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](http://wiki.gacrc.uga.edu)
Support: [https://wiki.gacrc.uga.edu/wiki/Getting_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help)
Web Site: [http://gacrc.uga.edu](http://gacrc.uga.edu)
Kaltura Channel: [https://kaltura.uga.edu/channel/GACRC/176125031](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. /work/phys4601/MyID: data storing space for individual user in a class
  3. /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/3.8.2-GCCcore-8.3.0`
  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:
   \[\text{ssh MyID@teach.gacrc.uga.edu}\]
2. Change directory to your scratch space: \[\text{cd /scratch/MyID}\]
3. Create a working subdirectory for a job: \[\text{mkdir workDir}\]
4. Change directory to workDir: \[\text{cd workDir}\]
5. Transfer data from local computer to workDir: use \text{scp} or WinSCP to connect Transfer node
   Transfer data on cluster to workDir: log on to Transfer node and then use \text{cp} or \text{mv}
6. Compile Fortran code \textit{mult.f} into a binary code
7. Make a job submission script in workDir: \[\text{nano sub.sh}\]
8. Submit a job from workDir: \[\text{sbatch sub.sh}\]
9. Check job status: \text{squeue --me} or Cancel a job: \text{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.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 ~$

4. Logged on!

5. Verify login using Duo
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:

- UGA MyID password
- Select DUO option
- Logged on!
Step2 - 4: cd to /scratch dir, make and cd into workDir

```
zhuofei@teach-sub1 ~$ cd /scratch/zhuofei
zhuofei@teach-sub1 zhuofei$ mkdir workDir
zhuofei@teach-sub1 zhuofei$ cd workDir/
zhuofei@teach-sub1 workDir$ ls
zhuofei@teach-sub1 workDir$
```

👉 cd command to change directory
👉 mkdir command to create a subdirectory
👉 cd command to change directory
👉 ls command to list contents of directory
👉 it is empty in workDir!
Step 5: 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/ .
```
Step 5 (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

Step5 (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@tcn26 workDir$ cp /usr/local/training/phys4601/mult.f .
zhuofei@tcn26 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@tcn26 workDir$ module load GCC/8.3.0
zhuofei@tcn26 workDir$ gfortran mult.f -o mult.x
zhuofei@tcn26 workDir$ ls
  mult.f mult.x
zhuofei@tcn26 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/training/phys4601/sub.sh . ➡ Copy sub.sh to your working dir
zhuofei@teach-sub1 workDir$ cat sub.sh ➡ Show contents of sub.sh

```bash
#!/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 $SLURM_SUBMIT_DIR
module load GCC/8.3.0
time ./.mult.x  # run the binary code you compiled in step 5 in this job
zhuofei@teach-sub1 workDir$ nano sub.sh ➡ Use nano modify sub.sh, e.g., email address
```
Step 8: Submit a job from workDir using sbatch

[Link to wiki page on submitting jobs](https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster#How_to_submit_a_job_to_the_batch_queue)

$$\text{sbatch sub.sh}$$

Submitted batch job 12099

**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

<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>12099</td>
<td>fsr4601</td>
<td>test</td>
<td>zhuofei</td>
<td>R</td>
<td>0:05</td>
<td>1</td>
<td>tcn18</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 12099
zhuofei@teach-sub1 workDir$ squeue --me
JOBID PARTITION NAME USER ST TIME NODES Nodelist(REASON)
```

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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
JobID  JobName   User       Partition  NodeList  AllocNodes  NTask  NCPUS  ReqMem  MaxVMSize  State   CPUPTime  Elapsed  Timelimit  ExitCode
-------- -------- --------- --------- -------- --------- ------ ------ ------- ---------- -------- --------- -------- ---------- --------
33561    test     zhuofei  fsr4601  tcn18     1         1          2Gn     COMPLETED 00:00:01 00:00:01 00:01:00  0

$ seff 33561  # Check computing resources used by a COMPLETED job
Job ID: 33561
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: 1.27 MB
Memory Efficiency: 0.06% of 2.00 GB
```
Step9 (Cont.): Check node info using sinfo

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

```
zhuofei@teach-sub1 workDir$ sinfo
PARTITION   AVAIL  TIMELIMIT  NODES  STATE  NODELIST
batch*      up    7-00:00:00   1  down*  tcn17
batch*      up    7-00:00:00  24   idle   tcn[1-16,18-25]
interactive up    7-00:00:00  5   idle   tcn[26-30]
gpu         up    7-00:00:00  1   idle   tcgn1
highmem     up    7-00:00:00  2   idle   tchmn[1-2]
fsr4601     up    1:00      1  down*  tcn17
fsr4601     up    1:00      24   idle   tcn[1-16,18-25]
fsr8602     up    10:00     1  down*  tcn17
fsr8602     up    10:00     24   idle   tcn[1-16,18-25]
```

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` or `sacct-gacrc-v` 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=END,FAIL
```
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)
GACRC Support
https://wiki.gacrc.uga.edu/wiki/Getting_Help

➢ 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!
GACRC Service Catalog

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.

**My Recent Requests**

- Class provision on the teaching cluster - phys8601-dlau
- Class provision on the teaching cluster - bomb8330 - njwoods
- Class provision on the teaching cluster - binf8211 - szhao, im43161
- MATLAB License Request
- Create clder lab group
Click to request