Job Management on LONI and LSU HPC clusters

Le Yan
HPC Consultant
User Services @ LONI
Outline

- Overview
  - Batch queuing system
  - Job queues on LONI clusters
- Basic commands
The Cluster Environment

- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously
Batch Queuing System

• A software that manages resources (CPU time, memory etc.) and schedules job execution
  • Linux clusters: **Portable Batch System**(PBS)
  • AIX clusters: **Loadleveler**

• A job can be considered as a user's request to use a certain amount of **resources** for a certain amount of **time**

• The batch queuing system determines
  • The order jobs are executed
  • On which node(s) jobs are executed
A Simplified View of Job Scheduling

- Map jobs onto the node-time space
  - Assuming CPU time is the only resource
- Need to find a balance between
  - Honoring the order in which jobs are received
  - Maximizing resource utilization
Backfilling

- A strategy to improve utilization
  - Allow a job to jump ahead of others when there are enough idle nodes
  - Must not affect the estimated start time of the job with the highest priority
- Enabled on all LONI and LSU HPC clusters
How Much Time Should I Ask for?

- Ask for an amount of time that is
  - Long enough for your job to complete
  - As short as possible to increase the chance of backfilling
Job Queues

- There are more than one job queue
- Each job queue differs in
  - Number of available nodes
  - Max run time
  - Max running jobs per user
  - ...
- The main purpose is to maximize utilization
Queue Characteristics – Queen Bee

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Total number of available nodes</th>
<th>Max running jobs per user</th>
<th>Max nodes per job</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>Workq</td>
<td>2 days</td>
<td>530</td>
<td>8</td>
<td>128</td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td></td>
<td>668</td>
<td></td>
<td>256</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td></td>
<td>668</td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td></td>
<td>668</td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
</tbody>
</table>
Queue Characteristics – Other LONI Linux Clusters

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Total number of available nodes</th>
<th>Max running jobs per user</th>
<th>Max nodes per job</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single</td>
<td>14 days</td>
<td>16</td>
<td>64</td>
<td>1</td>
<td>Single processor jobs</td>
</tr>
<tr>
<td>Workq</td>
<td>3 days</td>
<td>96</td>
<td>8</td>
<td>40</td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td>3 days</td>
<td>128</td>
<td>8</td>
<td>64</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td>3 days</td>
<td>64</td>
<td>NA</td>
<td>NA</td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td>3 days</td>
<td>64</td>
<td>NA</td>
<td>NA</td>
<td>Require permission</td>
</tr>
</tbody>
</table>
## Queue Characteristics – Tezpur

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Total number of available nodes</th>
<th>Max running jobs per user</th>
<th>Max nodes per job</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single</td>
<td>3 days</td>
<td>16</td>
<td>64</td>
<td>1</td>
<td>Single processor jobs</td>
</tr>
<tr>
<td>Workq</td>
<td></td>
<td>180</td>
<td>8</td>
<td>90</td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td></td>
<td>344</td>
<td>8</td>
<td>180</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td></td>
<td></td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td></td>
<td></td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
</tbody>
</table>
## Queue Characteristics – Philip

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Total number of available nodes</th>
<th>Max running jobs per user</th>
<th>Max nodes per job</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single</td>
<td>3 days</td>
<td>24</td>
<td>12</td>
<td>1</td>
<td>Single processor jobs</td>
</tr>
<tr>
<td>Workq</td>
<td></td>
<td>28</td>
<td></td>
<td></td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td></td>
<td>28</td>
<td></td>
<td>5</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Bigmem</td>
<td></td>
<td>5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Preempt</td>
<td></td>
<td></td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td></td>
<td></td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
</tbody>
</table>
## Queue Characteristics – LONI AIX Clusters

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Total number of available nodes</th>
<th>Max running jobs per user</th>
<th>Max nodes per job</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single</td>
<td>14 days</td>
<td>1</td>
<td>8</td>
<td>1</td>
<td>Single processor jobs</td>
</tr>
<tr>
<td>Workq</td>
<td>5 days</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td>14</td>
<td>14</td>
<td>NA</td>
<td>14</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td>6</td>
<td>NA</td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td>6</td>
<td>NA</td>
<td>NA</td>
<td></td>
<td>Require permission</td>
</tr>
</tbody>
</table>
### Queue Characteristics – Pelican

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Total number of available processors</th>
<th>Max running jobs per user</th>
<th>Max processors per job</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>SB5L</td>
<td>12 hours</td>
<td>42</td>
<td></td>
<td>1</td>
<td>Short single processor jobs</td>
</tr>
<tr>
<td>LB5L</td>
<td>14 days</td>
<td>42</td>
<td></td>
<td>1</td>
<td>Long single processor jobs</td>
</tr>
<tr>
<td>SP5L</td>
<td>4 hours</td>
<td>360</td>
<td>8</td>
<td>256</td>
<td>Short parallel jobs</td>
</tr>
<tr>
<td>MP5L</td>
<td>7 days</td>
<td>360</td>
<td></td>
<td>128</td>
<td>Medium parallel jobs</td>
</tr>
<tr>
<td>LP5L</td>
<td>14 days</td>
<td>360</td>
<td>4</td>
<td>64</td>
<td>Long parallel jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td>7 days</td>
<td>80</td>
<td>NA</td>
<td>64</td>
<td>Require permission</td>
</tr>
</tbody>
</table>
Basic Commands

- Queue querying
  - Check how busy the cluster is
- Job submission
- Job monitoring
  - Check job status (estimated start time, remaining run time etc.)
- Job manipulation
  - Cancel/hold jobs
Queue Querying – Linux Clusters

- **Command:** qfree
  - Show the number of free, busy and queued nodes

- **Command:** qfreeloni
  - Equivalent to run `qfree` on all LONI Linux clusters

```
[lyan1@louie2 ~]$ qfree
PBS total nodes: 128, free: 81, busy: 44, down: 3, use: 34%
PBS checkpt nodes: 128, free: 81, busy: 28
PBS workq nodes: 32, free: 16, busy: 16
```
### Queue Querying – AIX Clusters

#### Command: `llclass`

<table>
<thead>
<tr>
<th>Name</th>
<th>MaxJobCPU</th>
<th>MaxProcCPU</th>
<th>Free</th>
<th>Max</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>interactive</td>
<td>undefined</td>
<td>undefined</td>
<td>8</td>
<td>8</td>
<td>Interactive Parallel jobs running on interactive node</td>
</tr>
<tr>
<td>single</td>
<td>unlimited</td>
<td>unlimited</td>
<td>4</td>
<td>8</td>
<td>One node queue (14 days) for serial and up to 8-procesor parallel jobs</td>
</tr>
<tr>
<td>workq</td>
<td>unlimited</td>
<td>unlimited</td>
<td>51</td>
<td>56</td>
<td>Default queue (5 days), up to 56 processors</td>
</tr>
<tr>
<td>priority</td>
<td>unlimited</td>
<td>unlimited</td>
<td>40</td>
<td>40</td>
<td>priority queue resevered for on-demand jobs (5 days), up to 48 processors</td>
</tr>
<tr>
<td>preempt</td>
<td>unlimited</td>
<td>unlimited</td>
<td>40</td>
<td>40</td>
<td>preemption queue resevered for on-demand jobs (5 days), up to 48 processors</td>
</tr>
<tr>
<td>checkpoint</td>
<td>unlimited</td>
<td>unlimited</td>
<td>91</td>
<td>96</td>
<td>queue for checkpointing jobs (5 days), up to 104 processors, Job running on this queue can be preempted for on-demand job</td>
</tr>
</tbody>
</table>
Checking Loads on All LONI Clusters

- Check Loads on all LONI clusters at docs.loni.org
- Updated every 15 minutes

### Dell Linux Clusters

<table>
<thead>
<tr>
<th>System Name</th>
<th>Nodes</th>
<th>SMP Size</th>
<th>Total CPUs</th>
<th>Memory/Node</th>
<th>TFLOPS</th>
<th>Work Disk</th>
<th>Location</th>
<th>Load</th>
<th>Running jobs</th>
<th>Queued jobs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Queen Bee</td>
<td>680</td>
<td>8</td>
<td>5440</td>
<td>8 GB</td>
<td>50.7</td>
<td>58 TB</td>
<td>LSU</td>
<td></td>
<td>0</td>
<td>422</td>
</tr>
<tr>
<td>Erc</td>
<td>128</td>
<td>4</td>
<td>512</td>
<td>4 GB</td>
<td>4.772</td>
<td>9 TB</td>
<td>LSU</td>
<td>70</td>
<td>111</td>
<td></td>
</tr>
<tr>
<td>Oliver</td>
<td>128</td>
<td>4</td>
<td>512</td>
<td>4 GB</td>
<td>4.772</td>
<td>9 TB</td>
<td>ULL</td>
<td>16</td>
<td>13</td>
<td></td>
</tr>
<tr>
<td>Louie</td>
<td>128</td>
<td>4</td>
<td>512</td>
<td>4 GB</td>
<td>4.772</td>
<td>9 TB</td>
<td>Tulane</td>
<td>27</td>
<td>56</td>
<td></td>
</tr>
<tr>
<td>Poseidon</td>
<td>128</td>
<td>4</td>
<td>512</td>
<td>4 GB</td>
<td>4.772</td>
<td>9 TB</td>
<td>UNO</td>
<td>17</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Painter</td>
<td>128</td>
<td>4</td>
<td>512</td>
<td>4 GB</td>
<td>4.772</td>
<td>9 TB</td>
<td>LaTech</td>
<td>23</td>
<td>28</td>
<td></td>
</tr>
</tbody>
</table>

### IBM P5 Clusters

<table>
<thead>
<tr>
<th>System Name</th>
<th>Nodes</th>
<th>SMP Size</th>
<th>Total CPUs</th>
<th>Memory/Node</th>
<th>TFLOPS</th>
<th>Work Disk</th>
<th>Location</th>
<th>Load</th>
<th>Running jobs</th>
<th>Queued jobs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bluedawg</td>
<td>14</td>
<td>8</td>
<td>104</td>
<td>16 GB</td>
<td>0.85L</td>
<td>270 GB</td>
<td>LaTech</td>
<td></td>
<td>16</td>
<td>3</td>
</tr>
<tr>
<td>Ducky</td>
<td>14</td>
<td>8</td>
<td>104</td>
<td>16 GB</td>
<td>0.85L</td>
<td>270 GB</td>
<td>Tulane</td>
<td></td>
<td>7</td>
<td>0</td>
</tr>
<tr>
<td>Zeke</td>
<td>14</td>
<td>8</td>
<td>104</td>
<td>16 GB</td>
<td>0.85L</td>
<td>270 GB</td>
<td>ULL</td>
<td></td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Neptune</td>
<td>14</td>
<td>8</td>
<td>104</td>
<td>16 GB</td>
<td>0.85L</td>
<td>270 GB</td>
<td>UNO</td>
<td></td>
<td>9</td>
<td>8</td>
</tr>
<tr>
<td>LaCumbia</td>
<td>14</td>
<td>8</td>
<td>104</td>
<td>16 GB</td>
<td>0.85L</td>
<td>270 GB</td>
<td>SU</td>
<td></td>
<td>8</td>
<td>8</td>
</tr>
</tbody>
</table>
Job Types

• Interactive job
  • Set up an interactive environment on compute nodes for users
    • Advantage: can run programs interactively
    • Disadvantage: must be present when the job starts
  • Purpose: testing and debugging (Don't run your test jobs on the head node!)

• Batch job
  • Executed without user intervention using a job script
    • Advantage: the system takes care of everything
    • Disadvantage: can only execute one sequence of commands which cannot be changed after submission
  • Purpose: production run
Submitting Jobs –
Linux Clusters

• Interactive job
  • `qsub -I -V -l walltime=<hh:mm:ss>,nodes=<# of nodes>:ppn=4 -A <your allocation> -q <queue name>`
  • Add “-X” to enable X11 forwarding

• Batch job
  • `qsub <job script>`

• `ppn` must be either 4 (all Linux clusters except Queen Bee) or 8 (Queen Bee) except for serial jobs
PBS Job Script – Parallel Jobs

#!/bin/bash
#PBS -l nodes=4:ppn=4
#PBS -l walltime=24:00:00
#PBS -N myjob
#PBS -o <file name>
#PBS -e <file name>
#PBS -q checkpt
#PBS -A <loni_allocation>
#PBS -m e
#PBS -M <email address>

<shell commands>
mpirun -machinefile $PBS_NODEFILE -np 16 <path_to_executable> <options>
<shell commands>
### PBS Job Script – Serial Jobs

```bash
#!/bin/bash
#PBS -l nodes=1:ppn=1
#PBS -l walltime=24:00:00
#PBS -N myjob
#PBS -o <file name>
#PBS -e <file name>
#PBS -q single
#PBS -A <loni_allocation>
#PBS -m e
#PBS -M <email address>

<shell commands>
<path_to_executable> <options>
<shell commands>
```

- **Number of nodes and processor**
- **Maximum wall time**
- **Job name**
- **File name for standard output**
- **File name for standard error**
- **The only queue that accepts serial jobs**
- **Allocation name**
- **Send mail when job ends**
- **Send mail to this address**
Submitting Batch Jobs - AIX Clusters

- Batch job
  - `llsubmit <job script>`

```bash
#!/bin/sh
#@ job_type = parallel
#@ output = /work/default/username/$(jobid).out
#@ error = /work/default/username/$(jobid).err
#@ notify_user = youremail@domain
#@ notification = error
#@ class = checkpt
#@ wall_clock_limit = 24:00:00
#@ node_usage = shared
#@ node = 2
#@ total_tasks = 16
#@ initialdir = /work/default/username
#@ environment = COPY_ALL
#@ queue

<shell commands>
poe <path_to_executable> <options>
<shell commands>
```
Loadleveler Job Script – Serial Jobs

#!/bin/sh
#@ job_type = serial
#@ output = /work/default/username/$(jobid).out
#@ error = /work/default/username/$(jobid).err
#@ notify_user = youremail@domain
#@ notification = error
#@ class = checkpoint
#@ wall_clock_limit = 24:00:00
#@ initialdir = /work/default/username
#@ environment = COPY_ALL
#@ queue

<shell commands>
<path_to_executable> <options>
<shell commands>
Job Monitoring – Linux Clusters

- **Command:** `showstart <job_id>`
  - Check when a job is estimated to start
- Things that can change the estimated start time
  - Higher priority job gets submitted
  - Other jobs terminate earlier than the system expects
  - The system has trouble starting your job
Job Monitoring – Linux Clusters cont'd

- **Command:** `qstat <options> <job_id>
  - Show information on job status
  - All jobs are displayed if `<job_id>` is omitted
  - Show jobs submitted by a specific user: `qstat -u <username>`
  - Display in the alternative format: `qstat -a <job_id>`

- **Command:** `qshow <job_id>
  - Show information on a running job
    - On which node(s) the job is running
    - CPU load
Job Monitoring – AIX Clusters

• **Command:** `llq <options> <job_id>`
  - All jobs are displayed if `<job_id>` is omitted
  - Display detailed information: `llq -l <job_id>`
  - Check the estimated start time: `llq -s <job_id>`
  - Show jobs from a specific user: `llq -u <username>`

```
lyan1@l2f1n03$ llq
Id            Owner    Submitted   ST  PRI  Class       Running On
-------------- --------- ---------- ---- ---- --------- ------------
12f1n03.3697.0 collin    1/22 16:59  R  50  single    12f1n14
12f1n03.3730.0 jheiko    1/28 13:30  R  50  workq     12f1n10
12f1n03.3726.0 collin    1/26 08:21  R  50  single    12f1n14
12f1n03.3698.0 collin    1/22 17:00  R  50  single    12f1n14
12f1n03.3727.0 collin    1/26 08:21  R  50  single    12f1n14

5 job step(s) in queue, 0 waiting, 0 pending, 5 running, 0 held, 0 preempted
```
Job Monitoring – AIX Clusters

- **Command:** `showllstatus.py`
- **Show job status as well as node status**

```
lyan1@peg304$ showllstatus.py

<table>
<thead>
<tr>
<th>Node</th>
<th>Status</th>
<th>Load</th>
<th>Arch</th>
<th>Node</th>
<th>Status</th>
<th>Load</th>
<th>Arch</th>
</tr>
</thead>
<tbody>
<tr>
<td>ben2</td>
<td>Idle</td>
<td>0.05</td>
<td>Power4</td>
<td>pen15</td>
<td>Run</td>
<td>8.04</td>
<td>Power5</td>
</tr>
<tr>
<td>ben3</td>
<td>Run</td>
<td>0.27</td>
<td>Power4</td>
<td>pen16</td>
<td>Idle</td>
<td>2.07</td>
<td>Power5</td>
</tr>
<tr>
<td>ian1</td>
<td>Idle</td>
<td>0.40</td>
<td>Power4</td>
<td>pen17</td>
<td>Down</td>
<td>0.01</td>
<td>Power5</td>
</tr>
<tr>
<td>pen01</td>
<td>Run</td>
<td>8.00</td>
<td>Power5</td>
<td>pen18</td>
<td>Idle</td>
<td>0.00</td>
<td>Power5</td>
</tr>
<tr>
<td>pen02</td>
<td>Busy</td>
<td>16.06</td>
<td>Power5</td>
<td>pen19</td>
<td>Busy</td>
<td>5.74</td>
<td>Power5</td>
</tr>
<tr>
<td>pen03</td>
<td>Busy</td>
<td>15.99</td>
<td>Power5</td>
<td>pen20</td>
<td>Idle</td>
<td>0.00</td>
<td>Power5</td>
</tr>
</tbody>
</table>

...```

```
Step ID    Owner     Status | Class | Hosts | Queue Date | Disp. Date
ian1.77438.0 hypoxia    R      | MP5L  | 4     | 02/10 10:26| 02/10 10:26
ian1.77437.0 pradeep    R      | SB4L  | 1     | 02/10 10:25| 02/10 10:25
ian1.77431.0 eshi1362   R      | MP5L  | 2     | 02/10 09:13| 02/10 09:13
ian1.77419.0 jovi       R      | MP5L  | 1     | 02/09 22:22| 02/10 08:28
ian1.77418.0 jovi       R      | MP5L  | 1     | 02/09 22:22| 02/10 07:32
ian1.77417.0 jovi       R      | MP5L  | 1     | 02/09 22:22| 02/10 06:37
...```
Job Manipulation – Linux Clusters

- **Command:** `qdel <job_id>
  - Cancel a running or queued job
  - May take some time depending on the size of the job
- **Command:** `qhold <job_id>
  - Put a queued job on hold
- **Command:** `qrls <job_id>
  - Resume a held job
Job Manipulation – AIX Clusters

- **Command:** `llcancel <job_id>`
  - Cancel a running or queued job
- **Command:** `llhold <job_id>`
  - Put a queued job on hold
- **Command:** `llhold -r <job_id>`
  - Resume a held job
Exercise 1

- Compile the parallel program hello_mpi.f90
  - Located under /home/lyan1/traininglab/environment
  - To compile
    - Linux clusters: mpif90 -o <name of executable> hello_mpi.f90
    - AIX clusters: mpxlf90 -o <name of executable> hello_mpi.f90

- Run it within an interactive job session
  - Submit an interactive job
  - Run on the command line
    - Linux clusters: mpirun -np <# of cpus> <name of executable>
Exercise 2

- Run the same program as a batch job
  - Sample submission scripts can be found under the same directory
    - Linux clusters: submit.aix
    - AIX clusters: submit.linux
When Issues Arise

- User's Guide
  - HPC: http://www.hpc.lsu.edu/help
  - LONI: https://docs.loni.org/wiki/Main_Page

- Contact us
  - Email ticket system: syshelp@loni.org
  - Telephone Help Desk: 225-578-0900
  - Walk-in consulting session at Middleton Library
    - Tuesdays and Thursdays only
  - Instant Messenger (AIM, Yahoo Messenger, Google Talk)
    - Add “lsuhpchelp”
What's Next

• Introduction to MPI
  • Date: March 4, 2010
  • Time: 1:30pm
  • Location: 307 Frey