First in a series…

**MILLS HPC CLUSTER:**
Compile and Run
MPI Jobs

January 28, 2012
Mills Community Cluster

http://www.it.udel.edu/research-computing
Goals

- Compile an MPI program using OpenMPI wrappers
- Use Grid Engine script for OpenMPI wrappers with Infiniband
Review

Bash

- `.bashrc` - aliases and functions
- `.bash_profile` - environment and startup

Filesystem

- `/home` - 2G quota, backed up
- `/scratch` - duration of job only
- `/lustre` - large, shared, not backed up
Getting started

- Connect to mills
  
  `ssh -l username mills.hpc.udel.edu`

- Change to today's personal directory
  
  `cd $WORKDIR/$USER`
Possible Errors

- No such file or directory

  mkdir $WORKDIR/$USER

- Cannot create directory

  workgroup -g <investing_entity>
  mkdir $WORKDIR/$USER
Copy Examples

cp -r ~trainf/ex-day4 .
cd ex-day4
Message passing interface (MPI) allows programs to communicate between processors that use their own node’s memory address space.

OpenMPI is the most desirable MPI implementation to use on Mills.

MPI jobs inherently generate a considerable amount of network traffic between the processor cores.
QDR Infiniband

- **What is it?**
  - A switched fabric communications link with quad data rate (10 Gbit/s) using a 4X aggregate, implying a 40 Gbit/s connection

- **Features include**
  - High throughput, low latency, quality of service and failover, and is designed to be scalable

- Lustre uses Infiniband
Parallel Environments

- Show a list of defined parallel environments currently available
  
  `qconf -spl`

- Show your workgroup queues configured for parallel environments
  
  `qconf -sq $WORKGROUP* | egrep "(qname|pe_list)"`
Using MPI

- OpenMPI versions
  
  `vpkg_versions openmpi`

- MPI Exercises
  
  `https://computing.llnl.gov/tutorials/mpi/exercise.html`
Compile

- MPI wrappers
  
  mpicc, mpif90, mpif77, mpiCC/mpiCxx/mpic++

- The Open MPI Team *strongly* recommends using the wrapper compilers to compile and link MPI applications.
MPI wrappers for pgi

- Using VALET

  vpkg_require openmpi/1.4.4-pgi

- Show the flags necessary to compile and link pgi MPI C applications

  mpicc --showme:compile
  mpicc --showme:link
Example (cexample)

    cd cexample
    . sourceme-pgi
Example (fexample)

```bash
cd ../fexample
  . sourceme-pgi
```
Example (cmm)

cd ..;/cmm
. sourceme-pgi
Example (fmm)

cd ../fmm
. sourceme-pgi
Grid Engine

Three job script variants available in

- `/opt/templates/openmpi/`

1. **OpenIB Verbs (default)**
   - `openmpi-ibverb` or `openmpi`

2. **High-bandwidth Infiniband**
   - `openmpi-psm`

3. **Low-bandwidth Ethernet**
   - `openmpi-gige`
Example (cexample)

cd ..///cexample
qsub openmpi-pgi.qs
Example (fexample)

cd ..;/fexample
qsub openmpi-pgi.qs
Example (cmm)

cd ../cmm
qsub openmpi-pgi.qs
Example (fmm)

cd ../fmm
qsub openmpi-pgi.qs
Help?

- Consulting questions should be sent to the IT Support Center <consult@udel.edu>.
- If you make the first line of the e-mail message

  Type=Cluster-Mills

your question will be routed more quickly.