Introduction to HPC Using the New Cluster at GACRC

Georgia Advanced Computing Resource Center
University of Georgia
Zhuofei Hou, HPC Trainer
zhuofei@uga.edu
Outline

• What is GACRC?
• What is the new cluster at GACRC?
• How does it operate?
• How to work with it?
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)
- [https://wiki.gacrc.uga.edu/wiki/Getting_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (Support)
- [https://blog.gacrc.uga.edu](https://blog.gacrc.uga.edu) (Blog)
- [http://forums.gacrc.uga.edu](http://forums.gacrc.uga.edu) (Forums)
<table>
<thead>
<tr>
<th>Colleges &amp; Schools</th>
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<th>PIs</th>
<th>Users</th>
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<td>Carl Vinson Institute of Government</td>
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What is the new cluster at GACRC?

- Cluster Structural Diagram
- General Information
- Computing Resources
What is the new cluster – General Information

The new cluster is a Linux high performance computing (HPC) cluster:

- **64-bit CentOS 6.5** operating system

- User can login to:
  - Login node: `sapelo1.gacrc.uga.edu` (for login & job submission)
  - Transfer mode: `xfer2.gacrc.uga.edu` (for data transferring & compression)
  - Build node: `build1.gacrc.uga.edu` (for code compilation)

- **InfiniBand network** provides internodal communication:
  - compute nodes ↔ compute nodes
  - compute nodes ↔ storage systems, e.g., /home and /scratch
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

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

<table>
<thead>
<tr>
<th>Queue</th>
<th>Node Type</th>
<th>Total Nodes</th>
<th>Processor</th>
<th>Cores / Node</th>
<th>RAM (GB) / Node</th>
<th>GPU</th>
<th>GPU Cards / Node</th>
<th>InfiniBand</th>
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<tr>
<td>batch</td>
<td>AMD</td>
<td>120</td>
<td>AMD Opteron</td>
<td>48</td>
<td>128</td>
<td>N/A</td>
<td>N/A</td>
<td>Yes</td>
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<tr>
<td></td>
<td>HIGHMEM</td>
<td>3</td>
<td>AMD Opteron</td>
<td>48</td>
<td>512 (2)</td>
<td>N/A</td>
<td>N/A</td>
<td>Yes</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1024 (1)</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>GPU</td>
<td></td>
<td>2</td>
<td>Intel Xeon</td>
<td>16</td>
<td>128</td>
<td>NVIDIA K40m</td>
<td>8</td>
<td>Yes</td>
</tr>
</tbody>
</table>

**Peak Performance per Node:** 500 Gflops/Node

Home directory: 100 GB

Scratch directory on /lustre1: NO quota limit, auto-moving to /project, if no modification in 30 days!
How does it operate?
Node 167

**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

128 GB Shared RAM

**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

48 cores and 128 GB RAM per node
How to work with it?

Before we start:

• To get the new cluster to be your best HPC buddy, go to GACRC Wiki (http://wiki.gacrc.uga.edu) and GACRC Web (http://gacrc.uga.edu)

• To get the most effective and qualified support from us, go to GACRC Support (https://wiki.gacrc.uga.edu/wiki/Getting_Help)

• To work happily and productively, follow the new cluster’s Community Code of Conduct (CCOC)
How to work with it?

• Cluster’s CCOC:

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 it?

- 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 it – 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 UGA 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. We send you an invitation letter with instructions to start account initialization
4. With Step 3 finished successfully, we send you a welcome letter with whole package of information about your account created successfully
How to work with it – 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 it — Software Packages

- The cluster uses **environment modules** to define the various paths for software packages
- Current number of modules installed is ~70 and expanding daily!

**module avail** to list all modules available on the cluster:

<table>
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<tr>
<th>Module</th>
<th>Version</th>
<th>Location</th>
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<tbody>
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<tr>
<td>examl/3.011</td>
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<tr>
<td>expat/latest</td>
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<td>fastqc/latest</td>
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<td>zlib/gcc447/1.2.8</td>
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</table>
How to work with it – 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 it – Run Jobs

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

- Common commands you need:
  - `qsub`, `qstat`, `qdel`
  - `showq`, `checkjob`, etc.
How to work with it – Run Jobs

• How to submit a job? **Easy!**

```
[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 it – Run Jobs

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

```
#PBS -S /bin/bash  
#PBS -q batch  
#PBS -N testBlast  
#PBS -l nodes=1:ppn=1:AMD  
#PBS -l mem=20g  
#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 it – 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
```

- Number of nodes (1), number of cores/node (4), node type (AMD)
  - *Number of threads (4) = Number of cores requested (4)*

- Email to receive a summary of computing resources used by the job
- Receive an email when the job finishes (e)
- Standard error file (`testBlast.e1234`) will be merged into standard out file (`testBlast.o1234`)
How to work with it – 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

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

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

→ 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)*

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

Run raxmlHPC-MPI-AVX with 50 MPI processes (–np 50)
#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_SHAREDCONTEXTS_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 ➔ Run raxmlHPC-MPI-AVX with 50 MPI processes (--np 50)
How to work with it – 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 24h
- **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 batch
```

```
How to work with it – Run Jobs

- How to check resource utilization of a job? `qstat -f`
How to work with it – Run Jobs

• How to check resource utilization of a job? **checkjob**

```bash
$ checkjob 501280
Job 501280
AName: testJob
State: Idle
Creds: user:zhuofei group:rccstaff class:batch
WallTime: 00:00:00 of 02:00:00:00
SubmitTime: Thu Aug 20 11:39:13
   (Time Queued Total: 00:03:31 Eligible: 00:03:24)
TemplateSets: DEFAULT
Total Requested Tasks: 48
Req[0] TaskCount: 48 Partition: ALL
Opsys: --- Arch: --- Features: AMD
Dedicated Resources Per Task: PROCS: 1 MEM: 426M
node:kmdnode:rjsnode:rmcnodel:tcpnode:xqwnodel
SystemJID: 501280
Notification Events: JobStart,JobEnd,JobFail Notification Address: zhuofei@uga.edu
Node Rejection Summary: [CPU: 11][Features: 18][State: 125]
```
How to work with it – Run Jobs

- How to check queue status? **showq!**

```bash
[zhuefei@75-104 MPis]$ showq
active jobs--
----------------------------------
JOBID  USERNAME  STATE   PROCS       REMAINING   STARTTIME
481914  brant    Running   1          20:46:21     Fri Jun 12 11:32:23
481915  brant    Running   1          20:48:56     Fri Jun 12 11:34:58
481567  becton   Running  288        2:04:15:48   Wed Jun 10 15:01:50

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

eligible jobs--
-------------------
JOBID  USERNAME  STATE  PROCS  WCLIMIT  QUEUETIME
481821  joykai   Idle   48      50:00:00:00 Thu Jun 11 13:41:20
481813  joykai   Idle   48      50:00:00:00 Thu Jun 11 13:41:19
481811  joykai   Idle   48      50:00:00:00 Thu Jun 11 13:41:19
481825  joykai   Idle   48      50:00:00:00 Thu Jun 11 13:41:20

50 eligible jobs

blocked jobs--
-------------------
JOBID  USERNAME  STATE  PROCS  WCLIMIT  QUEUETIME

0 blocked jobs

Total jobs:  158
```
Thank You!