HIGH PERFORMANCE RESEARCH COMPUTING

- HPRC Primer -Introduction to Grace: An HPRC Resource

September 5, 2025



High Performance Research Computing



Table of Contents

By the end of this primer you will know

- What Grace is as well as its resources
- How to log in and manage files/storage
- How to load software modules
- How to run jobs on the clusters using the SLURM scheduler

Prerequisites to Primer:

- Have an HPRC account
- Basic knowledge of Linux



Grace Hardware

Grace is a 940-node Intel cluster from Dell with an InfiniBand HDR-100 interconnect, A100 GPUs, RTX 6000 GPUs and T4 GPUs. The 940 nodes are based on the Intel Cascade Lake processor.

48 cores/node

3TB Large Memory-80 cores/node Login Nodes: 10 GbE TAMU network connection

Resource	Count
Login Nodes	5
384GB memory general compute nodes	800
GPU - A100 nodes with 384GB memory	100
GPU - RTX 6000 nodes with 384GB memory	9
GPU - T4 nodes with 384GB memory	8
3TB Large Memory	8

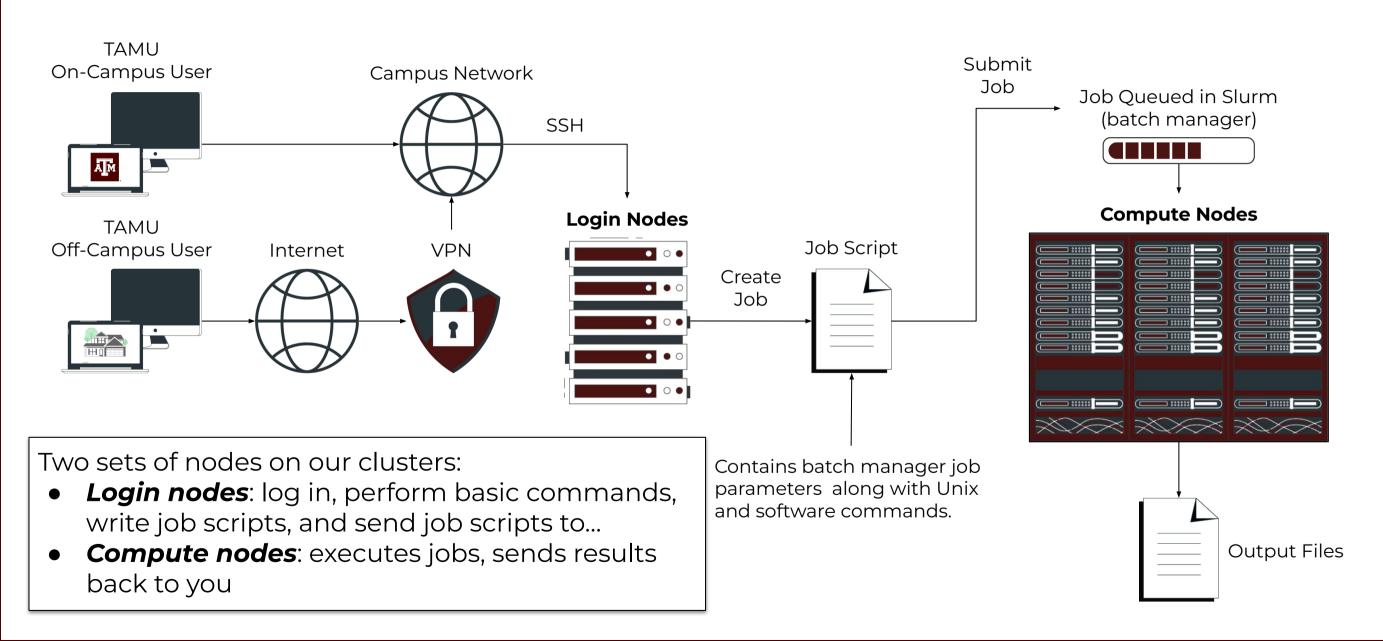


For more information:

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

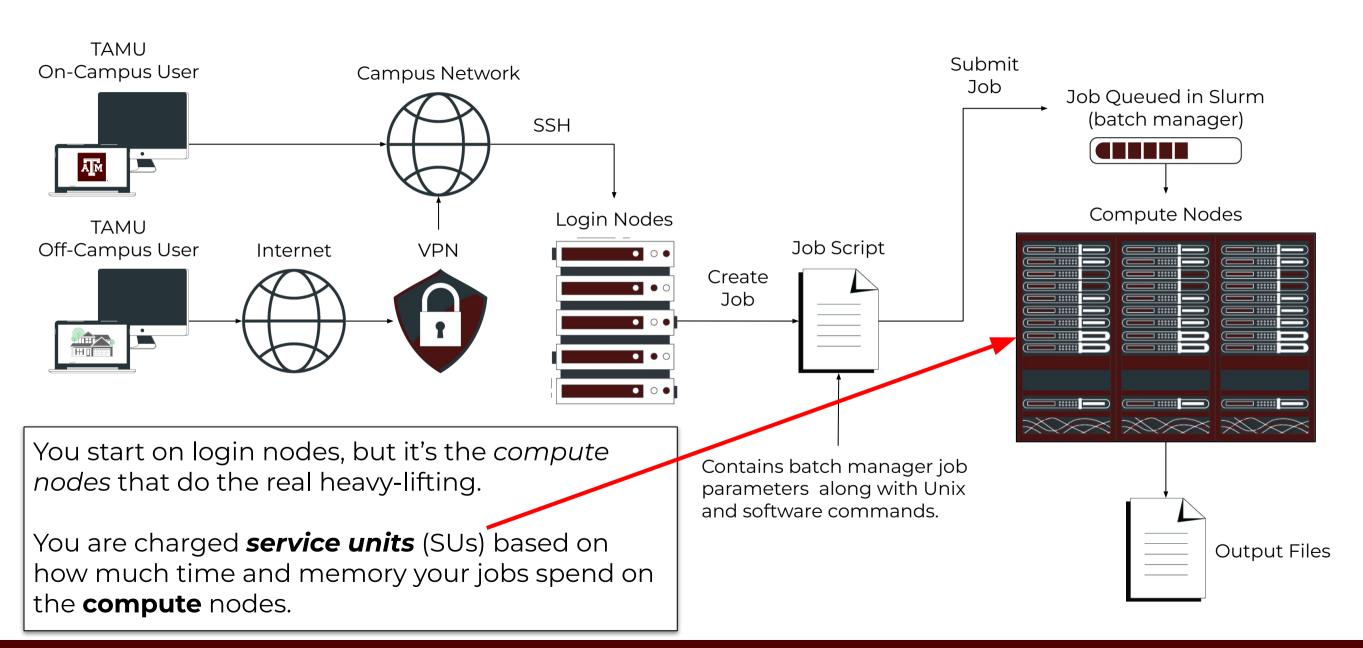


Computing on HPRC Clusters





Batch Jobs on HPRC Clusters

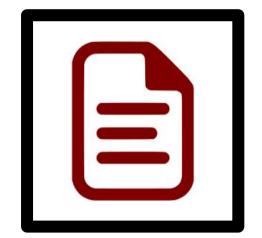




File Quotas and Resource Allocations

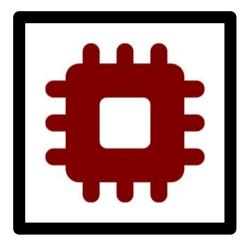
Two things to keep track of when computing

Quota



File Storage
File Count
File Space

<u>Allocation</u>

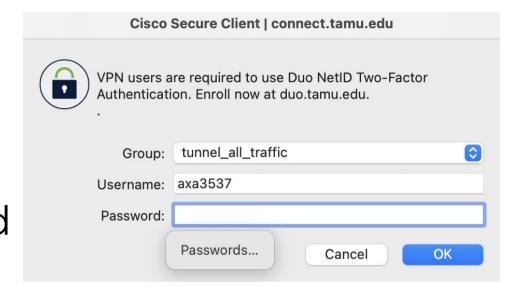


Computing Resources

Service Units (SUs)

Accessing Grace: Setup

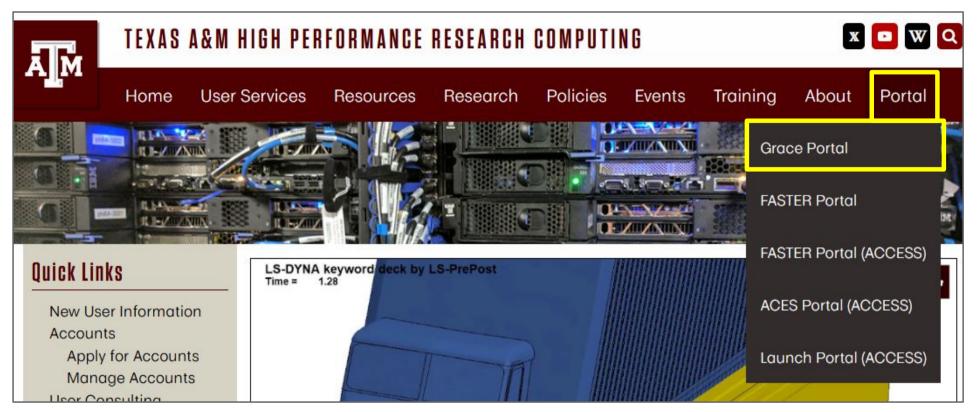
- If off-campus: Set up and start VPN (Virtual Private Network):
 - u.tamu.edu/VPnetwork
- Two-Factor Authentication required



- Today we'll access Grace via the online Portal, but
 you can also use ssh.

 ssh <NetID>@grace.hprc.tamu.edu
- See https://hprc.tamu.edu/kb/User-Guides/Grace/Access/ for more details.

Accessing Grace via the Portal



Access the HPRC portals through most web browsers:

- 1. Go to <u>portal.hprc.tamu.edu</u> or use the <u>Portal dropdown menu</u> on the HPRC homepage: <u>https://hprc.tamu.edu/</u>
- 2. Choose Grace Portal

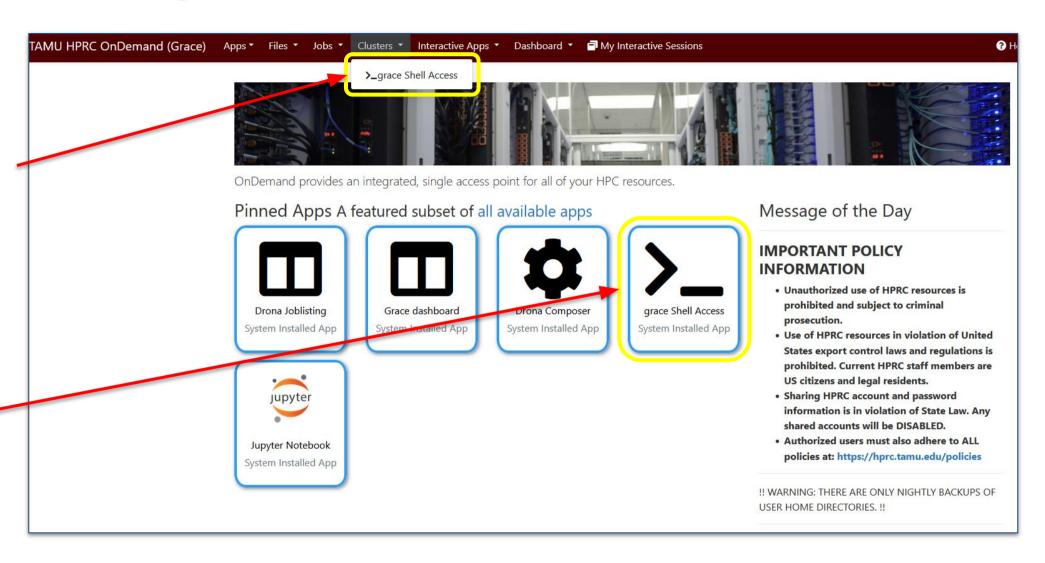
https://hprc.tamu.edu/kb/User-Guides/Grace/Access/



Accessing Grace via the Portal

Two ways to enter the Portal:

- (1) Select at the top:"Clusters" →"Grace Shell*Access"
- (2) Select in Main Menu: "Grace Shell Access"

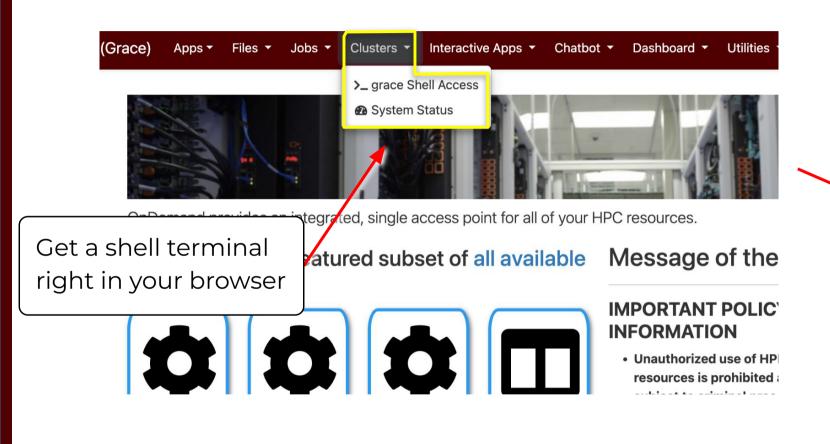


*shell is also called terminal or command line

https://hprc.tamu.edu/kb/User-Guides/Grace/Access/



Shell Access via the Portal





Hands-On Activity - 2 Minutes

Try to access a *shell** on Grace now, either through portal.hprc.tamu.edu or hprc.tamu.edu

*(also called terminal or command line)

What message do you see when you login?

Remember Grace has 5 login nodes. Which one does your command prompt say you were assigned?



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 nightly.
/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.

*Do NOT share your home or scratch directories.

Request a group directory for sharing files.

\$SCRATCH is shared between the FASTER and Grace clusters.

View file usage and quota limits in the shell using the command:

showquota

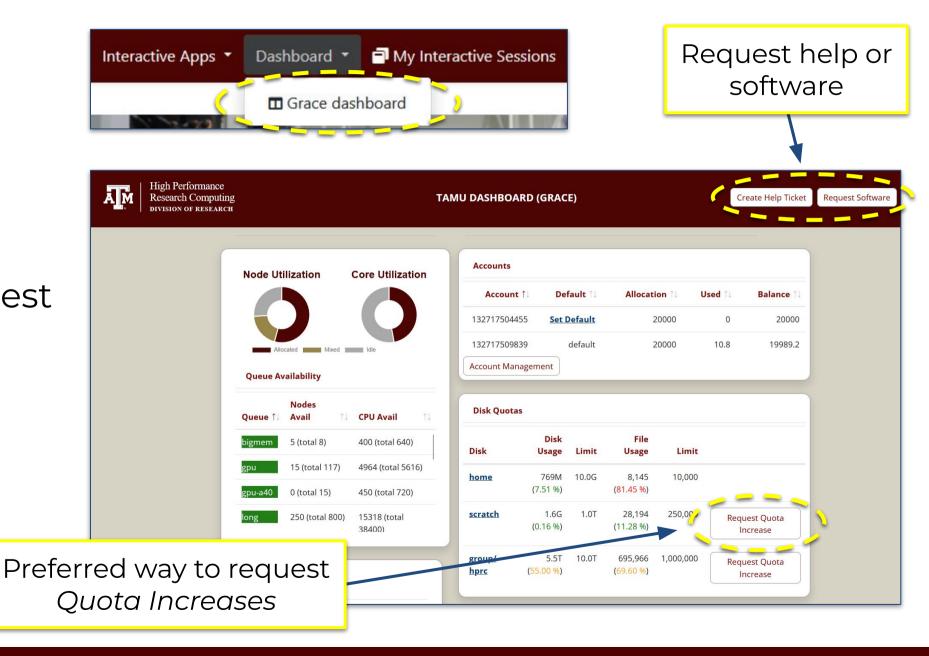
[axa3537@grace5 ~]\$ showquota				
Your current disk quotas are:				
Disk	Disk Usage	Limit	File Usage	Limit
/home/axa3537	681M	10.0G	6394	10000
/scratch/user/axa3537	2.0G	1.0T	52122	250000
/scratch/group/hprc	4.8T	10.0T	494939	1000000

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



Portal: Grace Dashboard

- Easily view <u>Cluster</u>
 <u>Utilization</u>, <u>Storage</u>
 <u>Quotas</u>, & <u>Allocation</u>
 <u>Balances</u>
- Ask for help and request software
- View current groups and job listings



Hands-On Activity - 2 Minutes

1. Please try to access dashboard now through the portal.

2. Check your quotas both on the command line and on the dashboard.

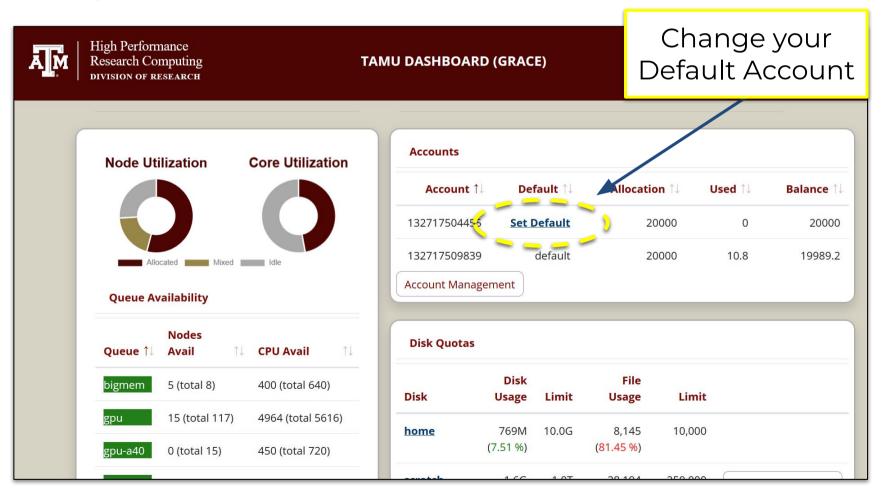
showquota



Checking Your Service Unit (SUs) Balance

- 1SU = 1 core/hr (GPUs are more expensive per-hour!)

 Visit https://hprc.tamu.edu/kb/User-Guides/AMS/#sus-for-jobs-requesting-gpus for more information
- SUs are charged to default account when none is specified.





Checking Your SUs in the Shell

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 | 2025 | N | 10000.00 | 0.00 | 10000.00 | Doe, John |

| 1428000243716 | 2025 | Y | 5000.00 | -71.06 | 4928.94 | Doe, Jane |

| 1258000247058 | 2025 | N | 5000.00 | -0.91 | 4999.09 | Doe, Jane |
```

Run myproject -d <Account#> to change default project account
 (replace <Account#> with your number!)

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



Checking Your SUs in the Shell

Run myproject -j to see SU usage for all jobs

ProjectAccount	JobID	JobArrayIndex	SubmitT		t of Jobs - Star	tTime	EndT	ime	Walltime	TotalSlots	UsedSUs
 132663473580	 15564194	 0	 2025-06-17 1	 0:39:31	2025-06-17	10:39:45	2025-06-17	10:43:03	 198	 1	0.06
132663473580	16029806	j 0	2025-08-05 1						j 82 j	1	0.02
132663473580	16030076	jø	2025-08-05 1	1:05:38	2025-08-05	11:05:54	2025-08-05	11:14:14	j 500 j	1	0.14
132663473580	16030256	jø	2025-08-05 1	1:14:56	2025-08-05	11:15:04	2025-08-05	11:23:14	490	1	9.94
132663473580	16030728	jø	2025-08-05 1	1:33:57	2025-08-05	11:34:08	2025-08-05	11:45:01	653	1	13.24
132663473580	16047456	jø	2025-08-06 1	5:58:38	2025-08-06	15:58:50	2025-08-06	16:19:44	1254	1	0.35
132663473580	16048154	jø	2025-08-06 1	6:49:31	2025-08-06	16:49:45	2025-08-06	17:49:48	3603	1	73.06
132663473580	16164088	jø	2025-08-15 1 ₁	4:51:00	2025-08-15	14:51:08	2025-08-15	14:51:54	46	1	0.01
								Total Job	 s: 8	 Total Usage:	96 . 82

Run myproject -h to see more options



Hands-On Activity - 2 Minutes

1. Use myproject to check the SU balance of your accounts.

2. Use the dashboard the check the same information.

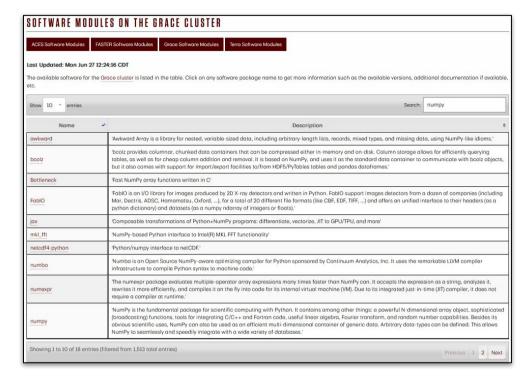


Software

 Search for software modules on <u>https://hprc.tamu.edu/software/grace/</u>



- See the Software Knowledge Base page <u>https://hprc.tamu.edu/kb/Software/</u>
 for instructions and examples
- License-restricted software
 - Contact <u>help@hprc.tamu.edu</u>



- Contact HPRC (can use the dashboard) for **software installation help/request**
 - User can install software in their home/scratch directory
 - Do NOT run the sudo command when installing software



Software: Application Modules

- Installed applications are made available with the module system
- Grace uses a *software hierarchy* inside the module system
- In this hierarchy, the user loads a compiler which then makes available Software built with the currently-loaded compiler

← shows which software is available module avail module load GCC/13.2.0 OpenMPI/4.1.6 ← load GCC compiler version 13.2.0 and OpenMPI version 4.1.6 ← show which software is available to use with the loaded module avail modules ← load PyTorch version 2.7.0 module load PyTorch/2.7.0 ← see what software you've loaded already

Module System Youtube Video → <u>www.youtube.com/watch?v=drxpbrOCPFw</u>



module list

Software: Modules and Toolchains

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

- intel/2024a
- o foss/2024a

(more than just these versions)

- GCCcore/13.3.0
- Other module commands:

```
module spider
module purge
```

- ← search for modules and their dependencies
- ← removes all loaded modules

good practice!

helpful: press q to quit module spider

Module System Youtube Video → <u>www.youtube.com/watch?v=drxpbrOCPFw</u>



Hands-On Activity - 5 Minutes

Remember:

module load

module purge

1. Please search for and load the following module:

OpenMPI/5.0.3

(Hint) Type this to show which compiler needs to be loaded:

module spider OpenMPI/5.0.3

(Hint) And check that it's been loaded with:

module list

2. Next remove (unload) all your current modules.

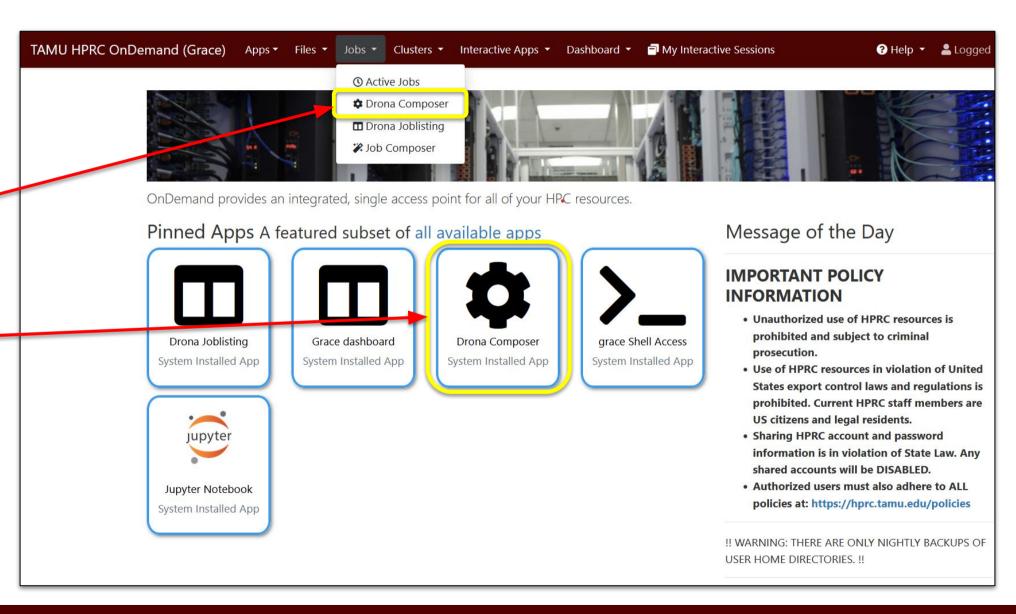
Module System Youtube Video → <u>www.youtube.com/watch?v=drxpbrOCPFw</u>

The Drona Composer

• A simple app to assist you with composing jobs

Two ways to get to Drona Composer:

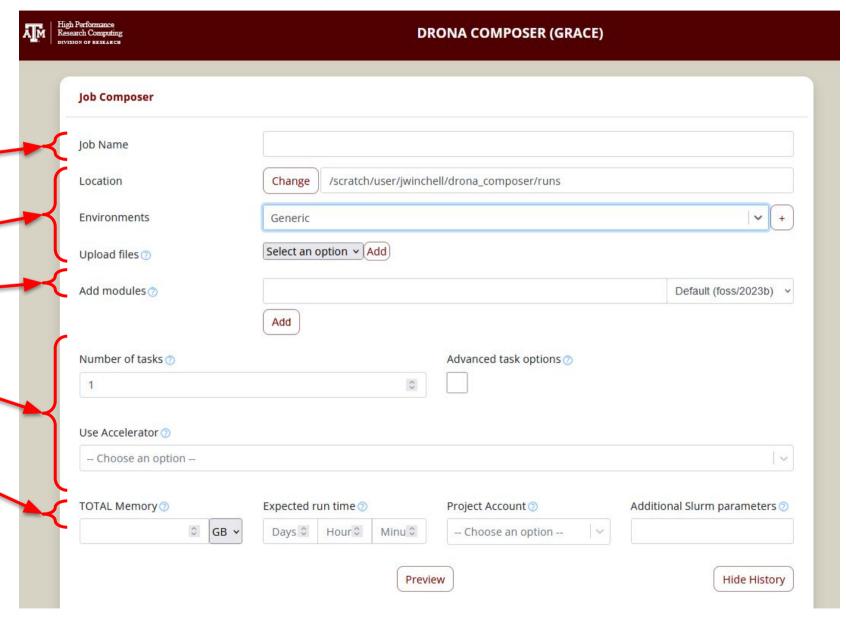
- (1) Select Drona Composer under "Jobs" tab
- (2) Select Drona Composer in Main Menu



The Drona Composer

Create your own jobs through the app:

- (1) Pick a job name
- (2) Choose location and environments
- (3) Add modules
- (4) Choose Resources
- (5) Choose Time



Sample Job Script Structure

```
#!/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 GCCcore/14.2.0 Python/3.13.1
# Run your program
python my program.py
```

These *parameters* describe your job to the Slurm job scheduler.

The lines starting with #SBATCH are NOT comments!

See the **Knowledge Base** for more info

ntasks = cores

Account number to be charged

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

(We will practice with job files in a few slides)!



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:
                         matching JOBID
  Check status
squeue -u netID
                            or
                                  squeue --me
JOBID
       NAME
                USER
                         PARTITION
                                                                   TIME LEFT
                                          CPUS
                                                STATE
                                                                             START TIME
                                    NODES
                                                        TIME
                                                                                              REASON
                                                                                                        NODELIST
6853258
                                                       3-07:36:50
                                                                  16:23:10
       jobname
                NetID
                         xlong
                                          96
                                                RUNNING
                                                                             2025-01-23T17:27:3
                                                                                               None
                                                                                                        c[180,202]
6853257 jobname
                                                                                                        c[523-524]
                         xlong
                                          96
                                                RUNNING
                                                        3-07:36:56 16:23:04
                                                                             2025-01-23T17:27:2 None
                someuser
```



Hands-On Activity

- 1. Navigate to /scratch/training/Intro-to-Grace
- 2. Copy hello_world.py to your home directory
- 3. Return to your home directory and submit the job file using **sbatch**.
- 4. Check that the job is running in a Slurm queue with **squeue**.
- 5. When your job completes, check the contents of the output file.



Batch Queues

- Job submissions are auto-assigned to batch queues based on the resources requested (e.g. number of cores/nodes and walltime limit)
- Use **sinfo** to check their status:

```
[NetID@grace2 ~]$ sinfo
PARTITION
                                                  NODES (A/I/O/T)
                                                                      CPUS (A/I/O/T)
               AVAIL
                       TIMELIMIT
                                       JOB SIZE
                                                  687/97/16/800
                                                                      30786/6758/856/38400
short*
                       2:00:00
                                       1-32
               up
medium
                       1-00:00:00
                                      1-128
                                                  687/97/16/800
                                                                      30786/6758/856/38400
               uр
                                                                      30786/6758/856/38400
long
                       7-00:00:00
                                      1-64
                                                  687/97/16/800
               up
                       21-00:00:00
                                      1-32
                                                  687/97/16/800
                                                                      30786/6758/856/38400
xlong
               up
                                      1-32
                                                  104/12/1/117
                                                                      895/4633/88/5616
                       12:00:00
vnc
               up
                       4-00:00:00
                                      1-32
                                                  104/12/1/117
                                                                      895/4633/88/5616
qpu
               up
                       2-00:00:00
                                      1 - 4
                                                  0/7/1/8
                                                                      0/560/80/640
bigmem
               up
                                      1-infinite 791/109/17/917 31681/11391/944/4401
staff
                       infinite
               up
                                      1-infinite 791/109/17/917 31681/11391/944/4401
special
                       7-00:00:00
               up
qpu-a40
                                                  15/0/0/15
                                                                      45/675/0/720
                       10-00:00:00
                                      1-15
               up
```

```
For the NODES and CPUS columns:

A = Active (in use by running jobs)

O = Offline (unavailable for jobs)

T = Total
```

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



Need Help?

First check the FAQ

- Grace User Guide
- 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



Job Submission and Tracking

Slurm queue command	Description
<pre>sbatch jobfile1</pre>	Submit jobfile to batch system
squeue [-u user_name] [-j job_id]	List jobs
scancel job_id	Kill a job
<pre>sacct -X -j job_id</pre>	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
<pre>lnu job_id</pre>	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

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



Continued Learning

Intro to HPRC Video Tutorial Series

HPRC's Knowledge Base





High Performance Research Computing

Give us feedback on the class with this survey:

https://u.tamu.edu/hprc_shortcourse_survey

Thank you

Questions?



HPRC Surve