Job Management on LONI and LSU HPC clusters

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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>3 days</td>
<td>180</td>
<td>8</td>
<td>90</td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td>3 days</td>
<td>344</td>
<td>8</td>
<td>180</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td></td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td></td>
<td>NA</td>
<td>NA</td>
<td>NA</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>NA</td>
<td></td>
<td></td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td></td>
<td>NA</td>
<td></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></td>
<td>8</td>
<td>Unpreemptable (default)</td>
</tr>
<tr>
<td>Checkpt</td>
<td>5 days</td>
<td>14</td>
<td></td>
<td>14</td>
<td>Preemptable jobs</td>
</tr>
<tr>
<td>Preempt</td>
<td>5 days</td>
<td>6</td>
<td>NA</td>
<td>NA</td>
<td>Require permission</td>
</tr>
<tr>
<td>Priority</td>
<td>5 days</td>
<td>6</td>
<td>NA</td>
<td>NA</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>32</td>
<td>8</td>
<td>1</td>
<td>Short single processor jobs</td>
</tr>
<tr>
<td>LB5L</td>
<td>14 days</td>
<td>28</td>
<td></td>
<td>1</td>
<td>Long single processor jobs</td>
</tr>
<tr>
<td>SP5L</td>
<td>4 hours</td>
<td>368</td>
<td></td>
<td>256</td>
<td>Short parallel jobs</td>
</tr>
<tr>
<td>MP5L</td>
<td>7 days</td>
<td>368</td>
<td></td>
<td>128</td>
<td>Medium parallel jobs</td>
</tr>
<tr>
<td>LP5L</td>
<td>14 days</td>
<td>368</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**: `qfreelon"`
  - Equivalent to run `qfree` on all LONI Linux clusters

```bash
[lyan1@louie2 ~]$ qfree
PBS total nodes: 128, free: 81, busy: 44, down: 3, use: 34%
PBS checkpoint 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-processor 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 reserved 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 reserved 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>0</td>
<td>422</td>
<td></td>
</tr>
<tr>
<td>Enc</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>16</td>
<td>3</td>
<td></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>7</td>
<td>0</td>
<td></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>1</td>
<td>0</td>
<td></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>9</td>
<td>8</td>
<td></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>8</td>
<td>8</td>
<td></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 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

```bash
#!/bin/bash

#PBS -l nodes=4:ppn=4
Number of nodes and processor

#PBS -l walltime=24:00:00
Maximum wall time

#PBS -N myjob
Job name

#PBS -o <file name>
File name for standard output

#PBS -e <file name>
File name for standard error

#PBS -q checkpt
Queue name

#PBS -A <loni_allocation>
Allocation name

#PBS -m e
Send mail when job ends

#PBS -M <email address>
Send mail to this address

<shell commands>

mpirun -machinefile $PBS_NODEFILE -np 16 <path_to_executable> <options>

<shell commands>
```
PBS Job Script – Serial Jobs

#!/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>`

```
#!/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 = 2,2
#@ 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

```bash
#!/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**

```bash
ychyan1@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>

```bash

```
... 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     esh1362  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](http://www.hpc.lsu.edu/help)
  - LONI: [https://docs.loni.org/wiki/Main_Page](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