Using computing resources at GACRC
An introduction to zcluster

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Outline

- GACRC
- zcluster Diagram
- How to Log on
- How to Transfer Files
- How to Submit a Job
- How to Find Support
- Important Rules
GACRC

- We are a high-performance computing (HPC) center at UGA
- We provide to the UGA research and education community an advanced computing environment:
  - HPC computing and networking infrastructure located at the Boyd Data Center
  - Comprehensive collection of scientific, engineering and business applications
  - Consulting and training services

http://gacrc.uga.edu/about/
**zcluster Diagram**

- **Node**: Computer for a specific function on cluster, e.g., login node, work nodes
- **Queue**: Organization of compute nodes for a specific computing need
- **Cluster**: Nodes + Drives, all connected by network
How to log on – Mac/Linux

1. Open Terminal utility
2. Type command line: `ssh username@zcluster.rcc.uga.edu`
   For example: `ssh s_01@zcluster.rcc.uga.edu`
3. You will be prompted for your `zcluster password` (when you type in the password, the prompt blinks and does not move)

On your first log on, use `passwd` command to change your temporary password to a permanent one!
How to log on – Windows

Download to install:

http://eits.uga.edu/hardware_and_software/software/

On your first log on, use `passwd` command to change your temporary password to a permanent one!

You will be prompted for your zcluster password after step 4.
Once You Log on

1. Your working environment is Linux

2. You are on login node

3. You are in your home directory: /home/student/courseID/username/
   for example: /home/student/BCMB8330/s_01/
How to Transfer Files – Mac/Linux

Local Computer ➔ zcluster; Type command in Terminal from your *local computer*

```bash
scp file s_01@zcluster.rcc.uga.edu:/home/student/BCMB8330/s_01
scp -r folder s_01@zcluster.rcc.uga.edu:/home/student/BCMB8330/s_01
```

zcluster ➔ Local Computer; Type command in Terminal from your *local computer*

```bash
scp s_01@zcluster.rcc.uga.edu:/home/student/BCMB8330/s_01/file.
scp -r s_01@zcluster.rcc.uga.edu:/home/student/BCMB8330/s_01/folder.
```
How to Transfer Files - Windows

1. Use Login node!
2. Host Name: zcluster.rcc.uga.edu
3. User Name: u_01
4. Port Number: 22
5. Authentication Method: <Profile Settings>
6. Local Name: /Library/StartupItems/ssh.plist
7. Remote Name: /home/student/BCMB8330/s_01

SSH Secure Shell 3.2.9 (Build 283)
Copyright (c) 2000-2003 SSH Communications Security Corp - http://www.ssh.com/
How to Submit a Job

• You need to create a *script* to make a *compute node* to know:
  ➢ Your working directory
  ➢ The software you want to run
  ➢ Any Linux commands you want the node to run

• Wiki Links:
  
  https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_zcluster
  
  https://wiki.gacrc.uga.edu/wiki/Software
  
  https://wiki.gacrc.uga.edu/wiki/Command_List
A Common Example – Running Samtools

- Samtools is a common utility in bioinformatics
- Script name: `sub.sh`
- Working directory: `/home/student/BCMB8330/s_01/workDir/

```
#!/bin/bash
# Linux default shell (bash)

cd ${HOME}/workDir
# Specify and enter (cd) a working directory

/usr/local/samtools/latest/samtools <command> [options]
# Run samtools
```

https://wiki.gacrc.uga.edu/wiki/Samtools
A Common Example – Submit Job

• Submit *sub.sh* to rcc-30d queue: Type command on command line from your working directory:

```
$ qsub -q rcc-30d sub.sh
```

Note: Once a job is submitted, you can logout from the cluster and log back in later to check status of job and to retrieve the results.
A Class (BCMB8330) Example – A Script Running AMBER

#!/bin/bash
# Linux default shell (bash)

cd /home/student/BCMB8330/s_01/workDir
# Specify and enter (cd) a working directory

source /usr/local/amber/14/amber.sh
# source Amber setup file

export LD_LIBRARY_PATH=/usr/local/cuda/5.0.35-gcc447/lib64:${LD_LIBRARY_PATH}

/usr/local/amber/14/bin/pmemd.cuda -O -i mdin -o mdout -p prmtop -c inpcrd
# run Amber

https://wiki.gacrc.uga.edu/wiki/AMBER
A Class (BCMB8330) Example – Submit Job

- Submit `sub.sh` to fsr3 GPU queue: Type command on command line from your working directory on zcluster:

```bash
$ qsub -q fsr3 -l cuda=1 sub.sh
```

use fsr3 queue

use 1 GPU card
Check Job Status

- **Type command on command line:** `qstat`

```bash
$ qstat

<table>
<thead>
<tr>
<th>job-ID</th>
<th>prior</th>
<th>name</th>
<th>user</th>
<th>state</th>
<th>submit/start at</th>
<th>queue</th>
<th>slots</th>
<th>ja-task-ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>9707321</td>
<td>0.50766</td>
<td>sub.sh</td>
<td>s_01</td>
<td>r</td>
<td>01/15/2017 13:39:23</td>
<td><a href="mailto:rcc-30d@compute-7-12.local">rcc-30d@compute-7-12.local</a></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>9707322</td>
<td>0.50383</td>
<td>sub.sh</td>
<td>s_01</td>
<td>Eqw</td>
<td>01/15/2017 13:39:23</td>
<td><a href="mailto:rcc-30d@compute-7-12.local">rcc-30d@compute-7-12.local</a></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>9707323</td>
<td>0.00000</td>
<td>sub.sh</td>
<td>s_01</td>
<td>qw</td>
<td>01/15/2017 13:39:28</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

r: Job is running
qw: Job is waiting in queue
Eqw: Job is in error state and pending
Cancel a Job

• Type command on command line: `qdel JobID`

```bash
$ qdel 9707322
$ qstat
job-ID  prior  name  user  state  submit/start at  queue  slots ja-task-ID
9707321  0.50766  sub.sh  s_01  r  01/15/2017 13:39:23  rcc-30d@compute-7-12.local  1
9707323  0.00000  sub.sh  s_01  qw  01/15/2017 13:39:28  1
```
Check Job Memory Usage

- For a running job: `qsj JobID`

```bash
$ qsj 9707368

job_number: 9707368
owner: s_110
cwd: /escratch4/s_110/s_110_Jan_28
hard_queue_list: rcc-30d
script_file: sub.sh
......
usage 1: cpu=00:01:27, mem=0.96498 GBs, io=0.00014, vmem=73.734M, maxvmem=75.734M
```

- For a finished jobs: `qacct -j JobID`

```bash
$ qacct -j 970732

qname rcc-30d
hostname compute-7-12.local
jobname sub.sh
jobnumber 9707323
......
cpu 183.320
mem 2.021
io 0.000
maxvmem 6.530G
```

Total Memory
How to Find Support


- **Password Reset** when you lost your password (Request needs to be validated by the instructor)
- **Job Troubleshooting:** Tell us details of your problem, please also include:
  - UserID and JobID
  - Working directory and script name
  - Working environment (queue/node/command you used)
  - Brief of your problem

**Note:**
It’s **USER**’s responsibility to make sure the **correctness of data** being used by jobs!
Important Rules

 Ø No Sharing User Account! ➔ Use your own user account

 Ø No Job Running on Login node! ➔ Submit job to batch queue
Useful Links

- GACRC Wiki: https://wiki.gacrc.uga.edu/wiki/Main_Page
- GACRC Software: https://wiki.gacrc.uga.edu/wiki/Software
- GACRC Support: http://gacrc.uga.edu/help/
- GACRC Training: https://wiki.gacrc.uga.edu/wiki/Training

Thank You!