

## Introduction to GACRC Teaching Cluster PHYS8601

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

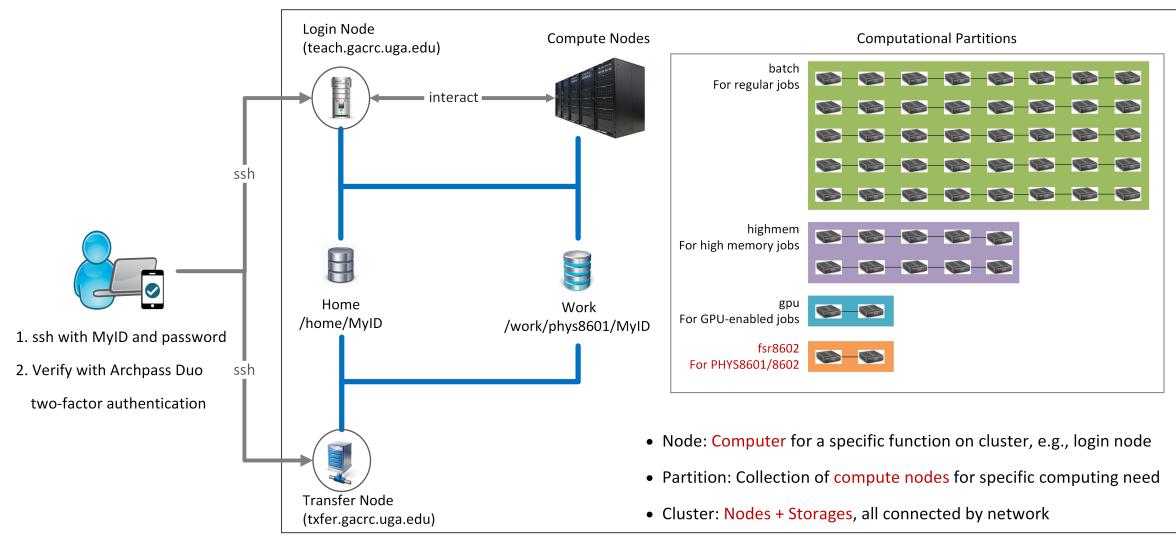
#### Wiki: http://wiki.gacrc.uga.edu

Support: <a href="https://wiki.gacrc.uga.edu/wiki/Getting\_Help">https://wiki.gacrc.uga.edu/wiki/Getting\_Help</a>

Web Site: http://gacrc.uga.edu

Kaltura Channel: <a href="https://kaltura.uga.edu/channel/GACRC/176125031">https://kaltura.uga.edu/channel/GACRC/176125031</a>

#### 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. /scratch/MyID: working space for running computational jobs
  - 3. /work/phys8601/MyID : data storing space for individual user in a class
  - 4. /work/phys8601/instructor\_data : data shared with class by the instructors
- Partitions for PHYS8601/8602 class: fsr8602



## 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

- 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 C code *mult.c* 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

### 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 <a href="https://eits.uga.edu/access">https://eits.uga.edu/access</a> and <a href="https://eits.uga.edu/access">security/infosec/tools/vpn/</a>



### 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...

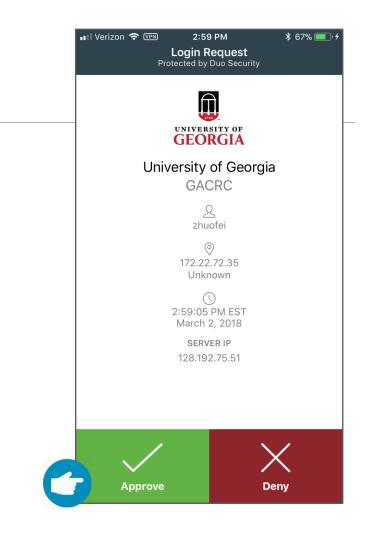
Password: 4 2. Enter your MyID password When you enter password, no stars or dots will show as you are typing. Please type password carefully!

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

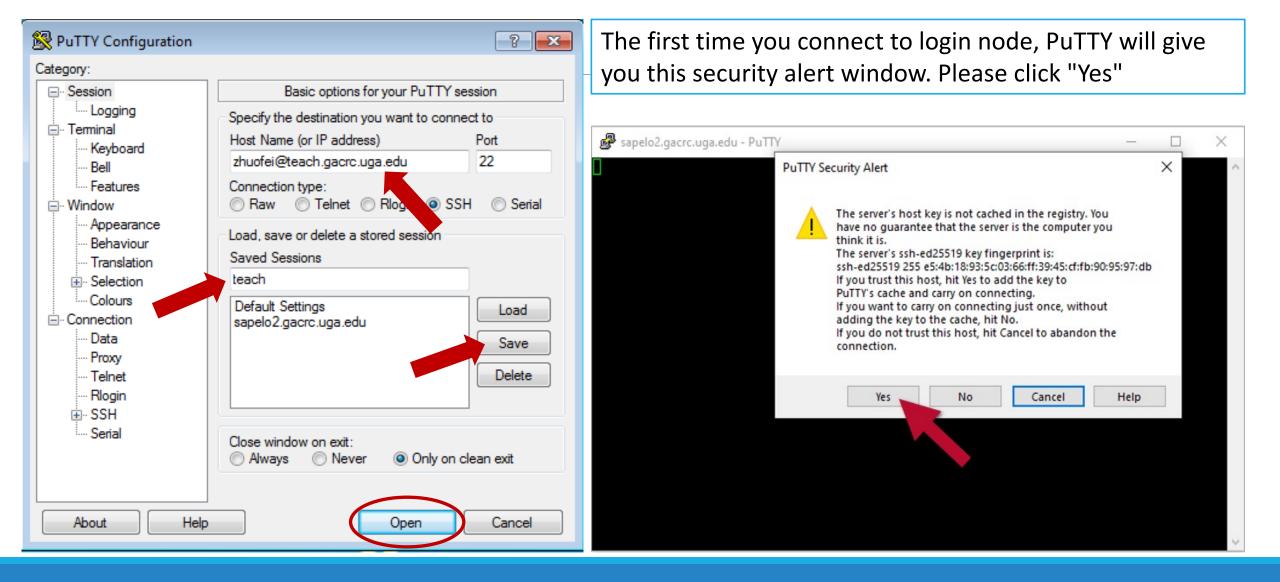
- 1. Download and install PuTTY: <u>https://www.putty.org/</u>
- 2. Detailed downloading and installation instructions:

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:

B zhuofei@teach-sub1:~		
🛃 Using username "zhuofei".	A	
Keyboard-interactive authentication prompts from server:		
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		
Passcode or option (1-5): 1 <- Select DUO option		
End 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 - 4: cd to /scratch dir, make and cd into workDir

# Step5: Transfer data from local computer to workDir - Mac/Linux <a href="https://wiki.gacrc.uga.edu/wiki/Transferring\_Files#Using\_scp\_2">https://wiki.gacrc.uga.edu/wiki/Transferring\_Files#Using\_scp\_2</a>

- 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

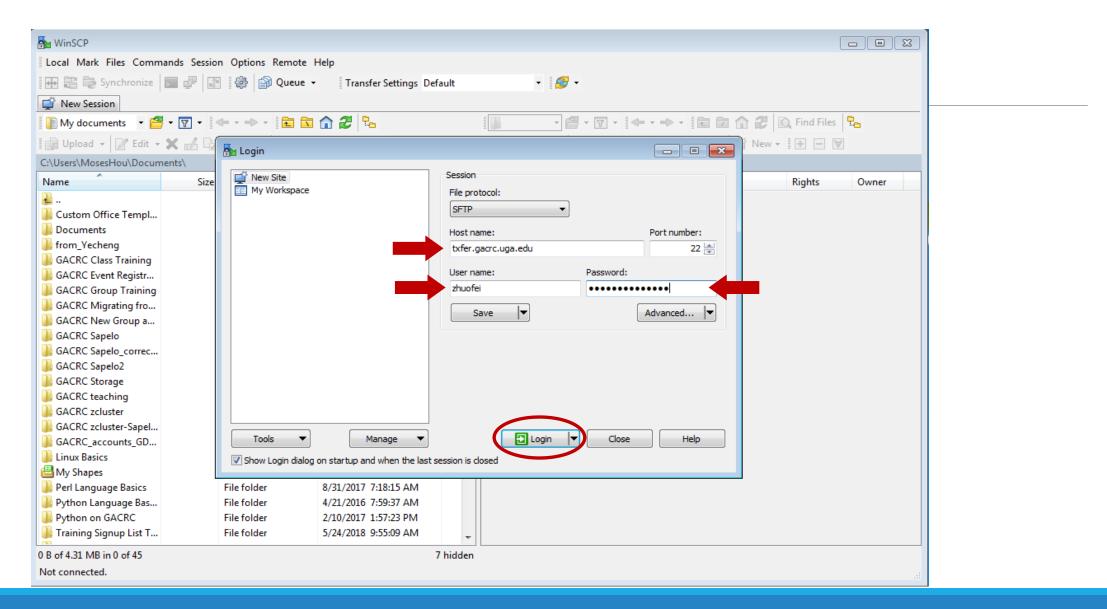
scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .

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

#### Step5 (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 <a href="https://winscp.net/eng/index.php">https://winscp.net/eng/index.php</a>
  - Default installation procedure is simple
- 3. Alternative FileZilla <u>https://wiki.gacrc.uga.edu/wiki/Transferring\_Files#Using\_FileZilla\_2</u>

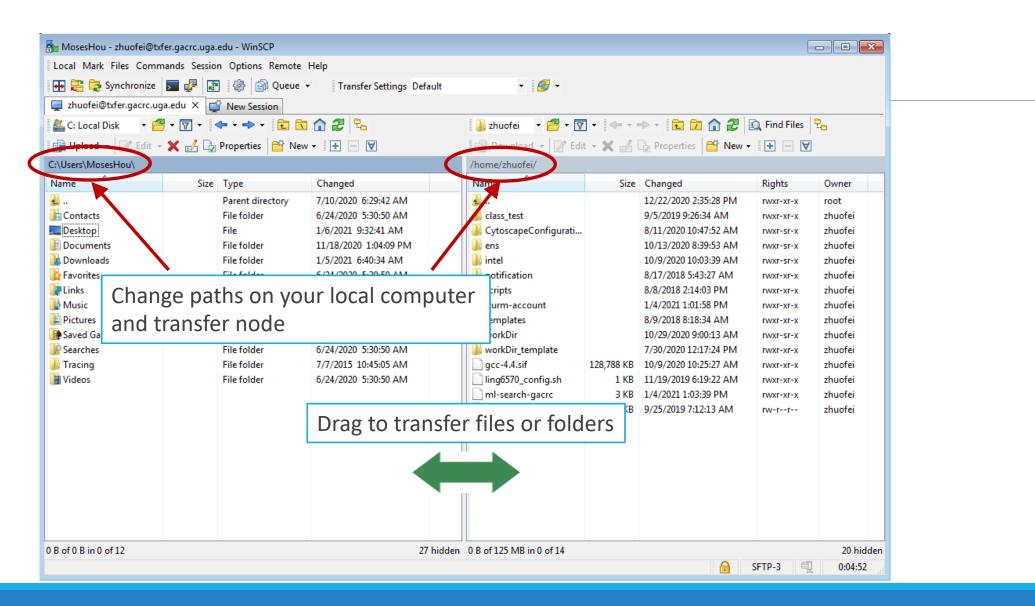
#### Step5 (Cont.) - Windows using WinSCP



#### Step5 (Cont.) - Windows using WinSCP

-											
🚵 zhuofei@xfer.gacrc.uga.eo	du - WinSCP										
Local Mark Files Commands Session Options Remote Help											
🖬 🕀 💱 Synchronize 📰 🧬 😰 🕼 🕼 Queue - 🛛 Transfer Settings Default - 🎉 -											
□ zhuofei@xfer.gacrc.uga.edu × □ New Session											
📗 My documents 🔹 🚰	- 🔽 - 🗇	> - 🔁 🔂	1 2 %		- 2 -	▼ - ◆	• - • • 🖻 🖬 🕻	🕈 🤁 🔯 Find Files	2		
🛙 🙀 Upload 👻 📝 Edit 👻	<b>X</b> - A Ba P	roperties 🏼 🕂 New			📓 Download 👻 📝						
C:\Users\MosesHou\Docume											
Name		T	Changed		Name		ing Channel	Dishts	Owner		
	Size	21	1				ize Changed	Rights	Owner		
<u>и</u>		Parent directory	Server prompt - zhuof	ei@xfer.gacr	rc.uga.edu	×					
Custom Office Templ	-	File folder	UGA DUO authenticatio	n is required f	for SSH/SCP access to						
Documents		File folder	GACRC systems.								
from_Yecheng		File folder File folder	UGA DUO is a two-facto								
GACRC Class Training			requires a password (or or device (second facto								
GACRC Event Registr	-	File folder File folder		or device (second factor) to successfully authenticate.							
GACRC Group Training		File folder File folder	If you are not enrolled in the UGA DUO service please visit the UGA DUO service self-service portal to enroll								
GACRC Migrating fro GACRC New Group a		File folder File folder		and configure or manage your DUO enabled devices.							
GACRC New Group a		File folder File folder	https://eits.uga.edu/ac	https://eits.uga.edu/access_and_security/infosec/tools/duo/portal/							
GACRC Sapelo correc	-	File folder File folder		For additional help with UGA DUQ authentication or to							
GACRC Sapelo_correc		File folder	For additional help with report an issue please v		thentication or to						
GACRC Sapeloz		File folder									
GACRC storage		File folder	https://eits.uga.edu/ac	cess_and_sec	curity/infosec/tools/archpass	/					
GACRC teaching		File folder File folder	Duo two-factor login fo	Duo two-factor login for zhuofei							
GACRC zcluster-Sapel		File folder	Enter a passcode or sel	act one of the	e fellowing options:						
GACRC_accounts_GD		File folder	Enter a passcoue or set	ectone of the	e rollowing options:						
Linux Basics		File folder	1. Duo Push to XXX-XX 2. Phone call to XXX-XX								
My Shapes		File folder	3. Phone call to XXX-XX	X-1925							
Perl Language Basics		File folder		4. Phone call to XXX-XXX-3535 5. SMS passcodes to XXX-XXX-5758							
Python Language Bas		File folder									
Python on GACRC	F	File folder	Passcode or option (1-5	j):							
Iraining Signup List T	F	File folder					Select L	OUO optio	n		
0 B of 4.31 MB in 0 of 45				ОК	Cancel	Help					
Not connected.											

#### Step5 (Cont.) - Windows using WinSCP





#### 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/phys8601/MyID
  - 3. /work/phys8601/instructor\_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

mv /work/phys8601/MyID/datafile /home/MyID/workDir

### Step6: Compile C code *mult.c* into a binary



zhuofei@teach-sub1 workDir\$ interact zhuofei@rb1-11 workDir\$ cp /usr/local/gacrc/training/phys8601/mult.c . zhuofei@rb1-11 workDir\$ cat mult.c /\* Program mult \* Multiple two integer numbers \*/ #include <stdio.h> int main(void) int i=3, j=4, iprod; FILE \*fp; fp = fopen("output.txt","w"); iprod=i\*j; fprintf(fp, "The product of %d and %d is %dn", i,j,iprod); fclose(fp); return 0; zhuofei@rb1-11 workDir\$ module load GCC/11.3.0 zhuofei@rb1-11 workDir\$ gcc mult.c -o mult.x zhuofei@rb1-11 workDir\$ ls mult.c mult.x zhuofei@rb1-11 workDir\$ exit

- ← Start an interactive session
- ← Copy source code to 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

#### Step7: Make a job submission script *sub.sh using nano*



Copy sub.sh to working dir

Show contents of sub.sh

zhuofei@teach-sub1 workDir\$ cp /usr/local/gacrc/training/phys8601/sub.sh . zhuofei@teach-sub1 workDir\$ cat sub.sh #!/bin/bash **#SBATCH** --job-name=test # Job name **#SBATCH** --partition=fsr8602 # Submit job to fsr8602 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=00:10:00 # Time limit hrs:min:sec; fsr8602 TIMELIMIT 10 min #SBATCH --output=log.%j # Standard output and error log #SBATCH --mail-user=MyID@uga.edu # Where to send mail

# Mail events (BEGIN, END, FAIL, ALL)

# run the binary code you compiled in step 5 in this job ← Use nano to modify sub.sh, e.g., email address

time ./mult.x

**#SBATCH** --mail-type=ALL

cd \$SLURM SUBMIT DIR

module load GCC/11.3.0

zhuofei@teach-sub1 workDir\$ nano sub.sh



### Step8: Submit a job from workDir using sbatch

\$ 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



### Step9: Check job status using squeue

https://wiki.gacrc.uga.edu/wiki/Monitoring\_Jobs\_on\_the\_teaching\_cluster

zhuofe	ei@teach-sub1	workDi	r\$ squeue	me					
JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST	(REASON)	
5230	fsr8602	test	zhuofei	R	0:01	1	rb1-3		
zhuofe	ei@teach-sub1	workDi	r\$ <mark>squeue</mark>	me -1					
Mon Ja	n 09 26:03:14	2024							
JOBID	PARTITION	NAME	USER	STATE		TIME TI	IME_LIMI	NODES N	ODELIST (REASON)
5230	fsr8602	test	zhuofei	RUNNING		0:01	1:00	1 r	b1-3

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

JopID	JobName Use	r Partition	NNode NCPUS	ReqMem	CPUTime	Elapsed	Timelimit	State	ExitCode	NodeList
5230	test zhuofe	i fsr8602	1 1	2G	00:00:01	00:00:01	00:01:00	COMPLETED	0:0	rb1-3

#### \$ 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

zhuofei@teach-sub1 workDir\$ <mark>sinfo</mark>										
PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST					
allnodes	up	infinite	1	mix	rb1-11					
allnodes	up	infinite	12	idle	c4-23,rb1-[1-10,12]					
batch	up	7-00:00:00	8	idle	rb1-[3-10]					
gpu	up	7-00:00:00	1	idle	c4-23					
highmem	up	7-00:00:00	2	idle	rb1-[1-2]					
Interactive	up	7-00:00:00	1	mix	rb1-11					
interactive	up	7-00:00:00	1	idle	rb1-12					
fsr4601	up	1:00	8	idle	rb1-[3-10]					
fsr8602	up	10:00	8	idle	rb1-[3-10]					

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\_utilizati on\_of\_a\_running\_or\_finished\_job

Option 1: seff for details of computing resource usage of a <u>finished</u> job

Option 2: sacct-gacrc for details of computing resource usage of a <u>running or finished</u> 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 <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
- Comula Job Coninter
- Sample Job Scripts:
- https://wiki.gacrc.uga.edu/wiki/Sample\_batch\_job\_submission\_scripts\_on\_the\_teaching\_cluster
- Linux Command: <a href="https://wiki.gacrc.uga.edu/wiki/Command\_List">https://wiki.gacrc.uga.edu/wiki/Command\_List</a>

#### 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!



Home IT Help Desks Projects/Workspaces Services Knowledge Base

Project Requests Ticket Requests My Favorites My Recent My Approvals Services A-Z Search

Service Catalog / Academics, Learning & Research / GACRC Service Catalog

#### **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 gacrchelp@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

Search the client portal

0 -

Class provision on the teaching cluster - phys8601dlandau

Class provision on the teaching cluster - bcmb8330 - rjwoods

Class provision on the teaching cluster - binf8211 - szhao, lm43161

MATLAB License Request

Create cider lab group

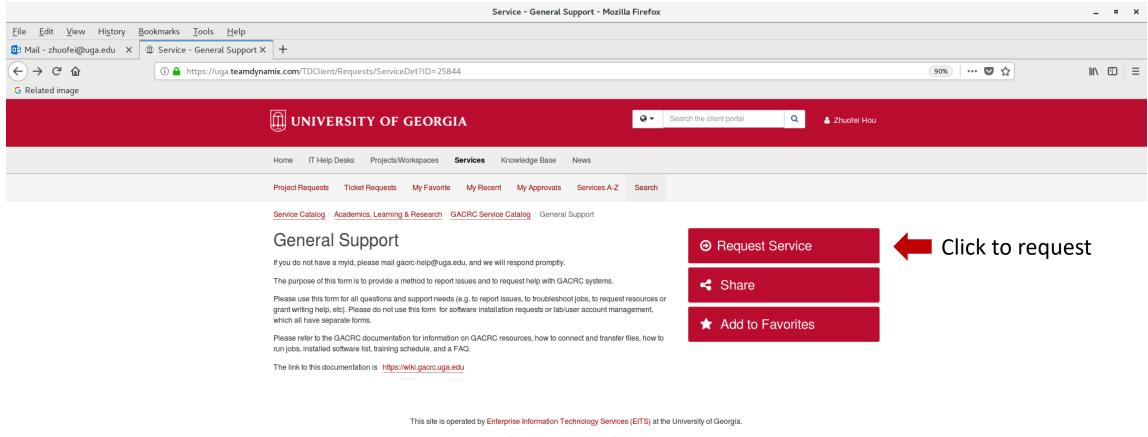
View All Recent Requests >

**Popular Services** 

Zhuofei Hou

Q

1/10/24



Privacy | Accessibility | Website Feedback

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

### **Need Support?** <u>http://help.gacrc.uga.edu</u>

