High Performance Computing:
Tools and Applications

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Lecture 14

MPI – Message Passing Interface

- MPI is used for distributed memory parallelism (communication between nodes of a cluster)
- Interface specification with many implementations
- Portability was a major goal
- Widespread use in parallel scientific computing
- Six basic MPI functions
  - `MPI_Init`, `MPI_Finalize`,
  - `MPI_Comm_size`, `MPI_Comm_rank`,
  - `MPI_Send`, `MPI_Recv`
- Many other functions…

MPI

- An MPI job consists of multiple *processes* running on multiple nodes, e.g., 1 or more processes per node.
- Processes do not share memory. MPI provides functions for passing messages between processes.
- If there are fewer processes than cores (usual case), then multiple threads are used in each process.

MPI Hello World!

```c
#include <stdio.h>
#include <mpi.h>

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

  MPI_Init(&argc, &argv);

  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  printf("Hello, world! from %d of %d\n", rank, size);

  MPI_Finalize();

  return 0;
```

Compiling MPI programs

Use `mpicc` which calls a compiler and links to appropriate libraries, etc.

```
mpicc    # wrapper around gcc
mpiicc   # wrapper around icc
mpiicpc  # wrapper around icpc
```

Running MPI programs

Use `mpirun -n <numproc> .... ./progname`

- `mpirun` will contact all nodes, set up communication between nodes, and run your program on all nodes
- Usually MPI jobs are run on multiple nodes of a cluster (1 or more processes per node), and multiple threads per MPI process

Running MPI programs on MIC

- We will use MPI to run multiple processes on a single coprocessor (although this is shared memory hardware)
- It is also possible to use MPI to run multiple processes on multiple coprocessors, and multiple coprocessors and CPU hosts, but we will not do this
- Run in native mode
  - compile on host using `mpiicc -mmic ...`
  - scp executable to coprocessor
  - log into coprocessor and use `mpirun`
- Run from the host
  - compile on host using `mpiicc -mmic ...`
  - scp executable to coprocessor
  - use `mpirun` but must also set `I_MPI_MIC`

```
I_MPI_MIC=1 mpirun -host mic0 -n 60 ~/progname
```

Blocking Send and Recv

- `MPI_Send`
  - Function does not return until send buffer can be reused
  - Does not imply the message has been sent
  - Must be assured that the receiver posts a receive call
- `MPI_Recv`
  - Function does not return until recv buffer contains received message
- Deadlock example (will deadlock if no buffering)
  - Two processes, each performs

```
Send(to other)
Recv(from other)
```

deadlock.c

```c
void main(int argc, char *argv[])
{
  int size, rank;
  double sum;
  double sendbuf[MSGLEN];
  double recvbuf[MSGLEN];
  MPI_Status status;

  MPI_Init(&argc, &argv);

  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  double val = (double) rank;
  sendbuf[0] = (double) rank;

  MPI_Send(sendbuf, MSGLEN, MPI_DOUBLE, (rank+1)%size,
    0, MPI_COMM_WORLD);

  MPI_Recv(recvbuf, MSGLEN, MPI_DOUBLE, (rank-1+size)%size,
    0, MPI_COMM_WORLD, &status);

  printf("Recv on node %d is %f\n", rank, recvbuf[0]);

  MPI_Finalize();
```

Non-blocking Send and Recv

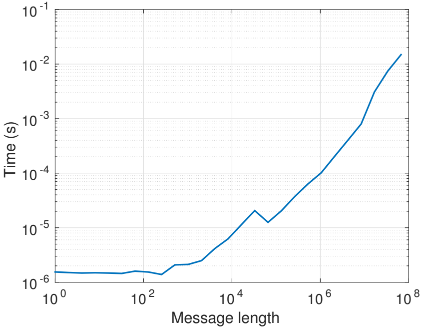
- `MPI_Isend`
  - Function returns immediately; the data may be buffered, and the message may not be sent yet
- `MPI_Irecv`
  - Function returns immediately; the message has not necessarily arrived
- `MPI_Wait`
  - Block until Isend/Irecv completes (buffer can only be used at this point)
- Allows overlap of communication with computation
- Easier to avoid deadlocks than using blocking calls
- Can combine blocking and non-blocking calls

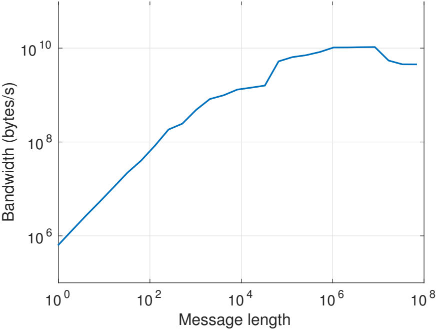
nonblocking.c

```
MPI_Request request;
MPI_Status status;

MPI_Irecv(recvbuf, length, MPI_CHAR, (rank-1+size)%size,
  0, MPI_COMM_WORLD, &request);

MPI_Send(sendbuf, length, MPI_CHAR, (rank+1)%size,
  0, MPI_COMM_WORLD);

MPI_Wait(&request, &status);
```

Measured latency and bandwidth

2 CPU Xeon host (bidirectional bandwidth, one pair of processes)

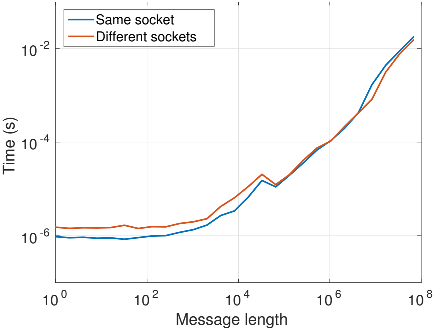




- latency is around 1 microsecond
- bandwidth is comparable to single thread memory bandwidth (MPI is using shared memory in this case)
- how does this curve change when multiple pairs are running?
- more efficient to send long messages than short messages (group your messages together if possible, unless you are pipelining computations)

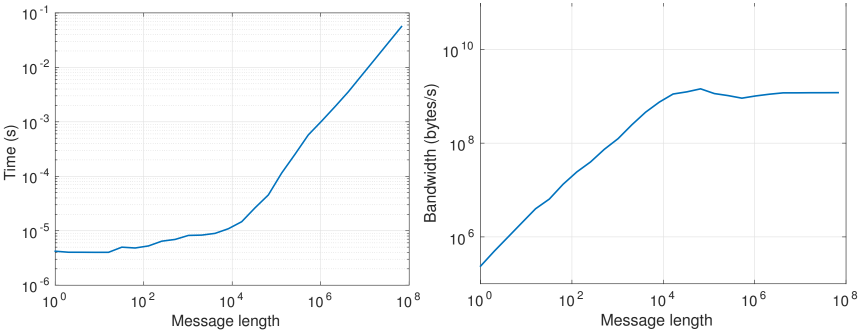
Measured latency and bandwidth

2 CPU Xeon host (bidirectional bandwidth, one pair of processes)



Measured latency and bandwidth

Xeon Phi coprocessor (bidirectional bandwidth, one pair of processes)



Eager and Rendezvous protocols

- Eager protocol: if the message is short, it is sent immediately and buffered on the receiver's side. On the receiver, the message is copied to the receive buffer when the receive is posted.
- Rendezvous protocol: if the message is long, a short message is first sent to the receiver to indicate that a send has been posted. The receiver sends the address of the receive buffer. The sender then sends the actual message.
- Kink in timing graph is due to the switchover from eager to rendezvous protocols.

MPI process pinning

- When using multiple MPI processes per node, it may be desirable to pin the processes to a socket, or to a set of cores
- Each MPI process may use multiple threads (within a socket or set of cores)
- Define a *domain* to be a non-overlapping set of logical cores
- A MPI process can be pinned to a domain; the threads in a process run on the logical cores of the domain (use `KMP_AFFINITY` to pin threads)
- Pinning can be accomplished with environment variables (also with the `mpirun` command, etc.)
- Set `I_MPI_DEBUG=4` to see how processes are pinned

MPI process pinning with environment variables

`I_MPI_PIN_DOMAIN` can take the following values:

- `core`
- `socket`
- `numa`
- `node`
- `cache1`
- `cache2`
- `cache3`
- numerical value, which is the *size* of the domain
- `omp` which sets the domain size to `OMP_NUM_THREADS`

MPI process pinning with environment variables

`I_MPI_PIN_ORDER` can take the following values:

- `scatter`
- `compact`
- `spread`
- `bunch`

Reference: https://software.intel.com/en-us/node/528819

Exercise 7 - Due Wed., Oct. 19, 10 pm

- Write a code to measure the maximum bandwidth between $2p$ processes on the coprocessor, for different message lengths, and for different values of p, e.g., 1, 2, 4, 8, 16, 30. (Use communication between pairs of processes.)
- At what value of p does the aggregate bandwidth for long messages no longer improve?
- For this value of p, plot the average time for sending a single message as a function of message length. Use lengths 1 byte, 2 bytes, 4 bytes, etc., up to 16 MB. Also plot the bandwidth (GB/s). Use log-log axes for both plots.