

Introduction to GACRC Teaching Cluster

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 (GACRC Wiki)
- https://wiki.gacrc.uga.edu/wiki/Getting_Help (GACRC Support)
- http://gacrc.uga.edu (GACRC Web)





Teaching Cluster

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/CourseID/MyID: data parking for individual user in the class (e.g., GENE4220)
 - 3. /work/CourseID/instructor_data: data shared with class by the instructors
- > Three Queues:
 - 1. batch: for running regular computational jobs
 - 2. highmem: for running high-memory jobs
 - 3. gpu: for running GPU jobs



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 <u>workDir</u> : use scp or SSH File Transfer to connect Transfer node Transfer data on cluster to <u>workDir</u> : log on to Transfer node and then use cp or mv
- 5. Make a job submission script in workDir : nano ./sub.sh
- 6. Submit a job from workDir: sbatch ./sub.sh
- 7. Check job status : squeue or Cancel a job : scancel JobID

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 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/ on how to enroll

More information: <u>https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_the_teaching_cluster</u>



ssh zhuofei@teach.gacrc.uga.edu 🛛 🗲 Log on

Step1 (Cont.) - Mac/Linux

Use Terminal utility on Mac or Linux!



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/infosec/tools/archpass/

Password: <- Input MyID password!

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. Phone call to XXX-XXX-3535

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

Passcode or option (1-5): 1 ← Select Duo login option!
Success. Logging you in...
Last login: Fri Aug 3 11:24:43 2018 from 172.22.72.35
[zhuofei@teach ~]\$ ← I am teaching cluster login node

Step1 (Cont.) - Windows

- 1. Download and install SSH Secure Utilities: <u>http://eits.uga.edu/hardware_and_software/software/</u>
- 2. You can use PuTTY as an alternative: <u>https://www.putty.org/</u>

Software Hardw	are and Software EITS – Mozilla Firefox	×	Download PUTTY - a free SSH and tainet client for Windows - Mozilla Firefox *			
<u>File Edit View History Bookmarks Tools Help</u>			<u>File Edit View History Bookmarks Tools Help</u>			
Running Jobs on Sapelo2 × 🖉 Software Hardware × 🔶			Running Jobs on Sapelo2 × Download PuTTY - a free ×	+		
(€) ▲ https://eits.uga.edu/hardware_and_software/software/	✓ C Q Search	☆ 自 ♥ ♣ 合 ♥ ☰	(https://www.putty.org			
QMF for Workstation						
Query and reporting tool set for IBM's DB2 relational data reports by providing a graphical user interface and deskto	pase management system. Facilitates the development printing capabilities.	of queries and	Anno Francesco Relation Anno Francesco Relation Anno Sector Relation Anno Sector Relation Anno Relation	Download PuTTY		
• Respondus 🔒			Distance Dis	PuTTY is an SSH and telnet client, developed originally by Simon Tatham for the Windows platform. PuTTY is open source software that is available with source code and is developed and supported by a group of		
A powerful tool for creating and managing exams that can	be printed to paper or published directly to eLearning	Commons.	Anne Anne Anne Anne Anne Anne Anne Anne	volunteers.		
SecureFTP			ans and and	You can download Pull I Y <u>nere</u> .		
A secure file transfer application that allows you to upload	/download files with a remote server. Compatible with	MyWeb/MyDrive.				
• SSH (Secure Shell Utilities for Windows)			Below suggestions a	re independent of the authors of PuTTY. They are not to be seen as endorsements by the PuTTY project.		
Software that allows you to connect securely to computers	on the internet. Supports secure file transfers.					
Turning Technologies				Bitvise SSH Client		
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• UGA Alert Desktop 🔒			Wer Mark Mark No. 10 Hard Ma	well as the following:		
This program will post a UGA Alert message at the bottom Alert.	of your computer screen when an emergency message	is issued by UGA		graphical SFTP file transfer; single-click Remote Desktop tunneling; auto-reconnecting capability; dwamic part forwarding through an integrated prove;		
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Host Name: teach.gacrc.uga.edu User Name: MyID Port Number: 22	8. Enter your UGA MyID password and click O	K
Not connected - press Enter or Space to connect 70x24	Connecting to teach.gacrc.uga.edu 70x24 🗱	- /



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9. Enter "push" and click OK	Approve Deny
Connecting to teach.gacrc.uga.edu 70x24	10. Verify login using Du



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	-	There was 1 failed login attempt since the last successful logi Last login: Sat Aug 18 16:21:12 2018 from 172.18.86.82 [zhuofei@teach ~]\$ 12. Logged on!	in.
Connecting to teach.gacrc.uga.edu 70x24		Connected to teach.gacrc.uga.edu SSH2 - aes128-cbc - hmac-sha1 - nr 70x24	

Step2 - 3: Create and change directory to workDir

```
[zhuofei@teach ~]$ ls< Is command to list folder's contents</td>[zhuofei@teach ~]$ mkdir workDir< mkdir command to create a subdirectory</td>[zhuofei@teach ~]$ lsworkDir[zhuofei@teach ~]$ cd workDir/[zhuofei@teach workDir]$ ls[zhuofei@teach workDir]$
```

Step4: 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 \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/ .

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster_.28txfer.gacrc.uga.edu.29







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4 SSH Secure Shell 3 Copyright (c) 2000 y Corp - http://ww This copy of SSH s version. This version does ctionality. Host Name: txfer.gacrc.uga.edu User Name: txfer.gacrc.uga.edu User Name: MyID Port Number: 22 Authentication Method: http://www.selfar.gacrc.uga.edu Port Number: 22 Authentication Method: http://www.selfar.gacrc.uga.edu Connect Connect Connect Connect Connect User Name: 22 Authentication Method: https://www.selfar.gacrc.uga.edu Connect Connect	SSH Secure Shell 3. Copyright (c) 2000- y Corp - http://www This copy of SSH Secure This version. This version does r ctionality. 8. Enter your UGA MyID password and click OK Steps 9 - 11 are the same as listed on page 13 - 14!
Not connected - press Enter or Space to connect 70x24	Connecting to teach.gacrc.uga.edu 70x24

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		© Recycle Bin System F., workDr emplate Folder 08/09/	2018
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12. Logged on!			
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Step4 (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/CourseID/MyID
 - 3. /work/CourseID/instructor_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

mv /work/gene4220/MyID/datafile /home/MyID/workDir

Step5: Make a job submission script in workDir using nano

\$ nano sub.sh	File Edit View Search Terminal GNU nano 2.0.9 hello nano! I am Zh	Heb Nuofei!	zhu File: sub.s	ofei@n124:/lustre1/zhuofei/workDir Sh		× Modified
nano is a small and friendly text editor on Linux.						
Ctrl-x to save file and quit from nano	AG Get Help AX Exit	∧O WriteOut ∧J Justify	<mark>^R</mark> Read File ^₩ Where Is	[New File] ^Y Prev Page ^V Next Page	<mark>∧K</mark> Cut Text ∧U UnCut Text	AC Cur Pos AI To Spell

Step5 (Cont).

• In /home/MyID/gene4220: Following files are available for all students

[pakala@teach gene4220]\$ ls ens ens.def ens.f ens.i01 ens.i02 ens.i12 ens.notes ens.notes~ ens.o00 ens.o01 ens.o02 ens.o04 ens.sh Makefile

- Compile source code before submitting the job:
 - gfortran compiler from GCC/4.4.7 to compile FORTRAN source code

[pakala@teach gene4220]\$ module load GCC/4.4.7

[pakala@teach gene4220]\$ ml

Currently Loaded Modules:

1) StdEnv 2) GMP/4.3.2 3) MPFR/2.4.2 4) GCC/4.4.7

[pakala@teach gene4220]\$ make ens

```
gfortran ens.f -o ens
```

Step5: Job Submission Script

#!/bin/bash

#SBATCH --job-name=ens_job #
#SBATCH --partition=batch #
#SBATCH --ntasks=1 #
#SBATCH --mem=4gb #
#SBATCH --time=168:00:00 #⁻

#SBATCH --output=log.%j.out

#SBATCH --error=log.%j.err

Job name
Partition (queue) name
Run on a single CPU
Job memory request
Time limit hrs:min:sec
Standard output log
Standard error log

cd \$SLURM_SUBMIT_DIR time ./ens

More Information: https://wiki.gacrc.uga.edu/wiki/Running Jobs on the teaching cluster



Step6: Submit a job from workDir using sbatch

[pakala@teach gene4220]\$ sbatch ens.sh
Submitted batch job 878

Tips: ens.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 the blast commands

Step7: Check job status using squeue

[pakal Thu Se	[pakala@teach gene4220]\$ squeue -1 Thu Sep 20 13:53:24 2018							
JOBID	PARTITIO	ON NAME	USER	STATE	TIME	TIME LIMI	NODES	NODELIST (REASON)
878	batch	ens_job	pakala	RUNNING	0:17	7-00:00:00	1	c1-38
[pakal	[pakala@teach gene4220]\$ squeue							
JOBID 878	PARTITION batch	NAME ens_job	USER <mark>ST</mark> pakala R	TIME 1 1:00	NODES NODI 1 c1-3	ELIST (REASON 38)	

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.

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

```
$ scontrol show job 878
   JobId=878 JobName=ens job
   UserId=pakala(1941) 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=00:06:01 TimeLimit=7-00:00:00 TimeMin=N/A
   SubmitTime=2018-09-20T13:53:07 EligibleTime=2018-09-20T13:53:07
   StartTime=2018-09-20T13:53:07 EndTime=2018-09-27T13:53:07 Deadline=N/A
   .....
   Partition=batch AllocNode:Sid=teach:15666
   NodeList=c1-38
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   • • •
   Command=/home/pakala/gene4220/ens.sh
   WorkDir=/home/pakala/gene4220
   StdErr=/home/pakala/gene4220/log.878.err
   StdOut=/home/pakala/gene4220/log.878.out
```

Step7 (Cont.): Cancel job using scancel

[pakala@teach gene4220]\$ squeue -1 Thu Sep 20 14:09:12 2018							
JOBID PARTITION 878 batch	NAME ens_job	USER pakala	STATE RUNNING	TIME 16:05	TIME_LIMI 7-00:00:00	NODES 1	NODELIST (REASON) c1-38
[pakala@teach gene4220]\$ scancel 878							
[pakala@teach gene Thu Sep 20 14:09:5	4220]\$ squ 1 2018	eue -l					
JOBID PARTITION	NAME	USER	STATE	TIME	rime_limi n	ODES NOI	DELIST (REASON)



Step7 (Cont.): Check node info using sinfo

\$ sinfo				
PARTITION	AVAIL	TIMELIMIT	NODES	STATE NODELIST
highmem	up	7-00:00:00	5	idle c1-[36-37,40],c2-[9-10]
gpu	up	1-00:00:00	1	idle c2-2
interq	up	1-00:00:00	3	idle c2-[4-6]
batch	up	7-00:00:00	39	idle c1-[1-35,38-39],c2-[11-12]

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



GACRC Wiki <u>http://wiki.gacrc.uga.edu</u>

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

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 c

luster .28txfer.gacrc.uga.edu.29

Linux Command: <u>https://wiki.gacrc.uga.edu/wiki/Command_List</u>

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

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
- ✓ Job ID
- \checkmark Job submission script and command you used to submit the job
- ✓ Your working directory on cluster
- Software Installation:
 - ✓ Specific name and version of the software
 - ✓ Download website
 - ✓ Supporting package information if have

Please note:

- In general only software widely used by the GACRC computing community will be centrally installed.
- 2. Make sure of the correctness of datasets being used by your jobs!





Request Support

* indicates Required fields.

Your Name *	First & Last
MyID *	myid
E-mail *	you@example.edu
Phone Number	411-555-1212
Brief Description	
Request Details *	(less than 2,000 characters)
Cluster	□ sapelo2 □ sapelo ☑ teach □ other Review

* For questions on cluster or software, please include the command/script used, working path and working nodes (interactive / queue name) if applicable.

* For software installation, please specify software name, version and include link to the software if applicable.

* Please review your message on the next page and then click the Submit button.



Thank You!