Introduction to HPRC Computing Resources

September 12, 2025

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High Performance
Research Computing
DIVISION OF RESEARCH

Outline

- **Introduction**
  - Setup
  - Usage Policies
  - HPRC Cluster Overview
- **Getting Started**
  - Accessing HPRC Clusters
  - HPRC Portal
- **Software Infrastructure**
  - Module System
  - Python Virtual Environments
- **Cluster Computing with Slurm**
- **Need Help?**

Introduction

Setup For This Course

To access the resources:

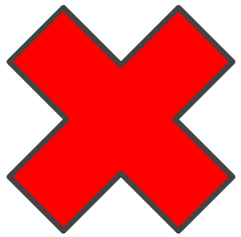
- HPRC Account: https://hprc.tamu.edu/user_services/#accounts
- TFA set up: https://it.tamu.edu/duo

To do the exercises:

- Basic Linux/Unix skills
  - Slides from our Linux short course are at: hprc.tamu.edu/training/intro_linux.html
  - Watch the relevant Introduction and Primer videos on our YouTube Channel: https://www.youtube.com/texasamhprc

Answers to frequently asked questions can be found on our Knowledge Base (KB): https://hprc.tamu.edu/kb/FAQ/Accounts

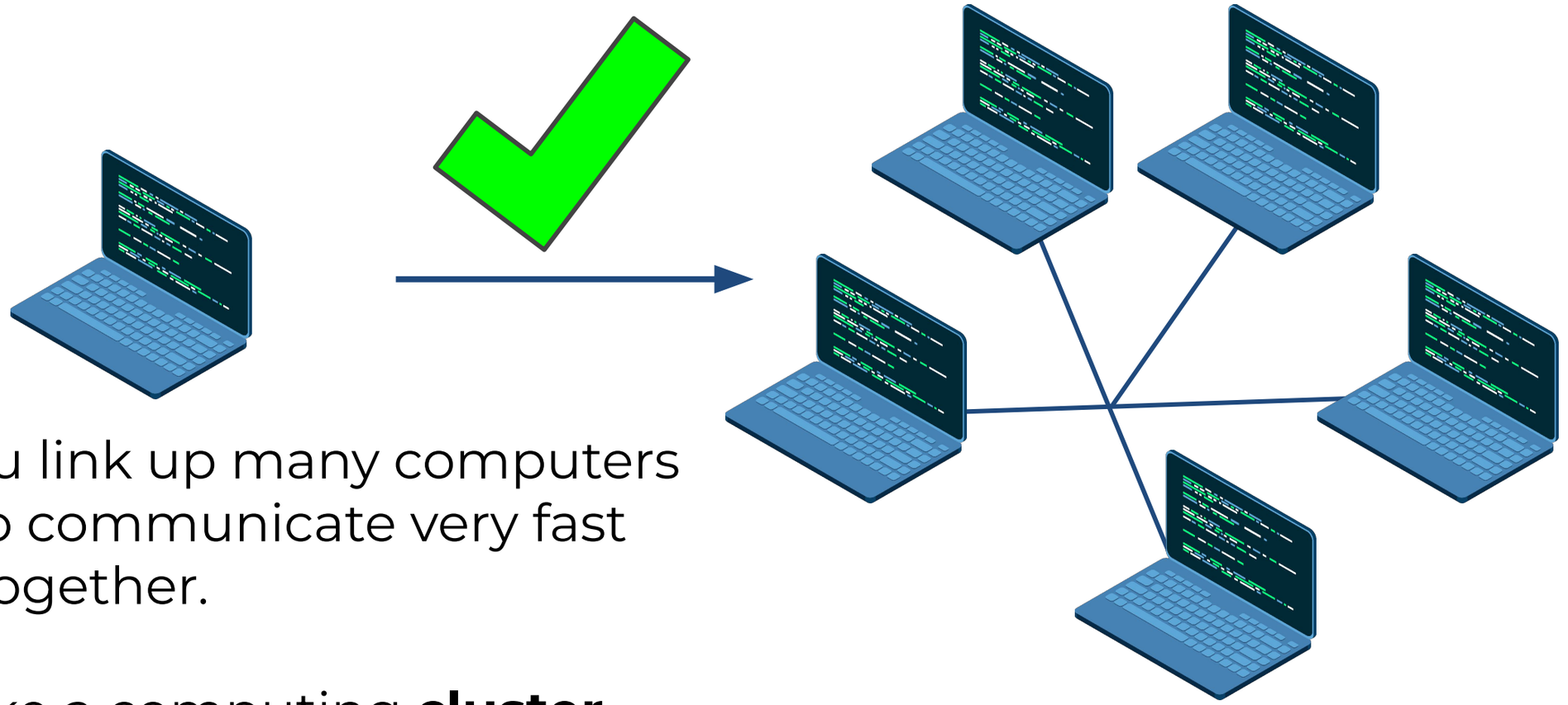
What is Supercomputing?



You have a workflow that's too big for your personal machine

...But you don't just get a bigger computer...

What is ~~Super~~Cluster computing?



Instead, you link up many computers (“nodes”) to communicate very fast and work together.

I.e. you make a computing **cluster.**

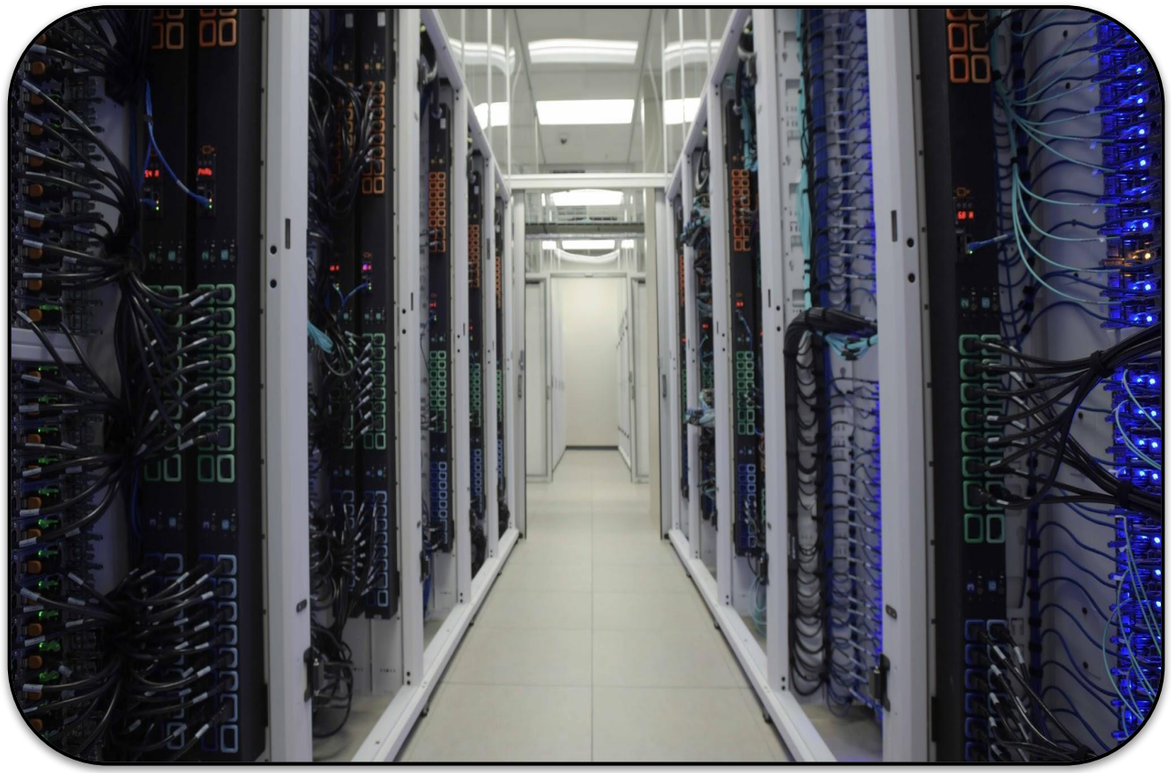
Clusters Are For You!

What kinds of problems are solved by cluster computing?

- Problems that are too big to fit in a laptop or workstation, due to limitation on memory, core count, gpu count, etc.
- Problems that scale well with more CPU cores or memory
- Single-threaded problems with many permutations
- Problems that require large high speed storage and/or interconnect

HPRC Clusters

- We operate five clusters
- Today we'll focus on just one: **Grace**
  - It is our largest cluster
  - It is dedicated for TAMU usage

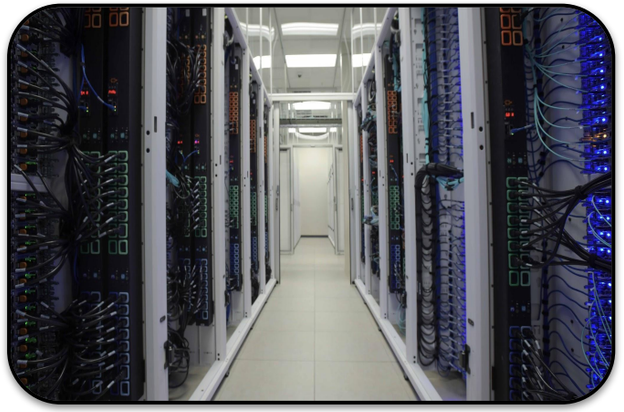


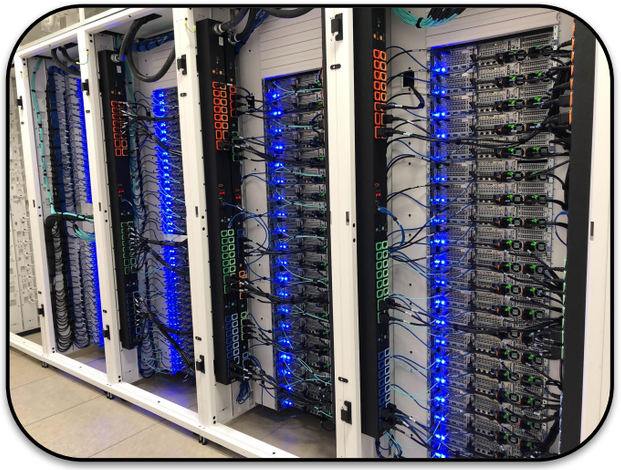
Others:

- Launch
- ViDaL
- FASTER
- ACES

See hprc.tamu.edu/resources for more info on all our clusters

Grace Overview

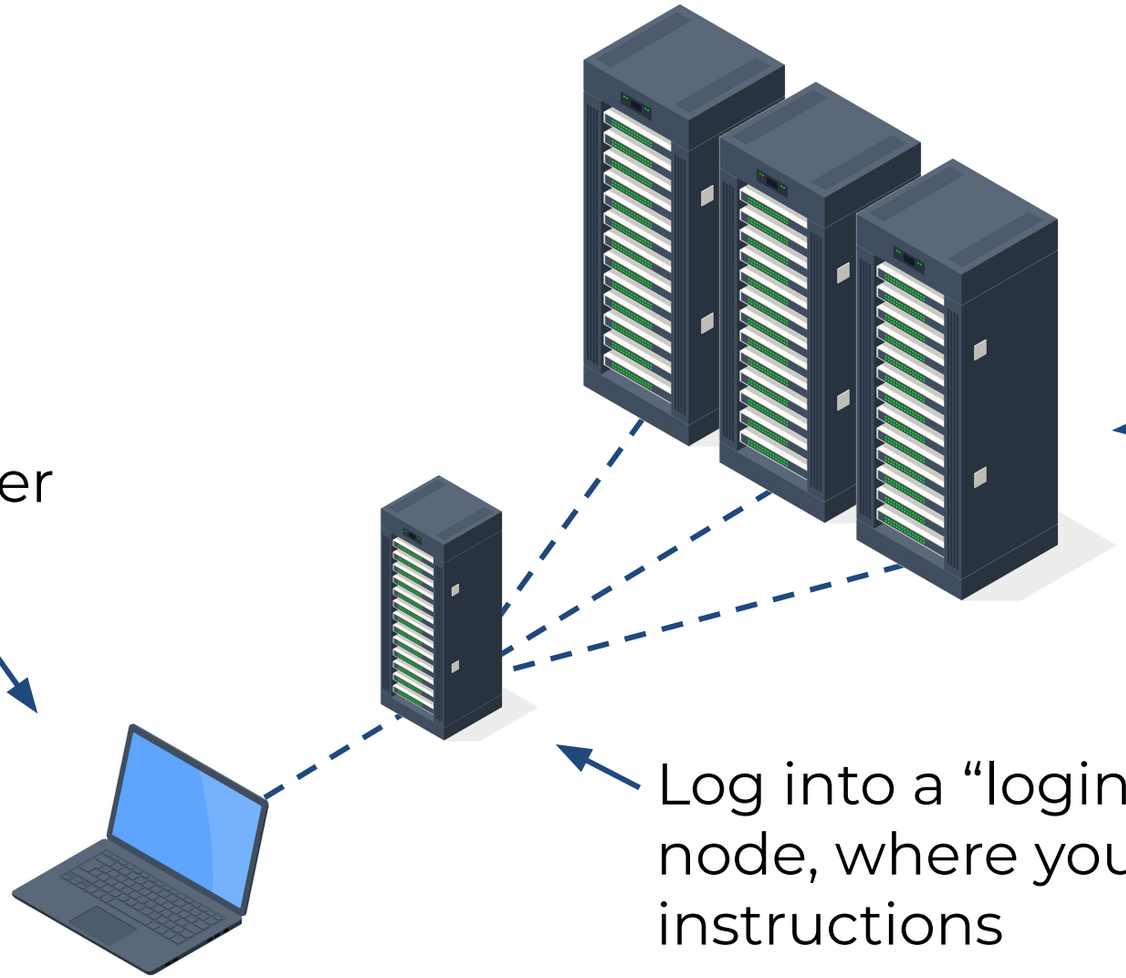




Host Name:	grace.hprc.tamu.edu
Operating System:	Linux (RHEL 8)
Total Compute Cores/Nodes:	45,376 cores 940 nodes
Compute Nodes:	800 48-core compute nodes 100 48-core GPU nodes, each with two A100s 9 48-core GPU nodes, each with two RTX 6000s 8 48-core GPU nodes, each with 4 T4s 15 48-core GPU nodes, each with two A40s 8 80-core large memory nodes, each with 3TB RAM
Interconnect:	Mellanox HDR 100 InfiniBand
Peak Performance:	6.3 PFLOPS

More details at: https://hprc.tamu.edu/kb/User-Guides/Grace

Computing on HPRC Clusters



You interact with your own computer

Make login node send instructions to “compute nodes” to do the heavy-lifting

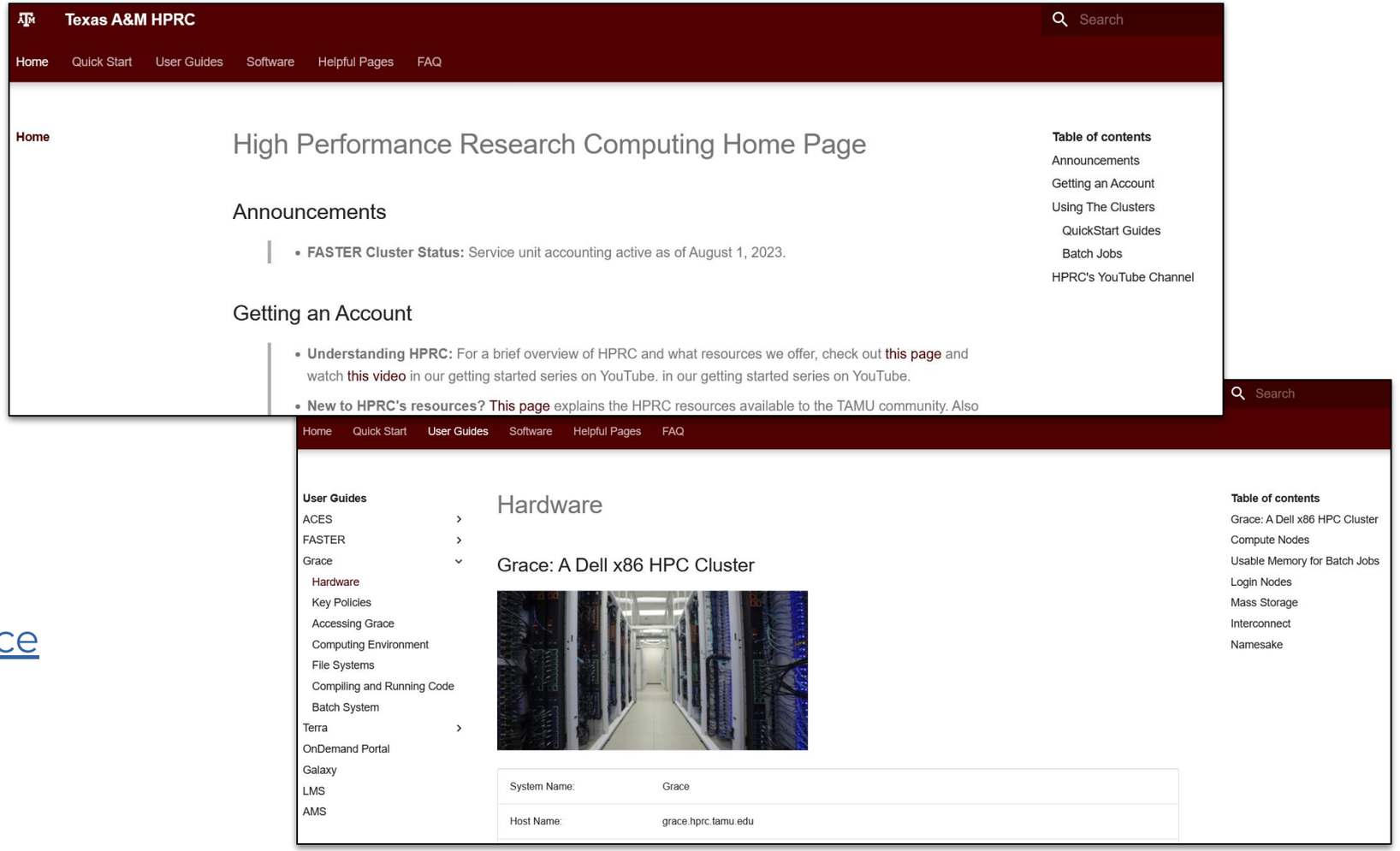
Log into a “login” node, where you write instructions

(This image is not to-scale: we have way more machines than this!)

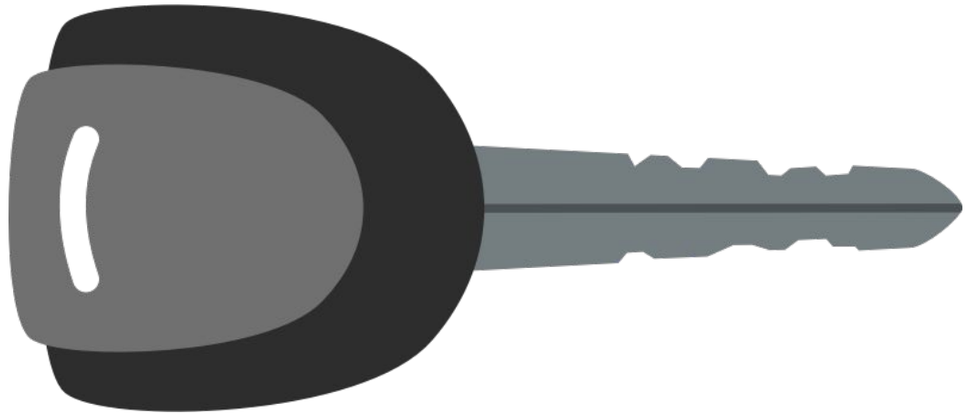
HPRC Knowledge Base

See our Knowledge Base for announcements, more hardware details, and more about the subjects we cover today.

hprc.tamu.edu/kb
hprc.tamu.edu/kb/User-Guides/Grace



Getting Started



Usage Policies
(Be a good compute citizen)

- It is illegal to share computer passwords and accounts by state law and university regulation.
- It is prohibited to use HPRC clusters in any manner that violates the United States export control laws and regulations, EAR & ITAR.
- Abide by the expressed or implied restrictions in using commercial software .

hprc.tamu.edu/policies

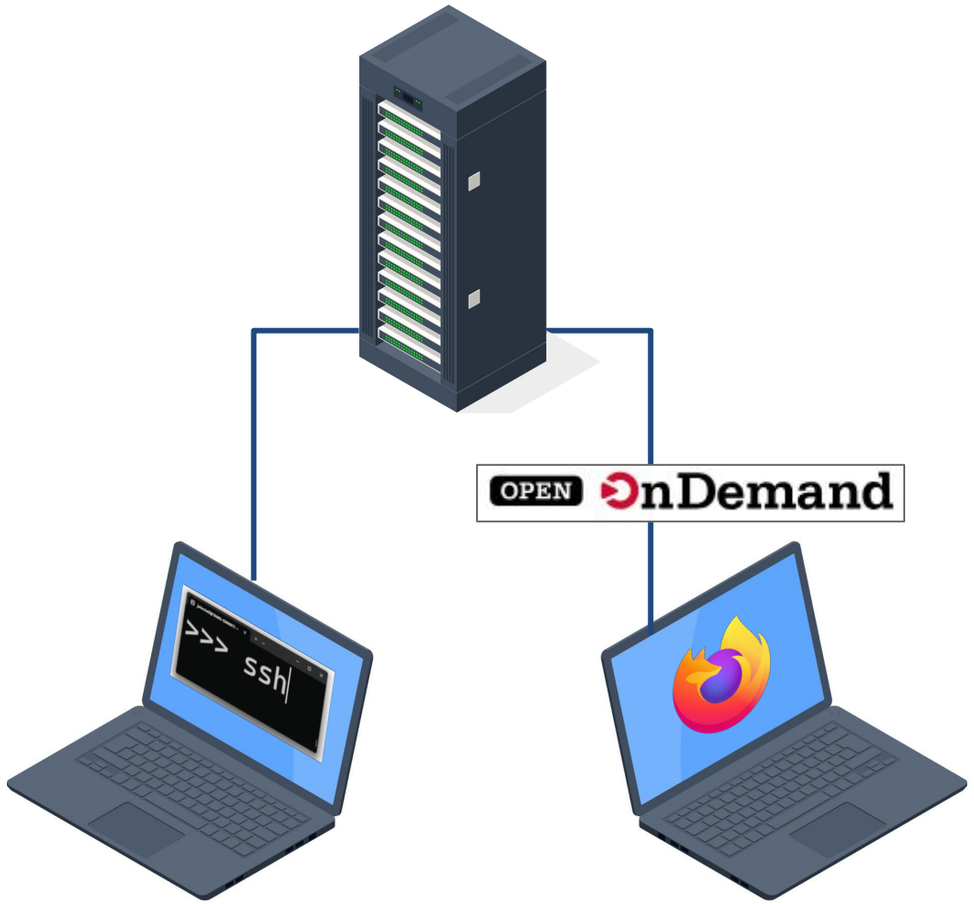
Getting on a Cluster

There are two ways you can access the Grace and FASTER clusters:

1. Using ssh (or related tools) on your local command line

2. Through the Open OnDemand portal in a web browser

If you like Linux, you can use option 1.
You can also use Linux in option 2
–but you don't have to!



Accessing Clusters 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* PowerShell Windows Command Prompt PuTTY SSH	Terminal*	Terminal*
* Recommended			

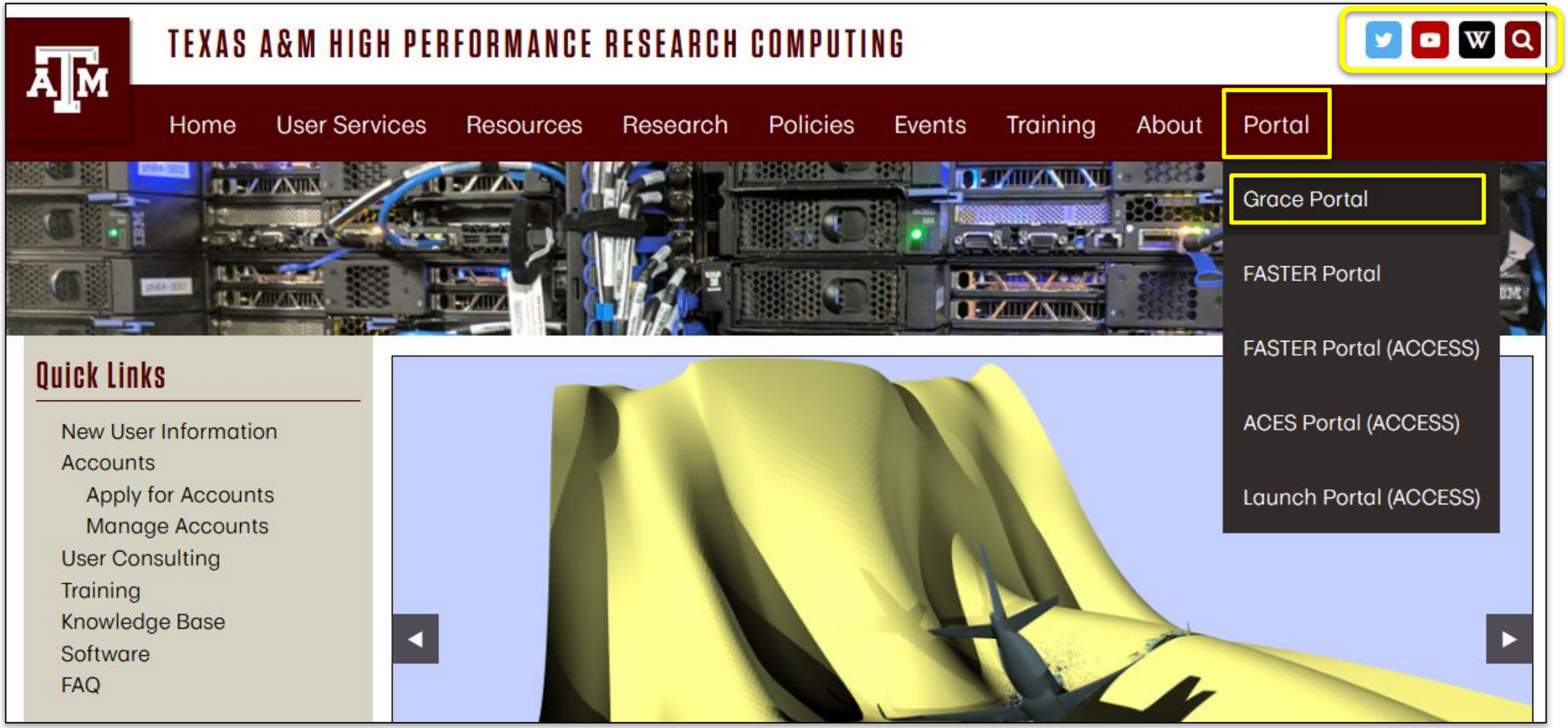
- If off-campus, connect with VPN first: u.tamu.edu/VPnetwork
- If on-campus or connected to VPN, log in with:

```
ssh NetID@grace.hprc.tamu.edu
```

Green box/highlights = text typed into a shell

Accessing Clusters via Portal

- (First, if you're off-campus, connect to TAMU VPN: u.tamu.edu/VPnetwork)
- HPRC webpage: hprc.tamu.edu: Portal dropdown menu



HPRC Portal

TAMU HPRC OnDemand (Grace) | Apps | Files | Jobs | Clusters | Interactive Apps | Dashboard | Utilities | My Interactive Sessions | Help | Logged in as jwinchell | Log Out

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

Pinned Apps A featured subset of all available apps

- Drona Composer (dev) — System Installed App
- Drona Composer — System Installed App
- Grace Dashboard (BETA) — System Installed App
- Grace Dashboard — System Installed App
- Chatbot — System Installed App
- grace Shell Access — System Installed App
- Jupyter Notebook — System Installed App

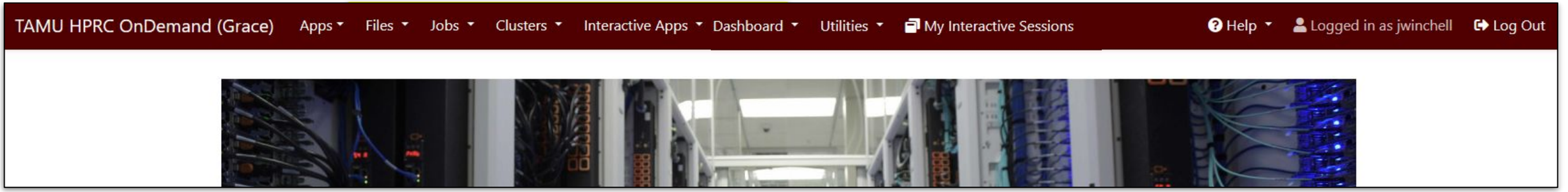
Message of the Day

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. Current HPRC staff members are US citizens and legal residents.**
- **Sharing HPRC account and password information is in violation of State Law. Any shared accounts will be DISABLED.**
- **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 Portal Overview



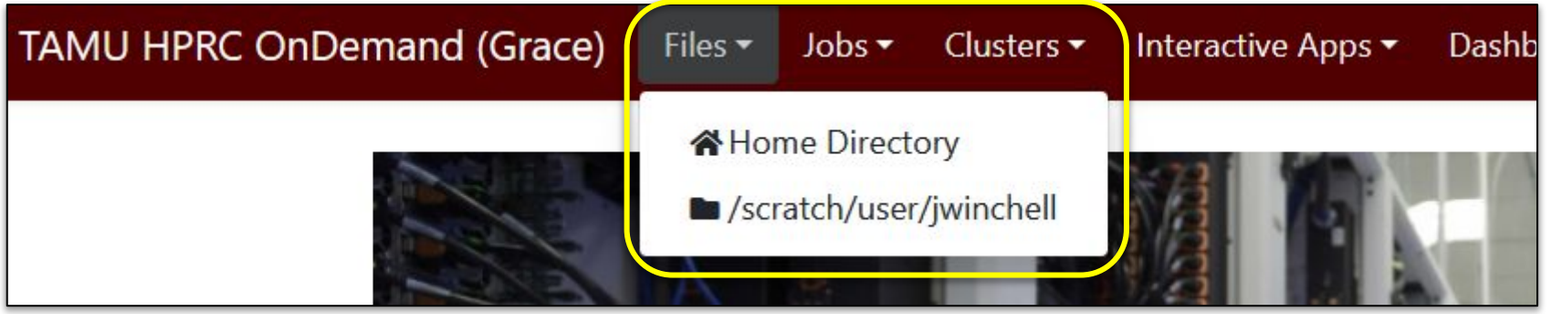
TAMU HPRC OnDemand (Grace): (click to return to portal homescreen)

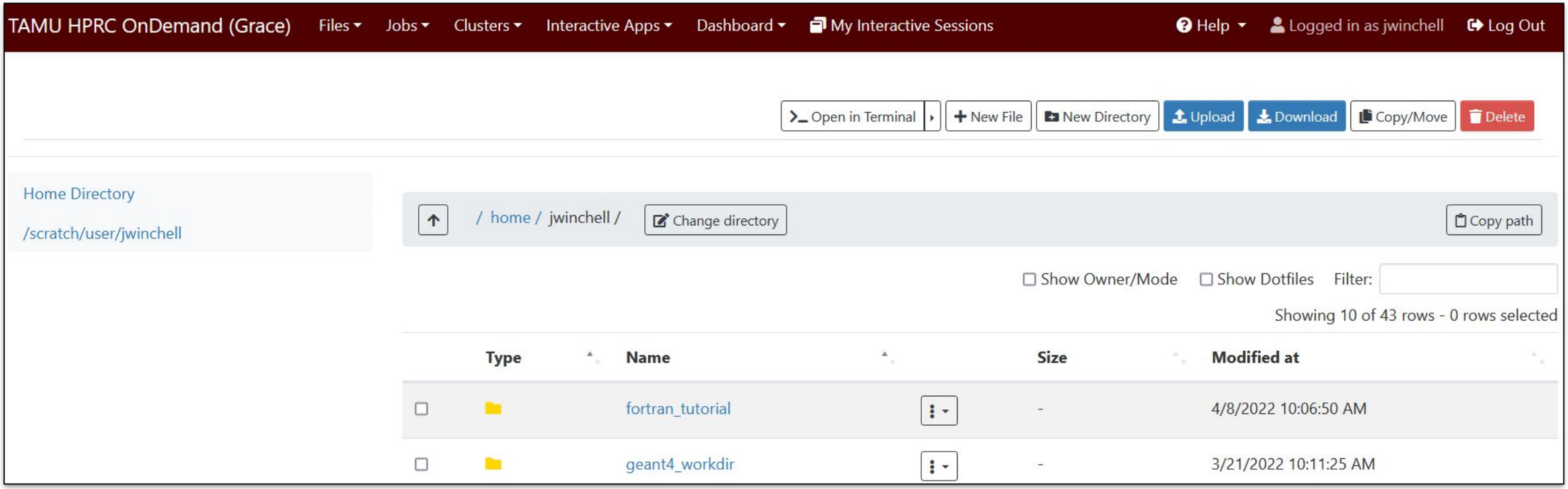
Apps:	collection of functions from other tabs
Files:	file browser on the cluster
Jobs*:	submit and monitor cluster jobs
Clusters:	open a shell terminal (command line) on a login node
Interactive Apps*:	start graphical software on a compute node
Dashboard:	view file quotas and computing account allocations
Utilities:	check cluster status
My Interactive Sessions*:	check interactive app status

(We'll talk about these three later)

Portal File Browser

The Portal includes a file browser in which you can do many of the things a terminal would do… or just launch a terminal.





File Systems and User Directories

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

`$SCRATCH` is shared between FASTER (TAMU/ACCESS) and Grace (TAMU) clusters.

View file usage and quota limits on the command line with: **`showquota`**

Do **NOT** share your home or scratch directories.

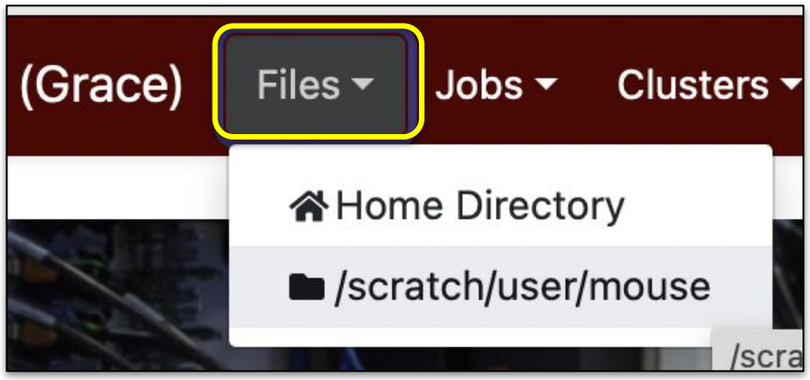
Request a group directory for sharing files using the portal Dashboard.

Note also: we are providing **work** space, not **storage** space.

Your data will be there as long as your account is active, but after that–no promises!

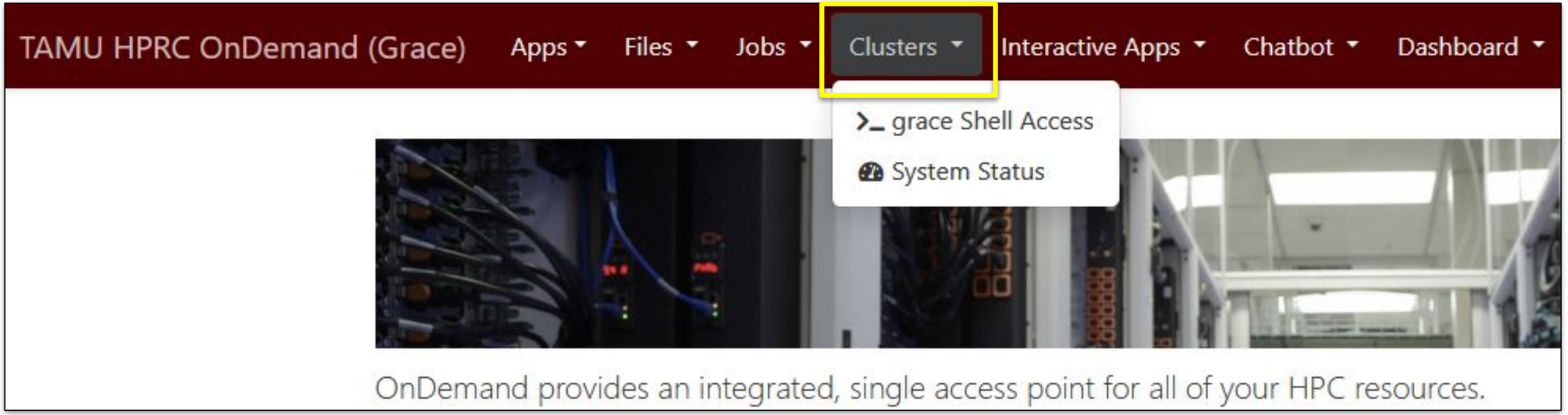
Hands-on Exercise

1. Enter your Scratch directory from the Portal:
   Files ➜ `/scratch/user/<NetID>`
2. Create or upload a file.
3. Move the file to your home directory.



Linux Command Line

- In Portal: “Clusters” dropdown ➜ “Shell Access”



Linux Command Line

```
********************************************************************************
This computer system and the data herein are available only for authorized
purposes by authorized users. Use for any other purpose is prohibited and may
result in disciplinary actions or criminal prosecution against the user. Usage
may be subject to security testing and monitoring. There is no expectation of
privacy on this system except as otherwise provided by applicable privacy laws.
Refer to University SAP 29.01.03.M0.02 Acceptable Use for more information.
********************************************************************************

Password:
Duo two-factor login for username

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...
Last login: Tue Sep  3 16:54:20 2025 from 128.194.35.38
```

Type in your NetID password (it won't show anything as you type)

Then sign in with TFA

Linux Command Line

```
      ========================================================================
   |          Texas A&M University High Performance Research Computing          |
   |                                                                            |
   | Website:              https://hprc.tamu.edu                                |
   | Consulting:           help@hprc.tamu.edu (preferred) or (979) 845-0219 |
   | ACES Documentation:    https://hprc.tamu.edu/kb/User-Guides/ACES      |
   | FASTER Documentation: https://hprc.tamu.edu/kb/User-Guides/FASTER    |
   | Grace Documentation:   https://hprc.tamu.edu/kb/User-Guides/Grace     |
   | Terra Documentation:   https://hprc.tamu.edu/kb/User-Guides/Terra     |
   | YouTube Channel:      https://www.youtube.com/texasamhprc            |
      ========================================================================

  **************************************************************************
 *                 === IMPORTANT POLICY INFORMATION ===                     *
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 *   Texas State Law. Any shared accounts will be DISABLED.                 *
 * - Authorized users must also adhere to ALL policies at:                  *
 *                       https://hprc.tamu.edu/policies/                        *
  **************************************************************************

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

      Please restrict usage to 8 CORES across ALL login nodes.
      Users found in violation of this policy will be SUSPENDED.

            To see these messages again, run the motd command.

Your current disk quotas are:
Disk                       Disk Usage    Limit  File Usage    Limit
/home/username                  899M    10.0G        7259    10000
/scratch/user/username        477.7G    1.0T       165425   250000
/scratch/group/group1          32.9T    60.0T     5322917   15000000
  * Quota increase for /scratch/group/group1 will expire on Aug 26, 2026
Type 'showquota' to view these quotas again.
username@login3:~$
```

Prints out a lot of text on successful login:

Message of the day & policy info

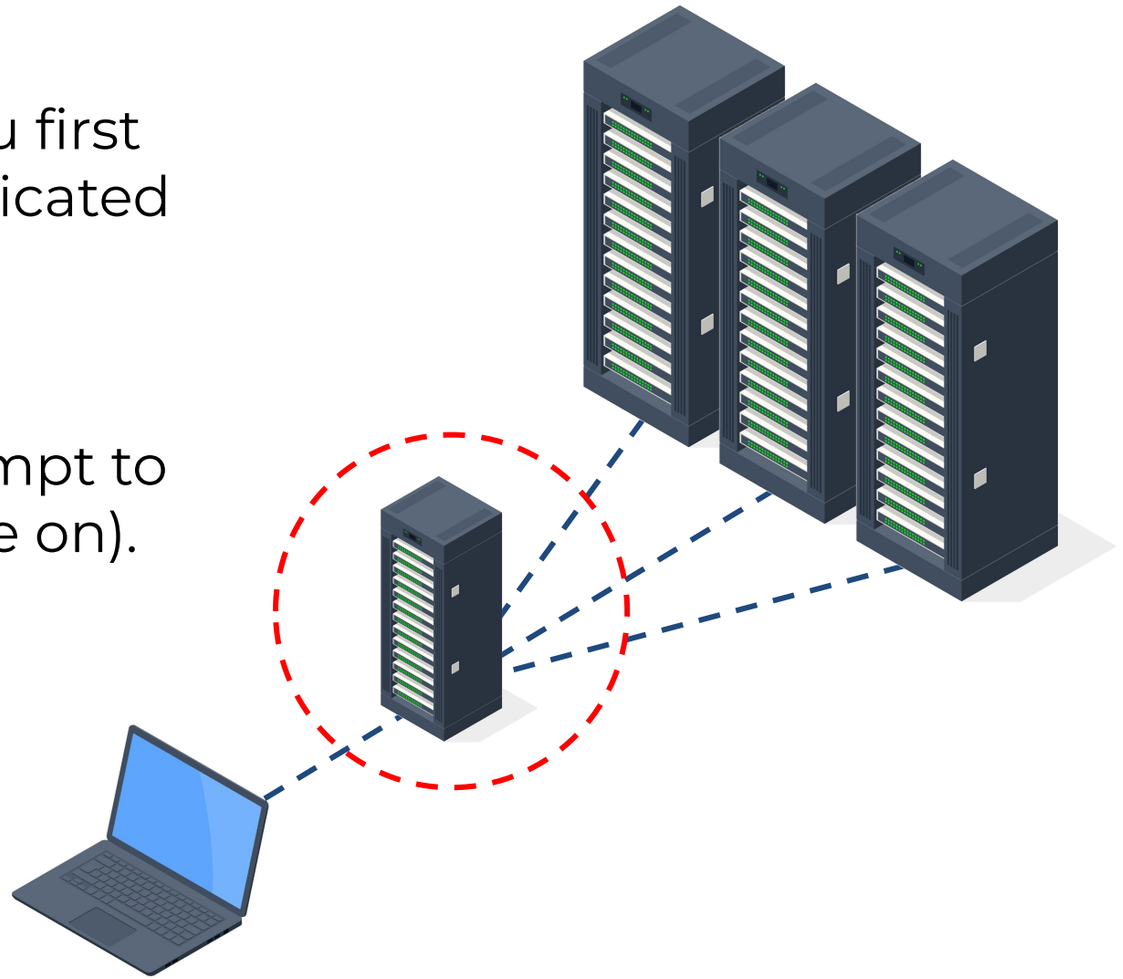
Your quota info

Command Prompt

Logged-In

Remember, when you first log in, you are on dedicated *login nodes*.

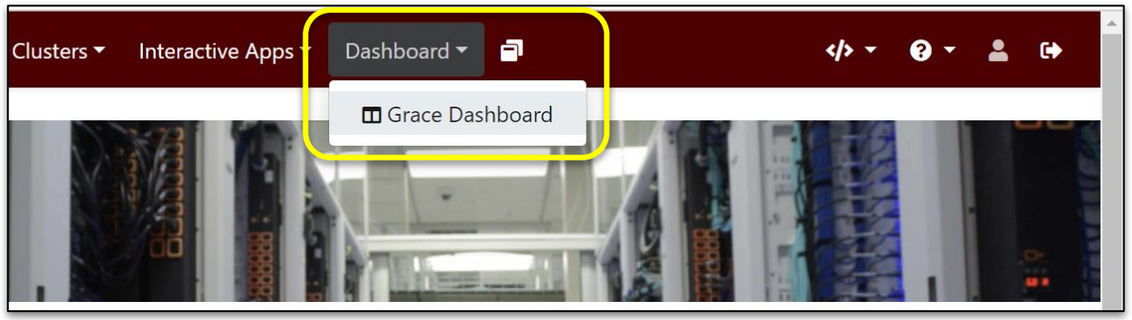
Grace has 5 of them (check your shell prompt to see which one you are on).



These are not for running big processes!
There are rules:

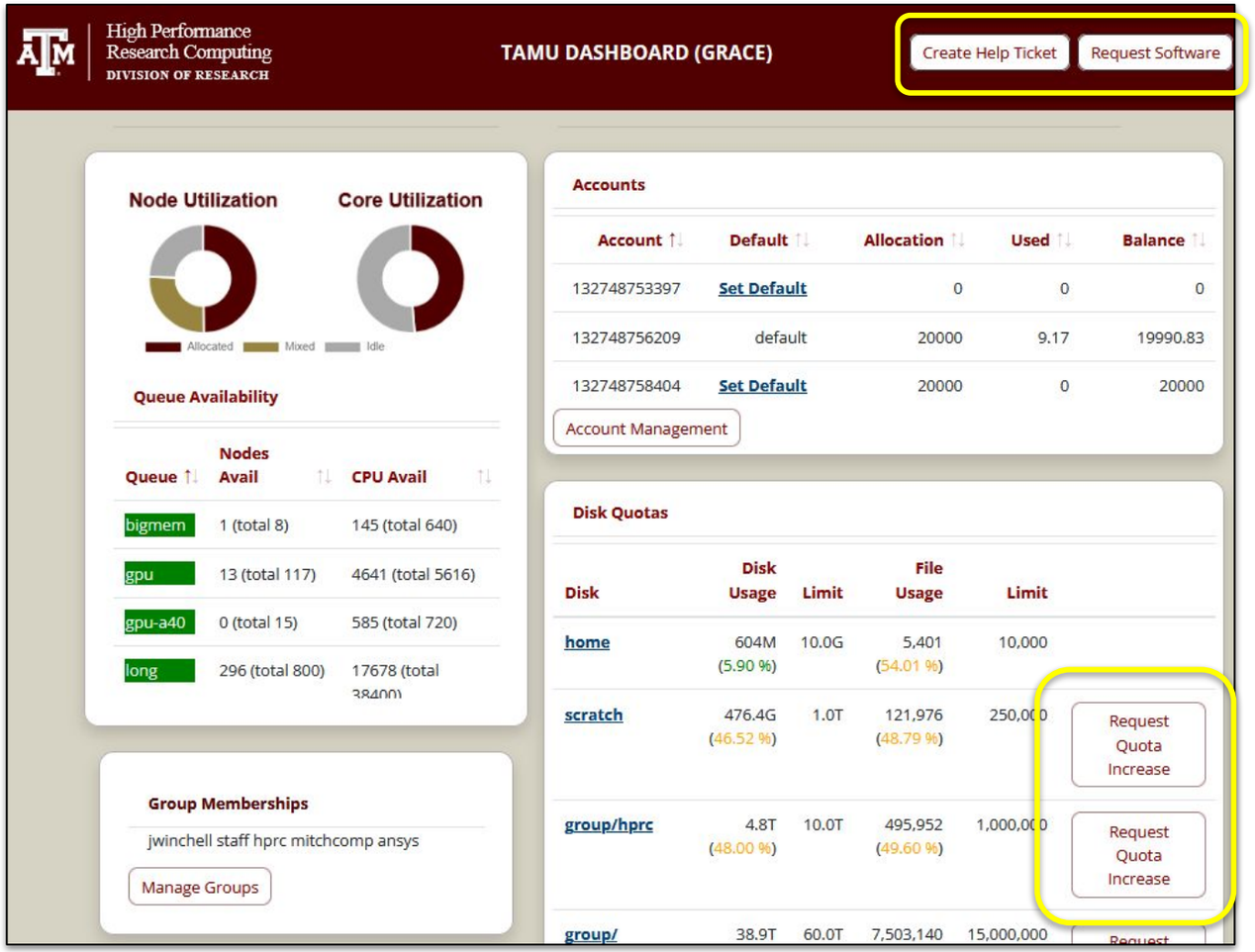
- No processes longer than 1 hr
- Sessions idle for 1 hr will be killed.
- Do not use more than 8 cores.
- Do not use `sudo`.

HPRC Portal Dashboard



Summarizes cluster status and your current usage

Note the buttons: these are the preferred way to request support!



Hands-on Exercise

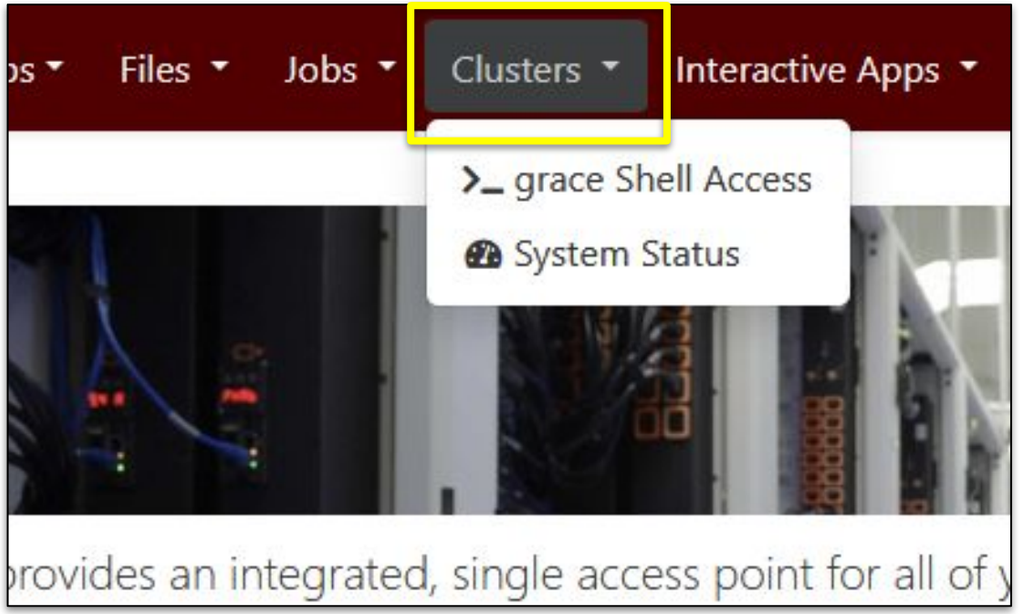
Check your file Quota:

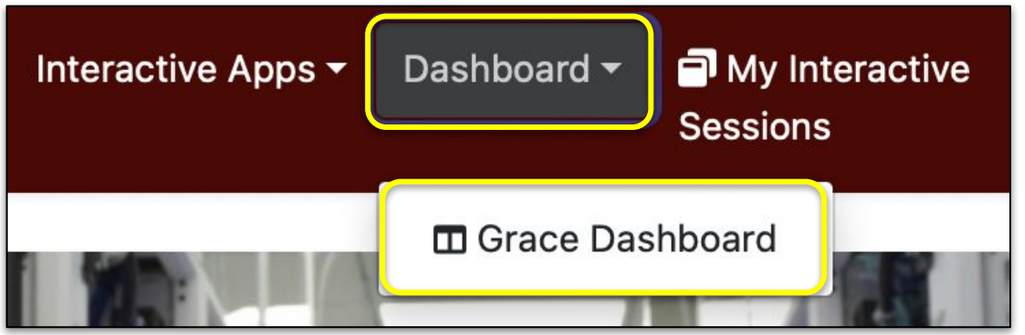
1. In the Portal:
   Dashboard ➜ Grace Dashboard

2. In the shell:
   (use `showquota`)

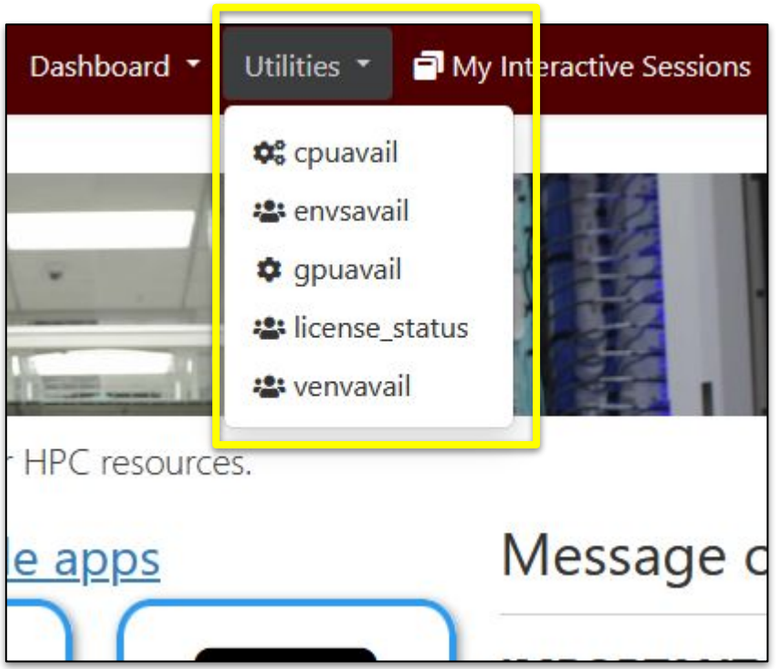
3. Locate your /scratch disk usage stats.

They should match!





Utilities



See availability of hardware, licenses, and environments.

(You can also call these on the command line)

Grace OnDemand Portal / Grace GPU Availability

Grace GPU Availability

This displays the CONFIGURATION of installed GPUs and the status of GPUs readily available for jobs.

GPUs and GPU nodes not in the AVAILABILITY table are busy with other jobs and will be available after jobs have completed.

Output generated: **2025-09-03 16:04:39**

```
$ gpuavail
```

CONFIGURATION	
NODE TYPE	NODE COUNT
gpu:a100:2	100
gpu:a40:3	15
gpu:rtx:2	9
gpu:t4:4	8

AVAILABILITY

Grace OnDemand Portal / Grace License Status

Grace License Status

Output generated: **2025-09-03 16:05:21**

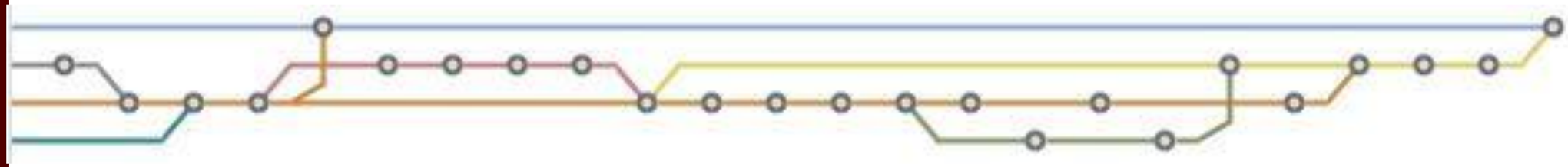
```
$ license_status -a
```

Abaqus | ANSYS | COMSOL | ConvergeCFD | ECLIPSE | FDTD | FEMZIP | FLOW3D | Hyperworks | Intel | INTERSECT | LS-DYNA | Madymo | Matlab | Matlab_MDCS | Metashape | MOE | Oasys | PGI_compilers | StarCCM | Schrodinger |

License status for Abaqus:

License Name	# Issued	# In Use	# Available
abaqus_teaching	320	0	320
abaqus_extended_teaching	40	0	40
cse_teaching	1	0	1

Software Infrastructure

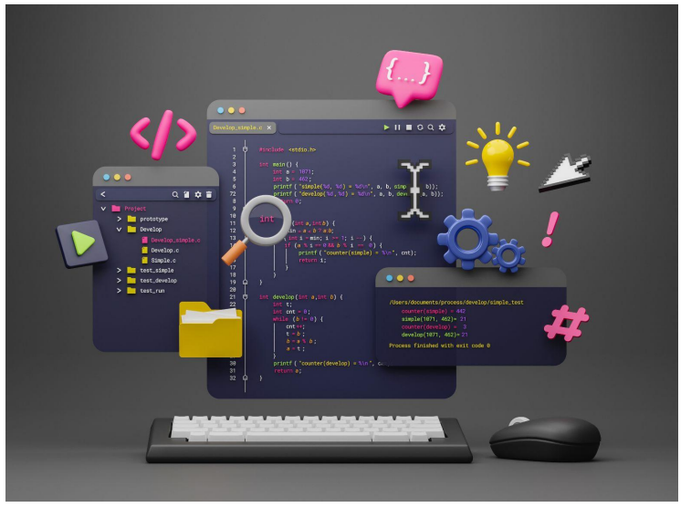


Software

- HPRC provides both pre-installed software and installation assistance.
- See the Software pages for instructions and examples:
  - hprc.tamu.edu/kb/Software
  - hprc.tamu.edu/software
- License-restricted software
  - Check on command line with `license_status` (example later)
  - Contact help@hprc.tamu.edu
- Contact us for software installation help/request (can use dashboard).
  - User can install software in their home/scratch directories.
  - Do NOT run the "`sudo`" command when installing software.

Computing Environment

- `PATH`: the location on disk where an executable or library may be found.
- Paths are saved as environment variables, so you can choose which libraries and executables will be used by modifying the variables.
- There is a lot of software, many versions, and many paths to manage.



..... How do you manage all these softwares?

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

Modules

Managing software versions using `lmod`

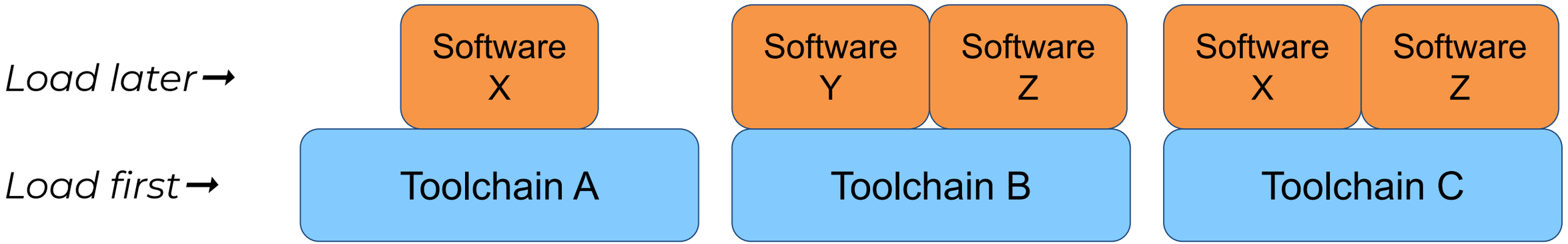
- Each version of a software, application, library, etc. is available as a module.
  - Module names have the format:

```
software-name/version[-dependency-version (optional)]
TensorFlow/2.11.0-CUDA-11.7.0
```

- Loading a module adds its location on disk to your `Path` environment variable.
  - You may have to load some of its dependencies, though

Modules

- Modules are organized *hierarchically*.
- The base modules that must be loaded before anything else are called “Toolchains”:
  - The same software may be available from multiple toolchains.
  - Do not mix up software from different toolchains!
- Loading the toolchain makes other modules available.



Modules: Search for Software

`module avail`

- Lists all available modules (may be slow).
- Navigation:
  -spacebar, arrows, or `j` and `k`
  -quit with `q`
- Case-sensitive search: `/`
- Use **`mla`** instead to save results to a file as well (will be named `module.avail.aces` or similar)

`module spider <word>`

- Case-sensitive search for modules with “word” in name.
- Provide an exact name to see dependencies.

```
jwinchell@login5:~$ module spider Python

----------------------------------------------------------------------------------------------------------------------------------
  Python:
----------------------------------------------------------------------------------------------------------------------------------
    Description:
      Python is a programming language that lets you work more quickly and integrate your systems more effectively.

     Versions:
        Python/2.7.18-bare
        Python/2.7.18
        Python/3.8.6
        Python/3.9.5-bare
        Python/3.9.5
        Python/3.9.6-bare
        Python/3.9.6
        Python/3.10.4-bare
        Python/3.10.4
        Python/3.10.8-bare
        Python/3.10.8
        Python/3.11.3
        Python/3.11.5
        Python/3.12.3
        Python/3.13.1
     Other possible modules matches:
        Biopython  Boost.Python  Brotli-python  GitPython  IPython  Python-bundle-PyPI  bx-python  cuda_python  flatbuffers-python
...
```

Modules: Manage Software

`module list`

- See what modules are loaded in your current session

`module load <module>`

- add <module> paths to the current environment variables

`module purge`

- Unload all modules

```
jwinchell@login5:~$ module list
No modules loaded
jwinchell@login5:~$ module load GCCcore/14.2.0
jwinchell@login5:~$ module list

Currently Loaded Modules:
  1) GCCcore/14.2.0

jwinchell@login5:~$ module purge
jwinchell@login5:~$ module list
No modules loaded
jwinchell@login5:~$
```

There is also a shorthand:

```
ml
ml <module>
ml purge
```

Module Usage Example

```
mla snakemake
```

Search for the software “snakemake”; it saves a file of available modules.

```
snakemake/5.26.1-Python-3.8.2
snakemake/6.1.0
snakemake/6.10.0
snakemake/7.22.0
snakemake/7.32.3
snakemake/8.4.2
```

Choose a specific version and use it to search for its dependencies.

```
module spider snakemake/8.4.2
```

```
----------------------------------------------------------------------------
  snakemake: snakemake/8.4.2
----------------------------------------------------------------------------
     Description:
     The Snakemake workflow management system is a tool to create reproducible and scalable data analyses.

     You will need to load all module(s) on any one of the lines below before the "snakemake/8.4.2" module is
available to load.

     GCC/12.3.0  OpenMPI/4.1.5
```

Load the base dependency module(s) first then the full module name.

```
module load GCC/12.3.0  OpenMPI/4.1.5 snakemake/8.4.2
```

Hands-on Exercise: Module Loading

1. `mla blast+` -See which versions of BLAST+ are available.
2. `ml BLAST+/2.16.0` -error! You cannot do that yet.
3. `module spider BLAST+/2.16.0` -Learn how to load this module.
4. `ml _____ BLAST+/2.16.0` -Fill in the blank (with the correct toolchains) to load this module.
5. `ml list` -List all loaded modules.
6. `ml GCC/10.2.0` -Change version of a loaded Toolchain module (GCC); notice the message about reloaded modules.
7. `ml list` -List all loaded modules.
8. `ml purge` -Remove all loaded modules.

Module Commands Summary

- Commonly-used module commands
- Note that on there are some shorthands for you to use.

Command	Shorthand	Description
`module avail`	`mla` *(saves a searchable file as well)*	See what modules can be loaded now.
`module spider`	`ml spider`	Search for modules and find dependencies.
`module list`	`ml`	See what modules have been loaded already.
`module load foo bar`	`ml foo bar`	Load specified modules.
`module unload foo bar` `module load baz goo`	`ml -foo -bar baz goo`	Load and unload specified modules.
`module purge`	`ml purge`	Unload all modules.

Module Usage Practices

- Most software installed as modules are available to all users.
- It's a good habit to unload unused modules before loading new modules: `module purge`
- It is recommended to load a specific software version instead of the defaults: `ml GCC/13.2.0` instead of `ml GCC`
- Avoid loading modules in your $HOME/.bashrc
- Avoid mixing toolchains when loading multiple modules at the same time. This usually leads to one of them not working.

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

Python and Virtual Environments

Python is a language which supports many external libraries in the form of extensions–called Python Packages.

Some commonly used packages:

•SciPy •NumPy •Jupyter notebook •Scikit-learn

Once you have loaded the appropriate Python module, you can install these additional packages yourself using the *Virtual Environment* feature. Instructions are on our KB:

https://hprc.tamu.edu/kb/Software/Python/#hprc-venv-management-tools

Our HPRC student workers have developed a “create_venv” tool to help!

Hands-on Exercise: Python Software Install

1.
```
ml purge
ml GCCcore/13.2.0 Python/3.11.5
```
-Set up the underlying Python module

2.
```
create_venv myEnv
```
-Use HPRC's *create_venv* tool; Create a virtual environment in $SCRATCH/virtual_envs

3.
```
source activate_venv myEnv
```
-Activate virtual environment.

4.
```
python -c "import pytime"
```
-Check if python-time is installed (it is not).

5.
```
pip install python-time
```
-Install python-time.

6.
```
python -c "import pytime; print(pytime)"
```
-Where is python-time installed?

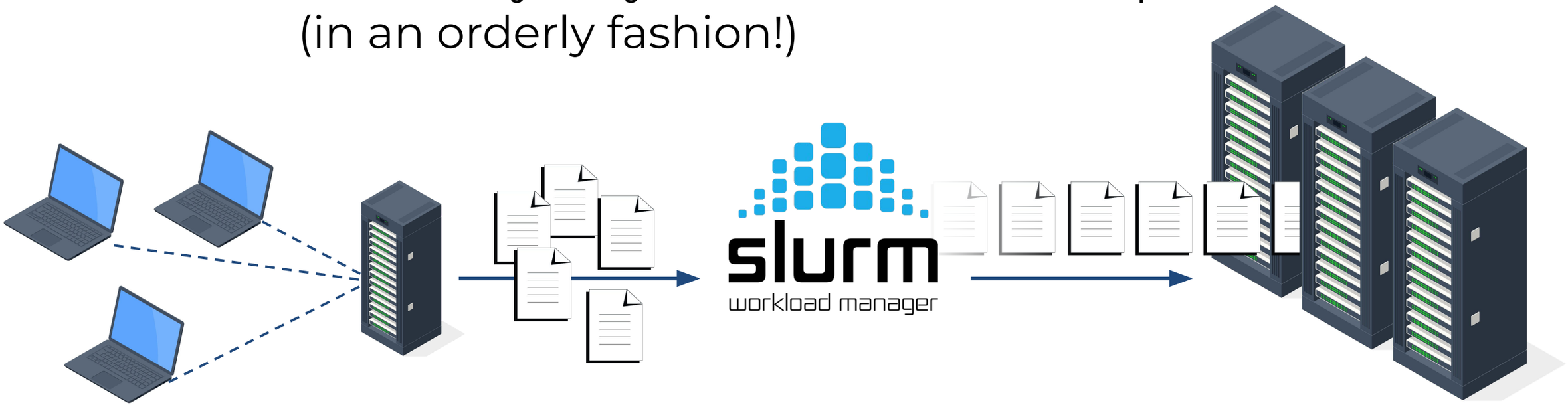
7.
```
deactivate
```
-Close virtual environment.

Cluster Computing

Batch Computing on HPRC Clusters: Overview

Since the cluster is a shared resource, jobs have to be moderated somehow so everyone has a turn. In short:

1. Write instructions on the login node
2. Give the instructions to Slurm
3. Slurm sends everybody's instructions to compute nodes (in an orderly fashion!)



Consumable Computing Resources

Computing resources are shared!

You will not be able to use an infinite amount!

- Resources external to jobs:
  - Service Unit (SU)
  - Software license/token
- Resources specified in a job file:
  - Processor cores
  - Memory
  - Wall time
  - GPU

Software Licenses

To check the availability of licensed software on the clusters, use the command **`license_status`**.

- List software the tool knows about:

```
license_status -l
```

- Help for this command:

```
license_status -h
```

- Find available license for "ansys":

```
license_status -s ansys
```

```
License status for ANSYS:
-------------------------------------------------------------
|License Name                |  # Issued|  # In Use|# Available|
-------------------------------------------------------------
|aa_mcad                     |        50|         0|         50|
|aa_r                        |        50|        32|         18|
|aim_mp1                     |        50|         0|         50|
|   ......                                                    |
-------------------------------------------------------------
```

Exact availability varies by license policy.
Contact us if you have questions.

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

Service Units

- Service Units (SUs) are part of our account management system (AMS).
- With a default (Basic) allocation, you start with 20,000 SUs.
- You are charged 1 SU per core-hour on the compute nodes.
  (Work on login nodes is not charged, but you cannot do big computing there!)
- You can check your SU balance on both:
  - The command line
  - The HPRC Portal

https://hprc.tamu.edu/kb/User-Guides/AMS
https://hprc.tamu.edu/kb/User-Guides/AMS/#service-unit

Check your (SU) Balance: Command Line

- List the SU Balance of your Account(s) with:

```
myproject
```

```
 ================================================================================
               List of YourNetID's Project Accounts
--------------------------------------------------------------------------------
|   Account    |    FY    | Default | Allocation |Used & Pending SUs|   Balance  |    PI    |
--------------------------------------------------------------------------------
|1228000223136|  2024    |       N|    10000.00|              0.00|    10000.00|Doe, John |
--------------------------------------------------------------------------------
|1428000243716|  2024    |       Y|     5000.00|            -71.06|     4928.94|Doe, Jane |
--------------------------------------------------------------------------------
|1258000247058|  2024    |       N|     5000.00|             -0.91|     4999.09|Doe, Jane |
--------------------------------------------------------------------------------
```

- Run **`myproject -d <Account#>`** to change default project account.

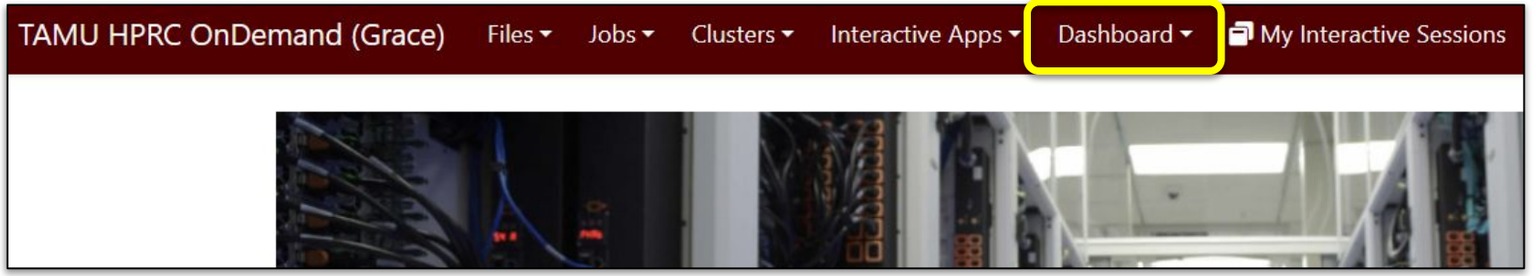
  (Replace <Account#> with your number!)

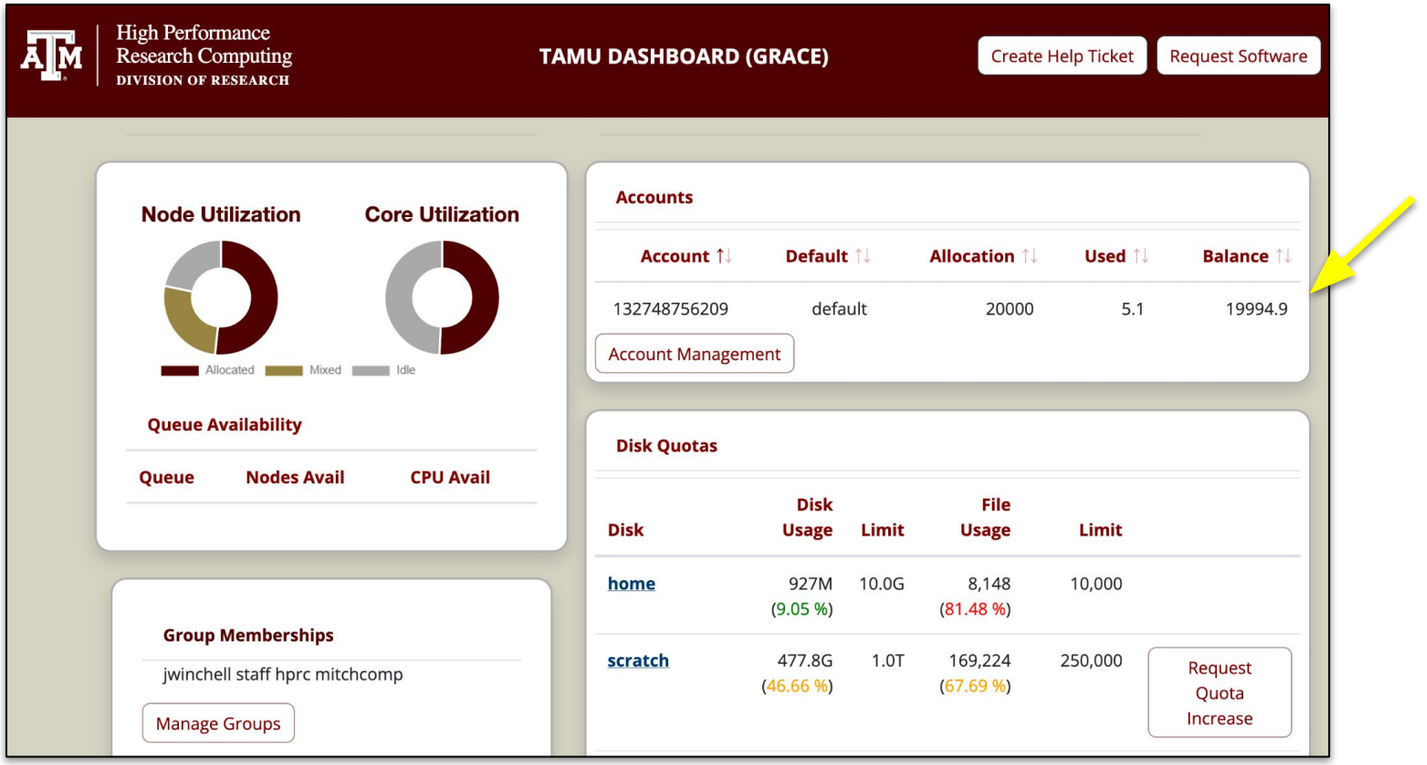
- Run **`myproject -h`** to see more options.

Check your (SU) Balance: Portal

SUs can also be checked in the Dashboard.

(The same place we checked file quotas previously)

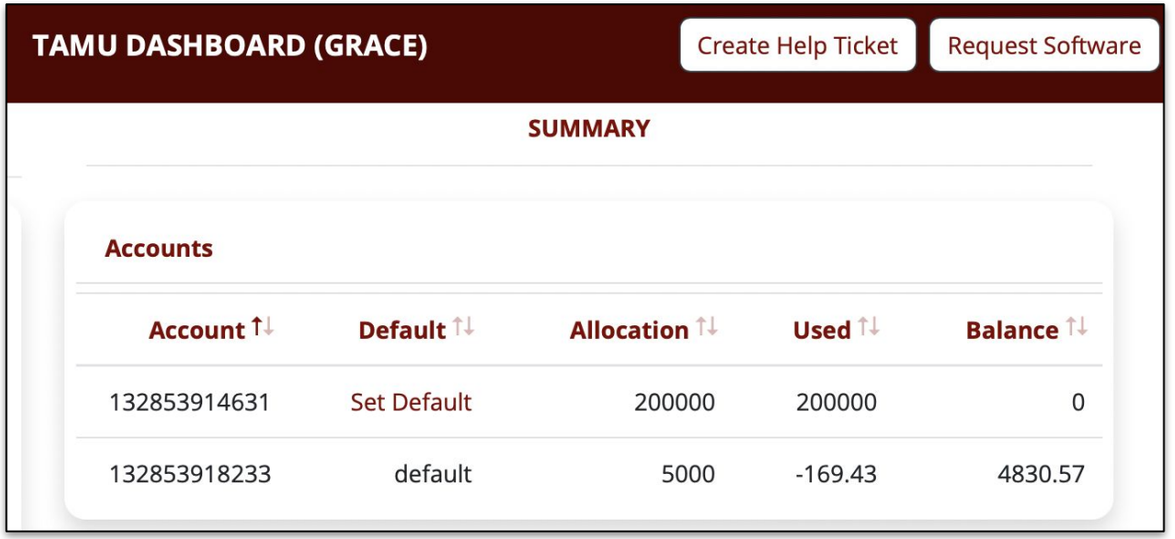




Hands-on Exercise

1. Check your SUs in both the command line and the Portal.
2. Check that you have a default account set.

```
myproject
```



Example Job Script

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=hello_world
#SBATCH --time=00:15:00
#SBATCH --ntasks=2
#SBATCH --ntasks-per-node=2
#SBATCH --nodes=1
#SBATCH --mem=3G
#SBATCH --output=hello_world_log.%j

# load required module(s)
module purge
module load GCCcore/13.2.0
module load Python/3.11.5
python hello_world.py

# Job Environment variables
echo $SLURM_JOBID
echo $SLURM_SUBMIT_DIR
echo $TMPDIR
echo $SCRATCH
```

These #SBATCH lines specify what resources you want to use, which in turn determine how many SUs you will be charged.

(Start with module purge; best practice to start with a clean environment)

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

Submit a Job and Check Job Status

Submit job

```
sbatch example01.job
```

```
Submitted batch job 6853258
(from job_submit) your job is charged as below
              Project Account: 122792016265
              Account Balance: 1687.066160
              Requested SUs:   3
```

Check status

```
squeue -u $USER
```

or

```
squeue --me
```

```
JOBID    NAME      USER      PARTITION  NODES  CPUS  STATE    TIME         TIME_LEFT  START_TIME          REASON     NODELIST
6853258  jobname   someuser   xlong       2     96   RUNNING  3-07:36:50   16:23:10   2024-01-23T17:27:3  None       c[180,202]
6853257  jobname   someuser   xlong       2     96   RUNNING  3-07:36:56   16:23:04   2024-01-23T17:27:2  None       c[523-524]
```

Hands-on Exercise

Submit a simple job file:

1. Navigate to `/scratch/training/Intro-to-Grace`, either on the command line or in the Portal's file browser.
2. Copy the files `hello_world.slurm` and `hello_world.py` to your home directory.
3. Return to your home directory yourself.
4. Submit the job file with: `sbatch hello_world.slurm`
5. Check the job's status with: `squeue -u $USER` or `squeue --me`
6. Check the output file (will be named like `hello_world_log.#`).

Job Environment Variables

Each job has access to several self-referential variables:

- **`$SLURM_JOBID`** = job ID
- **`$SLURM_SUBMIT_DIR`** = directory from which the job was submitted
- **`$TMPDIR`** = /work/job.$SLURM_JOBID

You can also still use non-Slurm variables like:

- **`$SCRATCH`** = /scratch/user/NetID

https://hprc.tamu.edu/kb/Helpful-Pages/Batch-Translation/#environment-variables

Important Batch Job Parameters

Slurm	Comment
`#SBATCH --time=HH:MM:SS`	Specifies the upper time limit for the job
`#SBATCH --ntasks=x`	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=xxxxM`
`or`
`#SBATCH --mem=xG`
	Sets the maximum amount of memory per *node*
	Can use M for MB or G for GB

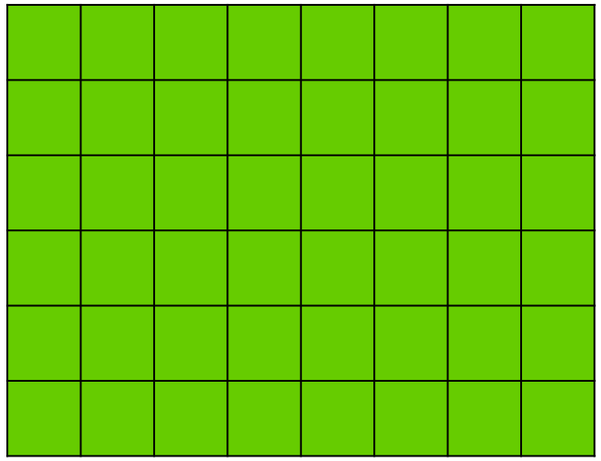
`#SBATCH --nodes=x`	Specifies the number of nodes to use

These usually all go in your job script file

https://hprc.tamu.edu/kb/Helpful-Pages/Batch-Translation/#job-specifications

Mapping Jobs to Cores per Node on Grace

A.

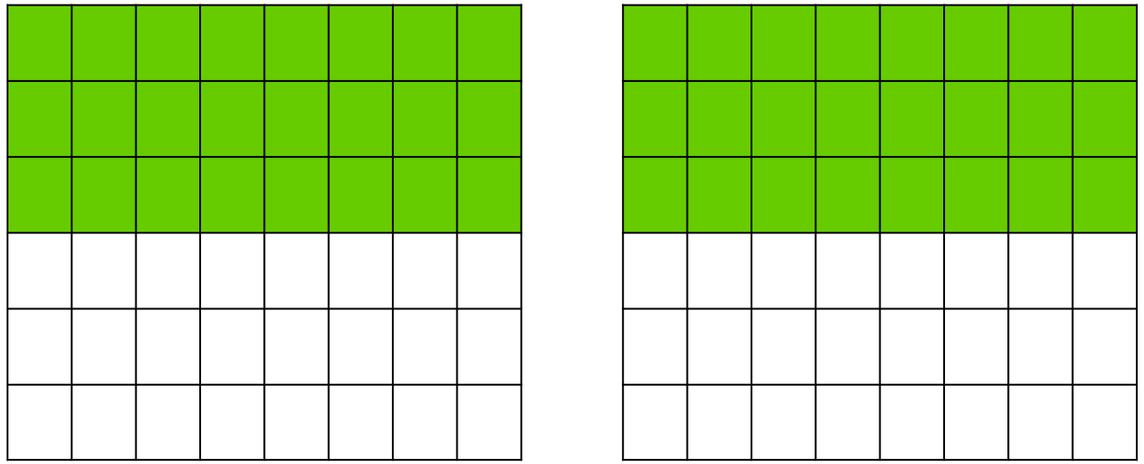


48 cores on
1 compute node

#SBATCH --ntasks=48
#SBATCH --tasks-per-node=48

Preferred Mapping
(if applicable)

B.



48 cores on
2 compute nodes

#SBATCH --ntasks=48
#SBATCH --tasks-per-node=24

Slurm Pop Quiz

```
#SBATCH --job-name=stacks_S2
#SBATCH --ntasks=80
#SBATCH --ntasks-per-node=20
#SBATCH --mem=40G
#SBATCH --time=48:00:00
#SBATCH --output stdout.%J
#SBATCH --error stderr.%J
```

How many nodes is this job requesting?

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

Job Memory Requests on Grace

- 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

- On 384GB nodes, usable memory is at most 360 GB.
  The per-process memory limit should not exceed ~7500 MB for a 48-core job.

- On 3TB nodes, usable memory is at most 2900 GB.
  The per-process memory limit should not exceed 37120 MB for a 48-core job.

Slurm: Examples of SUs charged based on Job Cores, Time and Memory Requested

An SU is equivalent to one core hour *or* a proportional amount of memory on the node for one hour.
On **Grace**: a typical node has 48 cores and 360 GB usable for jobs. (7.5 GB per core)

Number of Cores	GB of memory per core	Total Memory (GB)	Hours	SUs charged
1	7.5	7.5	1	1
24	1 *ask for more*	24	1	24
1	360	360	1	48
48	7.5	360	1	48

https://hprc.tamu.edu/kb/User-Guides/AMS/#service-unit

Slurm: SU Charges for GPU jobs

GPUs will use more SUs per hour than CPUs.

Effective GPU	SU charge per one hour (wall_time)
A100	72
RTX 6000	48
T4	24

gpuinfo

```
GPU      COMPUTE   CUDA     GB MEM   ARCH     SUs per GPU
a100     8.0       11.1+    40       Ampere   72
a40      8.6       11.1+    48       Ampere   48
rtx      7.5       10.0+    24       Ada      48
t4       7.5       10.0+    16       Turing   24
```

Job Submission and Tracking

Slurm commands	Description
`sbatch jobfile1`	Submit jobfile1 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
`pestat -u $USER`	Show resource usage for a running job
`seff job_id`	Check CPU/memory efficiency for a job

https://hprc.tamu.edu/kb/Helpful-Pages/Batch-Translation/#job-specifications

Batch Queues

- Job submissions are auto-assigned to batch *queues* (also called *partitions*) based on the resources requested:
  - number of cores/nodes and walltime limit
  - specific resources requested
- Some jobs can be directly submitted to a queue:
  - E.g. if gpu nodes are needed, use the gpu partition/queue:

  #SBATCH --partition=gpu
- Batch queue policies are used to manage the workload and may be adjusted periodically.

https://hprc.tamu.edu/kb/User-Guides/Grace/Batch/#batch-queues

Checking Resources for Jobs

`sinfo` `pestat` `maxconfig`

There are several tools available to check what you can use in your jobs...

Checking Resources for Jobs: Queues

sinfo pestat maxconfig

```
username@login1:~$ sinfo
PARTITION       AVAIL TIMELIMIT    JOB SIZE     NODES(A/I/O/T)      CPUS(A/I/O/T)
short*          up    2:00:00      1-32         711/0/89/800        33689/439/4272/38400
medium          up    1-00:00:00   1-128        711/0/89/800        33689/439/4272/38400
long            up    7-00:00:00   1-64         711/0/89/800        33689/439/4272/38400
xlong           up    21-00:00:00  1-32         711/0/89/800        33689/439/4272/38400
vnc             up    12:00:00     1-32         100/5/12/117        985/4055/576/5616
gpu             up    4-00:00:00   1-32         100/5/12/117        985/4055/576/5616
bigmem          up    2-00:00:00   1-4          7/0/1/8             560/0/80/640
staff           up    infinite     1-infinite   817/14/101/932      34689/5199/4848/4473
special         up    7-00:00:00   1-infinite   811/5/101/917       34674/4494/4848/4401
gpu-a40         up    4-00:00:00   1-15         6/9/0/15            15/705/0/720
```

Shows job queue status

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

Checking Resources for Jobs: Nodes

sinfo **pestat** maxconfig

```
username@login1:~$ pestat -p gpu -G
Print only nodes in partition gpu
GPU GRES (Generic Resource) is printed after each jobid
Hostname     Partition    Node Num_CPU  CPUload  Memsize  Freemem  GRES/node  Joblist
                          State Use/Tot  (15min)    (MB)     (MB)              JobID(JobArrayID) User GRES/job ...
g001             gpu         mix   2  48    1.94     368640   271338  gpu:a100:2 <jobID> <username> <gpus>
g002             gpu      drain*   0  48    0.00*    368640        0  gpu:a100:2
g003             gpu      drain*   0  48    0.01     368640   370427  gpu:a100:2
……
```

Shows status of nodes

Notable options:

- -p <partition name> show only a specific partition
- -u $USER show only specified user's jobs
- -G show "generic resources" (e.g. the gpus used)

Checking Resources for Jobs: SUs

sinfo pestat **maxconfig**

If you ask for too many resources, your job will not run. You can check beforehand:

```
username@login1:~$ maxconfig

  Grace partitions:   short  medium  long  xlong  vnc  gpu  bigmem  special  gpu-a40
  Grace GPUs in gpu partition:  a100:2  a40:3  rtx:2  t4:4

  Showing max parameters (cores, mem, time) for partition long

  CPU-billing * hours * nodes =   SUs
            48 *   168 *    1 = 8,064

#!/bin/bash
#SBATCH --job-name=my_job
#SBATCH --time=7-00:00:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=48
#SBATCH --mem=360G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j
```

Check specific partitions with:

maxconfig -p <partitionName>

Estimate the SUs a job will require with:

maxconfig -f <jobScriptName>

Job Summary: myjob

Command-line tool to show you details of a specific job:

myjob

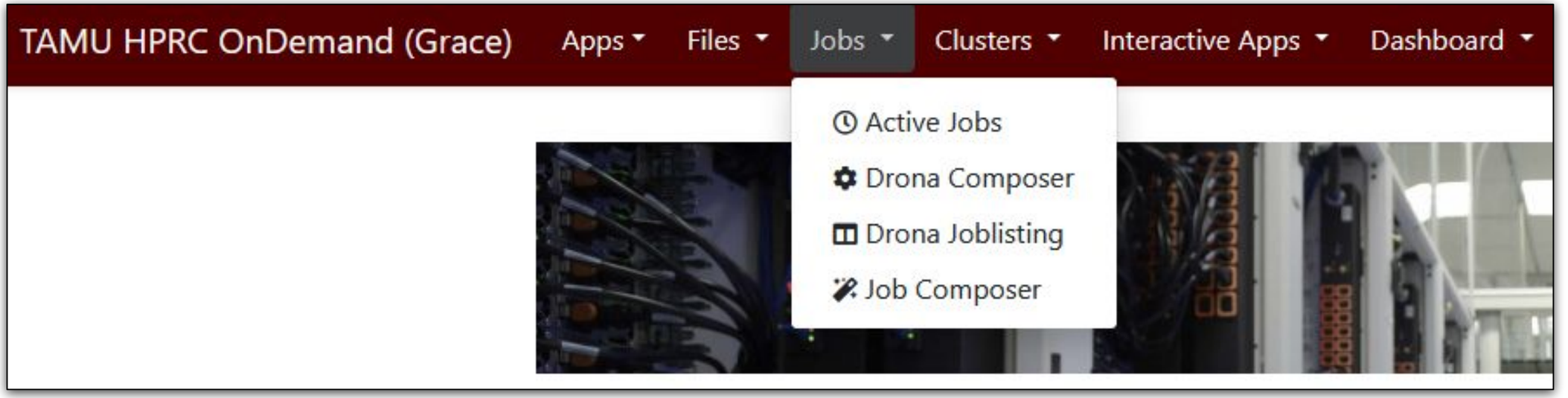
Shows, e.g.:

- Submission details
- Resource usage of finished jobs
- Status of pending job

```
[u.ab12345@aces-login2 ~]$ myjob 9814093

               Job ID: 9814093
              Cluster: grace
           User/Group: userid/userid
              Account: 123456789101
          SUs charged: 283.82
                State: COMPLETED (exit code 0)
            Partition: long
           Node Count: 1
             NodeList: c121
      Cores per node: 48
        CPU Utilized: 01:07:56
   CPU Efficiency: 0.42% of 11-08:28:00 core-walltime
         Submit time: 2025-02-24 17:32:41
          Start time: 2025-02-24 17:32:50
            End time: 2025-02-24 23:13:25
 Job Wall-clock time: 05:40:35
     Memory Utilized: 40.95 GB
   Memory Efficiency: 11.38% of 360.00 GB
            Job Name: parafold
Job Submit Directory: /scratch/user/netid/myproject
         Submit Line: sbatch run_parafold_grace.sh
```

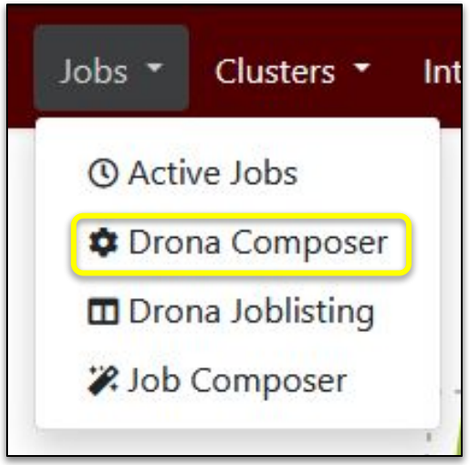
Portal Job Composers



Job management can also be done from the Portal.

- “Active Jobs” and “Job Composer” come with Open OnDemand
- The “Drona” options are developed by HPRC and have additional functionality

Drona Composer



Import additional environments

Select customizable environments or workflows

High Performance Research Computing
DIVISION OF RESEARCH

DRONA COMPOSER (GRACE)

Job Composer

Job Name

Location — Change — /scratch/user/jwinchell/drona_composer/runs

Environments — -- Choose an option -- — +

Preview

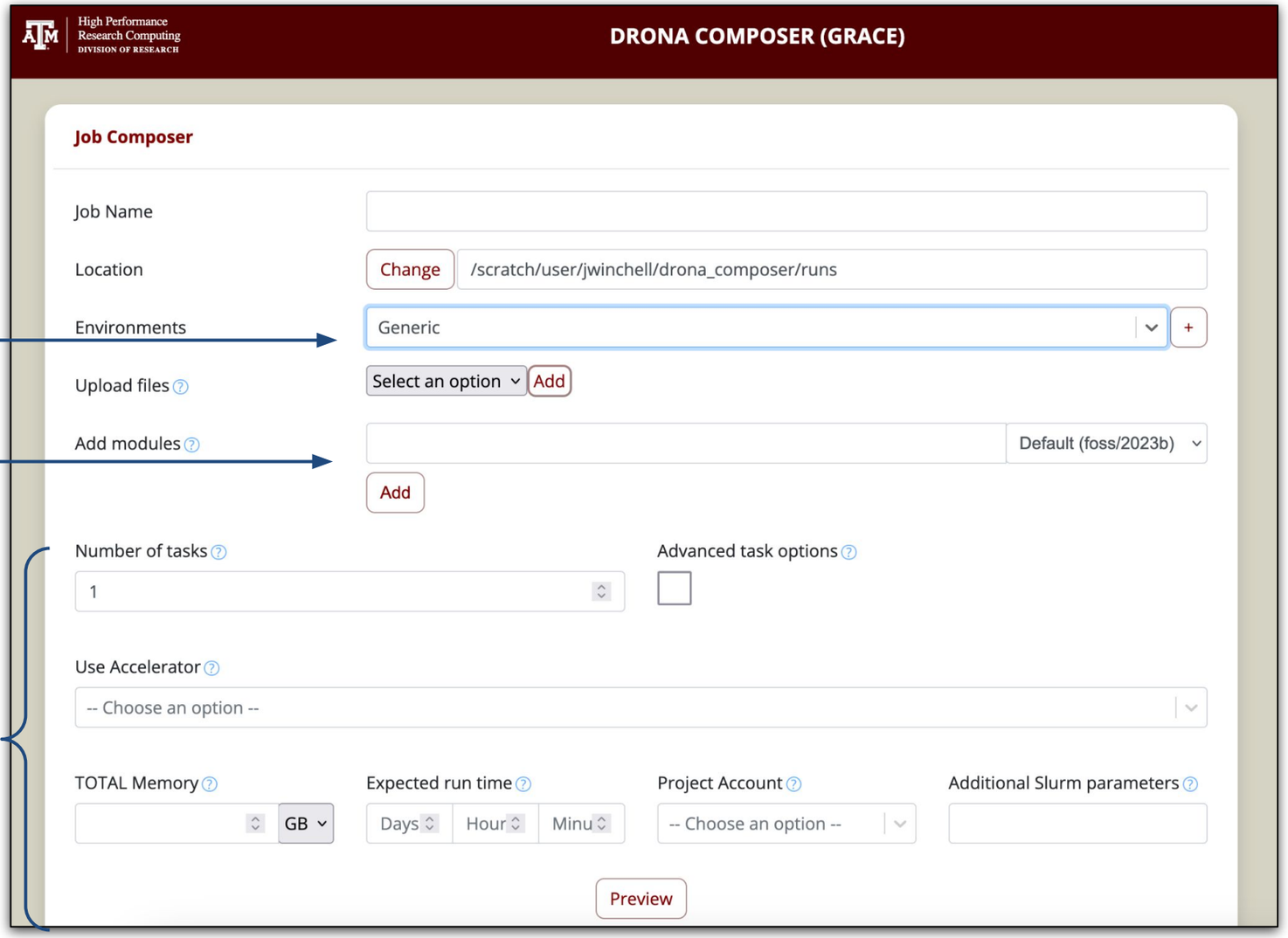
⚠ Cautions: Job files will overwrite existing files with the same name. The same principle applies for your executable scripts.

Drona Composer

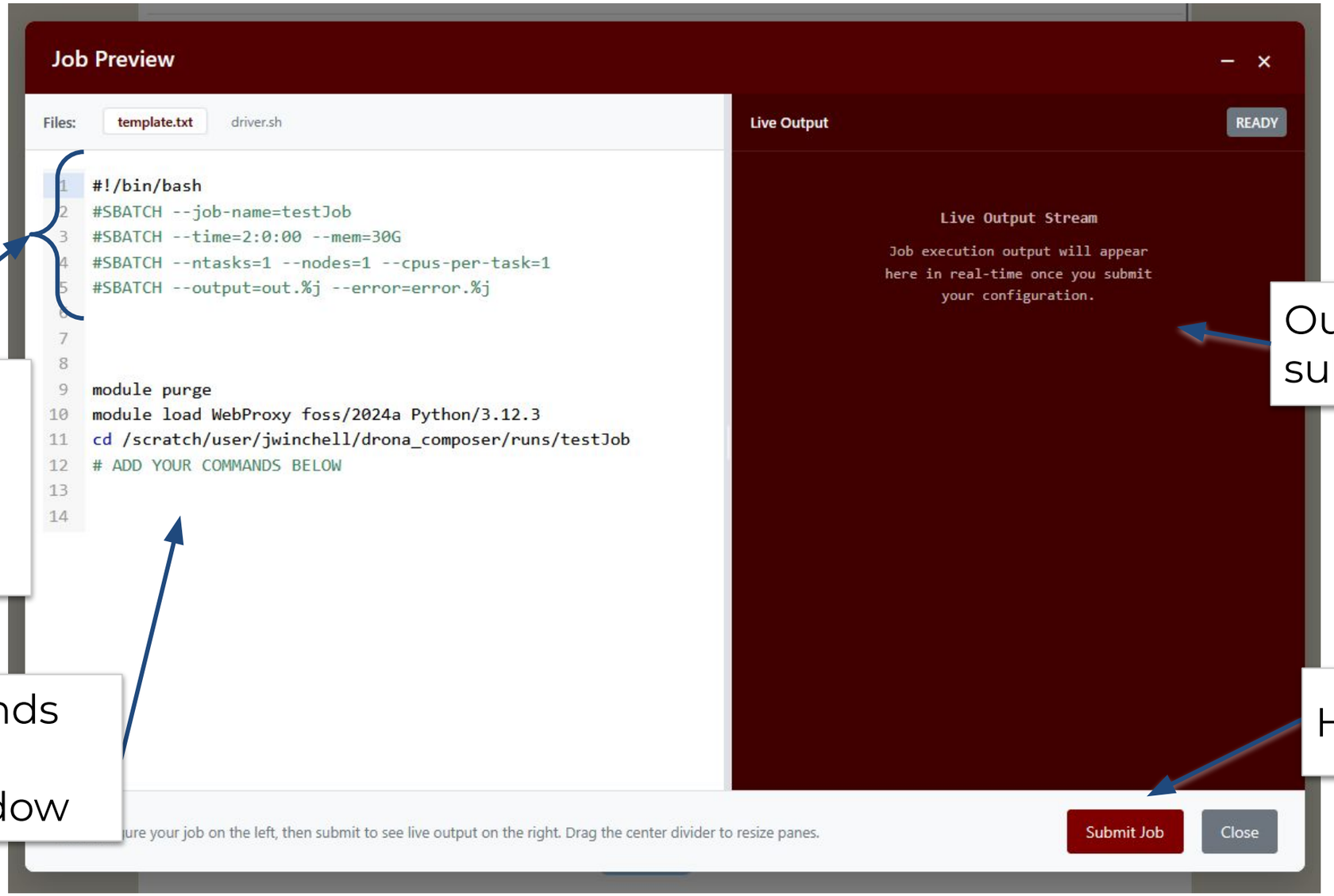
Generic environment to create custom Slurm batch job

Add modules for job

Fill out info that Slurm would need



Drona Composer



Generated Slurm directives and module loads

Add commands directly into editable window

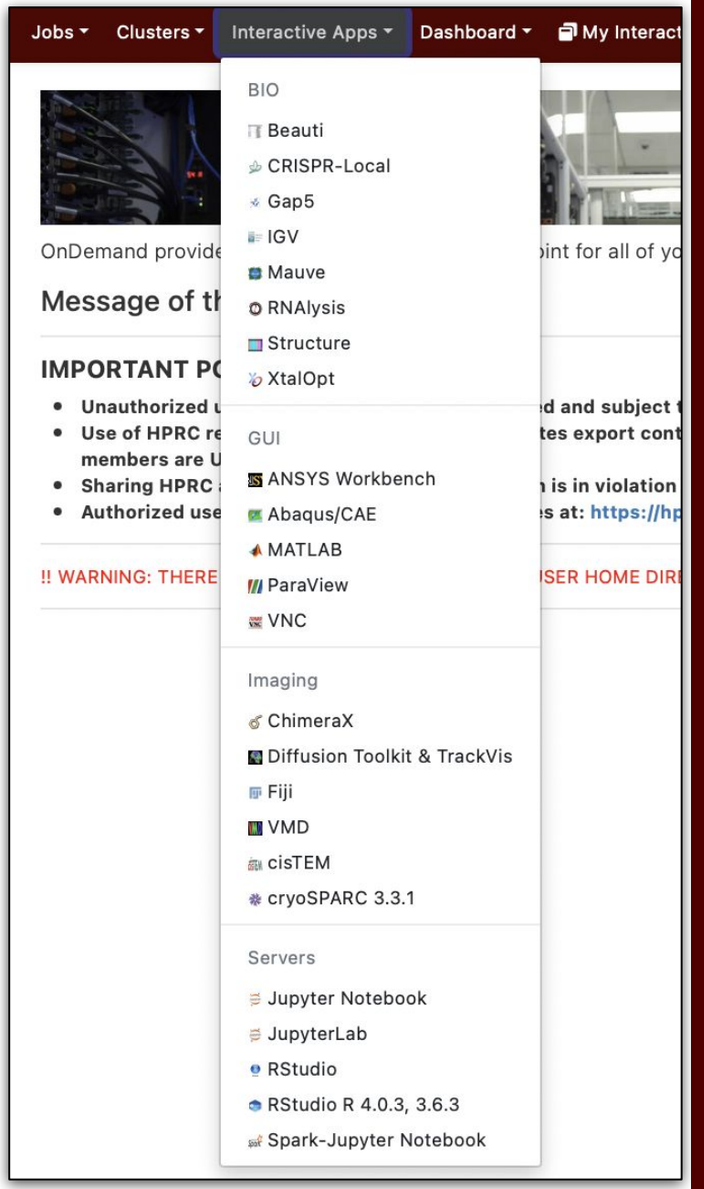
Output of job submission

Hit “Submit”

Other Type of Jobs

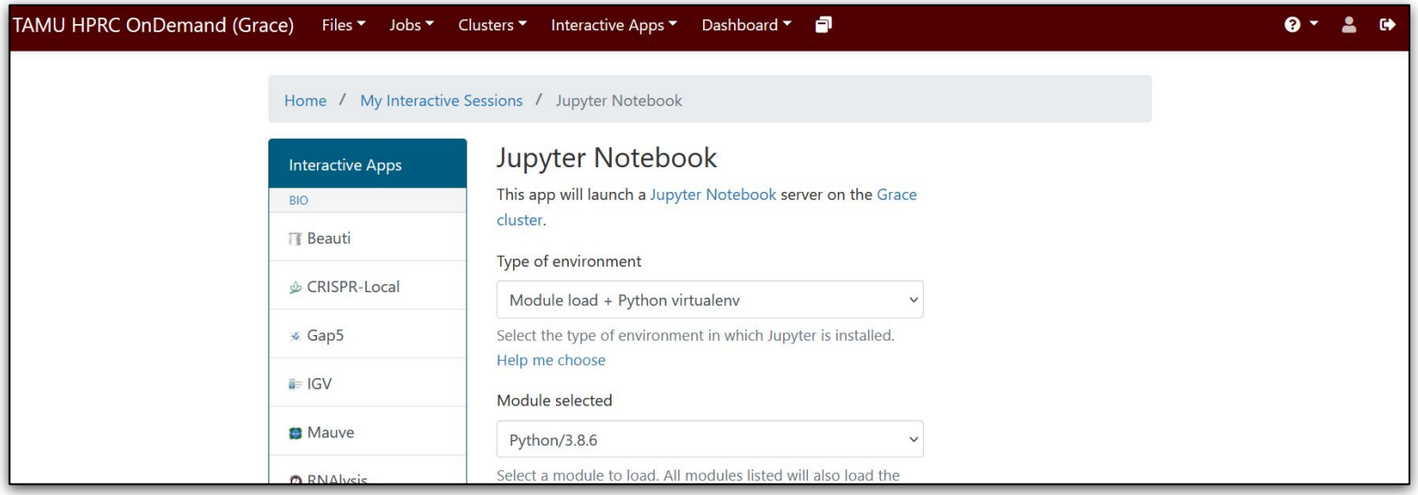
- Visualization:
  - portal.hprc.tamu.edu
  - Interactive Apps > choose application

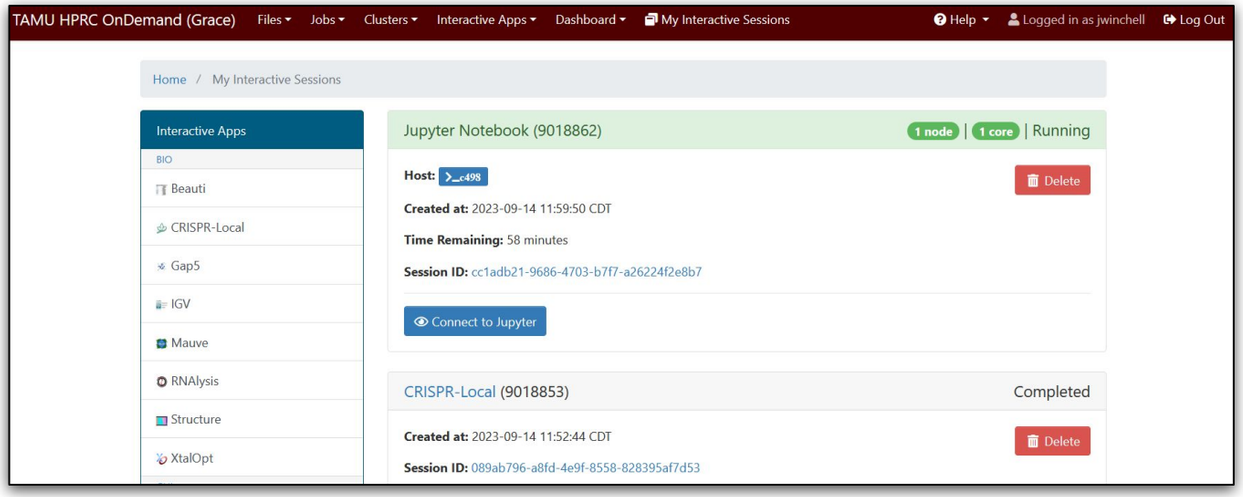
- Large number of concurrent single-core jobs
  - Check out *tamulauncher:*
    - Useful for running many single core commands concurrently across multiple nodes within a job
    - Can be used with serial or multi-threaded programs
    - If a tamulauncher job gets killed, you can resubmit the same job to complete the unfinished commands in the input file.
    - https://hprc.tamu.edu/kb/Software/tamulauncher



Interactive Apps

1. Select an app from the dropdown menu.
2. Specify environment and resources.
3. Hit “Launch” at the bottom.
4. On the “My Interactive Sessions” screen:
   a. wait for box to turn green
   b. connect to app
   c. quit from the app when you are done
   d. box should turn gray





Need Help?

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

- Grace User Guide https://hprc.tamu.edu/kb/User-Guides/Grace
- Email your questions to help@hprc.tamu.edu

Help us help you -- we need more info:

- Which Cluster
- 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

Remember you can start help requests from the Dashboard!

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Thank you

Questions?

Give us feedback on the class with this survey:
https://u.tamu.edu/hprc_shortcourse_survey

https://u.tamu.edu/hprc_shortcourse_survey

HPRC Survey

Batch Job Examples

Slurm Job File (Serial Example)

```
#!/bin/bash

##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
#SBATCH --mem=6G                    #Request 6GB per node
#SBATCH --output=Example1Out.%j       #Send stdout/err to "Example1Out.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##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

# this intel toolchain is just an example.  recommended toolchain is TBD
module purge
module load intel/2022a

# run your program
./helloworld.omp.C.exe
```

SUs = 1.5

Slurm Job File (multi core, single node)

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample2         # Set the job name to "JobExample2"
#SBATCH --time=6:30:00                    # Set the wall clock limit to 6hr and 30min
#SBATCH --nodes=1                      # Request 1 node
#SBATCH --ntasks-per-node=8            # Request 8 tasks(cores) per node
#SBATCH --mem=8G                       # Request 8GB per node
#SBATCH --output=Example2Out.%j        # Send stdout/err to "Example2Out.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456     # Set billing account to 123456  #find your account with "myproject"
##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/2022a

# run your program
mpirun ./helloworld.mpi.C.exe
```

SUs = 52

Slurm Job File (multi core, multi node)

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample3          # Set the job name to "JobExample3"
#SBATCH --time=1-12:00:00               # Set the wall clock limit to 1 Day and 12hr
#SBATCH --ntasks=8                      # Request 8 tasks (cores)
#SBATCH --ntasks-per-node=2             # Request 2 tasks(cores) per node
#SBATCH --mem=5G                        # Request 5GB per node
#SBATCH --output=Example3Out.%j         # Send stdout and stderr to "stdout.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456      # Set billing account to 123456 #find your account with "myproject"
##SBATCH --mail-type=ALL               # Send email on all job events
##SBATCH --mail-user=email_address    # Send all emails to email_address

# this intel toolchain is just an example.  recommended toolchain is TBD
module purge
module load intel/2022a

# run program with MPI
mpirun ./helloworld.mpi.C.exe
```

SUs = 288

Slurm Job File (serial GPU)

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample4          # Set the job name to "JobExample4"
#SBATCH --time=01:00:00                 # Set the wall clock limit to 1hr
#SBATCH --ntasks=1                      # Request 1 task (core)
#SBATCH --mem=5G                        # Request 5GB per node
#SBATCH --output=Example4Out.%j         # Send stdout and stderr to "Example4Out.[jobID]"
#SBATCH --gres=gpu:a100:1               # Request 1 A100 GPUs
#SBATCH --partition=gpu                 # Request the GPU partition/queue

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456     # Set billing account to 123456  #find your account with "myproject"
##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 CUDA/11.8.0

# run your program
my_cuda_enabled_program
```

SUs = 72

Slurm Job File (multi GPU)

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample5       # Set the job name to "JobExample4"
#SBATCH --time=01:00:00              # Set the wall clock limit to 1hr
#SBATCH --ntasks=2                   # Request 1 task (core)
#SBATCH --nodes=1
#SBATCH --mem=250G                   # Request 250GB per node
#SBATCH --output=Example4Out.%j      # Send stdout and stderr to "Example4Out.[jobID]"
#SBATCH --gres=gpu:a100:2            # Request 2 A100 GPUs
#SBATCH --partition=gpu              # Request the GPU partition/queue

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456     # Set billing account to 123456  #find your account with "myproject"
##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 CUDA/11.8.0

# run your program
my_cuda_enabled_program
```

SUs = 179

Modules: Toolchain Details

- Toolchains are combinations of compilers, MPI libraries, and highly optimized math libraries.
- Toolchain components are primarily either Intel or Open Source.

Example toolchains for C++ development:

Components	Open Source	Intel Source	Mixed Source
Compiler only	`GCCcore`	`iccifort`	-
Compiler + MPI	`gompi`	`iimpi`	`iompi`
Compiler + MPI + MKL, BLAS, FFTW, LAPACK	`foss`	`intel`	`iomkl`
Compiler + all of the above + CUDA Compiler	`fosscuda`	`intelcuda`	`iomklc`

Example usage:

```
module load foss/2022a
```

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