Introduction to HPC Using the New Cluster (Sapelo) at GACRC

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University of Georgia
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Outline

• What is GACRC?
• What is the new cluster (Sapelo) at GACRC?
• How does Sapelo operate?
• How to work with Sapelo?
What is GACRC?

Who Are We?
- Georgia Advanced Computing Resource Center
- Collaboration between the Office of Vice President for Research (OVPR) and the Office of the Vice President for Information Technology (OVPIT)
- Guided by a faculty advisory committee (GACRC-AC)

Why Are We Here?
- To provide computing hardware and network infrastructure in support of high-performance computing (HPC) at UGA

Where Are We?
- [http://gacrc.uga.edu](http://gacrc.uga.edu) (Web)
- [http://wiki.gacrc.uga.edu](http://wiki.gacrc.uga.edu) (Wiki)
- [http://gacrc.uga.edu/help/](http://gacrc.uga.edu/help/) (Web Help)
- [https://wiki.gacrc.uga.edu/wiki/Getting_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (Wiki Help)
<table>
<thead>
<tr>
<th>Colleges &amp; Schools</th>
<th>Depts</th>
<th>PIs</th>
<th>Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>Franklin College of Arts and Sciences</td>
<td>14</td>
<td>117</td>
<td>661</td>
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<tr>
<td>College of Agricultural &amp; Environmental Sciences</td>
<td>9</td>
<td>29</td>
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<td>College of Engineering</td>
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<td><strong>214</strong></td>
<td><strong>970</strong></td>
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<td><strong>1029</strong></td>
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## GACRC Users September 2015

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<th>PIs</th>
<th>Users</th>
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<td>Center for Applied Isotope Study</td>
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<td><strong>19</strong></td>
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What is the new cluster (Sapelo) at GACRC?

- Cluster Structural Diagram
- General Information
- Computing Resources
- Storage Environment
The New GACRC Linux HPC Cluster Structural Diagram

Network Connection Speed:
- InfiniBand
- 10 Gbit Ethernet
- 1 Gbit Ethernet

Aggregator Switch

Storage Switch

Top of Rack Switch

Login Switch

User

Icebreaker Storage
Node index: sn3
/project

Icebreaker Storage
Node index: sn[0-2]
/home
/usr/local
/db

Seagate Storage
Lustre Parallel File System
/lustre1

Transfer Node
xfer2.gacrcc.uga.edu
Build Node
build1.gacrcc.uga.edu
AMD Opteron 16-core processor, 64 GB RAM

Compute Nodes
Node index: n0, n1, n2, ..... n165, n166, n167
CPU: AMD Opteron / Intel Xeon multicore processors
GPU: NVIDIA Tesla (Kepler) K40m GPU cards
/scratch

Login Node (VMs)
sapelo1.gacrcc.uga.edu
Intel Xeon processor
What is the new cluster – General Information

Sapelo is a Linux high performance computing (HPC) cluster:

• OS: 64-bit CentOS 6.5

• You can login to:
  
  Login (username@sapelo1.gacrc.uga.edu) : login, edit script, submit jobs
  
  Transfer (username@xfer2.gacrc.uga.edu) : transfer, compress data
  
  Build (username@build1.gacrc.uga.edu) : compile, test
  
  Login \textit{Interactive Node} \text{qlogin} \text{Interactive Node} : run interactively, edit script, submit jobs

• Communication: \textbf{InfiniBand network}

  compute nodes $\leftrightarrow$ compute nodes $\leftrightarrow$ storage systems, e.g., /home and /lustre1
What is the new cluster – General Information

• Batch-queueing System:
  - Jobs can be started (submitted), monitored, and controlled
  - Determine which compute node is the best place to run a job
  - Determine appropriate execution priority for a job to run

• Sapelo:
  - Torque Resource Manager
  - Moab Workload Manager
### What is the new cluster – Computing Resources

<table>
<thead>
<tr>
<th>Queue</th>
<th>Node</th>
<th>Total</th>
<th>Processor</th>
<th>CPUs /Node</th>
<th>RAM (GB) /Node</th>
<th>Max RAM (GB) /Single-node Job</th>
<th>GPU</th>
<th>GPU Cards /Node</th>
<th>InfiniBand</th>
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<td>batch</td>
<td>AMD</td>
<td>120</td>
<td>AMD Opteron</td>
<td>48</td>
<td>128</td>
<td>126</td>
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<td>N/A</td>
<td>Yes</td>
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<td>HIGHMEM</td>
<td>3</td>
<td>48</td>
<td>AMD Opteron</td>
<td>512 (2)</td>
<td>504</td>
<td>504</td>
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<td>N/A</td>
<td>Yes</td>
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<td></td>
<td>1024 (1)</td>
<td>997</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GPU</td>
<td>2</td>
<td>Intel Xeon</td>
<td>16</td>
<td>128</td>
<td>126</td>
<td>NVIDIA K40m</td>
<td>Yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>abcnode (buy-in)</td>
<td>2</td>
<td>AMD Opteron</td>
<td>48</td>
<td>256</td>
<td>252</td>
<td>N/A</td>
<td>N/A</td>
<td></td>
<td>Yes</td>
</tr>
</tbody>
</table>

Peak Performance per Node: 500Gflops/Node

Home: /home/username: **100GB**

Global scratch: /lustre1/username: **NO quota limit, auto-moved to /project if no modification in 30 days!**
Layer 1: Node
- A standalone “computer in a box”
- Multiple processors, e.g. 4, sharing memory
- Local disk storage, network interface, etc.
- Networked into a cluster

Layer 2: Processor
- A single computing component
- Multicore processor, e.g. 12 cores

Layer 3: Core
- Central processing unit (CPU) reading and executing instructions independently
- Each core is assigned to a software thread

Node 167
- 128 GB Shared RAM
- 48 cores and 128 GB RAM per node
## What is the new cluster – Storage Environment

<table>
<thead>
<tr>
<th>4 Filesystems</th>
<th>Role</th>
<th>Quota</th>
<th>Accessible from</th>
<th>Intended Use</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>/home/username</code></td>
<td>Home</td>
<td>100GB</td>
<td>sapelo1.gacrc.uga.edu (Login) Interactive nodes (Interactive)</td>
<td>Highly static data being used frequently</td>
<td>Snapshots</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>xfer2.gacrc.uga.edu (Transfer) build1.gacrc.uga.edu (Build) compute nodes (Compute)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><code>/lustre1/username</code></td>
<td>Global Scratch</td>
<td>No Limit</td>
<td>Interactive nodes (Interactive) xfer2.gacrc.uga.edu (Transfer) compute nodes (Compute)</td>
<td>Temporarily storing large data being used by jobs</td>
<td>Auto-moved to /project if 30 days no modification</td>
</tr>
<tr>
<td><code>/iscratch/username</code></td>
<td>Local Scratch</td>
<td>250GB</td>
<td>Individual compute node</td>
<td>Jobs with heavy disk I/O</td>
<td>User to clean up</td>
</tr>
<tr>
<td><code>/project/abclab</code></td>
<td>Storage</td>
<td>Variable</td>
<td>xfer2.gacrc.uga.edu (Transfer)</td>
<td>Long-term data storage</td>
<td>Group sharing possible</td>
</tr>
</tbody>
</table>

Note: `/usr/local/apps` : Software installation directory  
/db : Bioinformatics database installation directory
## What is the new cluster – Storage Environment

<table>
<thead>
<tr>
<th>7 Main Functions</th>
<th>On/From-Node</th>
<th>Related Filesystem</th>
</tr>
</thead>
<tbody>
<tr>
<td>Login Landing</td>
<td>Login or Transfer or Build</td>
<td>/home/username (Home) <em>(Always!)</em></td>
</tr>
<tr>
<td>Batch Job Submitting</td>
<td>Login</td>
<td>/home/username (Home)</td>
</tr>
<tr>
<td></td>
<td>Interactive</td>
<td>/lustre1/username (Scratch) <em>(Suggested!)</em></td>
</tr>
<tr>
<td></td>
<td></td>
<td>/home/username (Home)</td>
</tr>
<tr>
<td>Interactive Job Running</td>
<td>Interactive</td>
<td>/lustre1/username (Scratch) <em>(Suggested!)</em></td>
</tr>
<tr>
<td></td>
<td></td>
<td>/home/username (Home)</td>
</tr>
<tr>
<td>Data Transferring, Archiving , and</td>
<td>Transfer</td>
<td>/lustre1/username (Scratch) <em>(Suggested!)</em></td>
</tr>
<tr>
<td>Compressing</td>
<td></td>
<td>/home/username (Home)</td>
</tr>
<tr>
<td>Job Data Temporarily Storing</td>
<td>Compute</td>
<td>/lscratch/username (Local Scratch)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>/lustre1/username (Scratch)</td>
</tr>
<tr>
<td>Long-term Data Storing</td>
<td>Transfer or Copy</td>
<td>/project/abclab</td>
</tr>
<tr>
<td>Code Compilation</td>
<td>Build</td>
<td>/home/username (Home)</td>
</tr>
</tbody>
</table>
How does Sapelo operate?
How to work with Sapelo?

Before we start:

• To get zcluster to be your best HPC buddy

GACRC Wiki: http://wiki.gacrc.uga.edu

GACRC Support: https://wiki.gacrc.uga.edu/wiki/Getting_Help
How to work with Sapelo?

To submit your ticket to GACRC?

- **Job Troubleshooting:**
  
  Please tell us details of your question or problem, including but not limited to:
  
  ✓ Your user name
  ✓ Your job ID
  ✓ Your working directory
  ✓ The queue name and command you used to submit the job

- **Software Installation:**
  
  ✓ Specific name and version of the software
  ✓ Download website
  ✓ Supporting package information if have

**Note:**

It’s USER’s responsibility to make sure the correctness of datasets being used by jobs!
How to work with Sapelo?

- On cluster, you are not alone....... Each user is sharing finite resources, e.g., CPU cycles, RAM, disk storage, network bandwidth, with other researchers. *What you do may affect other researchers on the cluster.*

6 rules of thumb to remember:

- **NO** jobs running on login node
- **NO** multi-threaded job running with only 1 core requested
- **NO** large memory job running on regular nodes
- **NO** long job running on interactive node
- **NO** small memory job running on large memory nodes
- Use the copy node for file transfer and compression
How to work with Sapelo?

- Start with the Cluster
- Connect & Login
- Software Packages
- Run Jobs
  - How to submit a job
  - How to make a job submission script
  - How to check job status, cancel a job, etc.
How to work with Sapelo – Start with the Cluster

• You need a User Account: UGAMyID@sapelo1.gacrc.uga.edu
  To create your account correctly, you must provide us with your official MyID, not a UGA MyID alias!
• To get a user account, follow 4 steps:

1. New user training (http://gacrc.uga.edu/help/training/)
2. Tell us your Name, UGA MyID, Lab name and PI’s name, via GACRC Support (https://wiki.gacrc.uga.edu/wiki/Getting_Help)
3. Invitation letter with instructions to start account initialization
4. Welcome letter with whole package of information about your account created successfully
How to work with Sapelo – Connect & Login

• Open a connection: Open a terminal and `ssh` to your account
  
  ```
  ssh zhuofei@sapelol.gacrc.uga.edu
  ```

  or
  
  ```
  ssh -X zhuofei@sapelol.gacrc.uga.edu
  ```

  (1 - `X` is for X windows application running on the cluster to be forwarded to your local machine

  2 If using Windows, use **SSH client** to open connection, get from UGA download software page)

• Logging in: You will be prompted for your **UGA MyID password**

  ```
  zhuofei@sapelol.gacrc.uga.edu’s password: 
  ```

  (3 On Linux/Mac, when you type in the password, the prompt blinks and does not move)

• Logging out: **exit** to leave the system

  ```
  [zhuofei@75-104 ~]$ exit
  ```
How to work with Sapelo – Software Packages

• The cluster uses **environment modules** to define the various paths for software packages
• Current number of modules installed is ~200 and expanding daily!
• **module avail** to list all modules available on the cluster:

```
$ module avail
```

<table>
<thead>
<tr>
<th>Module</th>
<th>Version</th>
<th>Installation Date</th>
<th>Latest</th>
<th>Type</th>
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</thead>
<tbody>
<tr>
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</tbody>
</table>
How to work with Sapelo – Software Packages

- **module list** to list which modules currently loaded:

  ```
  [zhuofei@75-104 ~]$ module list
  Currently Loaded Modules:
  1) StdEnv   2) moab/7.2.10
  ```

- **module load** to load the needed modules:

  ```
  [zhuofei@75-104 ~]$ module load ncbiblast+/2.2.29
  [zhuofei@75-104 ~]$ module load python/2.7.8
  [zhuofei@75-104 ~]$ module load R/3.1.2
  [zhuofei@75-104 ~]$ module list
  ```

  ```
  Currently Loaded Modules:
  1) StdEnv   2) moab/7.2.10   3) ncbiblast+/2.2.29   4) python/2.7.8   5) R/3.1.2
  ```

- **module unload** to remove the specific module:

  ```
  [zhuofei@75-104 ~]$ module unload R/3.1.2
  [zhuofei@75-104 ~]$ module list
  ```

  ```
  Currently Loaded Modules:
  1) StdEnv   2) moab/7.2.10   3) ncbiblast+/2.2.29   4) python/2.7.8
  ```
How to work with Sapelo – Run Jobs

• Components you need to run a job:
  ➢ *Software* already loaded. If not, used `module load`
  ➢ *Job submission script* to run the software, and specify computing resources:
    ✓ Number of nodes and cores
    ✓ Amount of memory
    ✓ Type of nodes
    ✓ Maximum wallclock time, etc.

• Common commands you need:
  ➢ `qsub`, `qdel`
  ➢ `qstat -f`, `showjobs`, `showq` etc.
How to work with Sapelo – Run Jobs

• How to submit a job?  *Easy!*

  ```bash
  [zhuofei@75-104 MPIs]$ qsub sub.sh
  ```

  *qsub* is to submit a job

  *sub.sh* is your **job submission script** specifying:
  - Number of nodes and cores
  - Amount of memory
  - Type of nodes
  - Maximum wallclock time, etc.

• How to make a job submission script?  *Next Page!*
How to work with Sapelo – Run Jobs

- **Example 1: Serial job script** *sub.sh* running NCBI Blast +

```bash
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=1:AMD
#PBS -l mem=20gb
#PBS -l walltime=48:00:00
cd $PBS_O_WORKDIR
module load ncbiblast+/2.2.29
time blastn [options] > outputfile
```

- **Linux shell** *(bash)*
- **Queue name** *(batch)*
- **Name of the job** *(testBlast)*
- **Number of nodes** *(1)*, **number of cores/node** *(1)*, **node type** *(AMD)*
- **Maximum amount of physical memory** *(20 GB)* used by the job
- **Maximum wall clock time** *(48 hours)* for the job, default 6 minutes
- **Use the directory from which the job is submitted as the working directory**
- **Load the module of ncbiblast+, version 2.2.29**
- **Run blastn with ‘time’ command to measure the amount of time it takes to run the application**
How to work with Sapelo – Run Jobs

• Example 2: **Threaded job script** *sub.sh* running NCBI Blast + with **4** threads

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=4:AMD
#PBS -l walltime=480:00:00
#PBS -l mem=20gb

#PBS -M jSmith@uga.edu
#PBS -m ae
#PBS -j oe

cd $PBS_O_WORKDIR

module load ncbiblast+/2.2.29

time blastn -num_threads 4 [options] > outputfile

⇒ Run blastn with 4 threads (-num_threads 4)
⇒ Number of nodes (**1**), number of cores/node (**4**), node type (**AMD**)

*Number of threads (4) = Number of cores requested (4)*

⇒ Email address to receive a notification for computing resources
⇒ Send email notification when job aborts (**a**) or terminates (**e**)
⇒ Standard error file (**testBlast.e1234**) will be merged into standard out file (**testBlast.o1234**)
How to work with Sapelo – Run Jobs

• Example 3: MPI job script `sub.sh` running RAxML with 50 MPI processes

```bash
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testRAxML
#PBS -l nodes=2:ppn=48:AMD
#PBS -l walltime=480:00:00
#PBS -l mem=20gb
#PBS -j oe

Number of nodes (2), number of cores/node (48), node type (AMD)
Total cores requested = 2 × 48 = 96

We suggest, Number of MPI Processes (50) ≤ Number of cores requested (96)

```bash
cd $PBS_O_WORKDIR

module load raxml/8.1.20
module load intel/15.0.2
module load openmpi/1.8.3/intel/15.0.2

To run raxmlHPC-MPI-AVX, MPI version using OpenMPI 1.8.3/Intel 15.0.2

```bash
mpirun –np 50 raxmlHPC-MPI-AVX [options] > outputfile
Run raxmlHPC-MPI-AVX with 50 MPI processes (–np 50)
```
```bash
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testRAxML
#PBS -l nodes=2:ppn=27:AMD
#PBS -l walltime=480:00:00
#PBS -l mem=20gb
#PBS -j oe

cd $PBS_O_WORKDIR

# Context Sharing
CONTEXTS=$(/usr/local/bin/set_contexts.sh $PBS_NUM_PPN)
if [[ "$?" -eq "0" ]]; then
    export PSM_SHARDEDCONTEXTS_MAX=$CONTEXTS
fi

module load raxml/8.1.20
module load intel/15.0.2
module load openmpi/1.8.3/intel/15.0.2

mpirun --np 50 raxmlHPC-MPI-AVX [options] > outputfile
```

ppn number (27) fewer than 48 MUST be a multiplier of 3!
How to work with Sapelo – Run Jobs

• How to check job status? **qstat**

```
[jSmith@75-104 MPIS]$ qstat
Job ID   Name         User   Time Use S Queue
---------- ------------------------------------------
481929.pbs testJob1    jSmith  900:58:0 C batch
481931.pbs testJob2    jSmith  04:00:03 R batch
481934.pbs testJob3    jSmith  0 C batch
```

Job status:
R: job is running
C: job completed (or crashed) and is not longer running. Jobs stay in this state for 1h
Q: job is pending, waiting for resources to become available

• How to cancel *testJob3* with jobID 481934? **qdel**

```
[zhuofei@75-104 MPIS]$ qdel 481934
[jSmith@75-104 MPIS]$ qstat
Job ID   Name         User   Time Use S Queue
---------- ------------------------------------------
481929.pbs testJob1    jSmith  900:58:0 C batch
481931.pbs testJob2    jSmith  04:00:03 R batch
481934.pbs testJob3    jSmith  0 C C batch
```

← Stay on list 1 hr
How to work with Sapelo – Run Jobs

• How to check computing resources?

Option 1: `qstat -f JobID` for running jobs or finished jobs in 1 hour

Option 2: `showjobs JobID` for finished jobs over 1 hour, but ≤ 7 days

Option 3: Email notification from finished jobs (completed, canceled, or crashed), if using:

```bash
#PBS -M jSmith@uga.edu
#PBS -m ae
```
How to work with it – Run Jobs

- **qstat -f JobID** for *running jobs* or *finished jobs in 1 hour*

```bash
[zhuofei@75-104 MPIs]$ qstat -f 699847
Job Id: 699847.pbs.scm
  Job_Name = testJob
  Job_Owner = zhuofei@uga-2f0f976.scm
  resources_used.cput = 00:11:55
  resources_used.energy_used = 0
  resources_used.mem = 411572kb
  resources_used.vmem = 6548528kb
  resources_used.walltime = 00:01:36
  job_state = C
  queue = batch
  Error_Path = uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.e699847
  exec_host = n165/0-23
  Output_Path = uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.o699847

Resource_List.mem = 5gb
Resource_List.nodect = 1
Resource_List.nodes = 1:ppn=24:AMD
Resource_List.walltime = 10:00:00

Variable_List = PBS_O_QUEUE=batch,PBS_O_HOME=/home/zhuofei, ...... , PBS_O_WORKDIR=/home/zhuofei/MPIs,
How to work with it – Run Jobs

- **showjobs JobID** for *finished jobs over 1 hour, but ≤ 7 days*

```bash
[zhuofei@75-104 MPIS]$ showjobs 699847
Job Id            : 699847.pbs.scm
Job Name          : testJob
Output File       : uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.o699847
Error File        : uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.e699847
Working Directory : /home/zhuofei/MPIs
Home Directory    : /home/zhuofei
Submit Arguments  : sub.sh
User Name         : zhuofei
Group Name        : rccstaff
Queue Name        : batch
Wallclock Limit   : 10:00:00
Wallclock Duration: 00:01:36
CPUTime           : 00:11:55
Memory Used       : 401.9Mb
Memory Limit      : 5gb
vmem Used         : 6.2Gb
Submit Time       : Wed Nov  4 12:02:22 2015
End Time          : Wed Nov  4 12:04:45 2015
Exit Code         : 0
Master Host       : n165
```
How to work with it – Run Jobs

- Email notification from **finished jobs (completed, canceled, or crashed)**
How to work with it – Run Jobs

- How to check queue status?

```
showq
```

<table>
<thead>
<tr>
<th>JOBID</th>
<th>USERNAME</th>
<th>STATE</th>
<th>PROCS</th>
<th>REMAINING</th>
<th>STARTTIME</th>
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<tbody>
<tr>
<td>481914</td>
<td>brant</td>
<td>Running</td>
<td>1</td>
<td>20:46:21</td>
<td>Fri Jun 12 11:32:23</td>
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<tr>
<td>481915</td>
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<td>Running</td>
<td>1</td>
<td>20:48:56</td>
<td>Fri Jun 12 11:34:58</td>
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<tr>
<td>481567</td>
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<td>Running</td>
<td>288</td>
<td>2:04:15:48</td>
<td>Wed Jun 10 15:01:50</td>
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</table>

108 active jobs       5141 of 5740 processors in use by local jobs (89.56%)
121 of 122 nodes active      (99.18 %)

<table>
<thead>
<tr>
<th>JOBID</th>
<th>USERNAME</th>
<th>STATE</th>
<th>PROCS</th>
<th>QUEUETIME</th>
</tr>
</thead>
<tbody>
<tr>
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<td>joykai</td>
<td>Idle</td>
<td>48</td>
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<td>48</td>
<td>50:00:00:00:00:00:00   Thu Jun 11 13:41:20</td>
</tr>
</tbody>
</table>

50 eligible jobs

Total jobs: 158
Thank You!