Advanced Topics in Numerical Analysis: High Performance Computing

MATH-GA 2012.001 & CSCI-GA 2945.001

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April 6, 2017

Outline

Organization

Summary from last class

Coding and running code time!

Organization

- Homework 4 due next week.
- Have you logged into Stampede and tried to run there? Please try asap (to give us time to work out issues).
- Final projects: Expect individual feedback for your projects in the next couple of days.
- Final project presentations: May 10/11 (most likely). Recall that you've to give a 10 minute presentation.
- And please come to your colleagues' presentations.

Organization

Planned material for remainder of course (you are welcome to give input!):

- Hybrid computing (MPI + OpenMP; today)
- GPU computing with OpenCL; possibly Intel Xeon Phi accelerators
- Algorithms: Multigrid (?) FMM (?)
- Tools: Some debugging; Visualization with paraview; load balancing tools (?)
- Homeworks: Expect either two more short homeworks, or one longer one.

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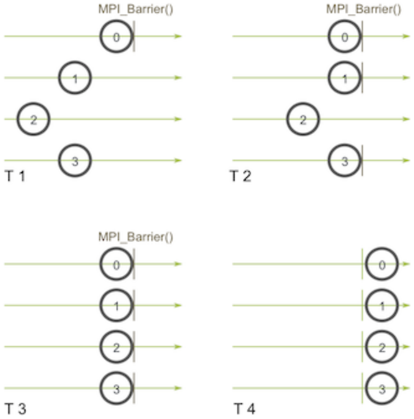
Coding and running code time!

MPI Barrier

Synchronizes all processes. Other collective functions implicitly act as a synchronization. Used for instance for timing.

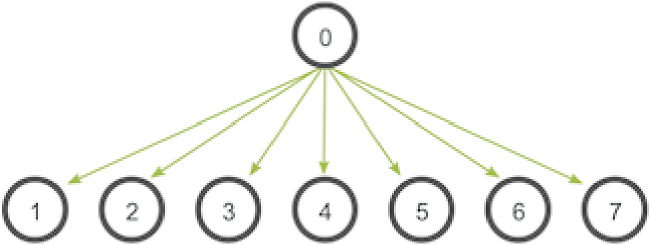
```
MPI_Barrier(MPI_Comm communicator)
```



MPI Broadcast

Broadcasts data from one to all processors. Every processor calls same function (although its effect is different).

```
MPI_Bcast(void* data, int count, MPI_Datatype
datatype, int root, MPI_Comm communicator)
```



Actual implementation depends on MPI library.

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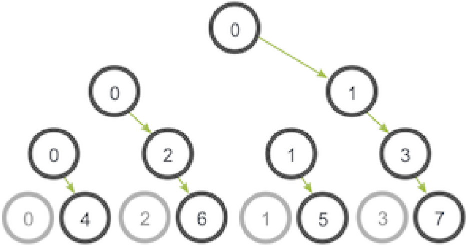


Actual implementation depends on MPI library.

MPI Reduce

Reduces data from all to one processors. Every processor calls same function.

```
MPI_Reduce(void* sendbuf, void* recvbuf, int count,
MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm
communicator)
```

Possible Reduce operators:

MPI_MAX: Returns the maximum element.

MPI_MIN: Returns the minimum element.

MPI_SUM: Sums the elements.

MPI_PROD: Multiplies all elements.

MPI_LAND: Performs a logical and across the elements.

MPI_LOR: Performs a logical or across the elements.

MPI_BAND: Performs a bitwise and across the bits of the elements.

MPI_BOR: Performs a bitwise or across the bits of the elements.

MPI_MAXLOC: Returns the maximum value and the rank of the process that owns it.

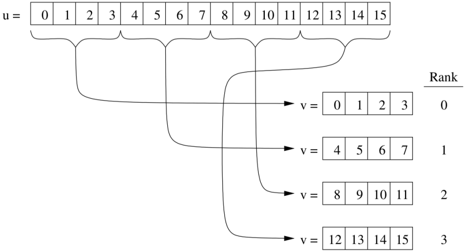
MPI_MINLOC: Returns the minimum value and the rank of the process that owns it.

`MPI_Allreduce()`: Provides result of reduction too all processors.

MPI Scatter

Broadcasts different data from one to all processors. Every processor calls same function.

```
MPI_Scatter(void* sendbuff, int sendcount,
MPI_Datatype sendtype, void* recvbuf, int recvcount,
MPI_Datatype recvtype, int root, MPI_Comm
communicator)
```



Send arguments must be provided on all processors, but sendbuf can be NULL. Send/recv count are per processor.

MPI Gather

Gathers different data from all to one processors. Every processor calls same function.

```
MPI_Gather(void* sendbuff, int sendcount, MPI_Datatype
sendtype, void* recvbuf, int recvcount, MPI_Datatype
recvtype, int root, MPI_Comm communicator)
```

Variant:

`MPI_Allgather()` gathers from all processors to all processors.

MPI_Bcast comparison

Let's compare a naive implementation of `MPI_Bcast` with the system implementation:

https://github.com/NYU-HPC17/lecture8

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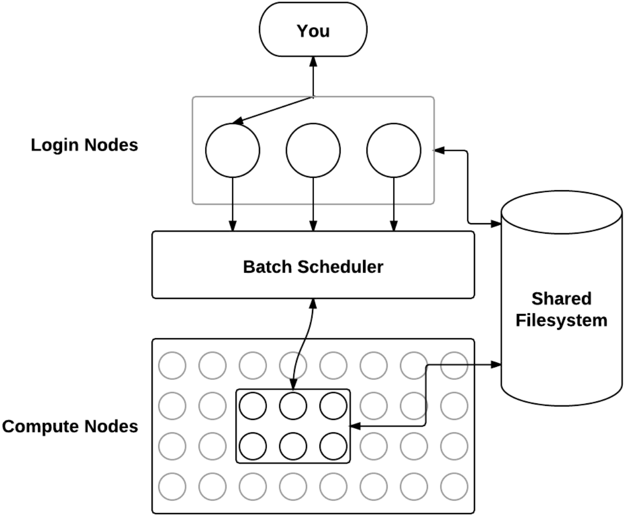
. . . and let's do it on Stampede!

Submitting jobs on Stampede

Overview of HPC cluster



Submitting jobs on Stampede

Stampede user guide:
`https://portal.tacc.utexas.edu/user-guides/stampede`

Batch facilities: SGE, LSF, SLURM. Stampede uses SLURM, and these are some of the basic commands:

- submit/start a job: `sbatch jobscript`
- see status of my job: `squeue -u USERNAME`
- cancel my job: `scancel JOBID`
- see all jobs on machine: `showq | less`

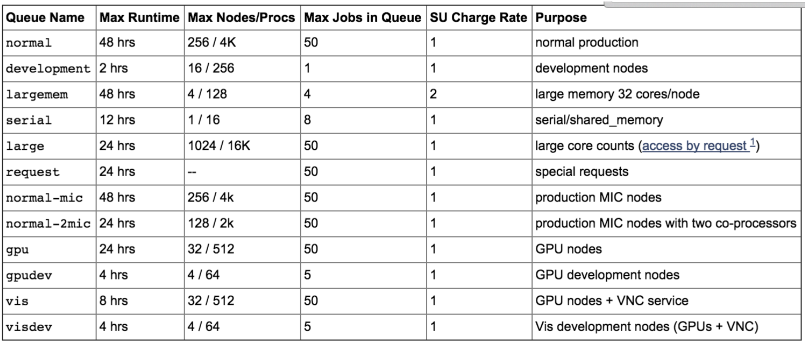
Submitting jobs on Stampede

Some basic rules:

- Don’t run on the login node!
- Don’t abuse the shared file system.

Submitting jobs on Stampede

Available queues on Stampede



Queue Name	Max Runtime	Max Nodes/Procs	Max Jobs in Queue	SU Charge Rate	Purpose
normal	48 hrs	256 / 4K	50	1	normal production
development	2 hrs	16 / 256	1	1	development nodes
largemem	48 hrs	4 / 128	4	2	large memory 32 cores/node
serial	12 hrs	1 / 16	8	1	serial/shared_memory
large	24 hrs	1024 / 16K	50	1	large core counts (access by request [1])
request	24 hrs	--	50	1	special requests
normal-mic	48 hrs	256 / 4k	50	1	production MIC nodes
normal-2mic	24 hrs	128 / 2k	50	1	production MIC nodes with two co-processors
gpu	24 hrs	32 / 512	50	1	GPU nodes
gpudev	4 hrs	4 / 64	5	1	GPU development nodes
vis	8 hrs	32 / 512	50	1	GPU nodes + VNC service
visdev	4 hrs	4 / 64	5	1	Vis development nodes (GPUs + VNC)

Submitting jobs on Stampede

Example job script (in git repo for lecture5)

```
#!/bin/bash
#SBATCH -J myMPI          \# job name
#SBATCH -o myMPI.o        \# output and error file name
#SBATCH -n 32             \# total number of mpi tasks
#SBATCH -p development    \# queue -- normal, development, etc.
#SBATCH -t 01:30:00       \# run time (hh:mm:ss) - 1.5 hours
#SBATCH --mail-user=username@tacc.utexas.edu
#SBATCH --mail-type=begin \# email me when the job starts
#SBATCH --mail-type=end   \# email me when the job finishes
ibrun ./a.out             \# run the MPI executable
```

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1D MPI Jacobi

- Blocking Send/Recv
- Nonblocking Send/Recv; overlapping computation and communication
- MPI-OpenMP hybrid on Stampede