Introduction to GACRC Teaching Cluster
PHYS4601/6601

Georgia Advanced Computing Resource Center (GACRC)
Enterprise Information Technology Services (EITS)
The University of Georgia
Outline

- GACRC
- Overview
- Working Environment
  - Two Nodes and Three Folders
  - Computational Partitions
  - Software
- Submit a Computational Batch Job
- GACRC Wiki and Support
GACRC

- A high-performance-computing (HPC) center at the UGA
- 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

Wiki: http://wiki.gacrc.uga.edu
Support: https://wiki.gacrc.uga.edu/wiki/Getting_Help
Web Site: http://gacrc.uga.edu
Kaltura Channel: https://kaltura.uga.edu/channel/GACRC/176125031
Note: You need to connect to the **UGA VPN** at first when accessing from outside of the UGA main campus.
Working Environment

https://wiki.gacrc.uga.edu/wiki/Systems#Teaching_cluster

- Two nodes, your "username" is your MyID for both of them:
  1. For batch job workflow, the host to log into is teach.gacrc.uga.edu
  2. For file transfers, the host to log into is txfer.gacrc.uga.edu

- Three folders:
  1. /home/MyID : working space for running computational jobs
  2. /scratch/MyID: working space for running computational jobs
  3. /work/phys4601/MyID : data storing space for individual user in a class
  4. /work/phys4601/instructor_data : data shared with class by the instructors

- Partitions for PHYS4601/6601 class: fsr4601
Working Environment (cont.)

- **Software**
  1. Software names are long and have a Easybuild toolchain name associated to it
  2. Complete module name: Name/Version-toolchain, e.g., Python/3.10.4-GCCcore-11.3.0
  3. Software names are case-sensitive!
    - `module spider pattern`: Search modules using a name pattern (case-insensitive)
    - `module load/unload moduleName`: Load/remove a module
    - `module avail`: List all available modules on the cluster
    - `module list`: List modules currently loaded
    - `module purge`: Remove all modules from working environment
Submit a Computational Batch Job

1. Log on to Login node using MyID and password, and two-factor authentication with Archpass Duo:
   `ssh MyID@teach.gacrc.uga.edu`
2. Change directory to your scratch space: `cd /scratch/MyID`
3. Create a working subdirectory for a job: `mkdir workDir`
4. Change directory to `workDir`: `cd workDir`
5. Transfer data from local computer to `workDir`: use `scp` or `WinSCP` to connect Transfer node
   Transfer data on cluster to `workDir`: log on to Transfer node and then use `cp` or `mv`
6. Compile Fortran code `mult.f` into a binary code
7. Make a job submission script in `workDir`: `nano sub.sh`
8. Submit a job from `workDir`: `sbatch sub.sh`
9. Check job status: `squeue --me` or Cancel a job: `scancel JobID`
Step 1: Log on to Login node
https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster

1. Teaching cluster access requires verification using two-factor authentication with Archpass Duo. If you are not enrolled in Archpass Duo, please refer to https://eits.uga.edu/access_and_security/infosec/tools/archpass_duo/ on how to enroll

2. If you are connecting from off-campus, please first connect to the UGA VPN and then connect to teach.gacrc.uga.edu. Information on how to use the VPN is available at https://eits.uga.edu/access_and_security/infosec/tools/vpn/
Step 1: Log on to Login node - Mac/Linux using ssh

1. Open **Terminal** utility

2. Type command line: `ssh MyID@teach.gacr.gacrc.uga.edu`

3. You will be prompted for your **UGA MyID password**

4. You will verify your login using **Archpass Duo** authentication
ssh zhuofei@teach.gacrc.uga.edu

1. use ssh to open connection

UGA DUO authentication is required for SSH/SCP access to GACRC systems. For additional help with UGA DUO authentication or to report an issue please visit: https://eits.uga.edu/access_and_security...

Password:

2. Enter your MyID password
   When you enter password, no stars or dots will show as you are typing. Please type password carefully!

Duo two-factor login for zhuofei

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-5758
2. Phone call to XXX-XXX-5758
3. Phone call to XXX-XXX-1925
4. SMS passcodes to XXX-XXX-5758 (next code starts with: 1)

Passcode or option (1-5): 1

3. Select Duo option

Success. Logging you in...

Last login: Mon Aug  3 11:11:58 2020 from 172.18.114.119
zhuofei@teach-sub1 ~$
Step1 (Cont.) - Windows using PuTTY

1. Download and install PuTTY: [https://www.putty.org/](https://www.putty.org/)

2. Detailed downloading and installation instructions:
   [https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY](https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY)

3. Detailed configuring and usage instructions:
   [https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY#Configuring_PuTTY](https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY#Configuring_PuTTY)
The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"
Next you will enter your UGA MyID password and initiate DUO authentication procedure:
Step2 - 4: cd to /scratch dir, make and cd into workDir

zhuofei@teach-sub1 ~$ cd /scratch/zhuofei  ➡️ cd command to change directory
zhuofei@teach-sub1 zhuofei$ mkdir workDir  ➡️ mkdir command to create a subdirectory
zhuofei@teach-sub1 zhuofei$ cd workDir/  ➡️ cd command to change directory
zhuofei@teach-sub1 workDir$ ls  ➡️ ls command to list contents of directory
zhuofei@teach-sub1 workDir$ it is empty in workDir!
Step5: Transfer data from local computer to workDir - Mac/Linux

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_scp_2

1. Connect to Transfer node (txfer.gacrc.uga.edu) in Terminal from your local computer
2. Use scp command: scp (-r) [Source] [Target]
3. Enter your MyID password, then select Duo option to verify connection

**E.g. 1**: use scp on local computer, from Local ➔ workDir on cluster

```
scp ./file zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir
scp -r ./folder/ zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir
```

**E.g. 2**: use scp on local computer, from workDir on cluster ➔ Local

```
scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .
scp -r zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/folder/ .
```
Step5 (Cont.) - Windows using WinSCP

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

1. You need to connect to cluster’s Transfer node (txfer.gacrc.uga.edu)

2. Use WinSCP on local computer
   - WinSCP can be downloaded from https://winscp.net/eng/index.php
   - Default installation procedure is simple

Step 5 (Cont.) - Windows using WinSCP
Step 5 (Cont.) - Windows using WinSCP

Select DUO option
Step 5 (Cont.) - Windows using WinSCP

Change paths on your local computer and transfer node:

Drag to transfer files or folders.
Step5 (Cont.): Transfer data on cluster to workDir

• Log on to Transfer node (txfer.gacrc.uga.edu)
  ✓ Mac/Linux: ssh MyID@txfer.gacrc.uga.edu (page 9-10)
  ✓ Windows: use PuTTY to log in MyID@txfer.gacrc.uga.edu (page 11-13)

• Directories you can access on transfer node:
  1. /home/MyID (Landing home)
  2. /work/phys4601/MyID
  3. /work/phys4601/instructor_data

• Transfer data between two folders on cluster using cp or mv, e.g.:
  
mv /work/phys4601/MyID/datafile /home/MyID/workDir
Step 6: Compile Fortran code *mult.f* into a binary

```
zhuofei@teach-sub1 workDir$ interact
zhuofei@rb1-11 workDir$ cp /usr/local/gacrc/training/phys4601/mult.f .
zhuofei@rb1-11 workDir$ cat mult.f
  Program mult
   C Multiplies two integer numbers
   implicit none
   integer i,j,iprod
   i=3
   j=4
   open(1, file='output.txt')
   iprod=i*j
   write(1,10)i,j,iprod
10 format('The product of ', i2, ' and ', i2, ' is ', i3)
   close(1)
   end
zhuofei@rb1-11 workDir$ module load GCC/11.3.0
zhuofei@rb1-11 workDir$ gfortran mult.f -o mult.x
zhuofei@rb1-11 workDir$ ls
  mult.f mult.x
zhuofei@rb1-11 workDir$ exit
```

- Start an interactive session
- Copy source code to your working dir
- Show contents of source code
- Load GCC compiler module
- Compile source code into a binary
- Binary is generated in your working dir
- Exit from interactive session
Step 7: Make a job submission script `sub.sh` using `nano`

```
zhuofei@teach-sub1 workDir$ cp /usr/local/gacrc/training/phys4601/sub.sh .  ➔ Copy sub.sh to working dir
zhuofei@teach-sub1 workDir$ cat sub.sh  ➔ Show contents of sub.sh
#!/bin/bash
#SBATCH --job-name=test  # Job name
#SBATCH --partition=fsr4601  # Submit job to fsr4601 partition
#SBATCH --ntasks=1  # Single task job
#SBATCH --cpus-per-task=1  # Number of cores per task
#SBATCH --mem=2gb  # Total memory for job
#SBATCH --time=00:01:00  # Time limit hrs:min:sec; fsr4601 TIMELIMIT 1 min
#SBATCH --output=log.%j  # Standard output and error log
#SBATCH --mail-user=MyID@uga.edu  # Where to send mail
#SBATCH --mail-type=ALL  # Mail events (BEGIN, END, FAIL, ALL)

cd $SLURM_SUBMIT_DIR
module load GCC/11.3.0
time ./mult.x  # run the binary code you compiled in step 5 in this job
zhuofei@teach-sub1 workDir$ nano sub.sh  # Use nano modify sub.sh, e.g., email address
```
Step 8: Submit a job from workDir using sbatch

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster#How_to_submit_a_job_to_the_batch_queue

$ sbatch sub.sh
Submitted batch job 5230

**Tips:** sub.sh is a job submission script for

1. specifying computing resources
2. loading compiler module using `module load`
3. running any Linux commands you want to run
4. running your binary code
Step 9: Check job status using squeue

[https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster)

```bash
zhuofei@teach-sub1 workDir$ squeue --me
```

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>ST</th>
<th>TIME</th>
<th>NODES</th>
<th>NODELIST(REASON)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5230</td>
<td>fsr4601</td>
<td>test</td>
<td>zhuofei</td>
<td>R</td>
<td>0:01</td>
<td>1</td>
<td>rb1-3</td>
</tr>
</tbody>
</table>

```bash
zhuofei@teach-sub1 workDir$ squeue --me -l
```

```bash
Mon Jan 09 26:03:14 2024
```

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>STATE</th>
<th>TIME</th>
<th>TIME_LIMI</th>
<th>NODES</th>
<th>NODELIST(REASON)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5230</td>
<td>fsr4601</td>
<td>test</td>
<td>zhuofei</td>
<td>RUNNING</td>
<td>0:01</td>
<td>1:00</td>
<td>1</td>
<td>rb1-3</td>
</tr>
</tbody>
</table>

Job State: R for Running; PD for PenDing; F for Failed

TIME: the elapsed time used by the job, not remaining time, not CPU time
Step9 (Cont.): Cancel job using scancel

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster#How_to_delete_a_running_or_pending_job

zhuofei@teach-sub1 workDir$ scancel 5230
zhuofei@teach-sub1 workDir$ squeue --me

JOBID PARTITION     NAME     USER ST    TIME NODES Nodelist(REASON)
Step9 (Cont.): Check job details using sacct-gacrc -X and seff

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster

$ sacct-gacrc -X

<table>
<thead>
<tr>
<th>JobID</th>
<th>JobName</th>
<th>User</th>
<th>Partition</th>
<th>NNode</th>
<th>NCPUS</th>
<th>ReqMem</th>
<th>CPUS/Time</th>
<th>Elapsed</th>
<th>Timelimit</th>
<th>State</th>
<th>ExitCode</th>
<th>NodeList</th>
</tr>
</thead>
<tbody>
<tr>
<td>5230</td>
<td>test</td>
<td>zhuofei</td>
<td>fsr4601</td>
<td>1</td>
<td>1</td>
<td>2G</td>
<td>00:00:01</td>
<td>00:00:01</td>
<td>00:01:00</td>
<td>COMPLETED</td>
<td>0:0</td>
<td>rb1-3</td>
</tr>
</tbody>
</table>

$ seff 5230  
# Check computing resources used by a COMPLETED job

Cluster: gacrc-teach
User/Group: zhuofei/gacrc-instruction
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 00:00:00
CPU Efficiency: 0.00% of 00:00:01 core-walltime
Job Wall-clock time: 00:00:01
Memory Utilized: 0.00 MB (estimated maximum)
Memory Efficiency: 0.00% of 2.00 GB (2.00 GB/node)
Step9 (Cont.): Check node info using sinfo

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster

<table>
<thead>
<tr>
<th>PARTITION</th>
<th>AVAIL</th>
<th>TIMELIMIT</th>
<th>NODES</th>
<th>STATE</th>
<th>NODELIST</th>
</tr>
</thead>
<tbody>
<tr>
<td>allnodes</td>
<td>up</td>
<td>infinite</td>
<td>1</td>
<td>mix</td>
<td>rb1-11</td>
</tr>
<tr>
<td>allnodes</td>
<td>up</td>
<td>infinite</td>
<td>12</td>
<td>idle</td>
<td>c4-23,rb1-[1-10,12]</td>
</tr>
<tr>
<td>batch</td>
<td>up</td>
<td>7-00:00:00</td>
<td>8</td>
<td>idle</td>
<td>rb1-[3-10]</td>
</tr>
<tr>
<td>gpu</td>
<td>up</td>
<td>7-00:00:00</td>
<td>1</td>
<td>idle</td>
<td>c4-23</td>
</tr>
<tr>
<td>highmem</td>
<td>up</td>
<td>7-00:00:00</td>
<td>2</td>
<td>idle</td>
<td>rb1-[1-2]</td>
</tr>
<tr>
<td>Interactive</td>
<td>up</td>
<td>7-00:00:00</td>
<td>1</td>
<td>mix</td>
<td>rb1-11</td>
</tr>
<tr>
<td>interactive</td>
<td>up</td>
<td>7-00:00:00</td>
<td>1</td>
<td>idle</td>
<td>rb1-12</td>
</tr>
<tr>
<td>fsr4601</td>
<td>up</td>
<td>1:00</td>
<td>8</td>
<td>idle</td>
<td>rb1-[3-10]</td>
</tr>
<tr>
<td>fsr8602</td>
<td>up</td>
<td>10:00</td>
<td>8</td>
<td>idle</td>
<td>rb1-[3-10]</td>
</tr>
</tbody>
</table>

idle = no cores in use; mix = some cores are still free; alloc = all cores are allocated
Obtain Job Details

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster#How_to_check_resource_utilization_of_a_running_or_finished_job

Option 1: `seff` for details of computing resource usage of a **finished** job

Option 2: `sacct-gacrc` for details of computing resource usage of a **running or finished** job

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

```
#SBATCH --mail-user=username@uga.edu
#SBATCH --mail-type=ALL
```
GACRC Wiki [http://wiki.gacrc.uga.edu](http://wiki.gacrc.uga.edu)
Kaltura Channel [https://kaltura.uga.edu/channel/GACRC/176125031](https://kaltura.uga.edu/channel/GACRC/176125031)

Connecting: [https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster)
Running Jobs: [https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster)
Monitoring Jobs: [https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster)
Transfer File:
[https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster_.28txfer.gacrc.uga.edu.29](https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster_.28txfer.gacrc.uga.edu.29)
Sample Job Scripts:
[https://wiki.gacrc.uga.edu/wiki/Sample_batch_job_submission_scripts_on_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Sample_batch_job_submission_scripts_on_the_teaching_cluster)
Linux Command: [https://wiki.gacrc.uga.edu/wiki/Command_List](https://wiki.gacrc.uga.edu/wiki/Command_List)
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 partition 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

Please note to make sure the correctness of datasets being used by your jobs!
Georgia Advanced Computing Resource Center (GACRC) service catalog.

If you would like to reach out to GACRC and do not have a UGA MyID, please send an email to gacrc-help@uga.edu, and we will respond promptly.

Categories (3)

**Services For Users**
- General user support, request software installation or update, request training.

**Services for PIs**
- For PIs only: Lab registration, user account creation/modification, class account requests, storage quota modifications.

**For GACRC Staff**
- For GACRC’s internal use only.
GACRC TEACHING CLUSTER NEW USER TRAINING WORKSHOP

Click to request