MPI Basics

- **Goal:** Overview of MPI
- **How to compile and run MPI programs**
- **Main MPI commands - examples**
- **See many other online resources available**
Where to find help

- Many tutorials and other documents including the MPI standard available online

- The openMPI latest documentation
  https://www.open-mpi.org/doc/current/

- The original MPI site:

- The LLNL link:
  https://computing.llnl.gov/tutorials/mpi/
#include <stdio.h>
#include <mpi.h>

int main(int argc, char *argv[]) {
    int nPEs, rank;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nPEs);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    printf("Hello from process %d out of %d \n", rank, nPEs);
    MPI_Finalize();
}
Comments:

- `#include <mpi.h>` is mandatory: contains MPI definitions, types, etc,
- `MPI_Init(.,.)` and `MPI_Finalize()` start and end MPI respectively
- `MPI_Comm_size` gives the number of processes
- `MPI_Comm_rank` gives the number of this process
- Note: all non-MPI functions/commands are local: e.g., printf will run on each PE.
Communicators

- A communicator defines a group of processes which communicate with each other.

- MPI_COMM_WORLD is the (default) communicator: an internal structure which includes all processes that are allowed to communicate with each other within this run.

- Ranks, sizes, are all relative to a communicator.

- Can define other communicators than MPI_COMM_WORLD by command MPI_Comm.

- Can work with communicators using various commands: MPI_Comm_group, MPI_Group_excl, MPI_Comm_create, ....
The “phixx cluster”

- A small cluster of 16 Xeon processors connected via a network
- Machines in the cluster: \( \text{phi01, phi02, \cdots, phi08} \)
- Login to any of these..
- System is dedicated to teaching parallel programming in CSE
Compiling, linking, and running a program

- On the phixx cluster - openmpi version 1.10.2 is loaded by default – but we will use version 1.3

- Instructions will be provided on how to load required modules, compiling, etc

[One note: It is important that *all nodes* run the same version!]

- For compiling: MPI provides mpicc for C and mpif77 (fortran 77), mpif90 (fortran 90 when installed) for fortran.

- For the “hello world” example:

  \[\text{mpicc -o hello.ex hello.c}\]

- For large programs use makefiles
Running a program

- in MPICH, and openMPI a program is run with `mpirun`:
  ```
  mpirun -np 2 hello.ex
  ```

A few options

- help: print mpi options
  ```
  mpirun -h[elp]
  ```

- use filename as host-file:
  ```
  mpirun -np 4 -machinefile < filename > executable.ex
  ```

- Note you will need a machinefile on the phixx cluster. [a default one will be made available].
Remember: hardest aspect of parallel programming is: Debugging

explore the use of MCA parameters (Modular Component Architecture) for debugging (and more) in

https://www.open-mpi.org/faq/?category=debugging

More information on the class web-site and/or canvas
Sends and Receives

Simplest types of communication yet there are several options. For example:

* Synchronous send
* Blocking send / blocking receive
* Non-blocking send / non-blocking receive
* Buffered send
*Blocking send* will complete (return) only when the buffered data has been sent or saved and it is safe to free or reuse send buffer.

*Synchronous blocking send:* Handshaking takes place between receiving and sending processes before actual send.

*Asynchronous blocking send:* data buffered until eventual delivery to receiving process.

*Blocking Receives* complete (return) after the data has arrived to receiving process.

*Non-blocking sends and receives* are similar - they return almost immediately. No waiting for communication to complete.
Non-blocking communications are useful when overlapping computation with communication

Non-blocking operations “request” the MPI library to perform the operation when possible. Cannot predict when this takes place

The application buffer (variable space, i.e., array to be sent) should not be changed until it is known that the requested non-blocking operation was performed

Can use “wait” routines and MPI Iprobe for this (see later)
Sends and Receives: Blocking send

\texttt{MPI\_Send\(\text{start},\text{count},\text{datatype},\text{dest},\text{tag},\text{comm}\)}

- **start** is a pointer to first entry of data to be sent
- **count** is the length of array
- **datatype** one of MPI's datatypes: \(\text{MPI\_INT, MPI\_FLOAT, MPI\_DOUBLE, etc,...}\)
- **dest** is the destination process
- **comm** is the communicator
- **tag** is a tag assigned to message so it is recognized by a matching receive.
There should be an associated receive. General form:

\[ \text{MPI} \text{Recv}(\text{start, count, datatype, source, tag, comm, status}) \]

- Start, count, datatype, comm, have the same meaning as in send
- \textit{source} is the rank of sending process
- \textit{tag} is the same as the tag used in the send
- Can also use:
  \textit{MPI_ANY_TAG} and / or \textit{MPI_ANY_SOURCE}
- \textit{status} is a struct of type \textit{MPI\_Status}
- The source, tag, and count of the message actually received can be retrieved from status.
MPI_Status status;
MPI_Recv( ... , &status );
... status.MPI_TAG;        <-- get tag
... status.MPI_SOURCE;     <-- get source
MPI_Get_count(&status,datatype,
               &count);         <-- get count

MPI_TAG, MPI_SOURCE useful in case when MPI_ANY_TAG
and/or MPI_ANY_SOURCE used in the receive

MPI_Get_count will tell us how much data of a particular type was
received [details shortly]
What is in the MPI_status struct?

MPI_SOURCE - id of processor sending the message

MPI_TAG - the message tag

MPI_ERROR - error status

MPI_LENGTH (Not accessible)

MPI_COMM - communicator,

➤ Other members reserved for internal implementation.
Can check that a message has arrived with MPI_Iprobe or MPI_Probe

```c
int MPI_Iprobe(int src, int tag, MPI_Comm comm, int* flag, MPI_Status stat)
```

- MPI_Probe is a blocking version of MPI_Iprobe
- Can loop-wait until message arrives
- Can retrieve the length of a message, with MPI_Get_count:

```c
int MPI_Get_count(MPI_Status *stat, MPI_Datatype dtyp, int *cnt)
```

Sets cnt to number of items in the message.
Example of usage: passing a variable-length string

```
int source = 0, tag = 100, len;
char *str;
MPI_Status status;
MPI_Probe(source, tag, MPI_COMM_WORLD, &status);
MPI_Get_count(&status, MPI_CHAR, &len);
if(len != MPI_UNDEFINED) str = malloc(len);
MPI_Recv(str, len, MPI_CHAR, source, tag,
          MPI_COMM_WORLD, &status)
```
Simple collective operations

\[ \text{MPI\_Bcast}(\text{start, count, datatype, root, comm}) \]

- Sends data from one process to all others.
- \text{start, count, datatype, comm} : as before
- \text{root}: origin (process \#) of broadcast

\[ \text{MPI\_Reduce}(\text{start, result, count, datatype, MPI\_OPE, root, comm}) \]

**\text{MPI\_OPE}:** OPE is one of MAX, MIN, SUM, PROD, LAND, BAND, LOR, BOR, LXOR, BXOR, MAXLOC, MINLOC

LAND = logical AND, BAND = bitwise AND. (Similarly for OR, XOR). \text{MPI\_MAXLOC, MPI\_MINLOC} : Find Max(min) and location of max (min)
Scatter and Gather

MPI_Scatter(void *sendbuf,int sendcnt,
    MPI_Datatype sendtyp,void *recvbuf,int recvcnt,
    MPI_Datatype recvtyp,int root,MPI_Comm comm )

➤ scatters sendcnt items in succession from sendbuf to processors 0. ... , p - 1.

➤ Arrays sent to each PE all have same length (sendcnt)

MPI_Gather (void *sendbuf,int sendcnt,
    MPI_Datatype sendtyp,void *recvbuf,int recvcnt,
    MPI_Datatype recvtyp,int root,MPI_Comm comm)

– mpi
**MPI Collective communication routines**

<table>
<thead>
<tr>
<th>Routine</th>
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<th>Routine</th>
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</thead>
<tbody>
<tr>
<td>Allgather</td>
<td>Allgatherv</td>
<td>Allreduce</td>
</tr>
<tr>
<td>Alltoall</td>
<td>Alltoallv</td>
<td>Bcast</td>
</tr>
<tr>
<td>Gather</td>
<td>Gatherv</td>
<td>Reduce</td>
</tr>
<tr>
<td>ReduceScatter</td>
<td>Scan</td>
<td>Scatter</td>
</tr>
<tr>
<td>Scatterv</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The 'v' versions: Scatterv, Gatherv, Allgatherv, Alltoallv, allow variable counts and shifts on the original array for each destination.

**Scatterv:**

- Process 0
- Process 1
- Process 2
- Process 3
Appendix: set-up for the phi cluster

- The nodes are called \textit{phi01, phi02, ..., phi08}
- You can login to any of them via \texttt{ssh phi0x.cselabs.umn.edu}
- You need to use mpi version 1.3 [others won't work]
  
  \begin{verbatim}
  module load hpc/openmpi
  \end{verbatim}

- Add this to your init shell file [e.g., in .cshrc or .bashrc]
- One key requirement is that you should be able to login to any node without requiring a password. Find out how to use ssh-keygen and enable ssh without passwords:

  \begin{verbatim}
  ssh-keygen -t rsa -P ""
cat ~/.ssh/id_rsa.pub > ~/.ssh/authorized_keys
  \end{verbatim}
You will need to add all the machines into `~/.ssh/known_hosts` file. For this you can ssh once to each machine. This will prevent prompts for confirmations each time you run something.

The next thing you will need is a hostfile needed by MPI [see examples provided] Here is a sample hostfile:

<table>
<thead>
<tr>
<th>Host Address</th>
<th>Slots</th>
</tr>
</thead>
<tbody>
<tr>
<td>phi01.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi02.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi03.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi04.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi05.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi06.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi07.cselabs.umn.edu</td>
<td>16</td>
</tr>
<tr>
<td>phi08.cselabs.umn.edu</td>
<td>16</td>
</tr>
</tbody>
</table>

Call it `hostfile` or `phi_cluster` for example

Run with, e.g.,

```bash
mpirun -np 32 -hostfile phi_cluster test.ex
```
Appendix: A few details and an example

Some function calls

Send-Receive Pairs

```c
#include <mpi.h>
int MPI_Send(const 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)
```

Broadcast

```c
#include <mpi.h>
int MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm)
```
Quoting from the documentation: (open-mpi.org):

MPI_Bcast broadcasts a message from the process with rank root to all processes of the group, itself included. It is called by all members of group using the same arguments for comm, root. On return, the contents of root’s communication buffer has been copied to all processes.

➤ Main point: no need to have a corresponding receive - but all nodes in comm must issue the same command (the communication is “collective”)

➤ What are MPI Data types?
## MPI Datatypes

<table>
<thead>
<tr>
<th>Type</th>
<th>Type</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_CHAR</td>
<td>MPI_C_COMPLEX</td>
<td></td>
</tr>
<tr>
<td>MPI_WCHAR</td>
<td>MPI_C_FLOAT_COMPLEX</td>
<td></td>
</tr>
<tr>
<td>MPI_SHORT</td>
<td>MPI_C_DOUBLE_COMPLEX</td>
<td></td>
</tr>
<tr>
<td>MPI_INT</td>
<td>MPI_C_LONG_DOUBLE_COMPLEX</td>
<td></td>
</tr>
<tr>
<td>MPI_LONG</td>
<td>MPI_C_BOOL</td>
<td></td>
</tr>
<tr>
<td>MPI_LONG_LONG_INT</td>
<td>MPI_LOGICAL</td>
<td></td>
</tr>
<tr>
<td>MPI_LONG_LONG</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MPI_SIGNED_CHAR</td>
<td>MPI_INT8_T, MPI_INT16_T</td>
<td></td>
</tr>
<tr>
<td>MPI_UNSIGNED_CHAR</td>
<td>MPI_INT32_T</td>
<td></td>
</tr>
<tr>
<td>MPI_UNSIGNED_SHORT</td>
<td>MPI_INT64_T</td>
<td></td>
</tr>
<tr>
<td>MPI_UNSIGNED_LONG</td>
<td>MPI_UINT8_T, MPI_UINT16_T</td>
<td></td>
</tr>
<tr>
<td>MPI_UNSIGNED</td>
<td>MPI_UINT32_T</td>
<td></td>
</tr>
<tr>
<td>MPI_FLOAT</td>
<td>MPI_UINT64_T</td>
<td></td>
</tr>
<tr>
<td>MPI_DOUBLE</td>
<td>MPI_BYTE</td>
<td></td>
</tr>
<tr>
<td>MPI_LONG_DOUBLE</td>
<td>MPI_PACKED</td>
<td></td>
</tr>
</tbody>
</table>
Example: Compute values of $e^x$

- No practical value: Only goal is to illustrate a pipelined computation and sends, receives, broadcasts.

- We will compute $exp(x)$ by its $n$-th Taylor series expansion and use Horner’s scheme:

  $$e^x \approx 1 + \frac{x}{1} \left( 1 + \frac{x}{2} \left( 1 + \frac{x}{3} \left( \cdots \left( 1 + \frac{x}{n} \right) \cdots \right) \right) \right)$$

- In Python this can be implemented as:

```python
x = some_value
n = some_value
val = 1.0
for i in range(n, 0, -1):
    val = 1.0 + (x/i) * val
print(val)
```
General procedure: Think of a linear array. For $n = 5$:

<table>
<thead>
<tr>
<th>West</th>
<th>MyId</th>
<th>East</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-----</td>
<td>1</td>
</tr>
</tbody>
</table>

Print Start

* Start: proc. $n - 1$ (last one) who sends value $val = 1 + (x/n)$ to West processor
* All other nodes: get $val$ from East; update; and:
* Send $val$ West *unless* MyId=0 in which case print.

➤ At first assume $x$ is set in each process
➤ Next: Assume $x$ is also sent along with $val$
➤ Next: Use a broadcast of $x$ instead
➤ Next: In the above only one process is active at a time. What if I need to compute a bunch of values $e^{x_0}$, $e^{x_1}$, $\cdots$ $e^{x_k}$
Example: Compute a sum of $n$ numbers

Generate/ read $n$ numbers, then scatter equal parts to each participating PE. Each PE computes a subsum then the whole sum is calculated by a reduction ($+$) of subsums.

```c
#include <mpi.h>
int MPI_Scatter(const void *sendbuf, int sendcnt, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
```

Explore also the nonblocking send and scatter

```c
#include <mpi.h>
int MPI_Isend(const void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm, MPI_Request *request)
```
int MPI_Iscatter(const void *sendbuf, int sendcnt,
MPI_Datatype sendtype, void *recvbuf,
int recvcount, MPI_Datatype recvtype,
int root, MPI_Comm comm, MPI_Request *request)

- Recall: nonblocking sends allow you to do some work while a
send is being processed. No need to wait until the send is completed.
Work can be done as long as we do not touch the buffer being sent.
Similarly for all non-blocking operations.

- Syntax for (regular) reduction operation

```c
#include <mpi.h>
int MPI_Reduce(const void *sendbuf, void *recvbuf,
int count, MPI_Datatype datatype, MPI_Op op,
int root, MPI_Comm comm)
```

- **MPI_Ireduce**: adds a MPI_Request *request at end.

- Common **MPI_Op’s**:
  - MPI_SUM, MPI_PROD, MPI_MAX, MPI_MIN