

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: <u>http://gacrc.uga.edu</u>

Kaltura Channel: <u>https://kaltura.uga.edu/channel/GACRC/176125031</u>

Teaching Cluster



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 your 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 module names matching a pattern (case-insensitive)
 - > module load moduleName: Load a module into your working environment
 - module avail : List all available software modules installed on cluster
 - > module list:List modules currently loaded
 - > module unload moduleName : Remove a module from working environment

Submit a Computational Batch Job

- 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 <u>workDir</u> : cd ./workDir
- 4. Transfer data from local computer to <u>workDir</u> : use scp or WinSCP to connect Transfer node Transfer data on cluster to <u>workDir</u> : log on to Transfer node and then use cp or mv
- 5. Compile Fortran code *mult.f* into a binary code
- 6. Make a job submission script in <u>workDir</u> : nano ./sub.sh
- 7. Submit a job from <u>workDir</u> : sbatch ./sub.sh
- 8. Check job status : squeue --me (-l) or Cancel a job : scancel JobID

Step1: Log on to Login node

https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster

- Teaching cluster access requires verification using two-factor authentication with Archpass Duo. If you are not enrolled in Archpass Duo, please refer to <u>https://eits.uga.edu/access and security/infosec/tools/archpass duo/</u> 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/



Step1: 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: 4 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 4 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: <u>https://www.putty.org/</u>
- 2. Detailed downloading and installation instructions:

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

Step1 (Cont.) - Windows using PuTTY



Step1 (Cont.) - Windows using PuTTY

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Next you will enter your UGA MyID password and initiate DUO authentication procedure:

P zhuofei@teach-sub1:~	
Jusing username "zhuofei".	
Keyboard-interactive authentication prompts from server:	
Password: 🗧 UGA MvID password	
Duo two-factor login for zhuofei	
Enter a passcode or select one of the following options:	
I = 1, Duo Bush to XXX-XXX-5758	
2. Phone call to XXX-XXX-5758	
3. Phone call to XXX-XXX-1925	
4. Phone call to XXX-XXX-3535	
5. SMS passcodes to XXX-XXX-5758	
Find of keyboard-interactive prompts from server	
Success. Logging you in	
Last login: Thu Jan 7 10:20:01 2021 from 128.192.240.123	
zhuofei@teach-sub1 ~\$ 🗧 🗲 Logged on!	
	~



Step2 - 3: Create and change directory to workDir

Step4: 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 \rightarrow 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 \rightarrow Local

scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .

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

Step4 (Cont.) - Windows using WinSCP https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

- 1. You need to connect to cluster's <u>Transfer node</u> (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
- 3. Alternative FileZilla <u>https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_FileZilla_2</u>

Step4 (Cont.) - Windows using WinSCP

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https://wiki.gacrc.uga.edu/wiki/Transferring Files#Using WinSCP 2



Step4 (Cont.) - Windows using WinSCP

💑 zhuofei@xfer.gacrc.uga.edu - WinSCP										
Local Mark Files Comma	ands Sessio	n Options Remote I	Help							
া 🕀 😰 🦆 Synchronize 📄 🖓 🕼 🎲 Queue 🔹 Transfer Settings Default 🔹 🎲										
📮 zhuofei@xfer.gacrc.uga.edu 🗙 🚅 New Session										
$1 My \text{ documents} \forall \stackrel{\text{def}}{=} \forall \nabla \forall $										
Upload - 📝 Edit - 🗶 🎜 🕞 Properties 🎒 New - 🗽 🗖 🔽										
Name	Siza	Type	Changed Name Size Changed Bights Owner							
	3126	Darent director:	Saniar manufer and a set of the s							
Custom Office Terrol		File folder								
		File folder	UGA DUO authentication is required for SSH/SCP access to							
from Vecheng		File folder	GAURE Systems.							
GACRC Class Training		File folder	UGA DUO is a two-factor authentication service which							
GACRC Event Registr		File folder	or device (second factor) to successfully authenticate.							
GACRC Group Training		File folder	If you are not enrolled in the LIGA DLIO service please							
GACRC Migrating fro		File folder	visit the UGA DUO service self-service portal to enroll							
GACRC New Group a		File folder	and configure or manage your DUO enabled devices.							
🌗 GACRC Sapelo		File folder	https://eits.uga.edu/access_and_security/infosec/tools/duo/portal/							
GACRC Sapelo_correc		File folder	For additional help with UGA DUO authentication or to							
GACRC Sapelo2		File folder	report an issue please visit:							
GACRC Storage		File folder	https://eits.uga.edu/access_and_security/infosec/tools/archpass/							
GACRC teaching		File folder	Due two factor logis for abustoi							
GACRC zcluster		File folder								
GACRC zcluster-Sapel		File folder	Enter a passcode or select one of the following options:							
GACRC_accounts_GD		File folder	1. Duo Push to XXX-XXX-5758							
Linux Basics		File folder	2. Phone call to XXX-XXX-5758 3. Phone call to XXX-XXX-1025							
My Shapes		File folder	4. Phone call to XXX-XXX-3535							
Peri Language Basics		File folder	5. SMS passcodes to XXX-XXX-5758							
Python Language Bas Python on GACPC		File folder	Passcode or option (1-5):							
Python on GACRC File folder										
0 B of 4.31 MB in 0 of 45										
Not connected.			the second se							

Step4 (Cont.) - Windows using WinSCP





Step4 (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

Step5: Compile Fortran code *mult.f* into a binary



zhuofei@teach-sub1 workDir\$ qlogin 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 i=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 moduleCompile source code into a binary



Step6: 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 #!/bin/bash **#SBATCH** --job-name=test # Job name **#SBATCH** --partition=fsr4601 # Submit job to fsr4601, which is PHYS4601/6601 partition **#SBATCH** --ntasks=1 # Single task job # Number of cores per task **#SBATCH** --cpus-per-task=1 #SBATCH --mem=2gb # Total memory for job #SBATCH --time=00:01:00 # Time limit hrs:min:sec; fsr4601 TIMELIMIT 1 min # Standard output and error log #SBATCH --output=log.%j #SBATCH -- mail-user=MyID@uga.edu # Where to send mail # Mail events (BEGIN, END, FAIL, ALL) **#SBATCH** --mail-type=ALL cd \$SLURM_SUBMIT_DIR module load GCC/8.3.0 # run the binary code you compiled in step 5 in this job time ./mult.x zhuofei@teach-sub1 workDir\$ nano sub.sh ← Use nano to make modifications to sub.sh, e.g., email address



Step7: 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 12099

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 binary code



Step7: Check job status using squeue

https://wiki.gacrc.uga.edu/wiki/Monitoring Jobs on the teaching cluster

zhuofei@teach-subl workDir\$ <mark>squeueme</mark>											
JOBID	PARTITION	NAME	USER S	Т	TIME	NODES	NODE	LIST(R	REASON)		
12099	fsr4601	test	zhuofei	R	0:05		1 tcn	18			
zhuofei@teach-sub1 workDir\$ <mark>squeueme -1</mark>											
Mon Ja	n 11 12:03:14	2021									
JOBID	PARTITION	NAME	USER	STATE		TIME	TIME_	LIMI	NODES	NODELIST (REASON)
12099	fsr4601	test :	zhuofei	RUNNING		0:11		1:00	1	tcn18	

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

Step7 (Cont.): Check job details using scontrol show job

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

```
zhuofei@teach-sub1 workDir$ scontrol show job 12099
JobId=12099 JobName=test
   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=00:00:23 TimeLimit=00:01:00 TimeMin=N/A
   .....
   Partition=fsr4601 AllocNode:Sid=10.31.32.252:92156
   NodeList=tcn18
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 RegB:S:C:T=0:0:*:*
   MinCPUsNode=1 MinMemoryNode=2G MinTmpDiskNode=0
   Command=/home/zhuofei/workDir/sub.sh
   WorkDir=/home/zhuofei/workDir
   StdErr=/home/zhuofei/workDir/log.12099
   StdOut=/home/zhuofei/workDir/log.12099
   MailUser=zhuofei@uga.edu MailType=BEGIN, END, FAIL, REQUEUE, STAGE OUT
```



Step7 (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)



Step7 (Cont.): Check node info using sinfo

https://wiki.gacrc.uga.edu/wiki/Monitoring Jobs on the teaching cluster

zhuofei@teach-sub1 workDir\$ <mark>sinfo</mark>								
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 Sapelo2#How to check resource utilization of a running or finished job

Option 1: scontrol show job JobID for details of a running or pending jobs

Option 2: seff for details of computing resource usage of a <u>finished</u> job

Option 3: sacct-gacrc or sacct-gacrc-v for details of computing resource usage of

a <u>running or finished</u> job

Option 4: Email notification from finished jobs (completed, canceled, or crashed), if using:

#SBATCH --mail-user=username@uga.edu

#SBATCH --mail-type=END, FAIL



GACRC Wiki <u>http://wiki.gacrc.uga.edu</u> Kaltura Channel <u>https://kaltura.uga.edu/channel/GACRC/176125031</u>

Connecting: <u>https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting to the teaching cluster</u>

Running Jobs: <u>https://wiki.gacrc.uga.edu/wiki/Running Jobs on the teaching cluster</u>

Monitoring Jobs: <u>https://wiki.gacrc.uga.edu/wiki/Monitoring Jobs on the teaching cluster</u> Transfer File:

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

Linux Command: 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

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.

My Recent Requests

home directory is not fully provisioned: ss57215

GACRC Sapelo2 New Lab/Use Account Request 2018-11-14_preTraining

GACRC Sapelo2 Cluster New Lab/Use Account Request 2018-11-05_preTraining

provision 5 user accounts for ugahelpdesk group

GACRC Sapelo2 New Lab/Use Account Request 2018-10-22_preTraining

View All Recent Requests >

Popular Services

EITS Help Desk Support Request

MyID Account Request

Change Request

02 Restricted VPN Access

Terry Classroom & Meeting Room Support

View All Popular Services >

My Recently Visited Services

Modify/Delete Account

Class Account Creation



Privacy | Accessibility | Website Feedback

https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalogSearch



Thank You!

Telephone Support

EITS Help Desk: 706-542-3106

Monday – Thursday: 7:30 a.m. – 7:30 p.m.

Friday: 7:30 a.m. – 6 p.m.

Saturday – Sunday: 1 p.m. – 7 p.m.

Georgia Advanced Computing Resource Center

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