Other MPI Features

- **Debugging and profiling.** MPI requires the availability of “hooks” that allow users to intercept MPI calls and thus define their own debugging and profiling mechanisms.
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- **Support for heterogeneous networks.** MPI programs can run on a heterogeneous network without the user having to worry about data type conversions.
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- **Processes and processors.** The MPI specification uses processes only. Thus the mapping of processes to processors is up to the implementation.
The Six Basic MPI Functions

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MPI History and Versions

- MPI versions: MPI-1, MPI-2, MPI-2.1, MPI-2.2, and MPI-3
- MPE (MPI Programming Environment): provides support for logging and visualization. Packaged with the MPI software in earlier versions, but now it is separated out.
- Freely available MPI implementations (with access to source code):
  - **MPICH.** The latest version of MPI implementation available for download from Argonne National Lab ([http://www.mpich.org](http://www.mpich.org)) that supports the full MPI standard.
  - On Fedora Linux install via
    ```
dnf install mpich*
    ```
    Note that this version doesn’t have MPE support in it. If you want that, then install the version discussed on the next slide.
MPI History and Versions (continued)

- **MPICH2.** MPICH2 was the newer version of MPICH-1, which has then been merged back with MPICH-1 to become MPICH (version 3). The download site for MPICH2 is shown below:

  http://www.mcs.anl.gov/research/projects/mpich2staging/
goodell/downloads/index.php?s=downloads

  Navigate to your Linux flavor and download the latest pre-built package there. For Fedora, the packages are also available on `onyx` under the `~amit/cs430/software` folder for your convenience.

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  We will use MPICH2 version 1.5 in this course.
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- **Open MPI.** Another implementation of full MPI standard. Available from http://www.open-mpi.org/. Also available via yum

  `yum install openmpi openmpi-devel`
Hello World in MPI

/*lab/MPI/hello_world/spmd_hello_world.c */
/* appropriate header files */
#include <asm/param.h> /* for MAXHOSTNAMELEN */
#include <mpi.h>

int main(int argc, char **argv)
{
    int pid;
    int nproc;
    char hostname[MAXHOSTNAMELEN];

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nproc);
    MPI_Comm_rank(MPI_COMM_WORLD, &pid);

    gethostname(hostname, 100);
    printf("Hello! I am %d of %d running on %s.\n", pid, nproc, hostname);

    MPI_Finalize();
    exit(0);
}
MPI Functions Introduced in the Example

- `int MPI_Init(int *argc, char ***argv)`
- `int MPI_Comm_size(MPI_Comm comm, int *size)`
- `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
- `int MPI_Finalize()`
Using MPICH in the Onyx cluster Lab

- Log in to the head node `onyx`. Acquire nodes from the scheduler: `pbsget -4`
- Run your mpi program with the `mpiexec` command. `mpiexec -n 4 hello_world`
- Exit and release all allocated nodes with the command: `exit`
Using MPICH on your computer

- **Setting up MPICH.** Assuming that it was installed via `yum`, there is no further setup required.

- **Running a MPI program**
  - Simply run your mpi program with the `mpiexec` command.
    ```bash
    mpiexec -n 4 hello_world
    ```
Building MPICH from source on your computer

- Download the tarball of either the MPICH or MPICH2 software. Unpack it somewhere you have enough space.
  
  `tar xzvf mpich-xyz.tar.gz`

- We recommend the following steps to build MPICH.
  
  `mkdir /usr/local/src/mpich2`
  `./configure --prefix=/usr/local/mpich --enable-romio 2>&1 | tee configure.log`
  `make 2>&1 | tee make.log`
  `sudo make install 2>&1 | tee install.log`

- For more details on installation, please read the instructions in the README file in the MPICH source.

- Add `/usr/local/mpich/bin` to your PATH.

- Add `/usr/local/mpich/share/man` in the `/etc/man.config` file to enable viewing man pages in KDE Konqueror.
MPI “Blocking” Send Call

- MPI “Blocking” send returns when “locally complete” – when the location used to hold the message can be safely altered without affecting the message being sent.

- int MPI_Send(void *buf, int count,
  MPI_Datatype datatype,
  int destination, int tag,
  MPI_Comm communicator);

- MPI_ANY_TAG is a wildcard value for tag.
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  ```

- **MPI_ANY_TAG** is a wildcard value for tag.
MPI Blocking Recv Call

- MPI blocking recv returns when a message is received.
- int MPI_Recv(void *buf, int count,
  MPI_Datatype datatype,
  int source, int tag,
  MPI_Comm communicator,
  MPI_Status *status);
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               MPI_Datatype datatype,
               int source, int tag,
               MPI_Comm communicator,
               MPI_Status *status);`
- `MPI_ANY_SOURCE` and `MPI_ANY_TAG` are wildcard values for destination and tag respectively.
Example Code Using Send and Recv

```c
MPI_Comm_rank(MPI_COMM_WORLD,&myrank); /* find rank */
if (myrank == 0) {
    int x = 12345;
    MPI_Send(&x, 1, MPI_INT, 1, msgtag, MPI_COMM_WORLD);
} else if (myrank == 1) {
    int x;
    MPI_Recv(&x, 1, MPI_INT, 0, msgtag, MPI_COMM_WORLD, status);
}
```
Let's Play Ping Pong

const int PROCESS_0 = 0;
const int PROCESS_1 = 1;
MPI_Comm_rank(MPI_COMM_WORLD,&myrank); /* find rank */
for (;;) {
    if (myrank == 0) {
        int x = 12345;
        MPI_Send(&x, 1, MPI_INT, PROCESS_1, msgtag, MPI_COMM_WORLD);
        MPI_Recv(&x, 1, MPI_INT, PROCESS_1, msgtag, MPI_COMM_WORLD, status);
    } else if (myrank == 1) {
        int x;
        MPI_Recv(&x, 1, MPI_INT, PROCESS_0, msgtag, MPI_COMM_WORLD, status);
        MPI_Send(&x, 1, MPI_INT, PROCESS_0, msgtag, MPI_COMM_WORLD);
    }
}
Example: Parallel Sum in MPI

For source code, see the folder MPI/parallel_sum. Four variations (assuming $p$ processes):

- **spmd_sum_0.c**: This version sends the $n$ numbers to all processes. Each process then adds its share and sends partial sum back to process 0, which then adds the $p$ partial sums to get the total sum. *This program gives incorrect answers.*
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- `spmd_sum_1.c`: Corrected version of `spmd_sum_0.c`.

- `spmd_sum_2.c`: Process 0 sends $n/p$ elements (for $p$ processes) to each process. Each process then adds its share and sends partial sum back to process 0, which then adds the $p$ partial sums to get the total sum.

- `spmd_sum_3.c`: Assumes that each process had $n/p$ elements to begin with. Each process then adds its share and sends partial sum back to process 0, which then adds the $p$ partial sums to get the total sum.
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Source Code for Parallel Sum in MPI

/* lab/MPI/parallel_sum/spmd_sum_mpi_0.c: */
/* appropriate header files */
#include <mpi.h>
const int PARTIAL_SUM = 1;

int add(int me, int n, int *data, int nproc)
{
    int i;

    int low = me *(n/nproc);
    int high = low +(n/nproc);
    int sum = 0;
    for(i=low; i<high; i++)
        sum += data[i];

    return(sum);
}
int main(int argc, char **argv)
{
    int i;
    int total = 0; /* total sum of data elements */
    int *partial_sums;
    int *data;
    int me, n, nproc;

    if (argc != 2) {
        fprintf(stderr,"Usage: %s <number of elements>
",argv[0]);
        exit(1);
    }

    n = atoi(argv[1]); // number of data elements
    data = (int *) malloc(sizeof(int)*n); // data array

    /* Start up MPI */
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nproc);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);

    if (me == 0) {
        /* Generate numbers to be summed up */
        for (i=0; i<n; i++)
            data[i] = 1;
    }
}
/* Broadcast initial data to other processes */
if( MPI_Bcast( data, n, MPI_INT, 0, MPI_COMM_WORLD)!= MPI_SUCCESS)
    fprintf(stderr, "Oops! An error occurred in MPI_Bcast()\n");

int result = add(me, n, data, nproc);
if (me == 0) {
    partial_sums = (int *)malloc(sizeof(int)*nproc);
    /* Process 0 gets its partial sum from local variable result */
    partial_sums[0] = result;
} else {
    /* Other processes send partial sum to the process 0 */
    MPI_Send(&result, 1, MPI_INT, 0, PARTIAL_SUM, MPI_COMM_WORLD);
}
if (me == 0) {
    printf("I got %d from %d\n", partial_sums[me], me);
    /* Wait for results from other processes */
    for (i=0; i<nproc-1; i++) {
        MPI_Recv(&partial_sums[i+1], 1, MPI_INT, i+1, PARTIAL_SUM,
                  MPI_COMM_WORLD, MPI_STATUS_IGNORE);
        printf("I got %d from %d\n", partial_sums[i+1], i+1);
    }
    /* Compute the global sum */
    for (i=0; i<nproc; i++)
        total += partial_sums[i];
    printf("The total is %d\n", total);
}
MPI_Finalize();
exit(0);
MPI Functions Introduced in the Parallel Sum Example

- `int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm);`
- `int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status);`
- `int MPI_Bcast(void *buf, int count, MPI_Datatype datatype, int root, MPI_Comm comm);`

- `MPI_ANY_SOURCE` and `MPI_ANY_TAG` are wildcard values.

- `double MPI_Wtime();` Time in seconds since some arbitrary point in the past.

- `double MPI_Wtick();` Time in seconds between successive ticks of the clock.
Visualization and Logging

- Link with the libraries `-llmpe -lmpe` to enable logging and the MPE environment. Then run the program as usual and a log file will be produced.
- The log file can be visualized using the `jumpshot` program that comes bundled with MPICH.
/* See complete example in lab/MPI/token-ring/token_ring_mpi.c */
void pass_the_token(int me, int nproc)
{
  int token, src, dest;
  int count = 1;
  const int TOKEN = 4;
  int msgtag = TOKEN;
  MPI_Status status;

  /* Determine neighbors in the ring */
  if (me == 0) src = nproc -1;
  else src = me - 1;

  if (me == nproc - 1) dest = 0;
  else dest = me + 1;

  if( me == 0 ) {
    token = dest;
    MPI_Send(&token,count, MPI_INT, dest, msgtag, MPI_COMM_WORLD);
    MPI_Recv(&token, count, MPI_INT, src, msgtag, MPI_COMM_WORLD, &status);
    printf("token ring done\n");
  } else {
    printf("received token ring on %d from %d \n",me, src);
    MPI_Recv(&token, count, MPI_INT, src, msgtag, MPI_COMM_WORLD, &status);
    MPI_Send(&token, count, MPI_INT,dest,msgtag,MPI_COMM_WORLD);
  }
}
Collective Operations, Communicators and Groups

- int MPI_Reduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm);
- int MPI_Allreduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, MPI_Comm comm);
- int MPI_Comm_group(MPI_Comm comm, MPI_Group *group);
- int MPI_Group_excl(MPI_Group group, int n, int *ranks, MPI_Group newgroup);
- int MPI_Group_free(MPI_Group *group);
- int MPI_Comm_create(MPI_Comm comm, MPI_Group group, MPI_Comm *newcomm);
- int MPI_Comm_free(MPI_Comm *comm);
Calculating $\pi$ using Monte Carlo Simulation

- The following code example calculates $\pi$ to a specified precision using a Monte Carlo simulation.
- This example illustrates the use of MPI groups and communicators. We designate one process to be the random number generator. All other processes form a separate group and communicator to do the simulation.
- The example also illustrates the use of the `MPI_AllReduce` function.
/* compute pi using Monte Carlo method */
/* appropriate header files */
#include <mpi.h>
#include <mpe.h>
#define CHUNKSIZE 1000
#define INT_MAX RAND_MAX
/* message tags */
#define REQUEST 1
#define REPLY 2
int main( int argc, char *argv[] )
{
    int iter, in, out, i, max, ranks[1], done;
    double x, y, Pi, error, epsilon;
    int numprocs, myid, server, totalin, totalout, workerid;
    int rands[CHUNKSIZE], request;
    MPI_Comm world, workers;
    MPI_Group world_group, worker_group;
    MPI_Status status;

    MPI_Init(&argc,&argv);
    world = MPI_COMM_WORLD;
    MPI_Comm_size(world,&numprocs);
    MPI_Comm_rank(world,&myid);
    server = numprocs-1; /* last proc is server */
    if (myid == 0)
        sscanf( argv[1], "%lf", &epsilon );
MPI_Bcast( &epsilon, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD );
MPI_Comm_group( world, &world_group );
ranks[0] = server;
MPI_Group_excl( world_group, 1, ranks, &worker_group );
MPI_Comm_create( world, worker_group, &workers );
MPI_Group_free(&worker_group);
if (myid == server) { /* I am the random number server */
    do {
        MPI_Recv(&request, 1, MPI_INT, MPI_ANY_SOURCE, REQUEST,
                  world, &status);
        if (request) {
            for (i = 0; i < CHUNKSIZE; ) {
                rands[i] = random();
                if (rands[i] <= INT_MAX) i++;
            }
            MPI_Send(rands, CHUNKSIZE, MPI_INT,
                     status.MPI_SOURCE, REPLY, world);
        }
    } while( request>0 );
}
} else {  /* I am a worker process */
    request = 1;
    done = in = out = 0;
    max = INT_MAX;  /* max int, for normalization */
    MPI_Send(&request, 1, MPI_INT, server, REQUEST, world);
    MPI_Comm_rank( workers, &workerid );
    iter = 0;

    ...
while (!done) {
    iter++;
    request = 1;
    MPI_Recv(rands, CHUNKSIZE, MPI_INT, server, REPLY, world, &status);
    for (i=0; i<CHUNKSIZE-1; ) {
        x = (((double) rands[i++])/max) * 2 - 1;
        y = (((double) rands[i++])/max) * 2 - 1;
        if (x*x + y*y < 1.0)
            in++;
        else
            out++;
    }
    MPI_Allreduce(&in, &totalin, 1, MPI_INT, MPISummon, workers);
    MPI_Allreduce(&out, &totalout, 1, MPI_INT, MPISummon, workers);
    Pi = (4.0*totalin)/(totalin + totalout);
    error = fabs( Pi-3.141592653589793238462643);
    done = (error < epsilon || (totalin+totalout) > 1000000);
    request = (done) ? 0 : 1;
    if (myid == 0) {
        printf( "\rpi = \%23.20f", Pi );
        MPI_Send(&request, 1, MPI_INT, server, REQUEST, world);
    } else {
        if (request)
            MPI_Send(&request, 1, MPI_INT, server, REQUEST, world);
    }
}  
MPI_Comm_free(&workers);
if (myid == 0) {
    printf( "\npoints: %d\nin: %d, out: %d, <ret> to exit\n",
            totalin+totalout, totalin, totalout );
    getchar();
}

MPI_Finalize();
exit(0);
Processes in Monte Carlo Simulation

Random Number Server

Monte Carlo Simulation Setup

Workers

World
A better way of splitting Communicators

```c
int MPI_Comm_split(MPI_Comm oldcomm, int color, int key, MPI_Comm newcomm);
```

Using the above function we can split the communicator in the Monte Carlo example as follows:

```c
color = (myid == server);
MPI_Comm_split(world, color, 0, &workers);
```
MPE Graphics

- Simple graphics capability is built in the MPE environment that comes with MPI.
- Allows users to draw points, lines, circles, rectangles as well as manipulate colors.
- Need to link in `-lmpe` and `-lX11` libraries.
The following shows the new code that was added to the previous example. Also we need to add 
\texttt{-lX11} linker option to link in the X Windows graphics library.

\begin{verbatim}
#include <mpe_graphics.h>

MPE_XGraph graph;

MPE_Open_graphics(&graph, MPI_COMM_WORLD, (char *)0, -1, -1, WINDOW_SIZE, WINDOW_SIZE, MPE_GRAPH_INDEPENDENT);

MPE_Draw_point(graph, (int) (WINDOW_SIZE/2 + x * WINDOW_SIZE/2), (int) (WINDOW_SIZE/2 + y * WINDOW_SIZE/2), MPE_BLUE);

MPE_Update(graph);

MPE_Close_graphics(&graph);
\end{verbatim}
Screenshot of Monte Carlo in Action
References


MPI Basic Calls Summary

int MPI_Init(int *argc, char ***argv)
int MPI_Comm_size(MPI_Comm comm, int *size)
int MPI_Comm_rank(MPI_Comm comm, int *rank)
int MPI_Finalize()
int MPI_Send(void *buf, int count, MPI_Datatype type, int dest, int tag, MPI_Comm comm)
int MPI_Recv(void *buf, int count, MPI_Datatype type, int src, int tag, MPI_Comm comm, MPI_Status *status)
int MPI_Bcast(void *buf, int count, MPI_Datatype type, int root, MPI_Comm comm)
int MPI_Reduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype type, MPI_Op op, int root, MPI_Comm comm)
int MPI_Allreduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype type, MPI_Op op, MPI_Comm comm)
double MPI_Wtime()
double MPI_Wtick()
Exercises

- Install a version of MPI on your personal computer (either MPICH or MPICH2). Check out the class code examples for MPI from the class repository and compile and run some of them on your system to test the MPI installation.

- Take the code snippet for the ping pong example and create an actual MPI program and test it.