

Iowa High Performance Computing Summer School

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Thank you



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Outline

- Welcome and Introductions
- Aims of this Summer School
- Comments
- Getting Online

Welcome and Introductions

- Students from a wide range of departments:
 - Chemistry
 - Computer Science
 - Economics
 - Electrical and Computer Engineering
 - Hydroscience and Engineering
 - Management Sciences
 - Mechanical Engineering
 - Molecular Pathology
 - Physics and Astronomy
 - Statistics and Actuarial Science
- Please Introduce yourselves:
 - Name
 - Department
 - Academic Status and Year (ex. graduate student, 3rd year)
 - High Performance Computing Experience

Aims of this Summer School

To enable you to apply parallel computing to your own research

General Comments:

- Much of this material may be familiar to you
- I plan to explain things from a very basic level to make sure this group from such diverse backgrounds can follow

Comments

A few comments before we get started are in order:

- 1) Terminology: Terminology in this field is *not* standardized.
 - This field is new and evolves rapidly.
- 2) HPC is valuable to a wide range of fields:
 - Many examples I use will come from the field of physics.
 - I will try to present the specific problems in a relatively abstract way so that you can consider them simply mathematical problems to be solved.
- 3) Software (programming) vs. Hardware (computers):
 - I am not going to talk a lot about different hardware options, but will focus on the software side, specifically how to design and implement parallel algorithms.

Comments

4) Common approaches vs. Exhaustive coverage:

- This will not be an exhaustive review of all possible HPC approaches
- I will focus on the most important and widely used approaches
- In particular, we will talk a lot about MPI and some about OpenMP

5) Specificity vs. Generality:

- I will try to strike a balance between specific examples, which are often most illuminating, vs. general considerations which may apply to a more wide variety of HPC applications

Getting Online

Each participant has accounts set up on several computers:
University of Iowa, Research Services:

- Research Clusters

 - `rs-001.its.uiowa.edu` (32 bit)

 - `rs-003.its.uiowa.edu` (64 bit)

Pittsburgh Supercomputing Center:

- Bigben: Cray XT3, 2068 compute nodes (4172 cores)

 - `bigben.psc.edu`

- Detailed information for running on bigben is available at

 - <http://www.psc.edu/machines/cray/xt3/>

- More detail follows below: getting online and submitting both interactive and batch jobs

Getting Online

Logging on:

- We use Secure Shell (ssh) to log on to remote computers from an xterm terminal:

```
ssh -X howes@bigben.psc.edu
```

- Enter your password at the prompt:

```
howes@bigben.psc.edu's password:
```

- The “`-x`” enables Xforwarding, so that you can pull up a window on your local terminal from an application on the remote machine

Transferring Files:

- We use Secure Copy (scp) to copy files to remote computers

```
scp localfile howes@bigben.psc.edu:~/remotefile
```

- “`~/`” denotes your home directory on the remote machine

Getting Online

Submitting Jobs on Bigben:

- Jobs can be run either interactively or in batch mode

Interactive Jobs:

- To reserve nodes for an interactive job, submit the command

```
qsub -I -q training -l walltime=10:00 -l size=2
```

where

`-I` denotes interactive mode

`-q training` denotes to submit to the queue “training”

`-l walltime=10:00` requests wallclock time in HH:MM:SS

`-l size=2` requests 2 cores

- The system will prompt you to wait for interactive session
[type `^C` (Ctrl-C) to cancel the request]

```
qsub: waiting for job 418954.phantom.psc.edu to start
```

- Once started, you can submit jobs using

```
pbsyod -size 2 ./hellompi
```

- `^D` terminates interactive session

Getting Online

Batch Jobs:

- Create a file `hellompi.pbs` with the following:

```
#!/bin/csh
#PBS -N hellompi
#PBS -o hellompi.log
#PBS -l size=4
#PBS -l walltime=10:00
#PBS -j oe
#PBS -q debug
set echo
cd $SCRATCH
cp $HOME/hellompi ./
pbsyod -size $PBS_O_SIZE ./hellompi
```

- To submit the job to the queue

```
qsub hellompi.pbs
```

- To delete the job from the queue

```
qdel 1234
```

where `1234` is the `jobid` of the job you want to kill

- To check queue, `qstat`