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



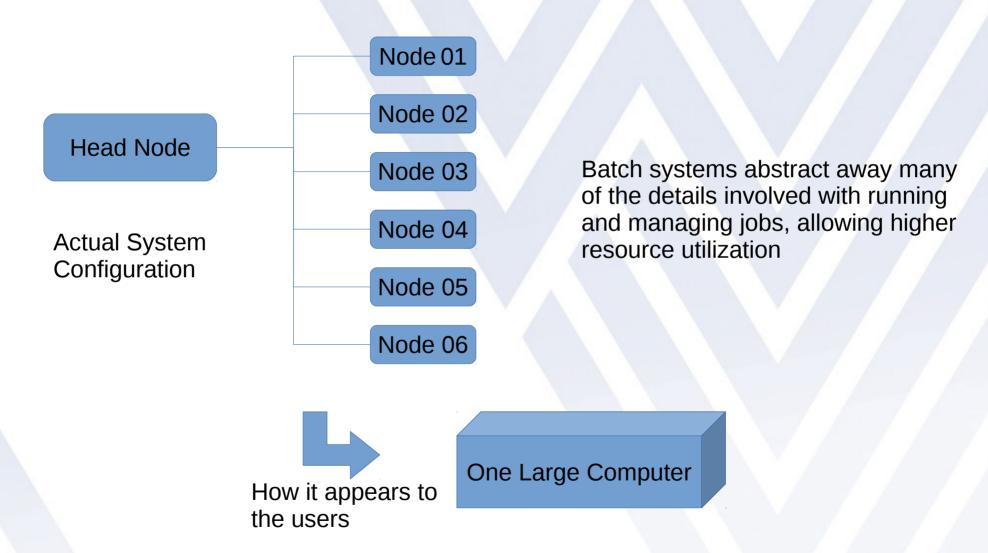
What is Torque, Moab and PBS?

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.

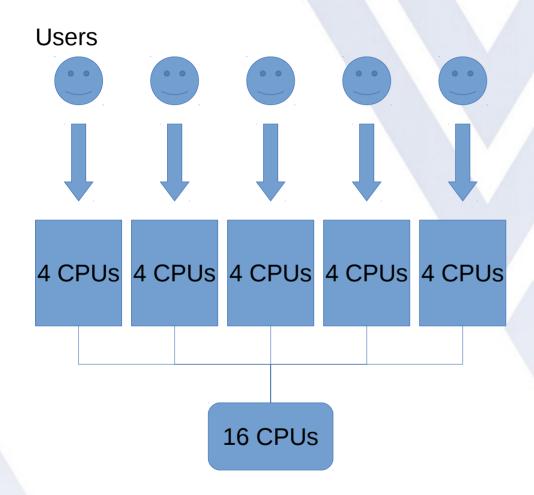


We Integrate Torque/Moab across computers to create a batch system





Accounting for User System Resource Requests



Since each user has it's 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

Phase	Controlled By	Phase Details
Creation	User	PBS submit script created by user that controls parameters of the job including walltime, CPUs need, memory, etc
Submission	User	User submission of the PBS submit script
Execution	System	Execution of commands
Finalization	System	Job completion; capture command outputs



What does a PBS script look like?

```
#!/bin/sh

#PBS -N localBlast
#PBS -I 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

PBS directives

Ver
Commands
```



Username on front of slide handout packet.

Login to Mountaineer (from command line):

ssh mountaineer.hpc.wvu.edu -l username

Password: training2014



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 -I 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>



Submit Job Script

qsub pbs_script.sh

Should get output response something similar to: 45521.mountaineer



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



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



Check to see your job running:

showq

often gives to 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>



Check your job's status:

checkjob <jobid>



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

Canceljob <jobid>



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 helpdesk@hpc.wvu.edu



Of course, you can always e-mail any of us directly

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