Introduction to GACRC Teaching Cluster

PHYS4601/6601

Georgia Advanced Computing Resource Center (GACRC)
EITS/University of Georgia
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Outline

• GACRC

• Overview

• Computing Resources
  ➢ Three Folders
  ➢ Three Computational Queues
  ➢ Software

• Submit Batch Job

• GACRC Wiki and Support
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://wiki.gacrc.uga.edu](http://wiki.gacrc.uga.edu) (GACRC Wiki)
- [https://wiki.gacrc.uga.edu/wiki/Getting_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (GACRC Support)
- [http://gacrc.uga.edu](http://gacrc.uga.edu) (GACRC Web)
Please note:
You need to connect to the UGA VPN when accessing from outside of the UGA main campus.

1. ssh with MyID and password
2. Verify with Archpass Duo two-factor authentication

- Node: Computer for a specific function on cluster, e.g., login node
- Queue: Collection of compute nodes for specific computing need
- Cluster: Nodes + Drives, all connected by network
Computing Resources

➢ Two Nodes:

1. Login node (MyID@teach.gacrc.uga.edu): for submitting computational jobs
2. Transfer node (MyID@txfer.gacrc.uga.edu): for transferring data files

➢ Three Directories:

1. /home/MyID: working space for computational jobs
2. /work/phys4601/MyID: data parking for individual user in the class
3. /work/phys4601/instructor_data: data shared with class by the instructors

➢ Queue for your class: fsr4601
Computing Resources (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/2.7.14-foss-2016b
  3. Software names are case-sensitive!
    - `module avail`: List all available software modules installed on cluster
    - `module load moduleName`: Load a module into your working environment
    - `module list`: List modules currently loaded
    - `module unload moduleName`: Remove a module from working environment
    - `ml spider pattern`: Search module names matching a pattern (case-insensitive)
Submit 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. Create a working subdirectory for a job: `mkdir ./workDir`

3. Change directory to `workDir`: `cd ./workDir`

4. Transfer data from local computer to `workDir`: use `scp` or `SSH File Transfer` to connect Transfer node
   
   Transfer data on cluster to `workDir`: log on to Transfer node and then use `cp` or `mv`

5. Compile your source codes `phys4601_mult.f` into binary

6. Make a job submission script in `workDir`: `nano ./phys4601_sub.sh`

7. Submit a job from `workDir`: `sbatch ./phys4601_sub.sh`

8. Check job status: `squeue` or Cancel a job: `scancel JobID`
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 **MyID password**

4. Teaching cluster access requires ID 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/](https://eits.uga.edu/access_and_security/infosec/tools/archpass_duo/) on how to enroll

More information: [https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster)
Step 1 (Cont.) - Mac/Linux

Using ssh in Terminal!

```plaintext
ssh zhuofei@teach.gacrc.uga.edu ➝ 1. Log on

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. 5. SMS passcodes to XXX-XXX-5758 (next code starts with: 1)

Passcode or option (1-5): 1 ➝ 3. Select Duo login option 1

Success. Logging you in...

Last login: Fri Aug 3 11:24:43 2018 from 172.22.72.35
[zhuofei@teach ~]$ ➝ 5. Logged on!
```
Step1 (Cont.) - Windows

1. Download and install SSH Secure Utilities: [http://eits.uga.edu/hardware_and_software/software/](http://eits.uga.edu/hardware_and_software/software/)
2. You can use PuTTY as an alternative: [https://www.putty.org/](https://www.putty.org/)
Step1 (Cont.) - Windows using SSH Secure Utilities

Please Note:
Authentication Method needs to be set as Keyboard Interactive in default <profile Setting>
Step 1 (Cont.) - Windows using SSH Secure Utilities

1. Host Name: teach.gacrc.uga.edu
2. User Name: MyID
3. Port Number: 22
4. Enter your UGA MyID password and click OK
Step 1 (Cont.) - Windows using SSH Secure Utilities

9. Enter “push” and click OK

10. Verify login using Duo
Step1 (Cont.) - Windows using SSH Secure Utilities

11. Click OK

12. Logged on!
Step 2 - 3: Create and change directory to `workDir`

```bash
[zhuofei@teach ~]$ ls
[zhuofei@teach ~]$ mkdir workDir
[zhuofei@teach ~]$ ls
workDir
[zhuofei@teach ~]$ cd workDir/
[zhuofei@teach workDir]$ ls
[zhuofei@teach workDir]$ ls
```

- `ls` command to list folder’s contents
- `mkdir` command to create a subdirectory
- `cd` command to change directory
- It is empty in `workDir!`
Step 4: Transfer data from local computer to workDir - Mac/Linux

1. Connect to Transfer node (MyID@txfer.gacrc.uga.edu) in Terminal on local computer
2. Type scp command: scp (-r) [Source] [Target]
3. Once you input MyID password, scp command will send “push” to your Duo Enrolled mobile device for verification

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

```bash
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

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

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster.28txfer.gacrc.uga.edu.29
Step 4 (Cont.) - Windows using SSH Secure Utilities

Please Note:
Authentication Method needs to be set as
Keyboard Interactive in default <profile Setting>
Step 4 (Cont.) - Windows using SSH Secure Utilities

1. Connect to Remote Host
2. Choose the Host Name: txfer.gacrc.uga.edu
3. Enter the User Name: MyID
4. Enter the Port Number: 22
5. Click on Connect

6. Enter your UGA MyID password and click OK

Steps 9 - 11 are the same as listed on page 13 - 14!
Step 4 (Cont.) - Windows using SSH Secure Utilities

12. Logged on!

13. Click yellow button

14. Change local and remote paths
Step 4 (Cont.) - Windows using SSH Secure Utilities

15. Drag data between local computer and remote cluster
Step 4 (Cont.): Transfer data on cluster to workDir

• Log on to Transfer node (MyID@txfer.gacrc.uga.edu)
  ✓ Mac/Linux: ssh MyID@txfer.gacrc.uga.edu (page 8-9)
  ✓ Windows: use SSH Secure Client app (page 14-16)

• Directories you can access on txfer:
  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 5: Compile your Fortran program `phys4601_mult.f` into binary

```fortran
[zhufei@teach ~]$ cat phys4601_mult.f
Program mult
C Multiples 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

[zhufei@teach ~]$ module load PGI/17.9
[zhufei@teach ~]$ pgf77 phys4601_mult.f -o phys4601_mult.x
[zhufei@teach ~]$ ./phys4601_mult.x
```

Note:
`phys4601_mult.f` is put in `/usr/local/training/phys`
You can copy it into your working directory for use
Step 6: Make a job submission script `phys4601_sub.sh`

```
#!/bin/bash
#SBATCH --job-name=testJob
#SBATCH --partition=fsr4601
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=2gb
#SBATCH --time=00:01:00
#SBATCH --output=log.%j
#SBATCH --mail-user=MyID@uga.edu
#SBATCH --mail-type=END,FAIL

cd $SLURM_SUBMIT_DIR

time ./phys4601_mult.x # run binary compiled in step 5
```

Note:
phys4601_sub.sh is put in /usr/local/training/phys
You can copy it into your working directory for use

More Information: [https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster)
Step7: Submit a job from workDir using sbatch

$ sbatch phys4601_sub.sh
Submitted batch job 139

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

1. specifying computing resources
2. loading software using `module load`
3. running any Linux commands you want to run
4. running your compiled binary
### Step 8: Check job status using `squeue`

```
$ squeue -l
Wed Aug  8 13:40:02 2018
JOBID PARTITION   NAME      USER     STATE    TIME   TIME_LIMIT NODES NODELIST
162  fsr4601   testJob   zhuofei   PENDING  0:00    00:01:00  1  (None)
160  fsr4601   testJob   zhuofei   RUNNING  0:02    00:01:00  1  c2-11
161  fsr4601   testJob   zhuofei   RUNNING  0:02    00:01:00  1  c2-11

$ squeue
JOBID PARTITION   NAME      USER  ST  TIME NODES NODELIST
162  fsr4601   testJob   zhuofei   PD  0:15  1  (None)
160  fsr4601   testJob   zhuofei   R   0:17  1  c2-11
161  fsr4601   testJob   zhuofei   R   0:17  1  c2-11
```

Common STATE: R for Running; PD for Pending; TO for TimedOut; S for Suspended; F for FAILED
TIME: the elapsed time used by the job, not remaining time, not CPU time.
Step8 (Cont.): Cancel job using `scancel`

```
$ squeue -l
Wed Aug  8 14:03:47 2018
JOBID PARTITION   NAME       USER    STATE     TIME   TIME_LIMI   NODES NODELIST
169 fsr4601 testJob  zhuofei  RUNNING  0:07   00:01:00   1 c1-38
168 fsr4601 testJob  zhuofei  RUNNING  0:10   00:01:00   1 c1-39

$ scancel 169

[zhuofei@teach workDir]$ squeue -l
Wed Aug  8 14:03:47 2018
JOBID PARTITION   NAME       USER    STATE     TIME   TIME_LIMI   NODES NODELIST
169 fsr4601 testJob  zhuofei  COMPLETE  0:15   00:01:00   1 c1-39
168 fsr4601 testJob  zhuofei  RUNNING  0:18   00:01:00   1 c1-38

$ squeue -l
Wed Aug  8 14:04:08 2018
JOBID PARTITION   NAME       USER    STATE     TIME   TIME_LIMI   NODES NODELIST
168 fsr4601 testJob  zhuofei  RUNNING  0:35   00:01:00   1 c1-38
```
Step8 (Cont.): Check job details using scontrol show job

$ scontrol show job 174

JobId=174  JobName=testJob
  UserId=zhuofei(1772)  GroupId=gacrc-instruction(21004)  MCS_label=N/A
  JobState=RUNNING  Reason=None  Dependency=(null)
  Requeue=1  Restarts=0  BatchFlag=1  Reboot=0  ExitCode=0:0
  RunTime=00:00:28  TimeLimit=00:01:00  TimeMin=N/A
  SubmitTime=2018-08-08T14:28:44  EligibleTime=2018-08-08T14:28:44
  StartTime=2018-08-08T14:28:44  EndTime=2018-08-08T16:28:44  Deadline=N/A
  ...
  Partition=fsr4601  AllocNode:Sid=teach:30986
  NodeList=c1-38
  NumNodes=1  NumCPUs=1  NumTasks=1  CPUs/Task=1  ReqB:S:C:T=0:0:*:*:
  ...
  Command=/home/zhuofei/workDir/sub.sh
  WorkDir=/home/zhuofei/workDir
  StdErr=/home/zhuofei/workDir/log.174
  StdOut=/home/zhuofei/workDir/log.174
Step8 (Cont.): Check node info using sinfo

```
$ sinfo

<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>highmem</td>
<td>up</td>
<td>7-00:00:00</td>
<td>5</td>
<td>idle</td>
<td>c1-[36-37,40],c2-[9-10]</td>
</tr>
<tr>
<td>gpu</td>
<td>up</td>
<td>1-00:00:00</td>
<td>1</td>
<td>down*</td>
<td>c2-2</td>
</tr>
<tr>
<td>interq</td>
<td>up</td>
<td>1-00:00:00</td>
<td>3</td>
<td>idle</td>
<td>c2-[4-6]</td>
</tr>
<tr>
<td>batch</td>
<td>up</td>
<td>7-00:00:00</td>
<td>39</td>
<td>idle</td>
<td>c1-[1-35,38-39],c2-[11-12]</td>
</tr>
<tr>
<td>fsr8602</td>
<td>up</td>
<td>10:00</td>
<td>39</td>
<td>idle</td>
<td>c1-[1-35,38-39],c2-[11-12]</td>
</tr>
<tr>
<td>fsr4601</td>
<td>up</td>
<td>1:00</td>
<td>39</td>
<td>idle</td>
<td>c1-[1-35,38-39],c2-[11-12]</td>
</tr>
</tbody>
</table>
```

idle = no cores in use; mix = some cores are still free; alloc = all cores are allocated
GACRC Wiki [http://wiki.gacrc.uga.edu](http://wiki.gacrc.uga.edu)

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)

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

Transfer File:

[https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster](https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster)

Linux Command: [https://wiki.gacrc.uga.edu/wiki/Command_List](https://wiki.gacrc.uga.edu/wiki/Command_List)

Training: [https://wiki.gacrc.uga.edu/wiki/Training](https://wiki.gacrc.uga.edu/wiki/Training)
GACRC Support
https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalog?CategoryID=11593

➢ **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

Please note to make sure the correctness of datasets being used by your jobs!
GACRC Service Catalog

Services (11)

Account Creation
For a research group's PI to request user accounts for group members on the GACRC computing systems.

Class Account Creation
For an instructor to request user accounts for students attending a course that will need to use GACRC computing systems.

Class Account Modification
For instructors to request changes to be made in previously requested class account.

Computing Lab Modification/Deletion

General Internal

General Support
Report issues and request help with GACRC systems, except for software installation requests and account/lab creation requests.

Lab Creation
For a research group's PI to register a computing lab on the GACRC computing systems

Modify/Delete Account
For PIs to request changes in or deletion of user accounts on GACRC computing systems.

Software Installation/Update
Request software and common application database (e.g. NCBI blast databases) installation and upgrade.
Click to request
General Support - Mozilla Firefox

UNIVERSITY OF GEORGIA

General Support

Report issues and request help with GACRC systems, except for software installation requests and account/fac creation requests.

Short Description *

Email *

MyID *

Phone Number *

Support Needed For

- [ ] Daliewy
- [ ] شمال
- [ ] Teaching Cluster
- [ ] Work Filesystem
- [ ] Home Filesystem
- [ ] Scratch Filesystem
- [ ] Project Filesystem
- [ ] We Nodes
- [ ] Other

Lab *

1/10/2019
Thank You!