Getting Started at NERSC: Running Jobs

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Jobs at NERSC

- Most jobs are parallel, using 10s to 100,000+ cores
- Production runs execute in batch mode
- Interactive and debug jobs are supported for up to 30 minutes
- Typically run times are a few to 10s of hours.
  - Each machine has different limits.
  - Limits are necessary because of MTBF and the need to accommodate 5,500 users’ jobs
- Also a number of ‘serial’ jobs
  - Typically some kind of pleasantly parallel simulation
What system is best for your job?

**Large-Scale Computing Systems**

**Hopper (NERSC-6): Cray XE6**
- 6,384 compute nodes, 153,216 cores
- 144 Tflop/s on applications; 1.3 Pflop/s peak

**Edison (NERSC-7): Cray XC30 Phase II**
- 5,200 compute nodes, 124,800 cores
- 236 Tflop/s on applications, 2.39 Pflop/s peak

**Midrange**
- Thousands of cores

**Carver**
- IBM iDataplex cluster, 1,202 nodes
- 9,984 cores; 106 TF

**PDSF (HEP/NP)**
- ~2K core cluster

**GenePool (JGI)**
- ~5K core cluster
- 2.1 PB Isilon File System

**NERSC Global Filesystem (NGF)**
- Uses IBM’s GPFS
  - 12.7 PB capacity
  - 150 GB/s of bandwidth

**Analytics & Testbeds**

**Dirac** 48 Fermi
- GPU nodes

**HPSS Archival Storage**
- 240 PB capacity
- 5 Tape libraries
- 200 TB disk cache
Login Nodes and Compute Nodes

- Each supercomputer has 3 types of nodes that you will use
  - Login nodes
  - Compute nodes
  - Job launcher or “MOM” nodes
- Login nodes
  - Edit files, compile codes, run UNIX commands
  - Submit batch jobs
  - Run short, small utilities and applications
- Compute nodes
  - Execute your application; dedicated to your job
  - No direct login access
- Job launcher or “MOM” nodes
  - Execute your batch script commands
  - Carver: “head” compute node; Hopper / Edison: shared “service” node; not a compute node
Launching Parallel Jobs

Login Node

MOM Node

Compute Nodes

qsub

aprun / mpirun
Launching Parallel Jobs

• A “job launcher” executes your code
  – Distributes your executables to all your nodes
  – Starts concurrent execution of N instances of your program
  – Manages execution of your application
  – On Hopper / Edison: the job launcher is called “aprun”
  – On Carver: “mpirun”

• Only the job launcher can start your job on compute nodes

• You can’t run the job launcher from login nodes
Submitting Batch Jobs

• To run a job on the compute nodes you must write a “batch script” that contains
  – Batch directives to allow the system to schedule your job
  – An aprun or mpi run command that launches your parallel executable

• Submit the job to the queuing system with the qsub command
  – %qsub my_batch_script
Hopper - Cray XE6

- 153,216 cores, 6,384 nodes
- "Gemini” interconnect
- 2 12-core AMD 'MagnyCours' 2.1 GHz processors per node
- 24 processor cores per node
- 32 GB of memory per node (384 "fat" nodes with 64 GB)
- 216 TB of aggregate memory
- 1.3 GB memory / core (2.7 GB / core on "fat" nodes) for applications
- /scratch disk quota of 5 TB
- 2 PB of /scratch disk
- Choice of full Linux operating system or optimized Linux OS (Cray Linux)
- PGI, Cray, Pathscale, GNU compilers
Hopper’s Nodes

• **Login Nodes**
  - Hopper's login nodes run a full Linux operating system and provide support services for the system. When you connect to Hopper with SSH, you land on the login nodes. These nodes are shared by many users; please do not run applications on the login nodes.

• **Compute Nodes**
  - The 6,384 compute nodes are dedicated to running scientific applications. A job is given exclusive access to each node it requests for the entirety of the job's run time. Since Hopper has 24 cores on each node, the minimum number of cores per job is 24.

• **Job Host (MOM) Nodes**
  - MOM nodes are servers that execute batch job commands. These nodes are shared by many users and thus are not intended for compute- or memory-intensive applications.
Sample Hopper Batch Script - MPI

```bash
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```
Job directives: instructions for the batch system

• Submission queue
• How many nodes to reserve for your job
• How long to reserve those nodes
• Optional: what to name STDOUT files, what account to charge, whether to notify you by email when your job finishes, etc.
Sample Hopper Batch Script - MPI

```bash
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

Change from home directory to job submission directory
Launches parallel executable on the compute nodes. Carries over (partial) login environment and controls how your executable accesses the memory on each processor.
Sample Hopper Batch Script - MPI

```bash
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

mppwidth is number of compute cores requested (/24 for number of nodes). Must match with number of tasks requested (-n)
#PBS -q debug
#PBS -l mppwidth=192
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 -N 12 ./my_executable

-N = number of tasks per node
 Might do this to get more memory / task
Hybrid OpenMP/MPI

#PBS –q regular
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
export OMP_NUM_THREADS=6
aprun -n 16 -d 6 -N 4 -S 1 ./hybrid.x

16 tasks (-n), 4 on each node (-N), 6 OpenMP threads / task (-d), separate tasks onto individual NUMA nodes (-S)
Many more examples on www.nersc.gov
Edison - Cray XC30

- Newest NERSC peta-flop machine
- Phase II just started August 23

- 124,800 cores, 5,200 nodes
- “Aries” interconnect
- 4 12-core Intel ‘IvyBridge’ 2.4 GHz processors per node
- 24 processor cores per node
- 64 GB of memory per node
- 333 TB of aggregate memory

- 2.7 GB memory / core for applications
- 6.4 PB of /scratch disk
- Choice of full Linux operating system or optimized Linux OS (Cray Linux)
- PGI, Cray, Pathscale, GNU compilers
- Still in testing
Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 -j 2 ./my_executable
```

Turn on hyperthreading (-j)
Carver - IBM iDataPlex

- 9,984 compute cores
- 1,202 compute nodes
- 2 quad-core Intel Nehalem 2.67 GHz processors per node
- 8 processor cores per node
- 24 GB of memory per node (48 GB on 80 "fat" nodes)
- 2.5 GB / core for applications (5.5 GB / core on "fat" nodes)
- InfiniBand 4X QDR

- NERSC global /scratch directory quota of 20 TB
- Full Linux operating system
- PGI, GNU, Intel compilers
```bash
#PBS -q debug
#PBS -l nodes=16:ppn=8
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
mpirun -n 128 ./myexecutable
```
Sample Carver Batch Script - OpenMP

`#PBS -q debug`
`
#PBS –l nodes=1:ppn=8`
`
#PBS –l walltime=00:10:00`
`
#PBS -N my_job`

`export OMP_NUM_THREADS=8`
`
cd $PBS_O_WORKDIR`
`
./myexecutable`

Number of threads
Interactive Parallel Jobs

- You can run small parallel jobs interactively for up to 30 minutes (ex. is for Hopper)

```bash
% qsub -I -q interactive -l mppwidth=48
[wait for job to start]
% cd $PBS_O_WORKDIR
% aprun -n 48 ./mycode.x
```
Serial Jobs

- Carver has a special queue for running serial jobs
  - A single process running on a single node
  - Each serial node can run up to 12 jobs from different users

```
#PBS -q serial
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
./myexecutable
```
Monitoring Your Job

• Once your job is submitted, it will start when resources are available

• Monitor it with
  – qstat –a
  – qstat –u username
  – showq
  – qs
  – NERSC web site “Queue Look”
  https://www.nersc.gov/users/live-status/global-queue-look/
  – NERSC web site “Completed Jobs”
  https://www.nersc.gov/users/job-logs-and-analytics/completed-jobs/
I qsub’d my job, but it’s not running!

• You are not alone!
How do we handle the demand?

That’s what the batch queue is for!

Your jobs will wait until the resources are available for them to run

Your job’s place in the queue is a mix of time and priority, so line jumping is allowed, but it may cost more
Job Limits

There are per user, per machine job limits. See the NERSC web site for details. Here are the limits on Hopper as of Sep. 3, 2013.

<table>
<thead>
<tr>
<th>Submit Queue</th>
<th>Execution Queue¹</th>
<th>Nodes</th>
<th>Processors</th>
<th>Max Wallclock</th>
<th>Relative Priority</th>
<th>Run Limit²</th>
<th>Queued Limit³</th>
<th>Queue Charge Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>interactive</td>
<td>interactive</td>
<td>1-256</td>
<td>1-6,144</td>
<td>30 mins</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
<td>debug</td>
<td>debug</td>
<td>1-512</td>
<td>1-12,288</td>
<td>30 mins</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>regular</td>
<td>reg_1hour</td>
<td>1-256</td>
<td>1-6,144</td>
<td>1 hr</td>
<td>5</td>
<td>8</td>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>reg_short</td>
<td>1-682</td>
<td>1-16,368</td>
<td>6 hrs</td>
<td>5</td>
<td>16</td>
<td>16</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>reg_long</td>
<td>1-64</td>
<td>1-1,536</td>
<td>96 hrs</td>
<td>6</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>reg_small</td>
<td>1-682</td>
<td>1-16,368</td>
<td>48 hrs</td>
<td>6</td>
<td>16</td>
<td>16</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>reg_med</td>
<td>683-2,048</td>
<td>16,369-49,152</td>
<td>36 hrs</td>
<td>6</td>
<td>4</td>
<td>4</td>
<td>0.6</td>
</tr>
<tr>
<td></td>
<td>reg_big</td>
<td>2,049-4,096</td>
<td>49,153-98,304</td>
<td>36 hrs</td>
<td>6</td>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>reg_xbig⁴</td>
<td>4,097-6,100</td>
<td>98,305-146,400</td>
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<td>6</td>
<td>2</td>
<td>2</td>
<td>0.6</td>
</tr>
<tr>
<td></td>
<td>--</td>
<td>1-384</td>
<td>1-9,216</td>
<td>24 hrs</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
<td></td>
<td>low</td>
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<td>1-16,392</td>
<td>24 hrs</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>0.5</td>
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<td>5</td>
<td>250</td>
<td>500</td>
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<td>1-16,392</td>
<td>6 hrs</td>
<td>8</td>
<td>2</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
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<td>premium</td>
<td>1-2,048</td>
<td>1-49,152</td>
<td>12 hrs</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>ccm_queue⁷</td>
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<td>1-16,368</td>
<td>96 hrs</td>
<td>4</td>
<td>16</td>
<td>16</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>ccm_int⁸</td>
<td>1-512</td>
<td>1-12,288</td>
<td>30 mins</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>iotask⁹</td>
<td>1-682</td>
<td>1-16,368</td>
<td>12 hrs</td>
<td>6</td>
<td>1</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>xfer¹⁰</td>
<td>--</td>
<td>--</td>
<td>12 hrs</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

Specify these queues (with #PBS –q queue_name)

NEVER these!
Tips for jobs

• Submit shorter jobs.
  – Checkpoint if possible
  – Take advantage of ‘backfill’ opportunities
  – Run jobs just before maintenance

• Make sure the wall clock time you request is accurate. As noted above, shorter jobs are easier to schedule. Many users unnecessarily enter the largest wall clock time possible as a default.
## Average Queue Wait Time

<table>
<thead>
<tr>
<th>Hours Requested</th>
<th>Nodes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;1</td>
<td>1.4</td>
<td>14</td>
<td>13</td>
<td>12</td>
<td>11</td>
<td>10</td>
<td>9</td>
<td>8</td>
<td>7</td>
</tr>
<tr>
<td>2</td>
<td>2.2</td>
<td>23</td>
<td>22</td>
<td>21</td>
<td>20</td>
<td>19</td>
<td>18</td>
<td>17</td>
<td>16</td>
</tr>
<tr>
<td>3</td>
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<td>31</td>
<td>30</td>
<td>29</td>
<td>28</td>
<td>27</td>
<td>26</td>
<td>25</td>
</tr>
<tr>
<td>4</td>
<td>4.2</td>
<td>41</td>
<td>40</td>
<td>39</td>
<td>38</td>
<td>37</td>
<td>36</td>
<td>35</td>
<td>34</td>
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<tr>
<td>5</td>
<td>5.3</td>
<td>51</td>
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<td>47</td>
<td>46</td>
<td>45</td>
<td>44</td>
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<td>6</td>
<td>6.4</td>
<td>61</td>
<td>60</td>
<td>59</td>
<td>58</td>
<td>57</td>
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<td>55</td>
<td>54</td>
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<tr>
<td>7</td>
<td>7.5</td>
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<td>69</td>
<td>68</td>
<td>67</td>
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<td>64</td>
</tr>
<tr>
<td>8</td>
<td>8.6</td>
<td>81</td>
<td>80</td>
<td>79</td>
<td>78</td>
<td>77</td>
<td>76</td>
<td>75</td>
<td>74</td>
</tr>
</tbody>
</table>

### Notes
- The table represents the average queue wait time in hours for different numbers of nodes and hours requested.
- The data is presented in a grid format, with each cell indicating the wait time for a specific combination of nodes and hours requested.
How Your Jobs Are Charged

• Your repository account is charged for each node your job was allocated for the entire duration of your job.
  – The minimum allocatable unit is a node. Hopper and Edison have 24 cores/node, so your minimum charge is $24 \times \text{walltime}$.

| MPP hours = (# nodes) \times (# cores / node) \times (\text{walltime}) \times (\text{queue charge factors}) |

  – mppwidth = 96 for 1 hour. MPP hours = (4) \times (24) \times (1 \text{ hour}) \times (1)
    MPP hours charged = 96 hours
  – Serial jobs on Carver are charged differently.

• If you have access to multiple repos, pick which one to charge in your batch script
  – #PBS -A repo_name
Charge Factors & Discounts

• Each machine has a “machine charge factor” (mcf) that multiplies the “raw hours” used
  – Hopper has mcf=1.0
  – Carver has mcf=1.5

• Queues have “priority charge factors” (pcf) and corresponding relative scheduling priorities
  – Premium pcf=2.0
  – Low pcf=0.5
  – Everything else pcf=1.0

• On Hopper only:
  – reg_med, reg_big, reg_xbig jobs get a 40% discount
More Information

NERSC Web pages

Hopper:
http://www.nersc.gov/users/computational-systems/hopper/running-jobs/

Edison:
http://www.nersc.gov/users/computational-systems/edison/running-jobs/

Carver:
http://www.nersc.gov/users/computational-systems/carver/running-jobs/

Contact NERSC Consulting:
- Toll-free 800-666-3772
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- Email consult@nersc.gov.