

Introduction to GACRC Teaching Cluster

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services(EITS)

The University of Georgia



Outline

- GACRC
- Overview
- Working Environment
 - Three Folders
 - Three Computational Partitions
 - Software on Cluster
- 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

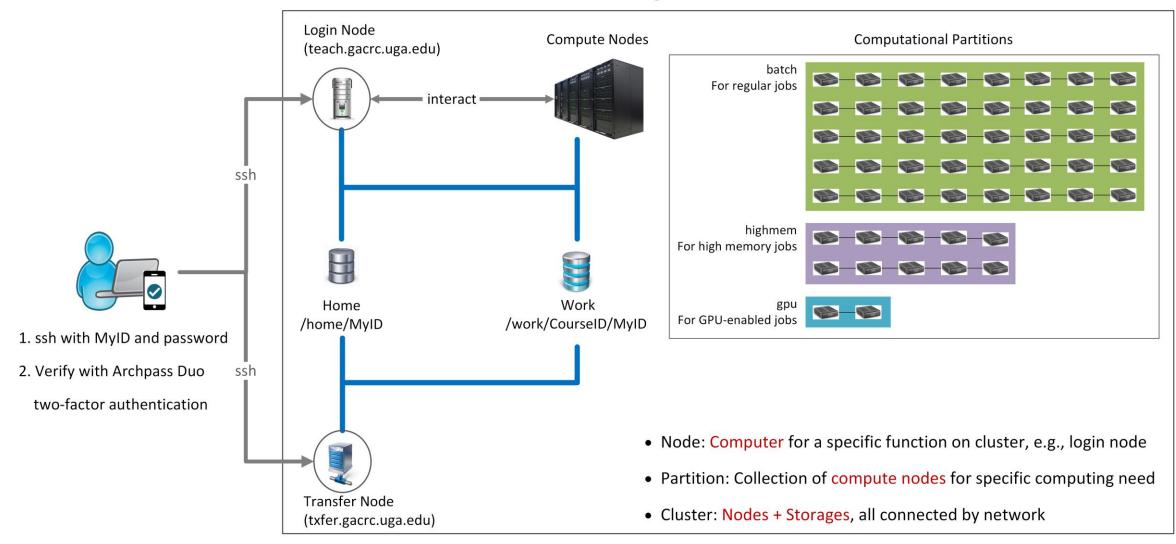
Wiki: http://wiki.gacrc.uga.edu

Support: https://wiki.gacrc.uga.edu/wiki/Getting-Help

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

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 Directories:
 - 1. /home/MyID : working space for running computational jobs
 - 2. /work/CourseID/MyID : data storing space for individual user in a class (e.g., /work/binf8211/MyID)
 - 3. /work/CourseID/instructor_data : data shared with class by the instructors
- Three Partitions:
 - 1. batch: for running regular computational jobs
 - 2. highmem: for running high-memory jobs
 - 3. gpu: for running GPU jobs



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 Batch Job

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

- 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 WinSCP to connect Transfer node Transfer data on cluster to workDir : 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 --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 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...

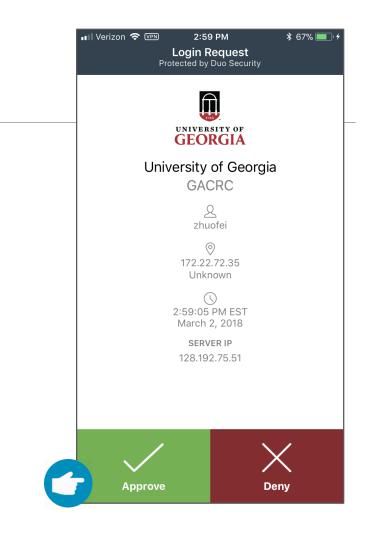
Password: 4 2. Enter your MyID password When you enter password, no stars or dots will show as you are typing. Please type password carefully!

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

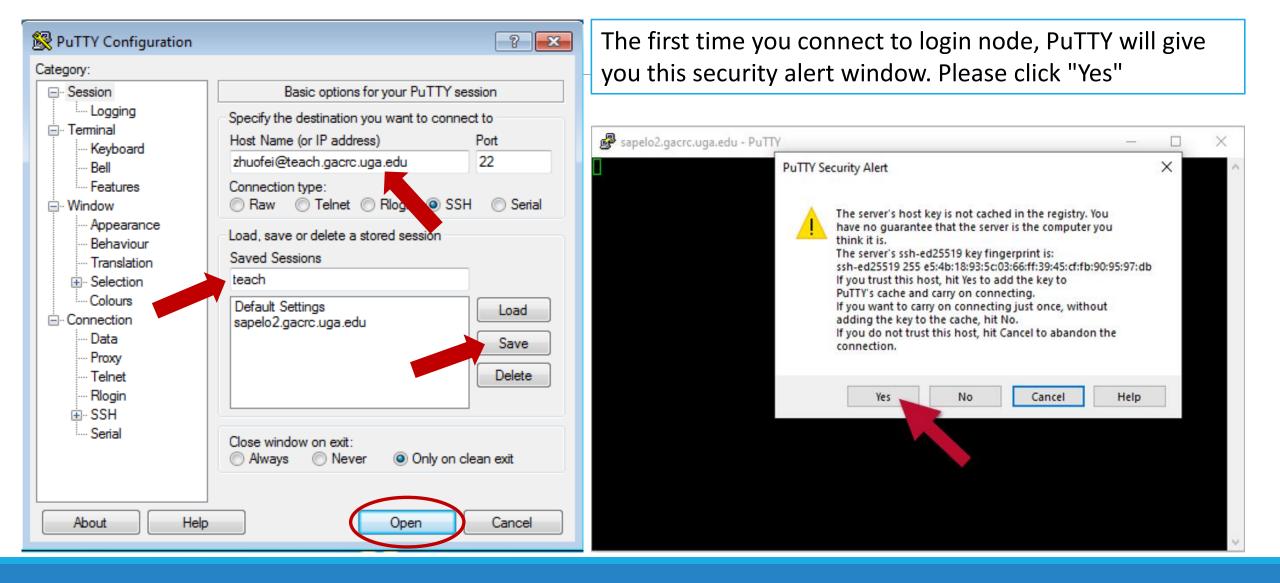
- 1. Download and install PuTTY: <u>https://www.putty.org/</u>
- 2. Detailed downloading and installation instructions:

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:

ے۔ ایس zhuofei@teach-sub1:~		
🛃 Using username "zhuofei".	A	
🚰 Keyboard-interactive authentication prompts from server:		
Password: - UGA 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		
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 - 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

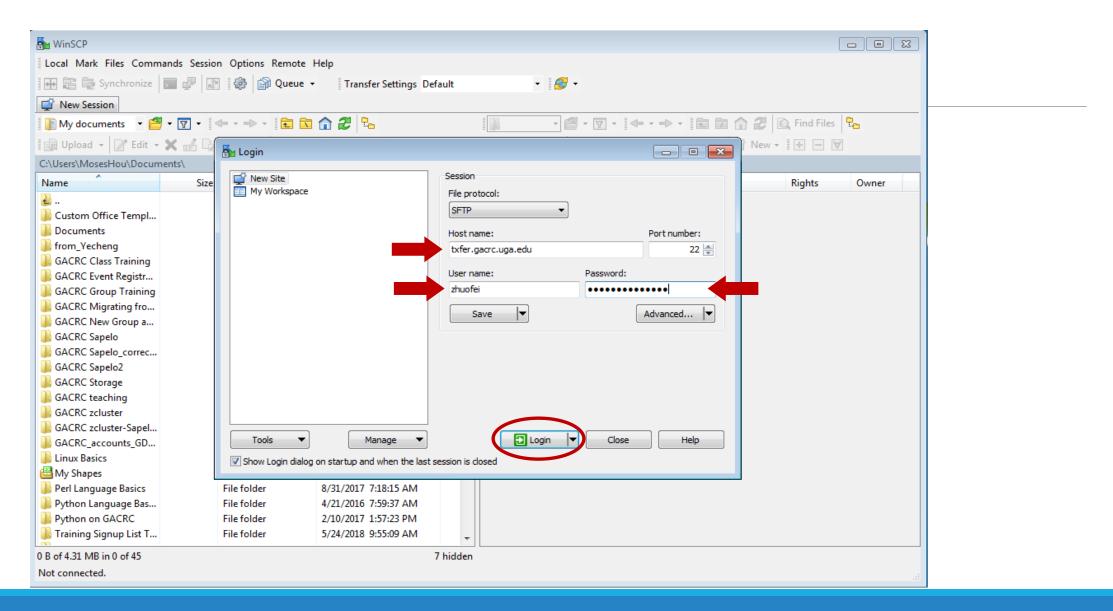
scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .

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

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 https://winscp.net/eng/index.php
 - Default installation procedure is simple
- 3. Alternative FileZilla https://wiki.gacrc.uga.edu/wiki/Transferring Files#Using FileZilla 2

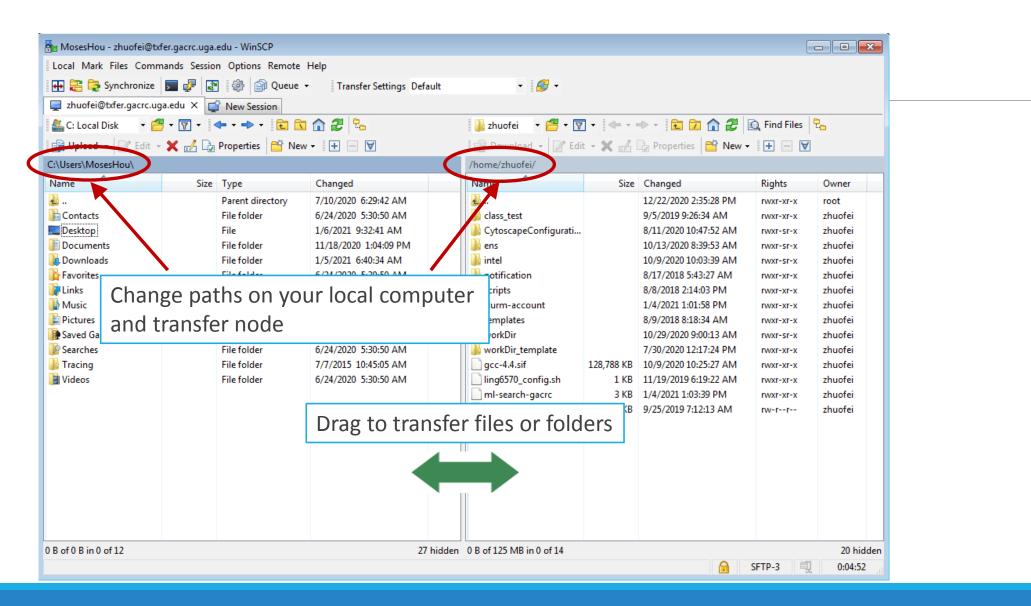
Step4 (Cont.) - Windows using WinSCP



Step5 (Cont.) - Windows using WinSCP

7												
🎦 zhuofei@xfer.gacrc.uga.e												
Local Mark Files Commands Session Options Remote Help												
🖩 🎛 🚔 Synchronize 📰 🕼 🎲 Queue 🗸 🛛 Transfer Settings Default 🔹 🧬												
📃 zhuofei@xfer.gacrc.uga.edu 🗙 🚅 New Session												
📗 My documents 🔹 音	- 🔽 -	🔶 - 🐟 - 🖹 🔂 🔂	a 🏠 🎜 🐾		• • • • • E	🗈 🏫 🤁 🔯 Find Files	2					
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C:\Users\MosesHou\Docum												
A				A			-					
Name	Size	Туре	-	Name	Size Changed	Rights	Owner					
L		Parent directory	Server prompt - zhuofei@xfer.gacro	rc.uga.edu	×							
🕌 Custom Office Templ		File folder	UGA DUO authentication is required for	for SSH/SCP access to								
bocuments		File folder	GACRC systems.									
b from_Yecheng		File folder	UGA DUO is a two-factor authentication	tion service which								
GACRC Class Training		File folder		requires a password (one factor) and a code, phone,								
GACRC Event Registr		File folder	or device (second factor) to successfu	fully authenticate.								
GACRC Group Training		File folder	If you are not enrolled in the UGA DU									
GACRC Migrating fro		File folder		visit the UGA DUO service self-service portal to enroll and configure or manage your DUO enabled devices.								
GACRC New Group a		File folder	2 2 .									
GACRC Sapelo		File folder	https://eits.uga.edu/access_and_sec	curity/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_sec	curity/infosec/tools/archpass/								
GACRC teaching		File folder	Due two factor logic for thus fai									
GACRC zcluster		File folder	Duo two-factor login for zhuofei									
GACRC zcluster-Sapel		File folder	Enter a passcode or select one of the	e 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									
🛗 My Shapes		File folder	 Phone call to XXX-XXX-1925 Phone call to XXX-XXX-3535 									
Perl Language Basics		File folder	5. SMS passcodes to XXX-XXX-5758									
Python Language Bas		File folder	Passcode or option (1-5):									
Python on GACRC		File folder				DUO ontio	n					
Training Signup List T		File folder				: DUO optio						
0 B of 4.31 MB in 0 of 45			ок	Cancel Help								
Not connected.												

Step5 (Cont.) - Windows using WinSCP





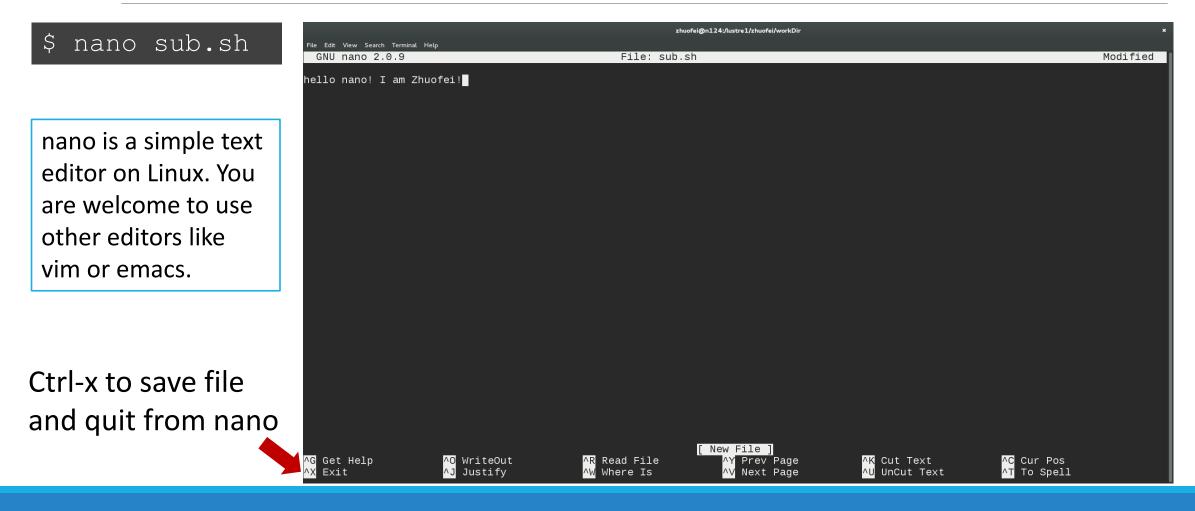
Step4 (Cont.): Transfer data on cluster to workDir

- 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/CourseID/MyID
 - 3. /work/CourseID/instructor_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

mv /work/binf8211/MyID/datafile /home/MyID/workDir

Step5: Make a job submission script in workDir using nano

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



Step5 (Cont.)

Сору

- 1. sample input data
- 2. job submission script

to your current working folder:

cp /usr/local/training/sample.fasta .

cp /usr/local/training/sub_blast.sh .

#!/bin/bash
#SBATCH --job-name=testBLAST
#SBATCH --partition=batch
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --cpus-per-task=4
#SBATCH --time=20gb
#SBATCH --time=2:00:00
#SBATCH --output=log.%j

#SBATCH --mail-user=MyID@uga.edu #SBATCH --mail-type=END,FAIL # Job name
Partition (queue) name
Single task job
Number of cores per task
Total memory for job
Time limit hrs:min:sec
Standard output and error log

Where to send mail# Mail events (BEGIN, END, FAIL, ALL)

cd \$SLURM_SUBMIT_DIR module load BLAST+/2.9.0-gompi-2019b time blastn -num_threads 4 -query sample.fasta -db /db/ncbiblast/nt/06042020/nt \ -out results.\${SLURM_JOB_ID} -outfmt 6 -max_target_seqs=2

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



Step6: 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_blast.sh

Submitted batch job 139

Tips: sub_blast.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

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

\$ squeue	me									
Wed Aug	8 13:40:	02 2018								
JOBID PAR	TITION	NAME	USER	S	TATE	TIME	TIME_LIMI	NODES	NODELIST	
162	batch	testBLAS	zhuofei	PEN	DING	0:00	2:00:00	1	(None)	
160	batch	testBLAS	zhuofei	RUN	NING	0:02	2:00:00	1	c2-11	
161	batch	testBLAS	zhuofei	RUN	NING	0:02	2:00:00	1	c2-11	
\$ squeue	me -l									
JOBID PAR	TITION	NAME	USER	ST	TIME	NODES	NODELIST			
162	batch	testBLAS	zhuofei	PD	0:15	1	(None)			
160	batch	testBLAS	zhuofei	R	0:17	1	c2-11			
161	batch	testBLAS	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.



Step7 (Cont.): Check job details using sacct-gacrc -X

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

\$ sacct	t-gacrc -X												
JobID	JobName	User	Partition	NodeList Allo	cNodes NTask	NCPUS	ReqMem	MaxVMSize	State	CPUTime	Elapsed	Timelimit	ExitCode
174	testBLAST	zhuofei	batch	tcn18	1	4	20Gn	RU	NNING	00:04:56	00:01:14	02:00:00	0:0

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

-	\$ squeueme -1 Wed Aug 8 14:03:47 2018										
JOBID	PARTITI(USER	STATE	TIME	TIME LIMI	NODES	NODELIST			
169	batch	testBLAS	zhuofei	RUNNING	2:07	2:00:00	1	c1-38			
168	batch	testBLAS	zhuofei	RUNNING	3:14	2:00:00	1	c1-39			
\$ scar	ncel 169										
[zhuoi	fei@teacl	h workDir]	\$ squeue	-1							
Wed Au	ıg 814	:03:47 201	8								
JOBID	PARTITI	ON NAME	USER	STATE	TIME	TIME_LIMI	NODES	NODELIST			
169	batch	testBLAS	zhuofei	COMPLETI	2:25	2:00:00	1	c1-39			
168	batch	testBLAS	zhuofei	RUNNING	3:32	2:00:00	1	c1-38			
\$ squeueme -1											
Wed Aug 8 14:04:08 2018											
JOBID	PARTITI	ON NAME	USER	STATE	TIME	TIME_LIMI	NODES	NODELIST			
168	batch	testBLAS	zhuofei	RUNNING	3:35	2:00:00	1	c1-38			



Step7 (Cont.): Check node info using sinfo

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

\$ 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]

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: squeue --me -l for details of a <u>running or pending</u> jobs

Option 2: sacct-gacrc -X for details of computing resource usage of a <u>running or finished</u> job

Option 3: seff for details of computing resource usage of a <u>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=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

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
- \checkmark 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

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 🕻

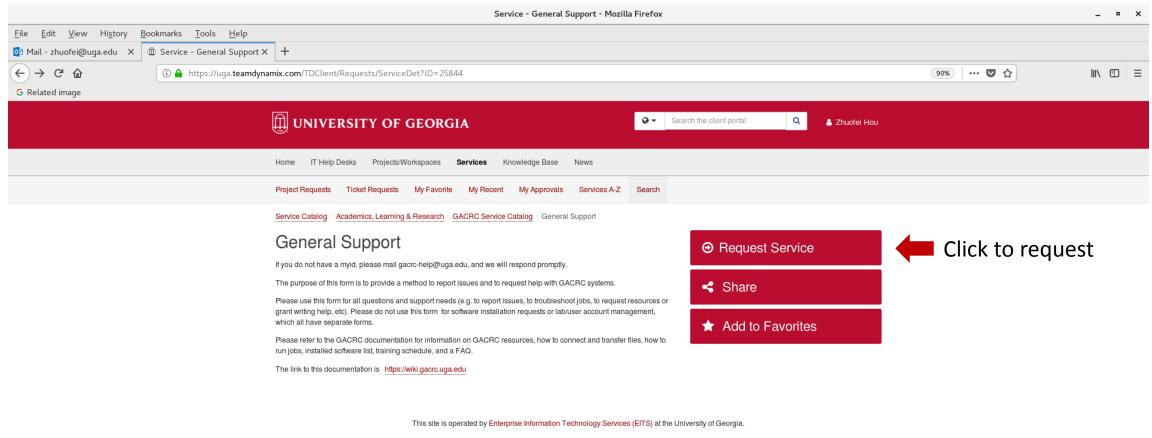
Popular Services

service catalog.

1/13/2022

Search the client portal Q

Zhuofei Hou



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

101-108 Computing Services building

University of Georgia

Athens, GA 30602

https://gacrc.uga.edu/