Outline

Hopper in blue; Jaguar in Orange; Kraken in Green

• XT5 Overview
• Creating and Submitting a Batch Job
• How a Job Is Launched
• Monitoring Your Job
• Queues and Policies
Cray XT5 Overview

Full Linux OS
- Login Node
- MOM Node
- etc...

CNL (no logins)
- Compute Node
- Compute Node
- Compute Node
- Compute Node
- etc...

No local disk

HPSS

Office of Science
U.S. Department of Energy

Joint Cray XT5 Workshop, UC Berkeley
February 1, 2010

NERSC only

$SCRATCH[1|2]
/tmp/work/$USER
/lustre/scratch/$USER
Running a Job on the XT5

1. Log in from your desktop using SSH
2. Compile your code or load a software module
3. Write a job script
4. Submit your script to the batch system
5. Monitor your job’s progress
6. Archive your output
7. Analyze your results
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• NERSC Queues and Policies
A job script is a text file. Create and edit with a text editor, like vi or emacs.

Directives specify how to run your job

UNIX commands run on a service node (Full Linux)

`code.x` runs in parallel on compute nodes

```bash
#PBS -l walltime=01:00:00
#PBS -l mppwidth=4096
#PBS -l mppnppn=8
#PBS -l size=4096
#PBS -q regular
#PBS -N BigJob
#PBS -V
#PBS -A mp999

cd $PBS_O_WORKDIR

echo "Starting at" `date`

aprun -n 4096 -N 8 ./code.x
```
Common Directives

Hopper

`#PBS -q queue_name`
Specify the *queue* in which to run.

`#PBS -l walltime=HH:MM:SS`
Specify the max *wallclock time* your job will use.

`#PBS -M email_address`
Specify the email address for notifications.

`#PBS -V`
Copy your current environment into batch environment.

`#PBS -A account`
Charge job to *account*.
Specifying Job Size

The fundamental schedulable unit on the XT5 is a compute node.

Your Torque/PBS directives tell the system how many compute nodes to reserve for your job.

You have exclusive access to a compute node. You “own” every node that is allocated for your job for the duration of your job.
Specifying Job Size

#PBS -l mppwidth=number_of_instances

Set mppwidth equal to the total number of copies of your executable to run in parallel.

#PBS -l mppnppn=instances_per_node

Set mppnppn equal to the # of instances to run per node.

#PBS -l size=cores

Set size equal to the # of cores that will be available for your job to use. Must be a multiple of 12
Sample Hopper Batch Script

```bash
#!/bin/bash -l
#PBS -q debug
#PBS -l mppwidth=384
#PBS -l mppnppn=8
###### NOTE: 48 nodes requested
#PBS -l walltime=00:30:00
#PBS -N myFirstTest
#PBS -M my_email@my_school.edu
#PBS -V

cd $PBS_O_WORKDIR

aprun -n 384 -N 8 ./a.out
```
Sample Jaguar/Kraken Script

```
#/bin/bash -l
#PBS -l size=384
##### NOTE: 384/12=32 nodes requested
#PBS -l walltime=00:30:00
#PBS -N myFirstTest
#PBS -M my_email@my_school.edu
#PBS -V

cd $PBS_O_WORKDIR

aprun -n 384 ./a.out
```
Running N tasks per node

Note that you never directly specify the number of nodes. It is implicit in your settings for `mppwidth` and `mppnppn` or `size`. You may want to run fewer tasks (instances) per node than there are cores per node to increase the memory available per MPI task.

```
#PBS -l mppwidth=512
#PBS -l mppnppn=2
```

This will allocate 256 nodes to run 512 tasks using 2 tasks per node. (Must be consistent with aprun options; see below)

```
#PBS -l size=768
```

This will always allocate 64 nodes (768/12). You will use aprun to control tasks/node (see below).
Submitting Jobs

Submit your job script with the qsub command.

```bash
nid04100% qsub script_name
```

The batch script directives (#PBS –whatever) can be specified on the qsub command line. For example:

```bash
nid04100% qsub -A account script_name
```

Use -A account (or repo) to specify the account to charge.

I recommend putting everything you care about explicitly in the batch script to avoid ambiguity and to have a record of exactly how you submitted your job.
Modifying Jobs

- `qdel <jobid>`: deletes queued job
- `qhold <jobid>`: holds job in queue
- `qrls <jobid>`: release held job
- `qalter <jobid> <options>`
  - You can modify some parameters
  - See “man qalter”
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Job Scheduling and Launch

Torque/PBS Batch Framework

- #PBS –l
- walltime=01:00:00
- #PBS –l mppwidth=4096
- #PBS –l mppnppn=2
- #PBS –q regular
- #PBS –N BigJob
- #PBS –V
- #PBS –A mp999
- cd $PBS_O_WORKDIR
- echo "Starting at" `date`
- aprun –n 4096 –N 2 ./code.x

ALPS Job Launch

- qsub
- STDOUT
- STDERR
- Obit – Completion Notification
- aprun arguments
- Run? Yes / No
- Reserve nodes
- Query machine status
- Run
- done

Moab - Scheduler

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Joint Cray XT5 Workshop, UC Berkeley
February 1, 2010
Parallel Job Launch - ALPS

ALPS = Application Level Placement Scheduler

my_executable aprun command

Full Linux

High Speed Seastar2 Network

Node 1

Node 2

Node 3

Node n

Full Linux

Login

High Speed Seastar2 Network

aprun –n instances my_executable

For MPI-only codes, this is equivalent to

aprun –n mpi_tasks my_executable
You use options to aprun to tell ALPS how to run your job

Tasks per compute node
- \texttt{-N [ 1-8 ]} Hopper
- \texttt{-N [ 1-12 ]} Jaguar, Kraken

Cores per Opteron
- \texttt{-S [ 1-4 ]} Hopper
- \texttt{-S [ 1-6 ]} Jaguar, Kraken

Opterons (or NUMA nodes, sockets) per compute node
- \texttt{-sn [ 1-2 ]}
CPU affinity

-cc[ cpu | numa_node | none ]
cpu: task bound to 1 core (default)
numa_node: task bound 1 Opteron
none: task can migrate to both

Memory affinity

-ss
Restrict memory access to within a NUMA node. Default: not set.

Defaults are fine in most cases; see “man aprun”
PBS Directives vs. aprun options

 aprun –n # must be consistent with
  #PBS –l mppwidth=#

 Ditto for –N and
  #PBS –l mppnppn

 Mismatches will cause job launch errors

 cd $PBS_O_WORKDIR
 echo “Starting at” `date`
 aprun –n 4096 –N 8 ./code.x
PBS Directives vs. aprun options

aprun –n value must be consistent with
   #PBS –l size

Size must be a multiple of 12

You will always get size/12 nodes

#PBS –l walltime=01:00:00
#PBS –l size=3072
###NOTE: 256 nodes
#PBS –N BigJob
#PBS –V
#PBS –A mp999

cd $PBS_O_WORKDIR

echo “Starting at” `date`

aprun –n 3072 ./code.x
Interactive Jobs

You can run interactive parallel jobs. It may not make semantic sense, but you can think of this as an interactive batch job: PBS/Torque. Moab, ALPS all participate.

```
% qsub -I -l mppwidth=24 -l walltime=30:00 Hopper
% qsub -I -l size=24 -A acct -l walltime=30:00 Jaguar, Kraken

... wait for prompt ...
```

When your prompt returns, you are on a service node, but you have compute nodes reserved for you so you can use `aprun` at the command line

```
nid04100% cd $PBS_O_WORKDIR
nid04100% aprun -n 24 ./mycode.x
```

`aprun` will fail if you don’t first use `qsub -I` to reserve compute nodes.
Job Notes

- Work out of $SCRATCH, /tmp/work/$USER, or /lustre/scratch/$USER.

- The job script itself executes on a service (MOM) node.

- All commands and serial programs (including hsi) therefore run on a shared node running a full version of Linux.

- You must use aprun to run anything on the compute nodes.
OpenMP

Each MPI task (instance) can create multiple OpenMP threads.

In most cases you will want 1 OpenMP thread per core.

You will need to use the proper PBS/Torque directives and aprun options.

Examples follow.
OpenMP on Hopper

Run using 4 MPI tasks per node and 2 OpenMP threads per task. Run 2 MPI tasks per socket.

```
#PBS –l walltime=00:30:00
#PBS –l mppwidth=1024
#PBS –l mppnppn=4
#PBS –l mppdepth=2
#PBS –q debug
#PBS –N BigOpenMPJob
#PBS –V

cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 2
aprun –n 1024 –N 4 –S 2 –d 2 ./OMPcode.x
```
OpenMP on Jaguar/Kraken

Run using 6 MPI tasks per node and 2 OpenMP threads per task. Run 3 MPI tasks per socket.

```
#PBS -l walltime=00:30:00
#PBS -l size=1008
#PBS -q debug
#PBS -N BigOpenMPJob
#PBS -V

cd $PBS_O_WORKDIR

setenv OMP_NUM_THREADS 2

aprun -n 1008 -N 6 -S 3 -d 2 ./OMPcode.x
```
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Monitoring Jobs

• Monitoring commands – each shows something different
  - showq – moab
  - qstat – torque
  - showstart – moab
  - checkjob – moab
  - apstat – ALPS
  - xtshowcabs/xtnodestat – Cray
  - qs – NERSC’s concatenation
showq (moab)

<table>
<thead>
<tr>
<th>JOBID</th>
<th>USERNAME</th>
<th>STATE</th>
<th>PROCS</th>
<th>REMAINING</th>
<th>STARTTIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>249696</td>
<td>ptr</td>
<td>Running</td>
<td>2</td>
<td>00:20:20</td>
<td>Tue Sep 18 14:21:13</td>
</tr>
<tr>
<td>249678</td>
<td>puj</td>
<td>Running</td>
<td>32</td>
<td>00:24:43</td>
<td>Tue Sep 18 13:55:36</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>JOBID</th>
<th>USERNAME</th>
<th>STATE</th>
<th>PROCs</th>
<th>WCLIMIT</th>
<th>QUEUETIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>249423</td>
<td>toussain</td>
<td>Idle</td>
<td>8192</td>
<td>3:00:00</td>
<td>Tue Sep 18 05:21:30</td>
</tr>
<tr>
<td>249424</td>
<td>toussain</td>
<td>Idle</td>
<td>8192</td>
<td>3:00:00</td>
<td>Tue Sep 18 05:21:35</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>JOBID</th>
<th>USERNAME</th>
<th>STATE</th>
<th>PROCs</th>
<th>WCLIMIT</th>
<th>QUEUETIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>248263</td>
<td>streuer</td>
<td>Hold</td>
<td>4096</td>
<td>12:00:00</td>
<td>Sat Sep 15 10:27:06</td>
</tr>
<tr>
<td>248265</td>
<td>streuer</td>
<td>Hold</td>
<td>2048</td>
<td>12:00:00</td>
<td>Sat Sep 15 10:27:06</td>
</tr>
</tbody>
</table>
### qstat –a (torque)

<table>
<thead>
<tr>
<th>Job ID</th>
<th>Username</th>
<th>Queue</th>
<th>Jobname</th>
<th>SessID</th>
<th>NDS</th>
<th>TSK</th>
<th>Memory</th>
<th>Time</th>
<th>S Time</th>
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<tr>
<td>248262.nid00003</td>
<td>streuer</td>
<td>reg_2048</td>
<td>td4</td>
<td>17483</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>R 10:03</td>
</tr>
<tr>
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<td>streuer</td>
<td>reg_2048</td>
<td>td4</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>H --</td>
</tr>
<tr>
<td>248265.nid00003</td>
<td>streuer</td>
<td>reg_1024</td>
<td>td1024</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>H --</td>
</tr>
<tr>
<td>248266.nid00003</td>
<td>streuer</td>
<td>reg_1024</td>
<td>td1024</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>H --</td>
</tr>
<tr>
<td>248806.nid00003</td>
<td>toussain</td>
<td>reg_2048</td>
<td>gen1</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>05:00</td>
<td>R 03:15</td>
</tr>
<tr>
<td>248826.nid00003</td>
<td>u4146</td>
<td>reg_512</td>
<td>B20_GE2_k1</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>Q --</td>
</tr>
<tr>
<td>248845.nid00003</td>
<td>toussain</td>
<td>reg_2048</td>
<td>spec1</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>05:00</td>
<td>Q --</td>
</tr>
<tr>
<td>248846.nid00003</td>
<td>toussain</td>
<td>reg_2048</td>
<td>gen1</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>05:00</td>
<td>Q --</td>
</tr>
<tr>
<td>248898.nid00003</td>
<td>u4146</td>
<td>reg_1024</td>
<td>BW_GE2_36k</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
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<td>Q --</td>
</tr>
<tr>
<td>248908.nid00003</td>
<td>u4146</td>
<td>reg_2048</td>
<td>VS2_GE2_k1</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>06:00</td>
<td>Q --</td>
</tr>
<tr>
<td>248913.nid00003</td>
<td>lijewski</td>
<td>reg_1024</td>
<td>doit</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>06:00</td>
<td>Q --</td>
</tr>
<tr>
<td>248929.nid00003</td>
<td>aja</td>
<td>reg_512</td>
<td>GT1024V4R</td>
<td>21124</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>R 08:51</td>
</tr>
<tr>
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<td>aja</td>
<td>reg_512</td>
<td>GT1024IR</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>12:00</td>
<td>Q --</td>
</tr>
</tbody>
</table>

**Blank**

**Random order**
Showstart (moab)

nid04100% showstart 249722.nid00003
job 249722 requires 8192 procs for 2:00:00

Estimated Rsv based start in 4:46:10 on Tue Sep 18 20:13:05
Estimated Rsv based completion in 6:46:10 on Tue Sep 18 22:13:05

Best Partition: hopper

May not be very useful, assumes that you are “top dog,” i.e., “next”? 
Compute node summary

<table>
<thead>
<tr>
<th>arch</th>
<th>config</th>
<th>up</th>
<th>use</th>
<th>held</th>
<th>avail</th>
<th>down</th>
</tr>
</thead>
<tbody>
<tr>
<td>XT</td>
<td>664</td>
<td>663</td>
<td>468</td>
<td>9</td>
<td>186</td>
<td>1</td>
</tr>
</tbody>
</table>

No pending applications are present

Total placed applications: 30

<table>
<thead>
<tr>
<th>Placed</th>
<th>Apid</th>
<th>ResId</th>
<th>User</th>
<th>PEs</th>
<th>Nodes</th>
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<th>State</th>
<th>Command</th>
</tr>
</thead>
<tbody>
<tr>
<td>148083</td>
<td>63</td>
<td>groucho</td>
<td>128</td>
<td>16</td>
<td>66h57m</td>
<td>run</td>
<td>cp_dis7_again</td>
<td></td>
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<tr>
<td>150341</td>
<td>301</td>
<td>freddy</td>
<td>512</td>
<td>64</td>
<td>12h45m</td>
<td>run</td>
<td>parsec.mpi</td>
<td></td>
</tr>
<tr>
<td>150422</td>
<td>1051</td>
<td>jyma</td>
<td>1</td>
<td>1</td>
<td>5h48m</td>
<td>run</td>
<td>tri.x</td>
<td></td>
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<tr>
<td>150433</td>
<td>1134</td>
<td>ynwu</td>
<td>32</td>
<td>4</td>
<td>5h35m</td>
<td>run</td>
<td>vasp</td>
<td></td>
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<tr>
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<td>1173</td>
<td>kokomoj</td>
<td>64</td>
<td>8</td>
<td>5h23m</td>
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<td>pw.x</td>
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<td>64</td>
<td>8</td>
<td>5h23m</td>
<td>run</td>
<td>pw.x</td>
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<tr>
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<td>1175</td>
<td>wanda23</td>
<td>64</td>
<td>8</td>
<td>5h16m</td>
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<td>pw.x</td>
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<td>jimmy</td>
<td>64</td>
<td>8</td>
<td>5h14m</td>
<td>run</td>
<td>vasp.5.mpi</td>
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<tr>
<td>150455</td>
<td>1206</td>
<td>afrankz</td>
<td>256</td>
<td>32</td>
<td>5h09m</td>
<td>run</td>
<td>namd2</td>
<td></td>
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<tr>
<td>150456</td>
<td>1209</td>
<td>tpaudel</td>
<td>112</td>
<td>14</td>
<td>4h59m</td>
<td>run</td>
<td>vasp5</td>
<td></td>
</tr>
</tbody>
</table>
### xtnodestat or xtshowcabs

<table>
<thead>
<tr>
<th>n3</th>
<th>mSennmmms</th>
<th>SqSqqq*q</th>
<th>wwwwSwww*</th>
<th>AAAAAAqq</th>
<th>wwwwwww</th>
<th>kkkkSmAA</th>
<th>wkkkSkk</th>
<th>kkkkSkkkSkk</th>
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</thead>
<tbody>
<tr>
<td>n2</td>
<td>k kkkkk</td>
<td>--kmm</td>
<td>kkk k-c</td>
<td>-----k-c</td>
<td>cccccccc</td>
<td>---c</td>
<td>ccccc</td>
<td>-- ---------</td>
</tr>
<tr>
<td>n1</td>
<td>e eeee</td>
<td>k kkkkk</td>
<td>eee ----</td>
<td>----------</td>
<td>--------</td>
<td>vvvv v-k</td>
<td>--ccc cc</td>
<td>ccvvvv v</td>
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<tr>
<td>c2n0</td>
<td>-S-----S</td>
<td>S-S*-e</td>
<td>--Skkk*</td>
<td>eeeeee-</td>
<td>k--------</td>
<td>---eeSee</td>
<td>-----S--</td>
<td>-------S-</td>
</tr>
<tr>
<td>n3</td>
<td>--S--j*j</td>
<td>----S-*</td>
<td>*jjjSjjc</td>
<td>---------</td>
<td>cccj-c</td>
<td>-----S-</td>
<td>cccccSc</td>
<td>cccc---S</td>
</tr>
<tr>
<td>n2</td>
<td>ii iiiii cc-</td>
<td>iiii iiiv</td>
<td>vvvvvvvv</td>
<td>-----</td>
<td>---vvvvv</td>
<td>v vvvvvv</td>
<td>v vvvvvv</td>
<td>v vvvvvvv</td>
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<td>ee eeee pp</td>
<td>ppppi e-</td>
<td>e ccppcppp</td>
<td>eeeeeeek</td>
<td>pppcc cc</td>
<td>kkkkkk k</td>
<td>ccffppp</td>
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<td>c1n0</td>
<td>ccSccc*c-</td>
<td>kkS---*</td>
<td>*ccccSc</td>
<td>ccccccSs</td>
<td>cccccSc</td>
<td>s----cSc</td>
<td>ccccccS</td>
<td></td>
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<td>SS--*---</td>
<td>ScccSccc</td>
<td>S----S-</td>
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<td>---------</td>
<td>S--------</td>
<td>S---------</td>
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<td>kkkyycc</td>
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<td>cccccckk k</td>
<td>kkyyc</td>
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<td>eec bdo oo</td>
<td>eeeeee eyyzzzzze</td>
<td>ccccc c</td>
<td>eCEEEEEE</td>
<td>exe eeyn</td>
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<td>c0n0</td>
<td>SSaA*a-g</td>
<td>SnbbSbfk</td>
<td>SrstuSuu</td>
<td>fddxnnnnn</td>
<td>u-----ttt</td>
<td>fdfdfzSB</td>
<td>dCDBBuSu uuBSBxxx</td>
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</table>

**Legend:**
- nonexistent node
- free interactive compute CNL
- free batch compute node CNL
- allocated, but idle compute node
- suspect compute node
- down compute node
- down or admindown service node
- admindown compute node
- system dedicated node (DVS)

**Available compute nodes:**
- 0 interactive, 202 batch

<table>
<thead>
<tr>
<th>Job ID</th>
<th>User</th>
<th>Size</th>
<th>Age</th>
<th>command line</th>
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<tbody>
<tr>
<td>a</td>
<td>150577</td>
<td>ynwu</td>
<td>2</td>
<td>0h15m</td>
</tr>
<tr>
<td>b</td>
<td>150445</td>
<td>peterpp</td>
<td>8</td>
<td>5h22m</td>
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<td>c</td>
<td>150078</td>
<td>mikre</td>
<td>128</td>
<td>22h35m</td>
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<td>d</td>
<td>150448</td>
<td>luckisg</td>
<td>8</td>
<td>5h29m</td>
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<tr>
<td>e</td>
<td>150341</td>
<td>jxhan</td>
<td>64</td>
<td>12h51m</td>
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<tr>
<td>f</td>
<td>150458</td>
<td>gfwu</td>
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<td>5h04m</td>
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qs (NERSC)

Jobs shown in run order.

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<tr>
<th>JOBID</th>
<th>ST</th>
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<th>NAME</th>
<th>SIZE</th>
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<th>USED</th>
<th>SUBMIT</th>
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<td>00:37:49</td>
<td>Sep 18 22:00:56</td>
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<td>MADmap_all</td>
<td>8192</td>
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<td>00:37:48</td>
<td>Sep 18 15:14:55</td>
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<td>spec1</td>
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<td>test.scrip</td>
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NERSC web queue display:
https://www.nersc.gov/nusers/status/queues/hopper/
Outline

• XT5 Overview
• Creating and Submitting a Batch Job
• How a Job Is Launched
• Monitoring Your Job
• Queues and Policies
Batch Queues & Policies

See web pages.

Hopper
http://www.nersc.gov/nusers/systems/hopper/running_jobs/queues.php

Kraken
http://www.nics.tennessee.edu/computing-resources/kraken/running-jobs/queues

Jaguar
http://www.nccs.gov/computing-resources/jaguar/running-jobs/scheduling-policy-xt5/