

HIGH PERFORMANCE RESEARCH COMPUTING

HPRC Primer

Introduction to FASTER and ACES: Composable Clusters

August 27, 2024



High Performance
Research Computing

DIVISION OF RESEARCH

ACES System Description

[ACES](#) (Accelerating Computing for Emerging Sciences) is a Dell cluster with a rich accelerator testbed:

Compute nodes	• 110 Intel Sapphire Rapids Nodes • 17 Intel Ice Lake Nodes • 1 AMD Rome Graphcore Node with 16 Mk2 Colossus GC200 IPU's • 1 Intel Ice Lake Graphcore Node with 16 Bow-2000 IPU's • 1 Intel Cascade Lake Node with 8 NEC Vector Engine Type 20B-P cards	
Accelerators	• 30 NVIDIA H100 GPUs (In 15 SPR nodes) • 4 NVIDIA A30 GPUs • 2 Bittware Agilex FPGAs • 2 Intel D5005 FPGAs	• 2 NextSilicon coprocessors • 48 Intel Optane Memory • 120 Intel GPU Max 1100 (Formerly Ponte Vecchio)
Interconnect	NVIDIA Mellanox NDR200 InfiniBand (MPI and storage) Liquid PCIe Gen4 Fabrics (composability), Gen 5 Fabrics (Coming Soon)	



The Intel Optane SSDs and all accelerators (except the Graphcore IPU's and NEC Vector Engines) are accessed using Liquid's composable framework via PCIe (Peripheral Component Interconnect express) Gen4 and Gen5 fabrics.

Visit <https://hprc.tamu.edu/kb/User-Guides/ACES/> for more details.

FASTER System Description

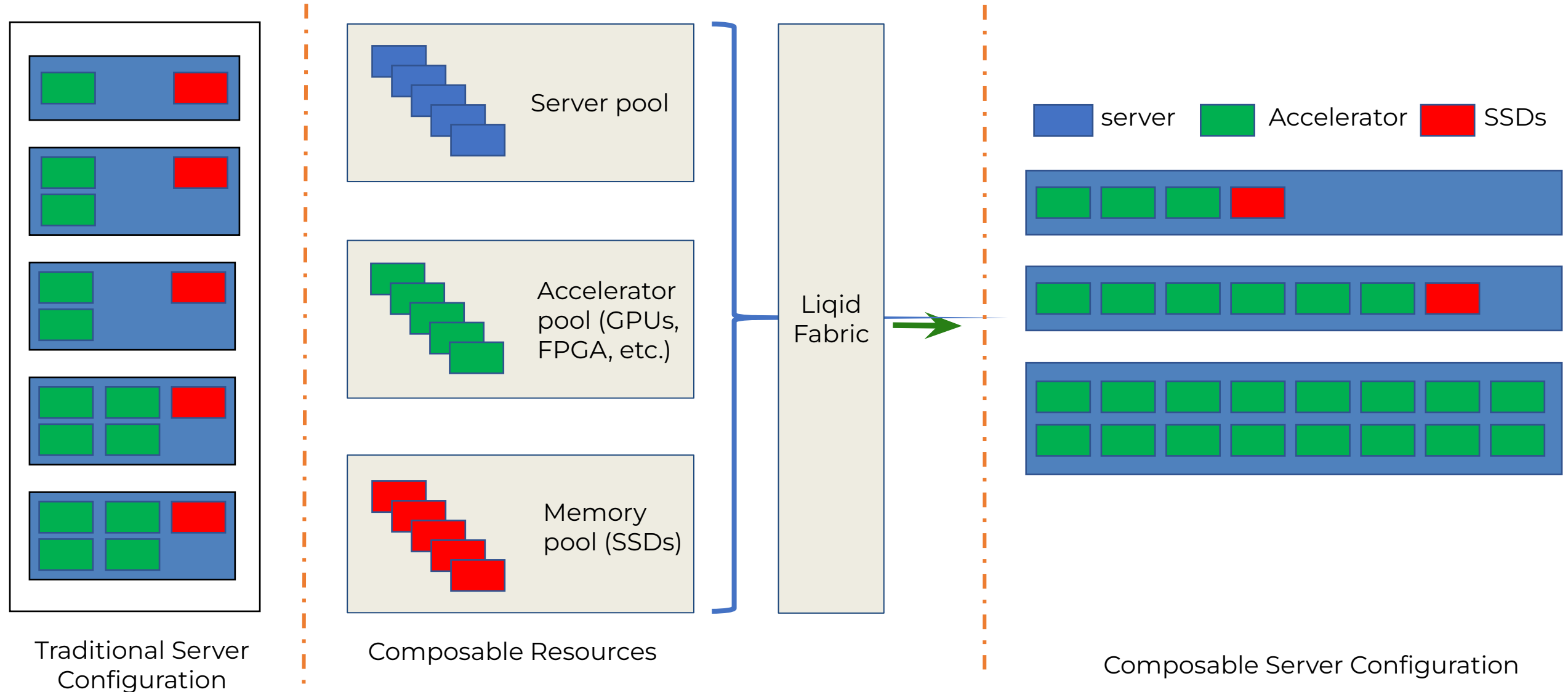
[FASTER](#) (Fostering Accelerated Sciences Transformation Education and Research) is a 180-node Intel cluster from Dell with an InfiniBand HDR-100 interconnect and Liquid PCIe Gen4 for composing the GPUs. NVIDIA A100, A10, A30, A40 and T4 GPUs are available. The 180 compute nodes are based on the Intel Ice Lake processor.

Node Type			
	Login	Compute	Large Memory
Quantity	3 (2 for TAMU, 1 for ACCESS)	180	1
CPU	2 32-core (64 cores) Intel Xeon 8352Y	2 32-core (64 cores) Intel Xeon 8352Y	2 32-core (64 cores) Intel Xeon 8352Y
Memory	256 GB	256 GB	1 TB
Additional Cluster Specifications			
Disk Space	3.84 TB NVMe (local, /tmp) 5PB DDN Lustre (global)		
Composable Accelerators	GPU: 200 T4 16GB; 40 A100 40GB; 10 A10 24GB; 4 A30 24GB; 8 A40 48GB		
Interconnect	Mellanox HDR100 InfiniBand (MPI and storage) Liquid PCIe Gen4 (resource composability)		



<https://hprc.tamu.edu/kb/Quick-Start/FASTER/>

Design: Composability at the Hardware Level



Pop Quiz



Which accelerators are available on ACES?

A. Intel PVC

B. H100

C. Graphcore IPUs

D. A30

E. A and B

F. All the above

Accessing FASTER/ACES via the HPRC Portal

- HPRC webpage: hprc.tamu.edu
 - FASTER USING TAMU: portal-faster.hprc.tamu.edu
 - FASTER USING ACCESS: portal-faster-access.hprc.tamu.edu
 - ACES USING ACCESS: portal-aces.hprc.tamu.edu

The screenshot shows the HPRC website interface. At the top is the Texas A&M logo and the text "TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING". Below this is a navigation bar with links: Home, User Services, Resources, Research, Policies, Events, Training, About, and Portal. The "Portal" link is highlighted with a yellow box. Below the navigation bar is a banner image of server racks. To the left of the banner is a "Quick Links" section with links: New User Information, Accounts, Apply for Accounts, and Manage Accounts. To the right of the banner is a dropdown menu for the "Portal" link, containing: Terra Portal, Grace Portal, FASTER Portal, FASTER Portal (ACCESS), and ACES Portal (ACCESS). The "FASTER Portal" is highlighted with a yellow box. A yellow arrow points from a box labeled "Use TAMU NetID" to the "FASTER Portal". Another yellow arrow points from a box labeled "Use ACCESS ID" to the "FASTER Portal (ACCESS)" and "ACES Portal (ACCESS)" options, which are grouped by a yellow bracket.

TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING

Home User Services Resources Research Policies Events Training About Portal

Terra Portal
Grace Portal
FASTER Portal
FASTER Portal (ACCESS)
ACES Portal (ACCESS)

Quick Links

New User Information
Accounts
Apply for Accounts
Manage Accounts

Use TAMU NetID

Use ACCESS ID

Using the ACES Portal - Shell Access



Convenient shell access anywhere with a web browser.



Starts an in-browser Linux terminal on ACES.

Accessing FASTER via SSH

- SSH (Secure SHell) allows users to establish a connection between their local machine and the TAMU HPRC clusters.
- SSH Programs

Operating System	Windows	MacOS	Linux
Programs	MobaXTerm* PuTTY SSH Windows Subsystem for Linux (WSL) Windows Command Prompt	Terminal*	Terminal*
* Recommended			

- SSH Command `ssh [NetID]@faster.hprc.tamu.edu`
- TAMU (on-campus: Duo 2FA; off-campus: [VPN](#) and Duo 2FA)
- ACCESS (ssh works differently for ACCESS users)
<https://hprc.tamu.edu/kb/User-Guides/FASTER/ACCESS-CI/>
- ACES cannot be accessed via SSH

Hands-On Activity - 2 Minutes

1. Please try to access ACES through the portal.
1. What message do you see when you log on to the shell?

File Systems and User Directories

Directory	Environment Variable	Space Limit	File Limit	Intended Use
/home/\$USER	\$HOME	10 GB	10,000	Small to modest amounts of processing.
/scratch/user/\$USER	\$SCRATCH	1 TB	250,000	Temporary storage of large files for on-going computations. Not intended to be a long-term storage area.

\$SCRATCH is shared between FASTER and Grace clusters.

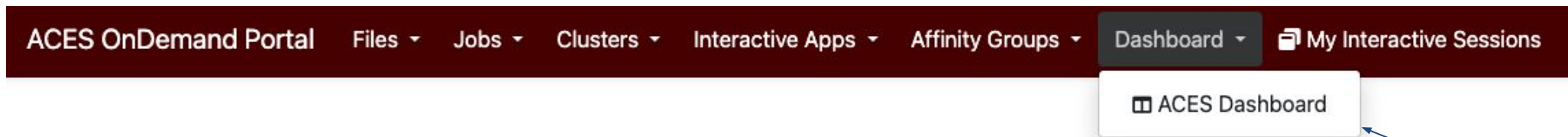
View file usage and quota limits using the command:

showquota

Do NOT share your home or scratch directories. Request a group directory for sharing files.

https://hprc.tamu.edu/kb/User-Guides/ACES/Filesystems_and_Files/

Using the Portal -Dashboard

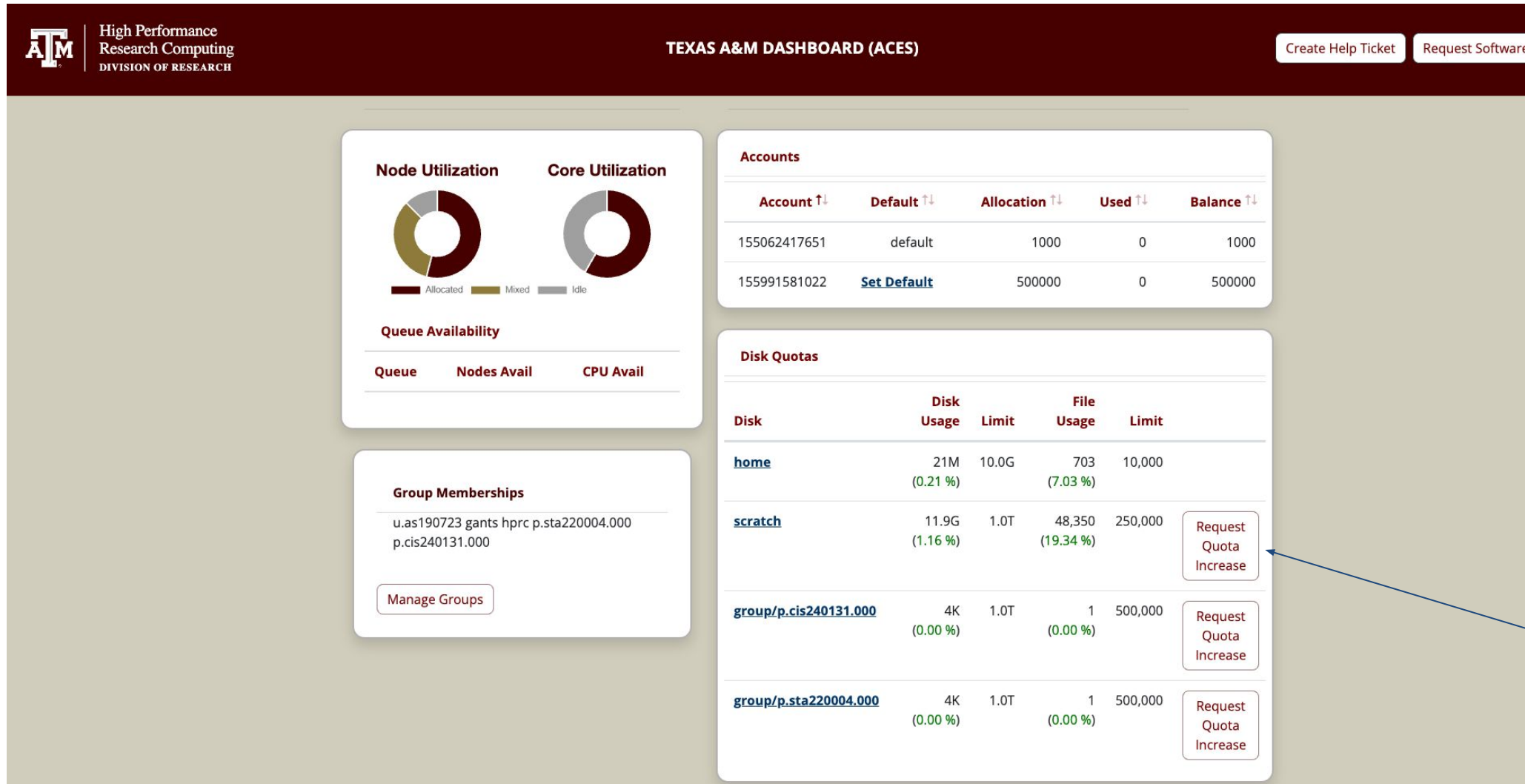


View your account
quota and projects



OOD Dashboard: ACES

Easily view Cluster utilization, Storage Quotas & Allocation Balances



Quota and file limit increases will only be considered for scratch directories

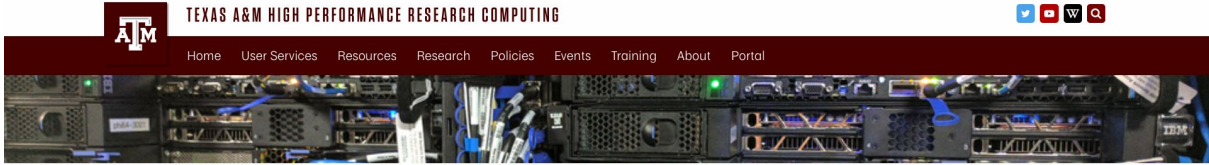
Preferred way to request *Quota Increases*

Hands-On Activity - 2 Minutes

1. Please try to access the dashboard now through the portal.
2. Where is the button to request a quota increase?

Software

- See the Software Knowledge Base page <https://hprc.tamu.edu/kb/Software/> for instructions and examples
- Search for software modules on <https://hprc.tamu.edu/software/aces/>
- License-restricted software
 - Contact help@hprc.tamu.edu
- Contact HPRC for software installation help/request
 - User can install software in their home/scratch directory
 - Do NOT run the `sudo` command when installing software



TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING

Home User Services Resources Research Policies Events Training About Portal

SOFTWARE MODULES ON THE ACES CLUSTER

(Last Updated: Thu Aug 15 14:22:54 CDT)

Name	Versions available	Description	Notes
ACTC	ACTC/1.1	'ACTC converts independent triangles into triangle strips or fans.'	
ANTLR	ANTLR/2.7.7-Java-11	'ANTLR, ANother Tool for Language Recognition, (formerly PCCTS) is a language tool that provides a framework for constructing recognizers, compilers, and translators from grammatical descriptions containing Java, C#, C++, or Python actions.'	
AOCC	AOCC/4.0.0	'AMD Optimized C/C++ & Fortran compilers (AOCC) based on LLVM 13.0.'	
APR	APR/1.7.0	'Apache Portable Runtime (APR) libraries.'	
APR-UTIL	APR-util/1.6.1	'Apache Portable Runtime (APR) util libraries.'	
ASE	ASE/3.20.1 ASE/3.22.1	'ASE is a python package providing an open source Atomic Simulation Environment in the Python scripting language. From version 3.20.1 we also include the ase-ext package. It contains optional reimplementations in C of functions in ASE. ASE uses it automatically when installed.'	
ATK	ATK/2.36.0 ATK/2.38.0	'ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications.'	

Software: Application Modules

- Installed applications are made available with the module system
- ACES uses a software hierarchy inside the module system
- In this hierarchy, the user loads a compiler “toolchain” which then makes available software built with that compiler toolchain

```
module list                # shows which software is ready
module load GCC/11.2.0     # load GCC compiler version 11.2.0
module list                # show which software is now ready
module load OpenMPI/4.1.1  # load OpenMPI version 4.1.1
module list                # show which software is now ready
```

Software: Modules and Toolchains

- Toolchains are what we call groups of compilers & libraries
- There is a variety of toolchains on the clusters:

```
intel/2023a  
foss/2024.05  
GCCcore/13.3.0
```

*(more than just these versions)
(varies by cluster, as well)*

- Module management:

```
module spider      # Search for modules and their dependencies  
module purge       # removes all loaded modules from environment
```

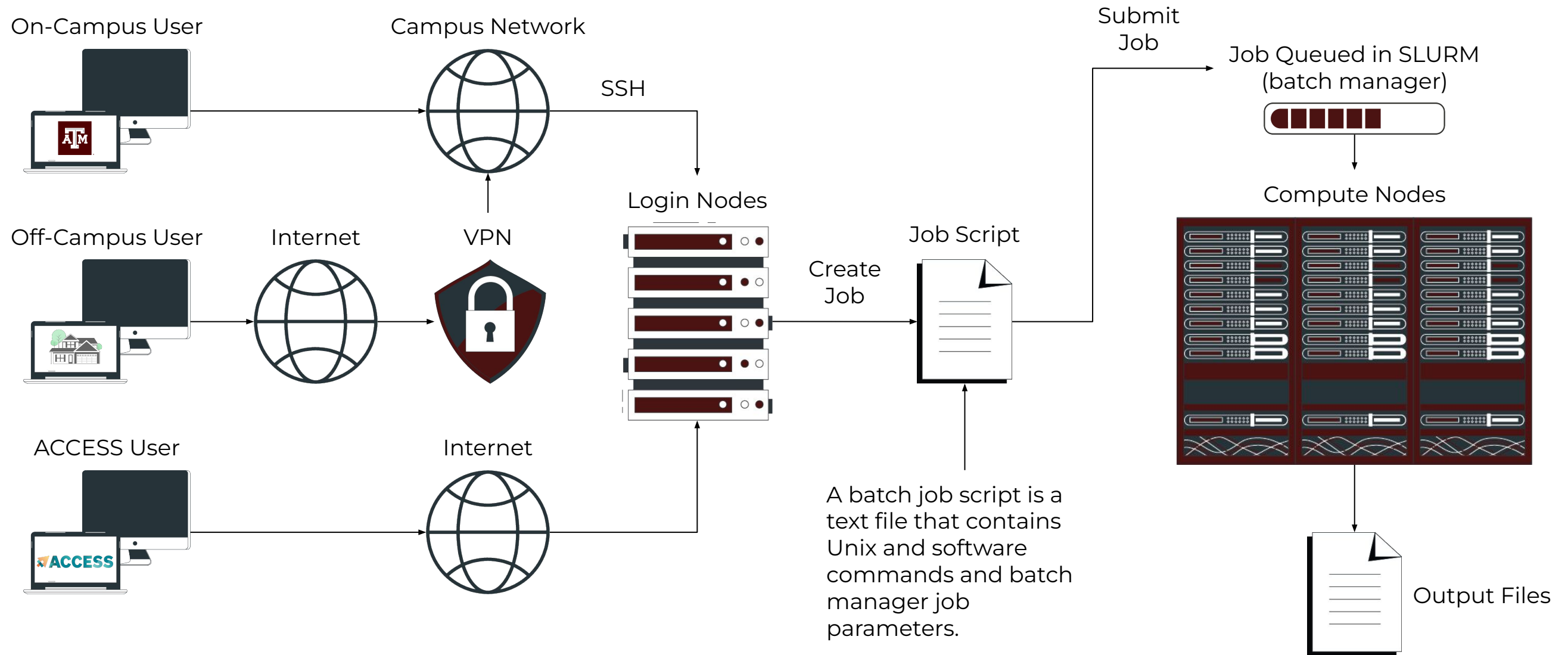
Hands-On Activity - 2 Minutes

1. Search for and load the following module:

```
GCC/12.3.0
```

1. Next remove all your current modules.

Batch Computing on HPRC Clusters



Batch Queues

- Job submissions are auto-assigned to batch queues based on the resources requested (e.g. cpu vs. gpu).
- Use 'sinfo' to check on their status:

```
[ashwin_k@faster1 ~]$ sinfo
PARTITION    AVAIL  TIMELIMIT  JOB_SIZE  NODES(A/I/O/T)  CPUS(A/I/O/T)
cpu*         up      7-00:00:00  1-32      83/21/12/116    5123/1533/768/7424
gpu          up      7-00:00:00  1-32      6/36/10/52      98/2590/640/3328
atasp        down    2-00:00:00  1         0/8/2/10        0/512/128/640
staff        up      2-00:00:00  1         89/65/24/178    5221/4635/1536/11392
```

FASTER

```
[u.ak118300@aces-login3 ~]$ sinfo
PARTITION    AVAIL  TIMELIMIT  JOB_SIZE  NODES(A/I/O/T)  CPUS(A/I/O/T)
cpu*         up      7-00:00:00  1-64      5/36/15/56      418/3518/1440/5376
gpu          up      2-00:00:00  1-15      14/0/2/16       29/1315/192/1536
pvc          up      2-00:00:00  1-15      2/7/11/20       96/768/1056/1920
atasp        up      2-00:00:00  1         0/3/1/4         0/288/96/384
bittware     up      2-00:00:00  1         0/2/0/2         0/192/0/192
d5005        up      2-00:00:00  1         0/2/0/2         0/192/0/192
gpu-hybrid   up      2-00:00:00  1-infinite 15/7/13/35     121/1991/1248/3360
```

ACES

For the NODES and CPUS columns:

A = Active (in use by running jobs)

I = Idle (available for jobs)

O = Offline (unavailable for jobs)

T = Total

Additional information:

<https://hprc.tamu.edu/kb/User-Guides/FASTER/Batch/#batch-queues>

DRONA COMPOSER - JOB SUBMISSION MADE EASY

DRONA COMPOSER (ACES)

Job Composer

Job Name

Location

Environments

Upload files (optional)

Add modules

Number of cores (if not sure, keep at 1)

Number of nodes (if not sure, leave as 0)

Use Accelerator

TOTAL Memory

Expected run time

Account (leave blank if using default?)

Additional Slurm parameters?

⚠ Cautions: Job files will overwrite existing files with the same name. The same principle applies for your executable scripts.

You can select environments.

You can add modules.

You can choose your choice of accelerator.

You can set the expected runtime.

Once you click on preview after filling the form, this is what you should see.

You can edit this script on the go.

Job Preview

run_command

driver

```
#!/bin/bash
# Template for a standard shell env

#SBATCH --job-name=asil_drona_composer_test_2
#SBATCH --time=24:0:00
#SBATCH --ntasks=1
#SBATCH --nodes=1
#SBATCH --mem-per-cpu=5000M
#SBATCH --output=out.%j
#SBATCH --error=error.%j
#SBATCH --partition=pvc --gres=pvc

module purge
module load WebProxy
module load foss/2023a Anaconda3/2024.02-1

cd /scratch/user/u.as190723/job_composer/asil_drona_composer_test_2

# ADD YOUR COMMANDS BELOW
```

Submit

Sample Job Script Structure

```
#!/bin/bash
```

```
##NECESSARY JOB SPECIFICATIONS
```

```
#SBATCH --job-name=JobExample1
```

```
#SBATCH --time=01:30:00
```

```
#SBATCH --ntasks=1
```

```
#SBATCH --nodes=1
```

```
#SBATCH --mem=2560M
```

```
#SBATCH --output=Example1Out.%j
```

These parameters describe your job to the job scheduler.
The lines starting with #SBATCH are NOT comments!

```
##OPTIONAL JOB SPECIFICATIONS
```

```
##SBATCH --account=123456
```

```
##SBATCH --mail-type=ALL
```

```
##SBATCH --mail-user=email_address
```

Account number to be charged
(if you're not using a default account).

```
# load required module(s)
```

```
module purge
```

```
module load GCCcore/11.3.0
```

```
module load Python/3.10.4
```

Whatever commands or scripts you want to run.
Here, we set up the modules we need for our environment and run a python program.

```
# Run your program
```

```
python my_program.py
```

Hands-On Activity

1. Navigate to `/scratch/training/Intro-to-ACES-Primer`

1. Copy “`hello_world.job`” to your home directory

Submit Your Job and Check Job Status

Submit job

```
sbatch example01.job
```

```
Submitted batch job 161997
(from job_submit) your job is charged as below
      Project Account: 122792016265
      Account Balance: 1687.066160
      Requested SUs:   3
```

Check status

```
squeue -u username
```

(or

```
squeue --me
```

 as a shortcut for your own jobs)

JOBID	NAME	USER	PARTITION	NODES	CPUS	STATE	TIME	TIME_LEFT	START_TIME	REASON	NODELIST
64039	somejob	someuser	medium	4	112	PENDING	0:00	20:00	2017-01-30T21:00:4	Resources	
64038	somejob	someuser	medium	4	112	RUNNING	2:49	17:11	2017-01-30T20:40:4	None	tnxt-[0401-0404]

Hands-On Activity - 5 Minutes

1. Create a submission file for a serial job; you can use the template shown previously or create your own.
2. Submit this job file using sbatch.
3. Check which queue the job is in.
4. When your job completes, check the contents of the ExOutput.txt file.

Check your Service Unit (SU) Balance

- List the SU Balance of your Account(s)

myproject

=====							
List of YourNetID's Project Accounts							
Account	FY	Default	Allocation	Used & Pending SUs	Balance	PI	
1228000223136	2023	N	10000.00	0.00	10000.00	Doe, John	
1428000243716	2023	Y	5000.00	-71.06	4928.94	Doe, Jane	
1258000247058	2023	N	5000.00	-0.91	4999.09	Doe, Jane	
=====							

- Run "myproject -d *Account#*" to change default project account
- Run "myproject -h" to see more options

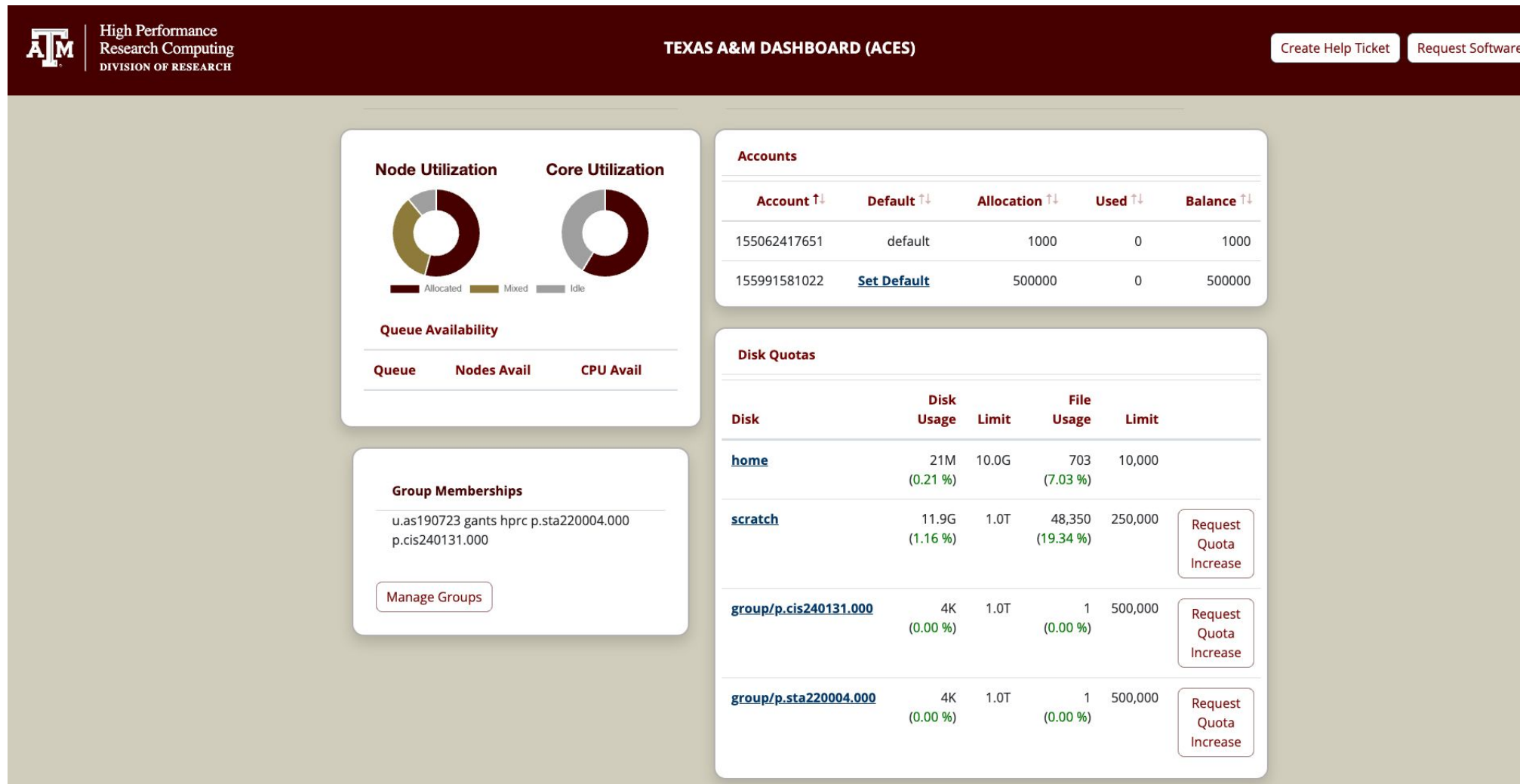
https://hprc.tamu.edu/kb/User-Guides/AMS/Service_Unit/

<https://hprc.tamu.edu/kb/User-Guides/AMS/UI/>

(reminder)

OOD Dashboard: ACES

Easily view Cluster utilization, Storage Quotas & Allocation Balances



Quota and file limit increases will only be considered for scratch directories

Preferred way to request *Quota Increases*

Hands-On Activity - 2 Minutes

1. Use myproject to check the SU balance of your accounts.
2. Use the dashboard to check the same information.

Need Help?

First check the FAQ: <https://hprc.tamu.edu/kb/FAQ/Accounts/>

- FASTER User Guide: <https://hprc.tamu.edu/kb/User-Guides/FASTER/>
- ACES User Guide: <https://hprc.tamu.edu/kb/User-Guides/ACES/>
- Email your questions to help@hprc.tamu.edu

Help us help you -- when you contact us, tell us:

- Which Cluster you're using
- Your username
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used if any
- Module(s) loaded if any
- Error messages
- Steps you have taken, so we can reproduce the problem



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Thank you.

Any questions?

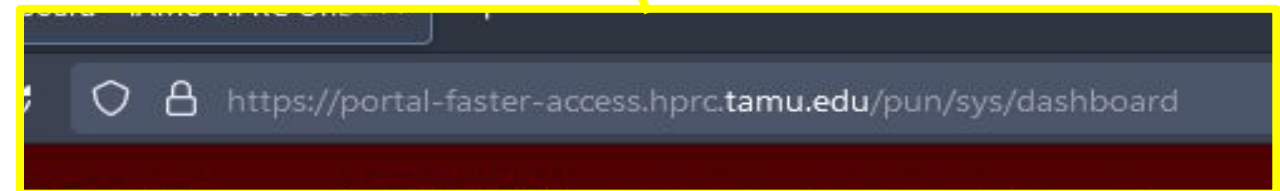
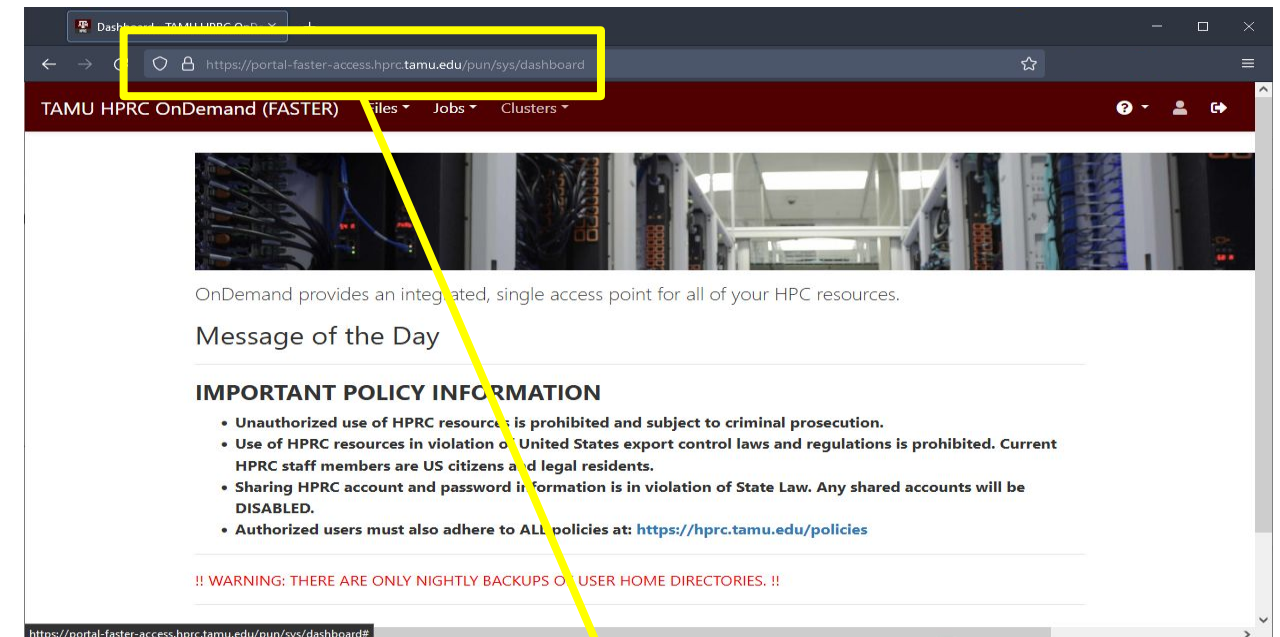
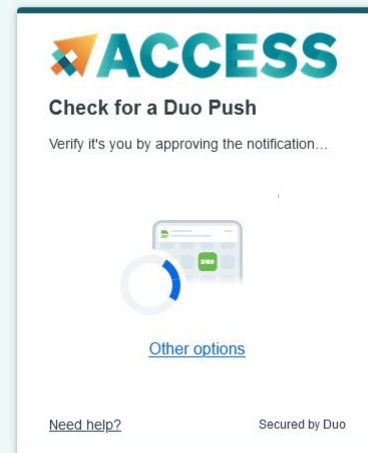
Composability on FASTER

- GPUs can be added to compute nodes on the fly by using the “gres” option in a Slurm script.
- A researcher can request up to 12 GPUs to create these CPU-GPU nodes.
- This approach allows for more flexibility and options for node types (CPU only, CPU + GPU) available to users.

Accessing FASTER via the HPRC Portal (ACCESS)

Complete the Duo Two-Factor Authentication prompt. Set-up the two-factor authentication if you have not already done so.

You will now have access to the FASTER portal.



Two-Factor Authentication

- Two-Factor Authentication (2FA) is required for access to all TAMU HPRC computing resources
- TAMU users enroll in Duo 2FA
 - <https://it.tamu.edu/duo/>
 - Authenticated through CAS (Central Authentication System)
- Users from other institutions may use a different 2FA system

Consumable Computing Resources

- Resources specified in a job file:
 - Processor cores
 - Memory
 - Wall time
 - GPU
- Service Unit (SU)
 - The “currency” with which you “pay” for computing resources.
 - Use "**myproject**" to check your balance

https://hprc.tamu.edu/kb/User-Guides/AMS/Service_Unit/

myproject

List of YourNetID's Project Accounts

Account	FY	Default	Allocation	Used & Pending SUs	Balance	PI
1228000223136	2023	N	10000.00	0.00	10000.00	Doe, John
1428000243716	2023	Y	5000.00	-71.06	4928.94	Doe, Jane

- Other resources:
 - Software license/token

- Use "**license_status**" to query

https://hprc.tamu.edu/kb/Software/useful-tools/License_Checker/

Find available license for "Matlab":

```
license_status -s Matlab
```

License status for Matlab:

License Name	# Issued	# In Use	# Available
Matlab	50	0	50

For more information about this command:

```
license_status -h
```

CRLF Line Terminators

Windows editors such as Notepad will add hidden Carriage Return Line Feed (CRLF) characters that will cause problems with many applications

```
cd $SCRATCH/batch_examples
```

```
file dos_text.txt
```

use file command to check

```
dos_text.txt: ASCII English text, with CRLF line terminators
```

```
cat -v dos_text.txt
```

use cat command to see CRLF characters

```
dos2unix dos_text.txt  
file dos_text.txt
```

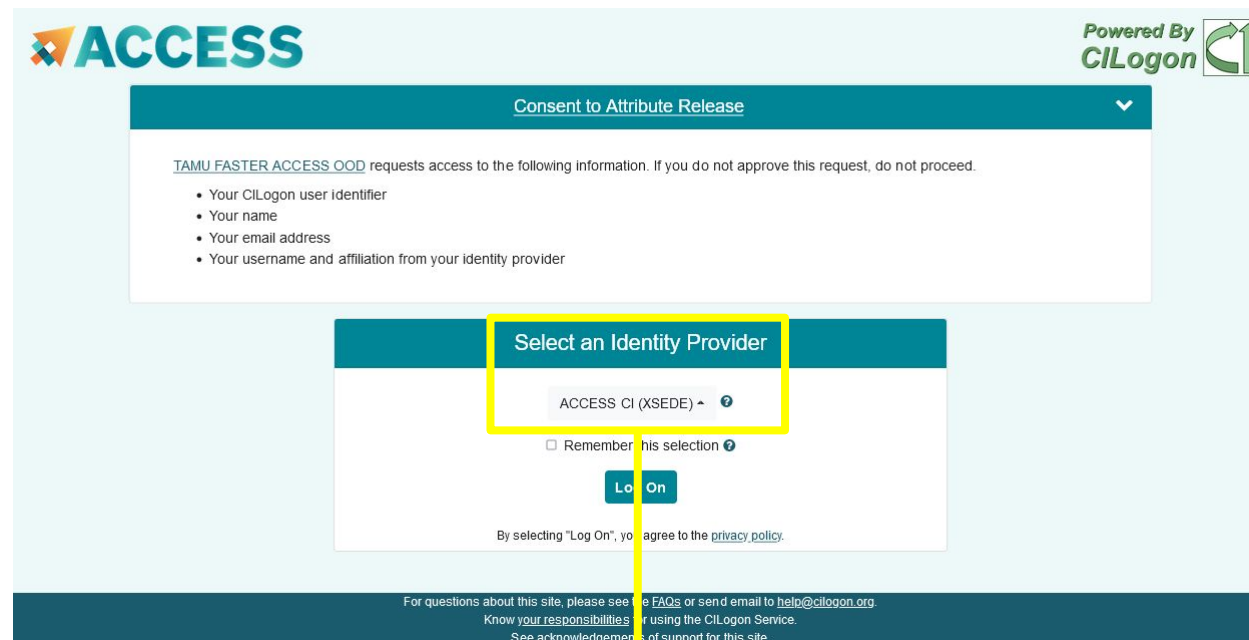
use dos2unix command to correct

```
dos_text.txt: ASCII English text
```

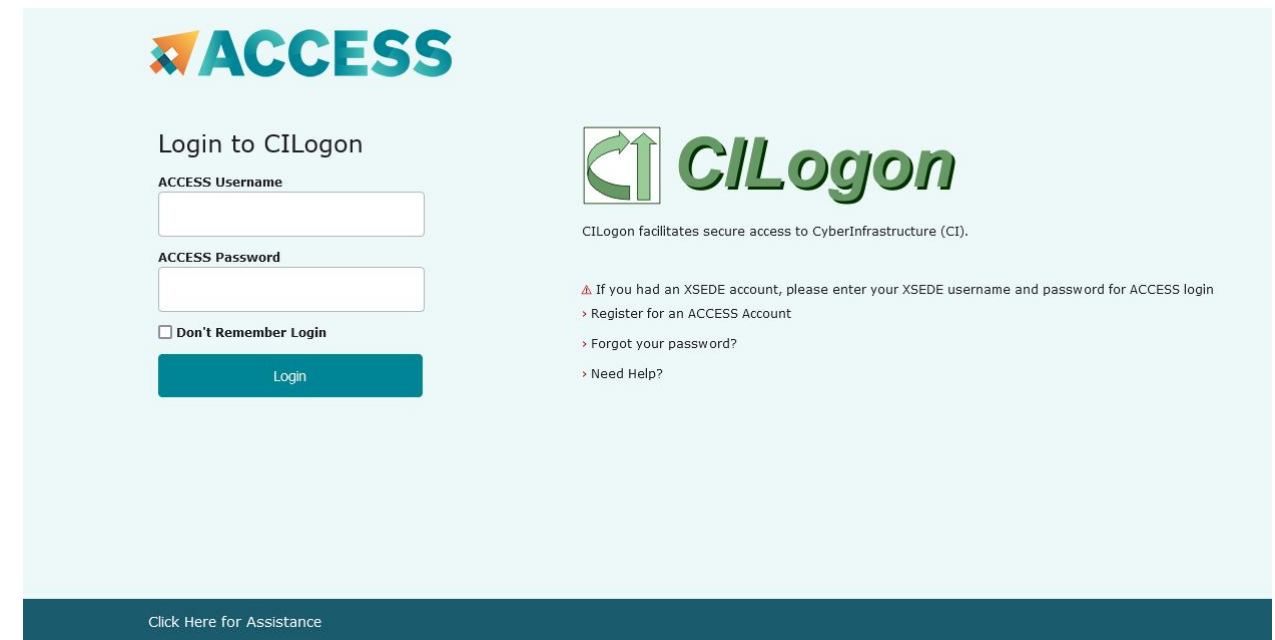
Accessing FASTER via the HPRC Portal (ACCESS)

Navigate to portal-faster-access.hprc.tamu.edu to get to the ACCESS CILogon OpenID Connect page.

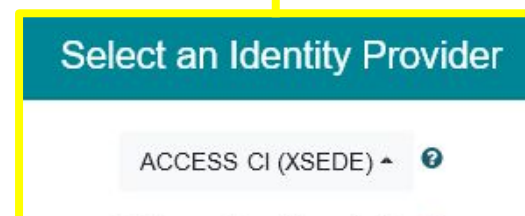
Log-in using your ACCESS credentials. Create an account if you do not already have one.



The screenshot shows the ACCESS CILogon OpenID Connect page. At the top, there is a teal header with the ACCESS logo and a 'Powered By CILogon' badge. Below the header, there is a 'Consent to Attribute Release' section with a dropdown arrow. The consent text states: 'TAMU FASTER ACCESS OOD requests access to the following information. If you do not approve this request, do not proceed.' The requested information includes: 'Your CILogon user identifier', 'Your name', 'Your email address', and 'Your username and affiliation from your identity provider'. Below the consent section, there is a 'Select an Identity Provider' dropdown menu. The dropdown is currently set to 'ACCESS CI (XSEDE)'. There is a 'Remember this selection' checkbox and a 'Log On' button. At the bottom, there is a note: 'By selecting "Log On", you agree to the privacy policy.' A yellow box highlights the 'Select an Identity Provider' dropdown menu.



The screenshot shows the ACCESS CILogon login page. At the top, there is a teal header with the ACCESS logo and a 'Powered By CILogon' badge. Below the header, there is a 'Login to CILogon' section. It contains a form with two input fields: 'ACCESS Username' and 'ACCESS Password'. There is a 'Don't Remember Login' checkbox and a 'Login' button. To the right of the login form, there is a CILogon logo and a description: 'CILogon facilitates secure access to CyberInfrastructure (CI)'. Below the description, there are links: 'If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login', 'Register for an ACCESS Account', 'Forgot your password?', and 'Need Help?'. At the bottom, there is a 'Click Here for Assistance' link.



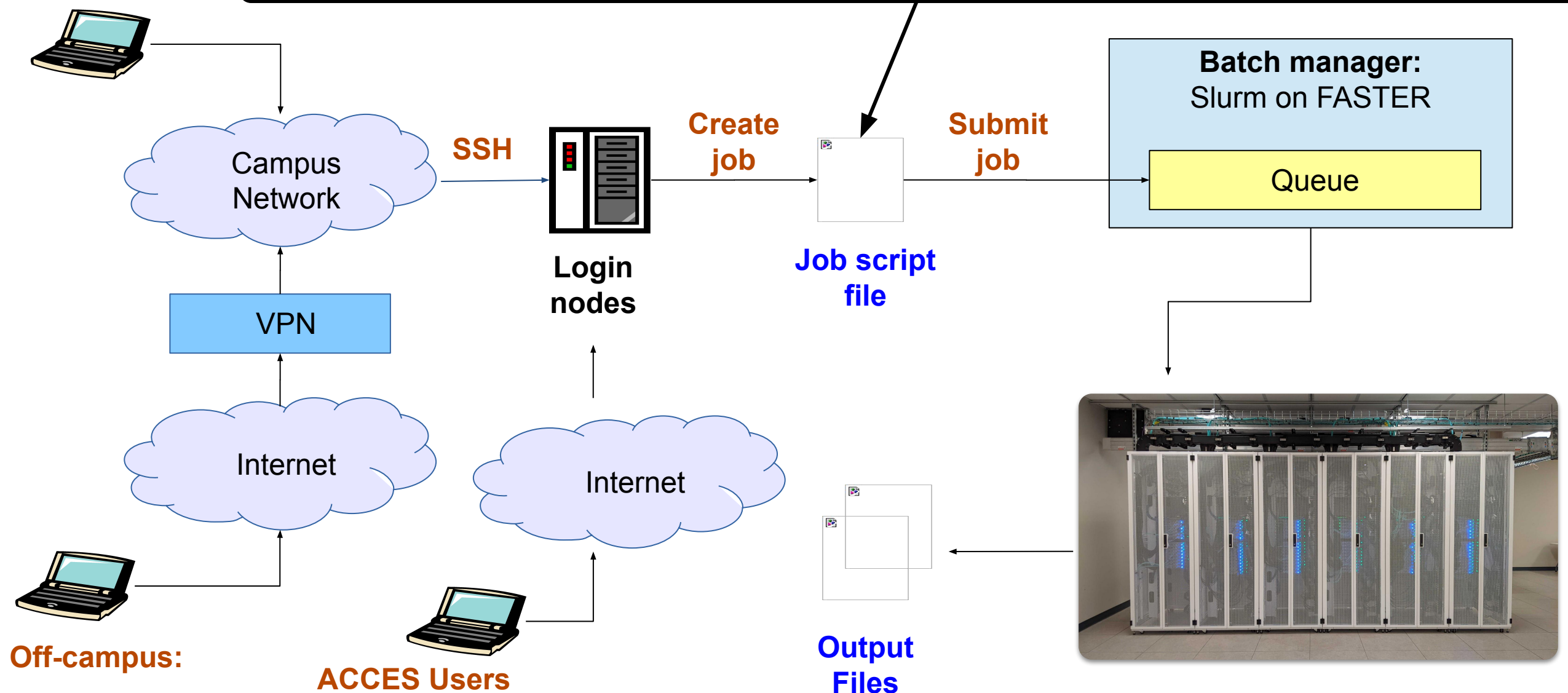
This is a close-up of the 'Select an Identity Provider' dropdown menu. The dropdown is currently set to 'ACCESS CI (XSEDE)'. There is a 'Remember this selection' checkbox and a 'Log On' button. A yellow box highlights the dropdown menu.

Select the Identity Provider appropriate for your account.

Batch Computing on HPRC Clusters

On-campus:

A batch job script is a text file that contains Unix and software commands and Batch manager job parameters

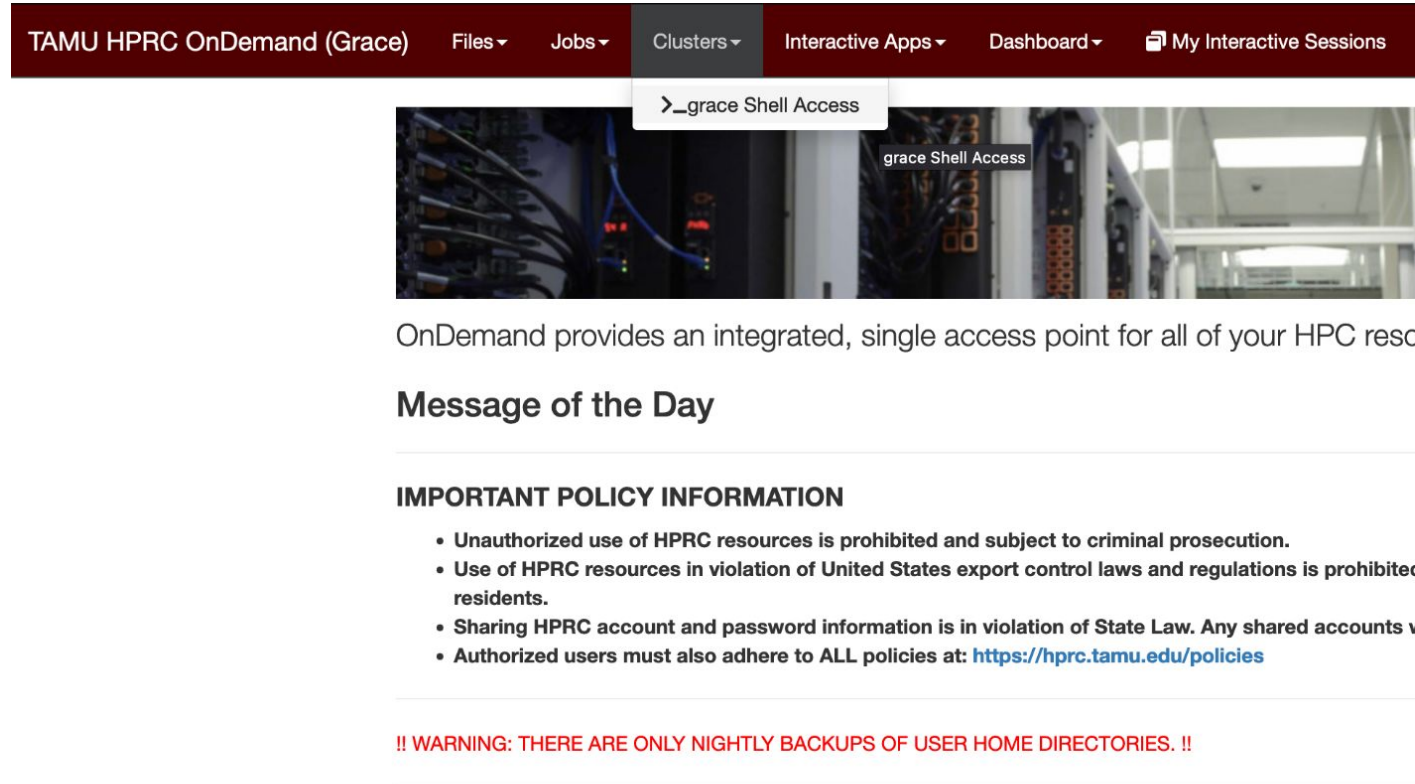


Accessing FASTER: via the Portal

- Access through (most) web browsers:

portal.hprc.tamu.edu

Top Banner Menu “Clusters” -> “FASTER Shell Access”



TAMU HPRC OnDemand (Grace) Files Jobs Clusters Interactive Apps Dashboard My Interactive Sessions

>_grace Shell Access

grace Shell Access

OnDemand provides an integrated, single access point for all of your HPC resolu

Message of the Day

IMPORTANT POLICY INFORMATION

- Unauthorized use of HPRC resources is prohibited and subject to criminal prosecution.
- Use of HPRC resources in violation of United States export control laws and regulations is prohibited. residents.
- Sharing HPRC account and password information is in violation of State Law. Any shared accounts wi
- Authorized users must also adhere to ALL policies at: <https://hprc.tamu.edu/policies>

!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!

hprc.tamu.edu/wiki/HPRC:Access

FASTER

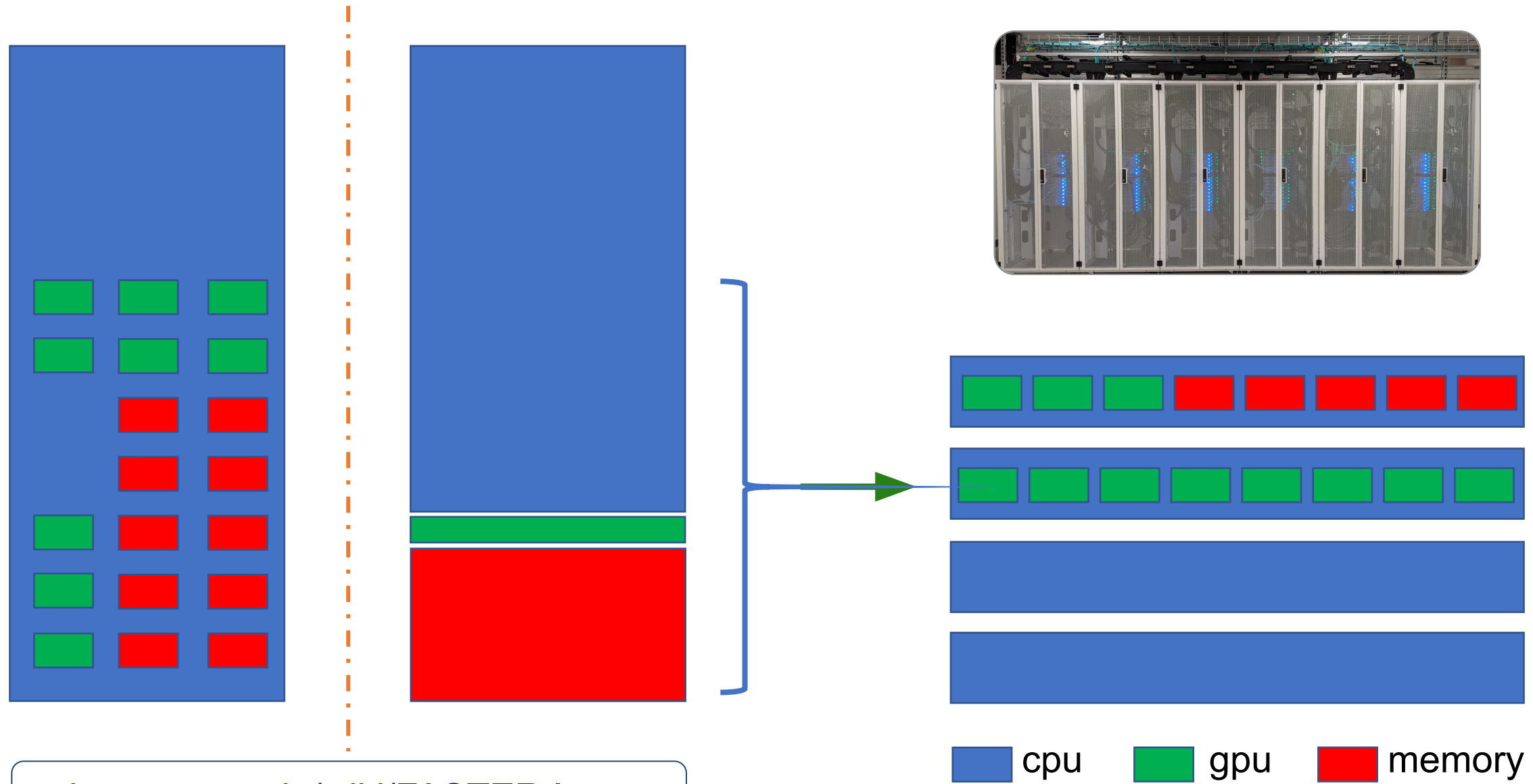
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Additional Cluster Specifications			
Disk Space	3.84 TB NVMe (local, /tmp); 5PB DDN Lustre (global)		
Composable Accelerators	GPU: 200 T4 16GB; 40 A100 40GB; 10 A10 24GB; 4 A30 24GB; 8 A40 48GB FPGA: 2 Intel D5005 PAC		
Interconnect	Mellanox HDR100 InfiniBand (MPI and storage) Liquid PCIe Gen4 (GPU composability)		



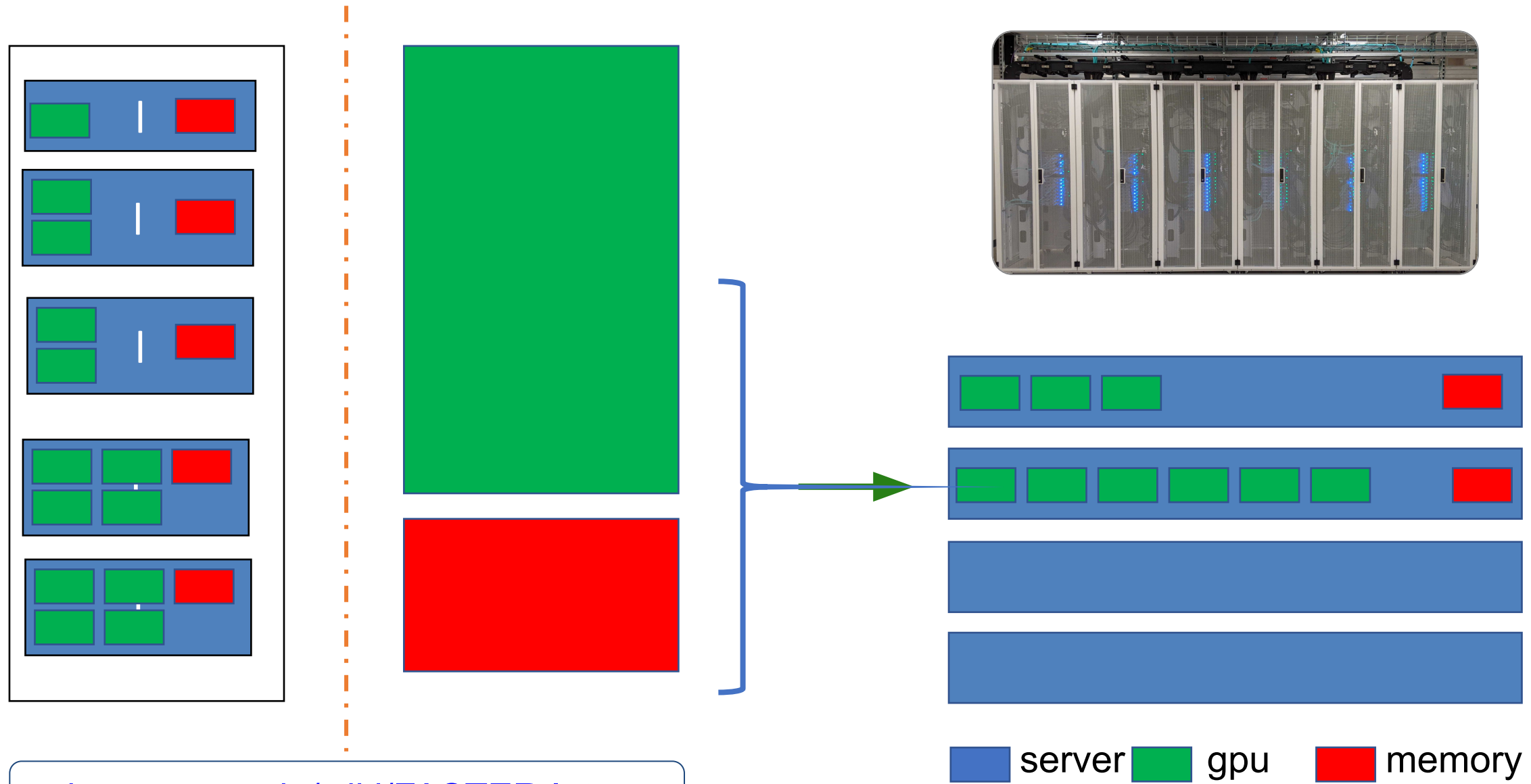
For more information:

Composability at the Hardware Level



hprc.tamu.edu/wiki/FASTER:Intro

Composability at the Hardware Level



hprc.tamu.edu/wiki/FASTER:Intro

Accessing FASTER via SSH (TAMU)

- SSH command is required for accessing FASTER:
 - On campus: `ssh userNetID@faster.hprc.tamu.edu`
 - Off campus:
 - Set up and start VPN (Virtual Private Network): u.tamu.edu/VPnetwork
 - Then: `ssh userNetID@faster.hprc.tamu.edu`
 - *Two-Factor Authentication* enabled for CAS, VPN, SSH
- SSH programs for Windows:
 - MobaXTerm (preferred, includes SSH and X11)
 - PuTTY SSH
 - Windows Subsystem for Linux
- FASTER has 3 login nodes. Check the bash prompt.

Login sessions that are idle for **60** minutes will be closed automatically
Processes run longer than **60** minutes on login nodes will be killed automatically.
hprc.tamu.edu/wiki/HPRC:Access

Do not use more than 8 cores on the login nodes!

High Performance Research Computing | hprc.tamu.edu

Accessing FASTER via SSH

- SSH (Secure SHell) allows users to establish a connection between their local machine and the TAMU HPRC clusters.
- SSH Programs

Operating System	Windows	MacOS	Linux
Programs	MobaXTerm* PuTTY SSH Windows Subsystem for Linux (WSL)	Terminal*	Terminal*
* Recommended			

- SSH Command
 - TAMU (on-campus: Duo TFA; off-campus: [VPN](#) and Duo TFA)

```
ssh userNetID@faster.hprc.tamu.edu
```
 - ACCESS ([additional steps required](#))

```
ssh -J [username]@faster-jump.hprc.tamu.edu:8822 [username]@login.faster.hprc.tamu.edu
```
- Additional information: <https://hprc.tamu.edu/wiki/HPRC:Access>

Two-Factor Authentication (TAMU)

- Duo NetID two-factor authentication to enhance security (it.tamu.edu/duo/)
 - All web login (howdy, portal.hprc.tamu.edu, Globus) through CAS
 - VPN to TAMU campus (since Oct 1st, 2018)
 - SSH/SFTP to HPRC clusters (since Nov 4th, 2019)
- See instructions in two-factor wiki page (hprc.tamu.edu/wiki/Two_Factor)
- SSH clients work with Duo
 - ssh command from Linux, macOS Terminal, Windows cmd
 - MobaXterm for Windows (click on “Session” icon or via local session: hit “enter” 3 times and wait for “Password:” prompt)
 - Putty for Windows
- SFTP clients work with Duo
 - scp/sftp command from Linux, macOS Terminal, Windows cmd
 - WinSCP for Windows
 - Cyberduck for macOS
- Not all software supports SSH+Duo: SFTP in Matlab

hprc.tamu.edu/wiki/Two_Factor

Example: SSH login with Duo

```
$ ssh userNetID@faster.hprc.tamu.edu
*****
*
... warning message (snipped) .....
*****
*
Password:
Duo two-factor login for userNetID

Enter a passcode or select one of the following
options:

1. Duo Push to XXX-XXX-1234
2. Phone call to XXX-XXX-1234
3. SMS passcodes to XXX-XXX-1234

Passcode or option (1-3): 1
Success. Logging you in...
```


Accessing FASTER via SSH (ACCESS)

Rough outline, fixing later (Shaina):

Generate pub key

Submit pubkey to keys@hprc.tamu.edu

Make sure it is pub key not private key

Wait for approval email

Log in via jump host

Sample Job Script Structure (FASTER)

```
#!/bin/bash
##NECESSARY JOB SPECIFICATIONS
#SBATCH --export=NONE
#SBATCH --get-user-env=L
#SBATCH --job-name=JobExample1
#SBATCH --time=01:30:00
#SBATCH --ntasks=1
#SBATCH --mem=2G
#SBATCH --output=stdout.%j

##OPTIONAL JOB SPECIFICATIONS
#SBATCH --account=123456
#SBATCH --mail-type=ALL
#SBATCH --mail-user=email_address

# load required module(s)
module purge
module load Python/3.7.0-intel-2018b

./my_program.py
```

These parameters describe your job to the job scheduler

Account number to be charged

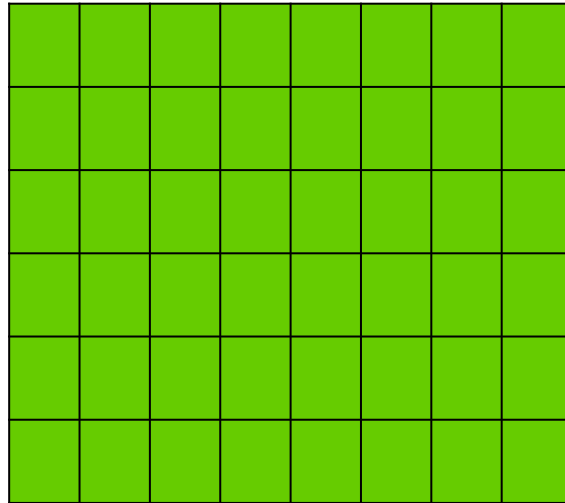
This is single line comment and not run as part of the script

Load the required module(s) first

This is a command that is executed by the job

Mapping Jobs to Cores per Node on FASTER

A.

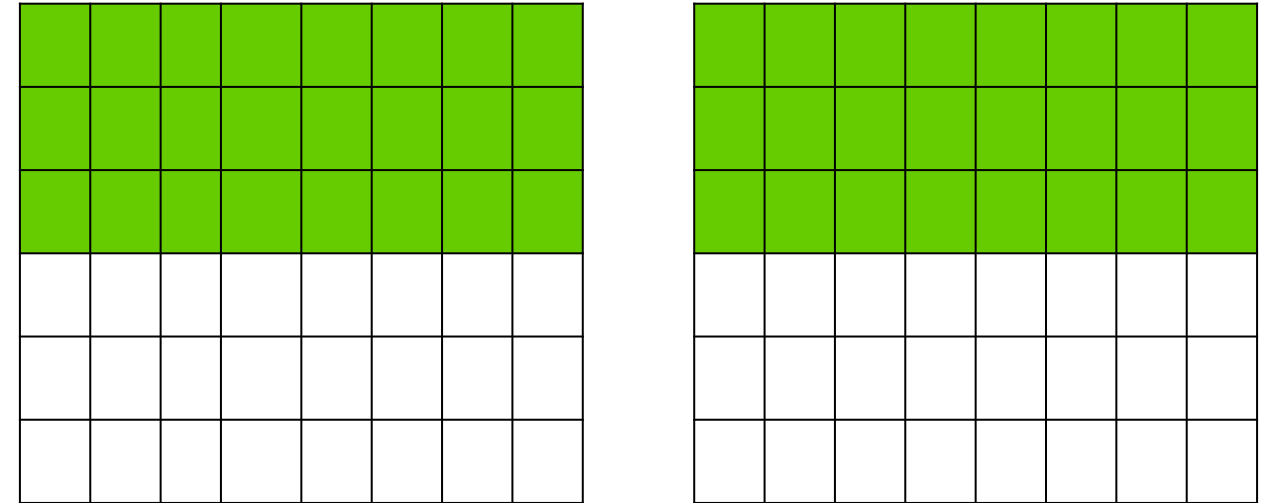


64 cores on
1 compute node

#SBATCH --ntasks=64
#SBATCH --tasks-per-node=64

Preferred Mapping
(if applicable)

B.



64 cores on
2 compute nodes

#SBATCH --ntasks=64
#SBATCH --tasks-per-node=32

Important Batch Job Parameters

FASTER	Comment
#SBATCH --export=NONE #SBATCH --get-user-env=L	Initialize job environment.
#SBATCH --time=HH:MM:SS	Specifies the time limit for the job.
#SBATCH --ntasks=NNN	Total number of tasks (cores) for the job.
#SBATCH --ntasks-per-node=XX	Specifies the maximum number of tasks (cores) to allocate per node
#SBATCH --mem=nnnnM or #SBATCH --mem=nG (memory per NODE)	Sets the maximum amount of memory (MB). G for GB is supported on FASTER

hprc.tamu.edu/wiki/HPRC:Batch_Translation

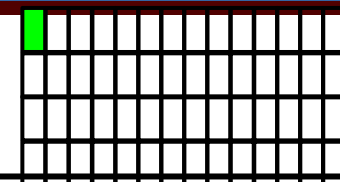
Pop Quiz

```
#SBATCH --export=NONE
#SBATCH --get-user-env=L
#SBATCH --job-name=stacks_S2
#SBATCH --ntasks=80
#SBATCH --ntasks-per-node=20
#SBATCH --mem=40G
#SBATCH --time=48:00:00
#SBATCH --output=/scratch/user/dylan/stdout.%J
#SBATCH --error stderr.%J
```

How many nodes is this job requesting?

- A. 1600
- B. 80
- C. 20
- D. 4

FASTER Job File (Serial Example)



```
#!/bin/bash
##ENVIRONMENT SETTINGS; CHANGE WITH CAUTION
#SBATCH --export=NONE          # Do not propagate environment
#SBATCH --get-user-env=L       # Replicate login environment

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample1 # Set the job name to "JobExample1"
#SBATCH --time=01:30:00        # Set the wall clock limit to 1hr and 30min
#SBATCH --ntasks=1             # Request 1 task (core)
#SBATCH --mem=2G               # Request 2GB per node
#SBATCH --output=stdout.%j     # Send stdout and stderr to "stdout.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
#SBATCH --account=123456       # Set billing account to 123456
#SBATCH --mail-type=ALL        # Send email on all job events
#SBATCH --mail-user=email_address # Send all emails to email_address

# load required module(s)
module purge
module load intel/2018b

# run your program
./myprogram
```

SUs = 1.5

Job Memory Requests on FASTER

Specify memory request based on memory per node:

#SBATCH --mem=xxxxM # memory per node in MB

or

#SBATCH --mem=xG # memory per node in GB

Job Submission and Tracking

FASTER command	Description
sbatch jobfile	Submit jobfile to batch system
squeue [-u user_name] [-j job_id]	List jobs
scancel job_id	Kill a job
sacct -X -j job_id	Show information for a job (can be when job is running or recently finished)
sacct -X -S YYYY-HH-MM	Show information for all of your jobs since YYYY-HH-MM
lnu job_id	Show resource usage for a job
pestat -u \$USER	Show resource usage for a running job
seff job_id	Check CPU/memory efficiency for a job

hprc.tamu.edu/wiki/HPRC:Batch_Translation

Job submission issue: insufficient SUs

```
$ sbatch myjob
sbatch: error: (from job_submit) your account's balance is
not sufficient to submit your job
      Project Account: 123940134739
      Account Balance: 382.803877
      Requested SUs:    18218.6666666667
```

What to do if you need more SUs

Ask your PI to transfer SUs to your account

Apply for more SUs (if you are eligible, as a PI or permanent researcher)

Resource Composability on FASTER

- GPUs can be added to a job when it is submitted by using the “gres” option in a SLURM script.
- A researcher can request up to 12* GPUs on these CPU-GPU nodes.
- This approach allows for more flexibility and options for node types (CPU only, CPU + GPU) available to users.

* Subject to change

Batch Queues

```
[ashwin_k@faster1 ~]$ sinfo
PARTITION    AVAIL  TIMELIMIT  JOB_SIZE  NODES(A/I/O/T)  CPUS(A/I/O/T)
cpu*         up      7-00:00:00  1-32      83/21/12/116    5123/1533/768/7424
gpu          up      7-00:00:00  1-32      6/36/10/52      98/2590/640/3328
atsp        down    2-00:00:00   1        0/8/2/10        0/512/128/640
staff        up      2-00:00:00   1        89/65/24/178    5221/4635/1536/11392
```

FASTER

```
[u.ak118300@aces-login3 ~]$ sinfo
PARTITION    AVAIL  TIMELIMIT  JOB_SIZE  NODES(A/I/O/T)  CPUS(A/I/O/T)
cpu*         up      7-00:00:00  1-64      5/36/15/56      418/3518/1440/5376
gpu          up      2-00:00:00  1-15      14/0/2/16       29/1315/192/1536
pvc          up      2-00:00:00  1-15      2/7/11/20       96/768/1056/1920
atsp        up      2-00:00:00   1        0/3/1/4         0/288/96/384
bittware     up      2-00:00:00   1        0/2/0/2         0/192/0/192
d5005        up      2-00:00:00   1        0/2/0/2         0/192/0/192
gpu-hybrid   up      2-00:00:00  1-infinite 15/7/13/35     121/1991/1248/3360
```

ACES

For the NODES and CPUS columns:

A = Active (in use by running jobs) I = Idle (available for jobs)

O = Offline (unavailable for jobs) T = Total

Additional information:

<https://hprc.tamu.edu/kb/User-Guides/FASTER/Batch/#batch-queues>

- Job submissions are auto-assigned to batch queues based on the resources requested (e.g. cpu vs. gpu).
- Use 'sinfo' to check on their status: