Interacting with Moab/Torque using PBS directives

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Outline

(1) What is Torque, Moab and PBS?

(2) Batch Computer Systems

(3) Basic Job Flow within a Batch System

(4) Creating PBS scripts [Exercise]

(5) Checking on a Job/Canceling a Job [Exercise]

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What is Torque, Moab and PBS?

Torque is a Resource Manager

“...Provides low-level functionality to start, hold, cancel and monitor jobs.”

- Torque v4.1.7 Manual
  Adaptive Computing
What is Torque, Moab and PBS?

Moab is a Work-load Manager (job scheduler)

“The scheduler tracks resources and dedicates requested resources to a particular jobs, which prevents use of such resources by other jobs.”

- Moab v7.1.6 Manual
  Adaptive Computing
What is Torque, Moab and PBS?

Portable Batch System (PBS)

A job scheduler originally developed by NASA in the early 1990s that Torque/Moab is based on. As such, Torque/Moab uses PBS directives (commands) to receive job requests from users.
We Integrate Torque/Moab across computers to create a batch system.

Batch systems abstract away many of the details involved with running and managing jobs, allowing higher resource utilization.
Accounting for User System Resource Requests

Since each user has its own terminal, a system needs to be in place to ensure two users do not get the same CPUs, or more CPUs than the system total is used at any one time.
Basic Job Flow when using Torque/Moab Batch Systems

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<td>PBS submit script created by user that controls parameters of the job including walltime, CPUs need, memory, etc...</td>
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What does a PBS script look like?

```bash
#!/bin/sh

#PBS -N localBlast
#PBS -l nodes=1:ppn=2,walltime=240:00:00
#PBS -M user@my.organization.com
#PBS -m ea

source ~/.bashrc
cd $HOME/work/dir
sh myBlast.sh -i -v
```
Exercise: Create a PBS Script

Login to Mountaineer (from command line):

```bash
ssh mountaineer.hpc.wvu.edu -l username
```

Password: training2014
Exercise: Create a PBS Script

Write the PBS file:

```
touch pbs_script.sh
vi pbs_script.sh
```

Enter insert mode by pressing the 'i' key

```
#!/bin/sh

#PBS -N pbs_trial
#PBS -l nodes=1:ppn=1,walltime=01:00:00
#PBS -q training
#PBS -m ae
#PBS -M youremail@address.com

echo “This message will go to standard output file”
echo “This message will go to standard error file” >&2
```

Save and quit file by hitting esc key, followed by :wq <enter>
Exercise: Create a PBS Script

Submit Job Script

qsub pbs_script.sh

Should get output response something similar to: 45521.mountaineer
Exercise: Create a PBS Script

Check Output:
ls -l

At the completion of jobs, Moab outputs files as:
JOB_NAME.oJOBID and JOB_NAME.eJOBID

Cat both output files (one at a time):
cat pbs_trial.oJOBID
cat pbs_trial.eJOBID
Exercise: Run a longer job and check job status

Edit PBS file to execute a different set of commands:

```
vi pbs_script.sh
```

Using arrow keys place cursor on the first echo line. Press '2dd' in the keyboard. Now enter insert mode with the 'i' key

```
source ~/.bashrc
cd $HOME
./infinite_loop
```

Press the 'esc' key to exit insert mode. Type ':wq' to save and exit file.

```
qsub pbs_script.sh
```
Exercise: Run a longer job and check job status

Check to see your job running:

showq

often gives too much output, try piping into less

showq | less

Use the 'q' key to exit less. Or you can explicitly view just your jobs

showq -u <username>
Exercise: Run a longer job and check job status

Check your job's status:

`checkjob <jobid>`

This jobs command will never end, it's bugged code that stalls indefinitely. You can cancel the job using:

`Canceljob <jobid>`
Exercise: Run a longer job and check job status

Just as in slide 13, you should check to see if Moab gave you output files.
Further Information

Man Pages:
  man qsub
  man pbs_resources_linux

SRF HPC Wiki:
  http://wiki.hpc.wvu.edu

OsTicket or E-mail:
  http://helpdesk.hpc.wvu.edu
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