

# HIGH PERFORMANCE RESEARCH COMPUTING

**- HPRC Primer -**

## Introduction to Grace: An HPRC Resource

*January 30, 2026*



High Performance  
Research Computing

DIVISION OF RESEARCH



High Performance Research Computing | [hprc.tamu.edu](http://hprc.tamu.edu)

# 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

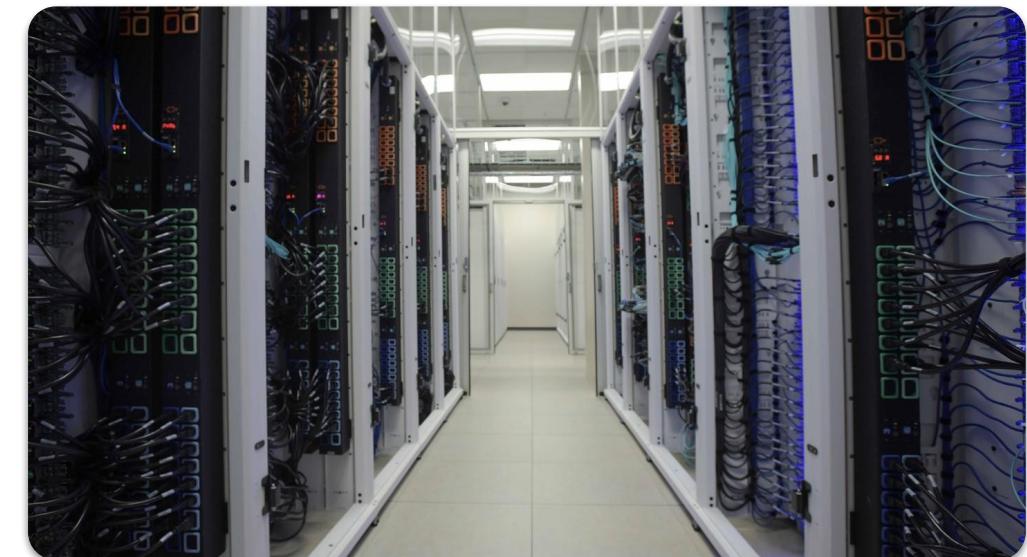
# Grace Hardware

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

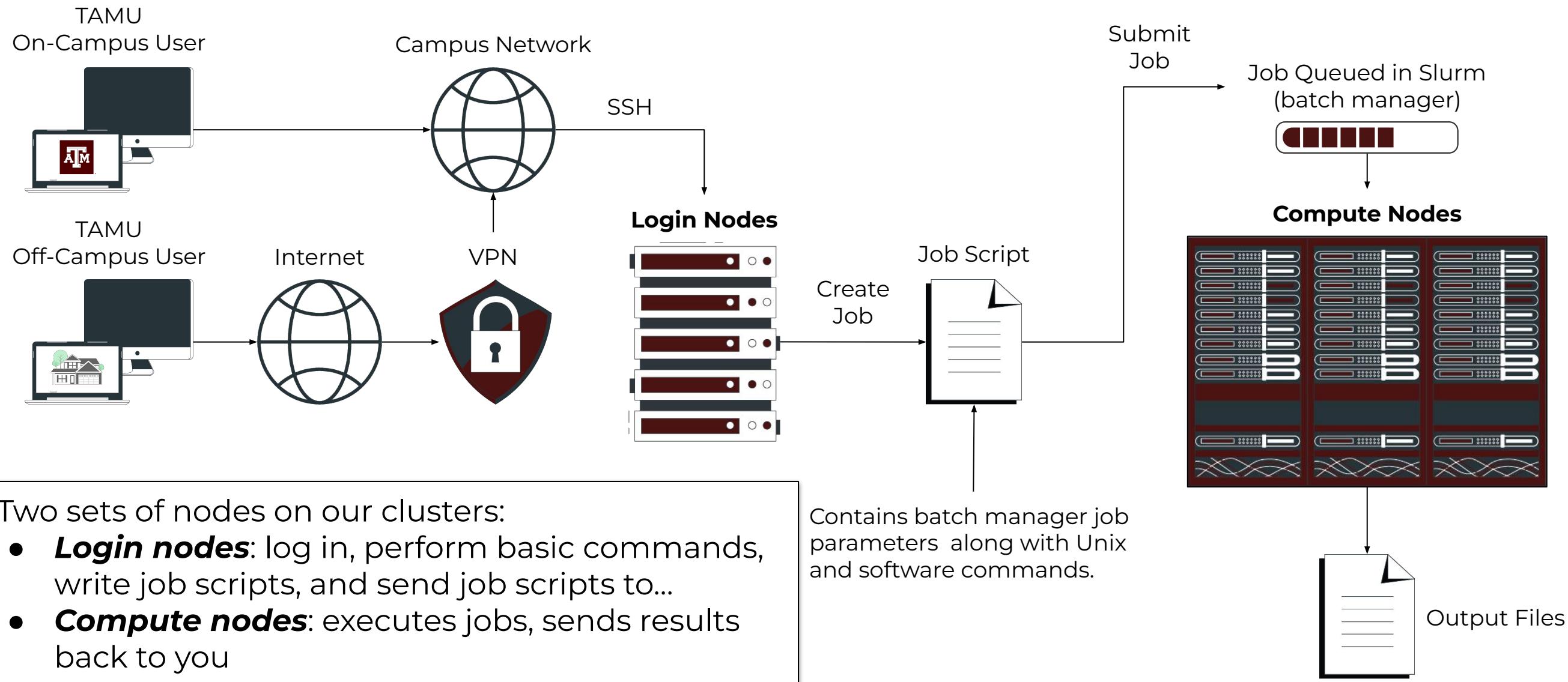
Resource	Count
Login Nodes	5
384GB memory general compute nodes	800
GPU - A100 nodes with 384GB memory	100
GPU - RTX 6000 nodes with 384GB memory	9
GPU - T4 nodes with 384GB memory	8
3TB Large Memory	8



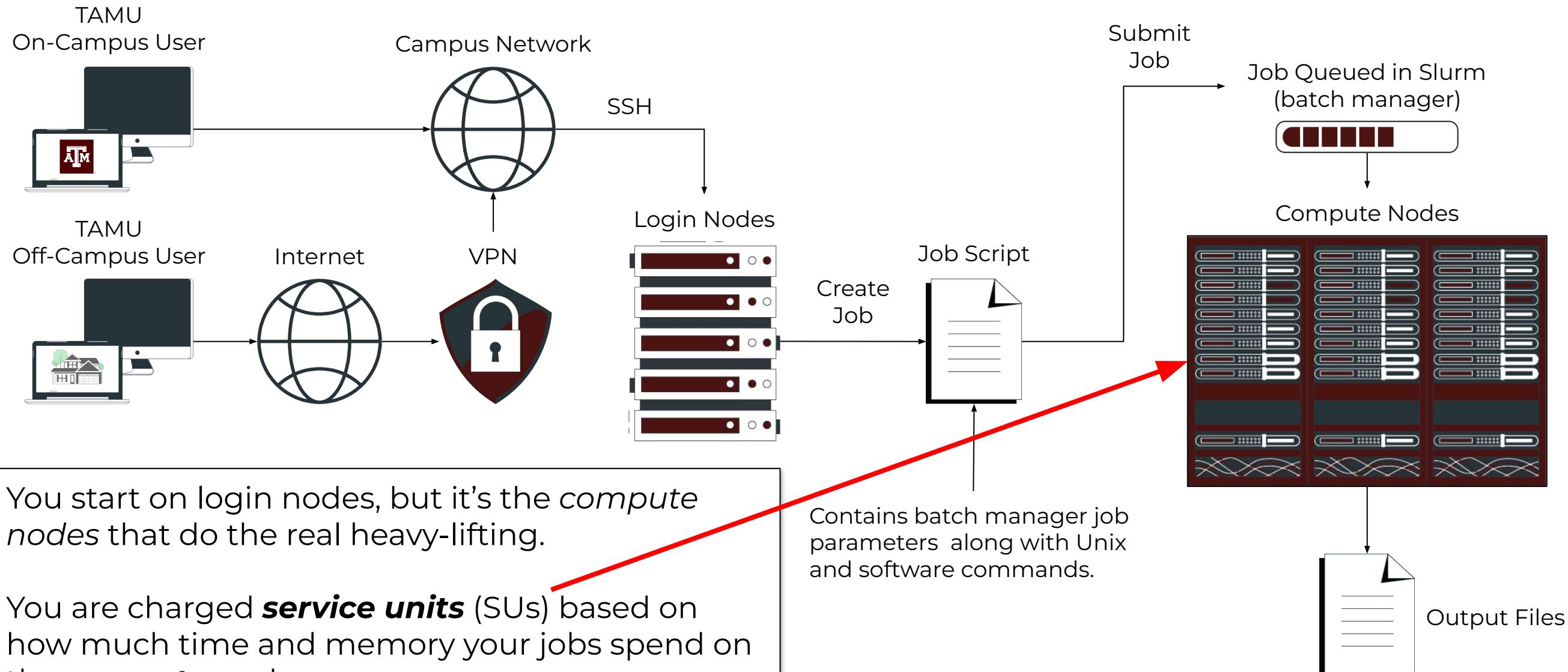
For more information:

<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

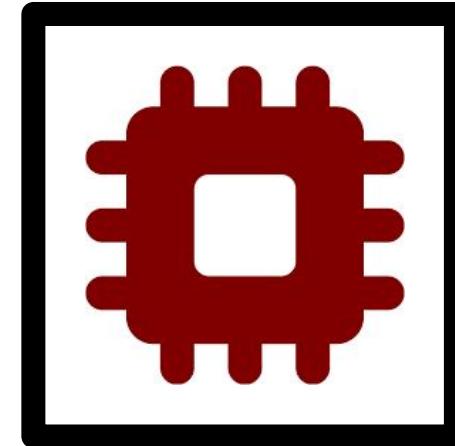


File Storage

*File Count*

*File Space*

Allocation

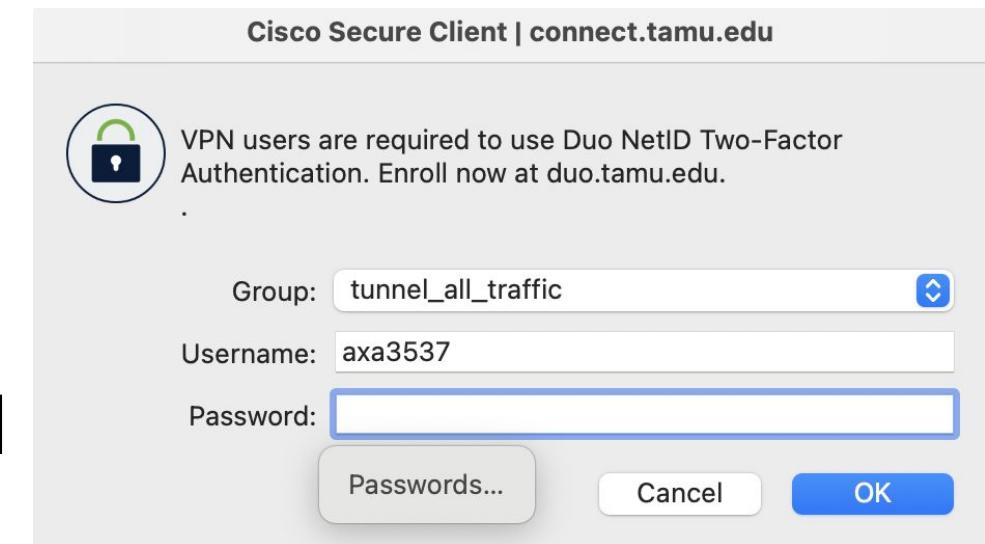


Computing Resources

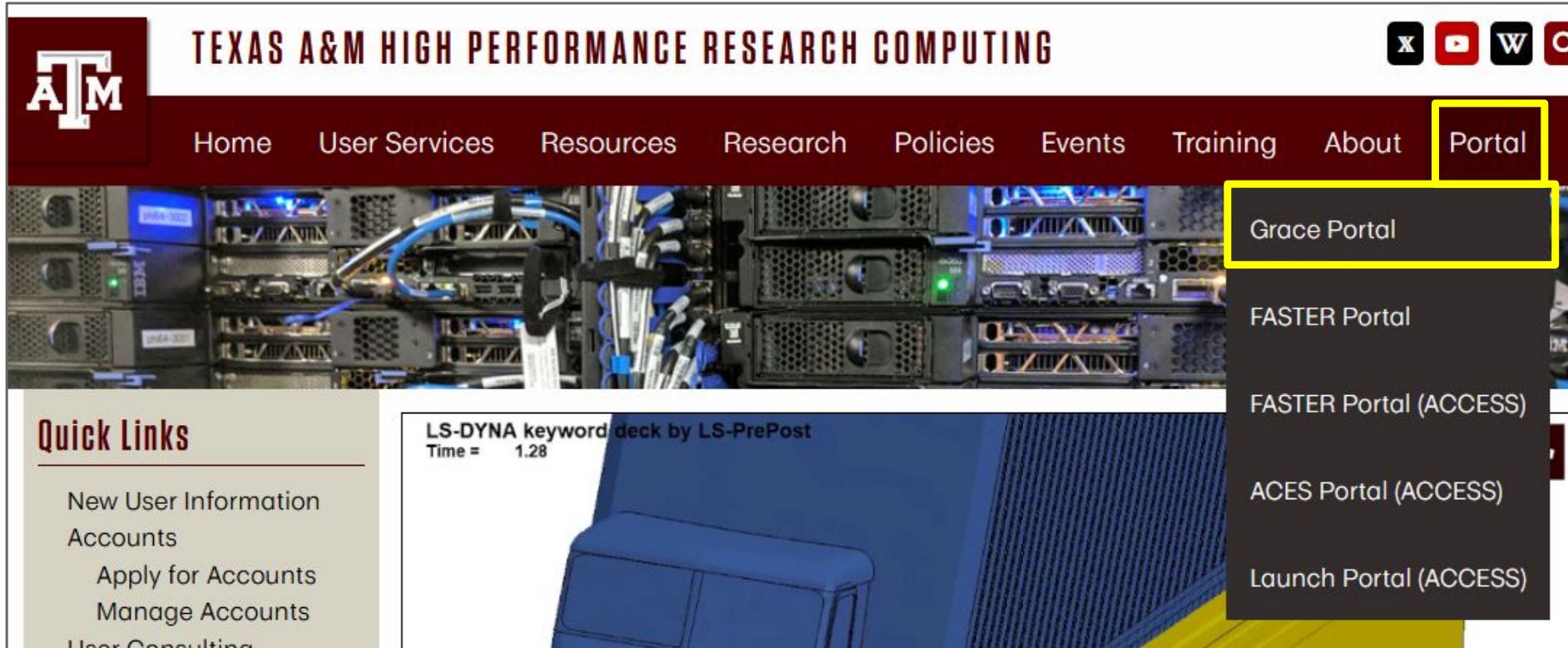
*Service Units (SUs)*

# Accessing Grace: Setup

- If off-campus: Set up and start VPN (Virtual Private Network):  
[u.tamu.edu/VPnetwork](http://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:

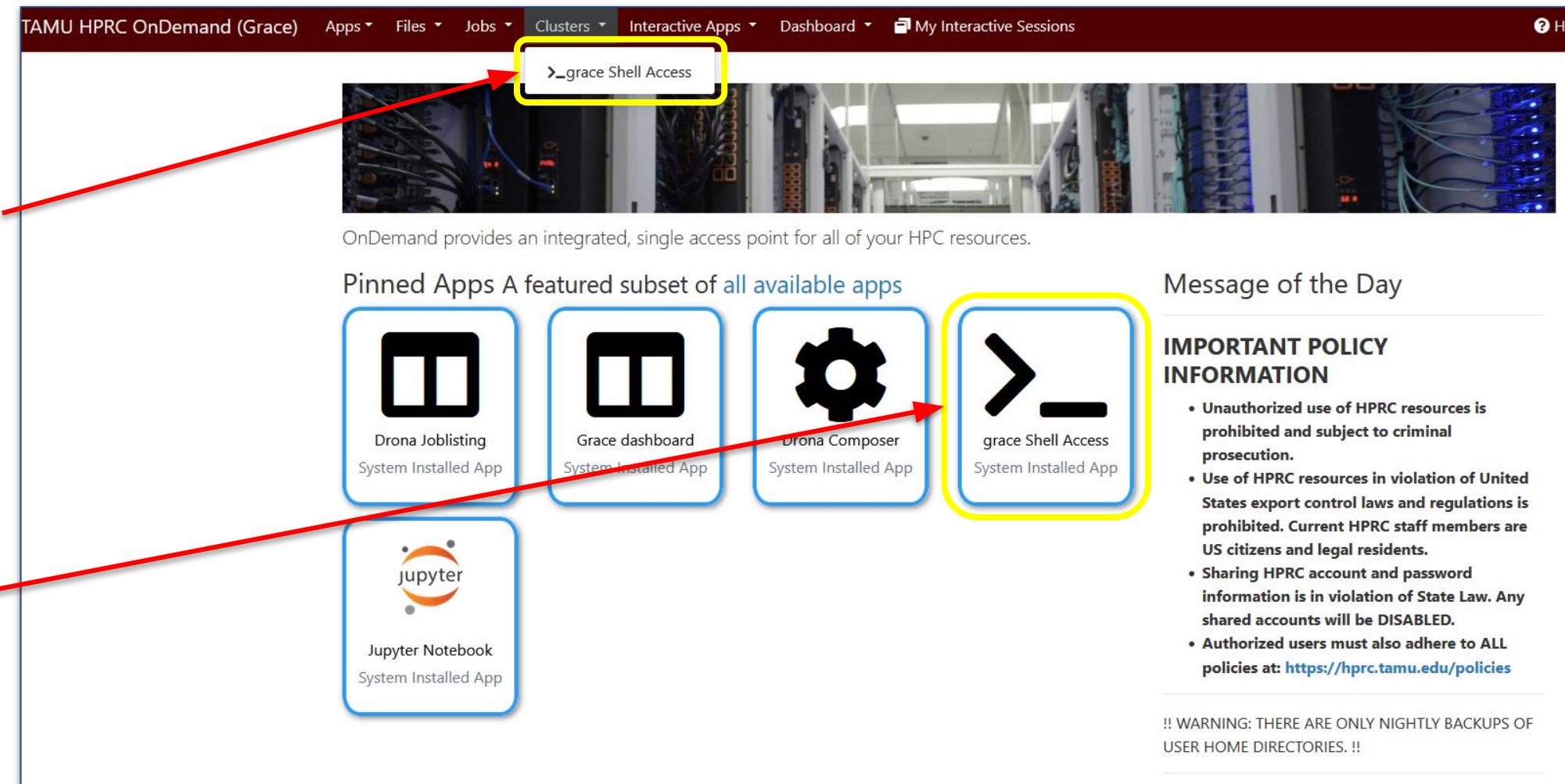
1. Go to [portal.hprc.tamu.edu](https://portal.hprc.tamu.edu) or use the Portal dropdown menu on the HPRC homepage: <https://hprc.tamu.edu/>
2. Choose **Grace Portal**

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

# Accessing Grace via the Portal

Two ways to enter the Portal:

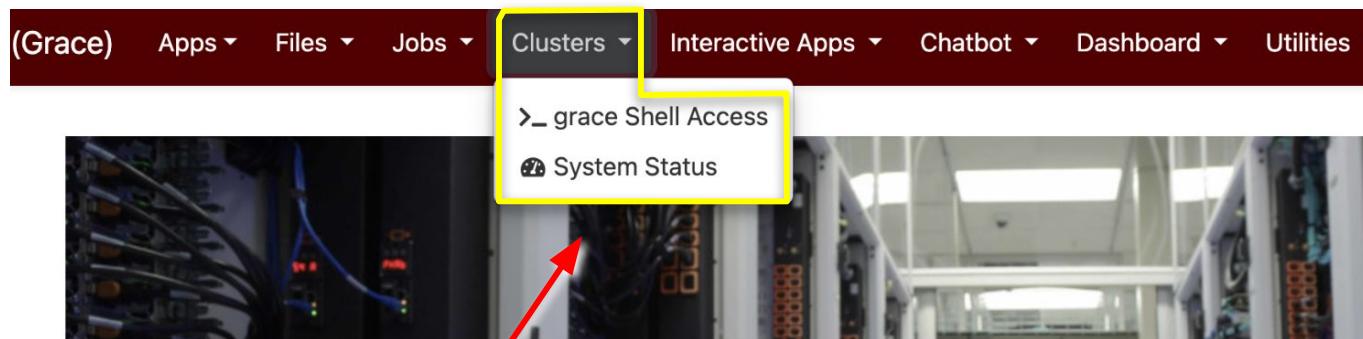
- (1) Select at the top:  
“Clusters” →  
“Grace Shell\*  
Access”
  
- (2) Select in Main  
Menu:  
“Grace Shell  
Access”



\*shell is also called *terminal* or *command line*

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

# Shell Access via the Portal



Get a shell terminal right in your browser

Integrated, single access point for all of your HPC resources.

Featured subset of **all available**

Message of the Day

**IMPORTANT POLICY INFORMATION**

- Unauthorized use of HPC resources is prohibited

```
Host: login.gracelocal
*****
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.
*****
Last login: Thu Aug 21 13:32:56 2025 from 10.73.4.63
=====
Texas A&M University High Performance Research Computing
=====
| Consulting:      help@hprc.tamu.edu (preferred) or (979) 845-0219
| Website:        https://hprc.tamu.edu
| Knowledgebase:  https://hprc.tamu.edu/kb/
| YouTube Channel: https://www.youtube.com/texasamhprc
=====

*****
* === 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.
* - Sharing HPRC account and password information is in violation of
*   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/axa3537  681M    10.0G  6394    10000
/scratch/user/axa3537  2.0G    1.0T  52122   250000
/scratch/group/hprc  4.8T   10.0T  494939  1000000
* Quota increase for /scratch/group/hprc will expire on Dec 31, 2026
Type 'showquota' to view these quotas again.
[axa3537@grace1 ~]$
```

# Hands-On Activity - 2 Minutes

Try to access a *shell*\* on Grace now, either through  
[portal.hprc.tamu.edu](http://portal.hprc.tamu.edu) or [hprc.tamu.edu](http://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/](https://hprc.tamu.edu/kb/User-Guides/Grace/Filesystems_and_Files/)

# Portal: Grace Dashboard

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

The screenshot shows the TAMU Dashboard (Grace) interface. At the top, there are navigation links: 'Interactive Apps', 'Dashboard' (which is the active tab), and 'My Interactive Sessions'. A yellow dashed box highlights the 'Dashboard' tab. On the right side of the header, there are buttons for 'Create Help Ticket' and 'Request Software', also highlighted with a yellow dashed box. The main content area is divided into several sections: 'Node Utilization' and 'Core Utilization' (both donut charts), 'Queue Availability' (table showing nodes and CPU availability for queues like bigmem, gpu, gpu-a40, and long), 'Accounts' (table showing account details like 132717504455 and 132717509839), 'Disk Quotas' (table showing disk usage and limits for home, scratch, and group/hprc), and a 'Request Quota Increase' section (with arrows pointing to the 'Request Quota Increase' buttons in the 'scratch' and 'group/hprc' rows). A yellow box at the bottom left points to the 'Request Quota Increase' section with the text 'Preferred way to request Quota Increases'.

# 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

- 1 SU = 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.

The screenshot shows the TAMU Dashboard (GRACE) interface. On the left, there are two donut charts: 'Node Utilization' and 'Core Utilization'. Below them is a table for 'Queue Availability' showing nodes and CPU availability for 'bigmem', 'gpu', and 'gpu-a40' queues. On the right, there is a section titled 'Accounts' with a table showing two accounts: 132717504455 and 132717509839. The account 132717504455 is highlighted with a yellow dashed circle around the 'Set Default' button. A yellow box with the text 'Change your Default Account' is overlaid on the top right of the dashboard. A blue arrow points from the text box to the 'Set Default' button. The 'Accounts' table has columns: Account, Default, Allocation, Used, and Balance. The 'Disk Quotas' section below shows disk usage for the 'home' disk.

Account	Default	Allocation	Used	Balance
132717504455	Set Default	20000	0	20000
132717509839	default	20000	10.8	19989.2

Disk	Disk Usage	File Usage	Limit
home	769M (7.51 %)	8,145 (81.45 %)	10,000

# 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/#UI>

<https://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

```
[axa3537@grace3 ~]$ myproject -j 132663473580
```

List of Jobs											
ProjectAccount	JobID	JobArrayIndex	SubmitTime	StartTime	EndTime	Walltime	TotalSlots	UsedSUs			
132663473580	15564194	0	2025-06-17 10:39:31	2025-06-17 10:39:45	2025-06-17 10:43:03	198	1	0.06			
132663473580	16029806	0	2025-08-05 10:55:15	2025-08-05 10:55:31	2025-08-05 10:56:53	82	1	0.02			
132663473580	16030076	0	2025-08-05 11:05:38	2025-08-05 11:05:54	2025-08-05 11:14:14	500	1	0.14			
132663473580	16030256	0	2025-08-05 11:14:56	2025-08-05 11:15:04	2025-08-05 11:23:14	490	1	9.94			
132663473580	16030728	0	2025-08-05 11:33:57	2025-08-05 11:34:08	2025-08-05 11:45:01	653	1	13.24			
132663473580	16047456	0	2025-08-06 15:58:38	2025-08-06 15:58:50	2025-08-06 16:19:44	1254	1	0.35			
132663473580	16048154	0	2025-08-06 16:49:31	2025-08-06 16:49:45	2025-08-06 17:49:48	3603	1	73.06			
132663473580	16164088	0	2025-08-15 14:51:00	2025-08-15 14:51:08	2025-08-15 14:51:54	46	1	0.01			
										Total Jobs: 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  
<https://hprc.tamu.edu/software/grace/>
- See the Software Knowledge Base page  
<https://hprc.tamu.edu/kb/Software/>  
for instructions and examples
- License-restricted software
  - Contact [help@hprc.tamu.edu](mailto:help@hprc.tamu.edu)
- 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 Modules on the Grace Cluster	
ACES Software Modules   FASTER Software Modules   Grace Software Modules   Terra Software Modules	
Last Updated: Mon Jun 27 12:24:16 CDT	
The available software for the Grace cluster is listed in the table. Click on any software package name to get more information such as the available versions, additional documentation if available, etc.	
Show	10 entries
<input type="text" value="Search: numpy"/>	
Name	Description
awkward	'Awkward Array is a library for nested, variable-sized data, including arbitrary-length lists, records, mixed types, and missing data, using NumPy-like idioms.'
boolz	'boolz provides columnar, chunked data containers that can be compressed either in-memory and on disk. Column storage allows for efficiently querying tables, as well as for cheap column addition and removal. It is based on NumPy, and uses it as the standard data container to communicate with boolz objects, but it also comes with support for import/export facilities to/from HDF5/PyTables tables and pandas dataframes.'
Bottleneck	'Fast NumPy array functions written in C'
FabIO	'FabIO is an I/O library for images produced by 2D X-ray detectors and written in Python. FabIO support images detectors from a dozen of companies (including Mar, Dectris, ADSC, Hamamatsu, Oxford, ...), for a total of 20 different file formats (like CBF, EDF, TIFF, ...) and offers an unified interface to their headers (as a python dictionary) and datasets (as a numpy ndarray of integers or floats).'
jax	'Composable transformations of Python+NumPy programs: differentiate, vectorize, JIT to GPU/TPU, and more'
mkl_fft	'NumPy-based Python interface to Intel(R) MKL FFT functionality'
netcdf4-python	'Python/numpy interface to netCDF.'
numba	'Numba is an Open Source NumPy-aware optimizing compiler for Python sponsored by Continuum Analytics, Inc. It uses the remarkable LLVM compiler infrastructure to compile Python syntax to machine code.'
numexpr	'The numexpr package evaluates multiple-operator array expressions many times faster than NumPy can. It accepts the expression as a string, analyzes it, rewrites it more efficiently, and compiles it on the fly into code for its internal virtual machine (VM). Due to its integrated just-in-time (JIT) compiler, it does not require a compiler at runtime.'
numpy	'NumPy is the fundamental package for scientific computing with Python. It contains among other things: a powerful N-dimensional array object, sophisticated (broadcasting) functions, tools for integrating C/C++ and Fortran code, useful linear algebra, Fourier transform, and random number capabilities. Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases.'

# 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

```
module avail
```

← shows which software is available

```
module load GCC/13.2.0 OpenMPI/4.1.6
```

← load GCC compiler version 13.2.0 and OpenMPI version 4.1.6

```
module avail
```

← show which software is available to use with the loaded modules

```
module load PyTorch/2.7.0
```

← load PyTorch version 2.7.0

```
module list
```

← see what software you've loaded already

Module System Youtube Video → [www.youtube.com/watch?v=drxpbrOCPFw](https://www.youtube.com/watch?v=drxpbrOCPFw)

# 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
  - 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 → [www.youtube.com/watch?v=drxpbrOCPFw](https://www.youtube.com/watch?v=drxpbrOCPFw)

# 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 → [www.youtube.com/watch?v=drxpbrOCPFw](https://www.youtube.com/watch?v=drxpbrOCPFw)

# 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 screenshot shows the TAMU HPRC OnDemand (Grace) web interface. At the top, there is a navigation bar with links for Apps, Files, Jobs (which is the active tab, indicated by a dropdown menu), Clusters, Interactive Apps, Dashboard, and My Interactive Sessions. A 'Logged' user icon is also present. The main content area has a banner stating "OnDemand provides an integrated, single access point for all of your HPC resources." Below this is a section titled "Pinned Apps A featured subset of all available apps" which lists five apps: Drona Joblisting, Grace dashboard, Drona Composer (which is highlighted with a yellow box and a red arrow), grace Shell Access, and Jupyter Notebook. To the right, there is a "Message of the Day" and a "IMPORTANT POLICY INFORMATION" section with a list of rules, and a warning at the bottom about backups.

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

Pinned Apps A featured subset of all available apps

- Drona Joblisting System Installed App
- Grace dashboard System Installed App
- Drona Composer** 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. !!

# 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

The screenshot shows the 'Job Composer' interface for the Drona Composer (GRACE) application. The interface is divided into several sections:

- Job Name:** A text input field with a 'Change' button and a default value of '/scratch/user/jwinchell/drona\_composer/runs'.
- Location:** A dropdown menu set to 'Generic'.
- Environments:** A dropdown menu set to 'Generic'.
- Upload files:** A button to upload files.
- Add modules:** A button to add modules.
- Number of tasks:** A dropdown menu set to '1'.
- Advanced task options:** A checkbox.
- Use Accelerator:** A dropdown menu set to '-- Choose an option --'.
- TOTAL Memory:** A dropdown menu set to 'GB'.
- Expected run time:** A dropdown menu set to 'Days'.
- Project Account:** A dropdown menu set to '-- Choose an option --'.
- Additional Slurm parameters:** A text input field.

At the bottom right are 'Preview' and 'Hide History' buttons.

# 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: 3
```

Check status

matching JOBID

```
squeue -u netID
```

or

```
squeue --me
```

JOBID	NAME	USER	PARTITION	NODES	CPUS	STATE	TIME	TIME_LEFT	START_TIME	REASON	NODELIST
6853258	jobname	NetID	xlong	2	96	RUNNING	3-07:36:50	16:23:10	2025-01-23T17:27:3	None	c[180,202]
6853257	jobname	someuser	xlong	2	96	RUNNING	3-07:36:56	16:23:04	2025-01-23T17:27:2	None	c[523-524]

# Hands-On Activity

1. Navigate to `/scratch/training/Intro-to-Grace`
2. Copy `hello_world.slurm` and `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:

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

For the NODES and CPUS columns:

A = Active (in use by running jobs)

O = Offline (unavailable for jobs)

I = Idle (available 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](mailto: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
<b>sbatch</b> jobfile1	Submit jobfile1 to batch system
<b>squeue</b> [-u user_name] [-j job_id]	List jobs
<b>scancel</b> job_id	Kill a job
<b>sacct -x -j job_id</b>	Show information for a job (can be when job is running or recently finished)
<b>sacct -x -s YYYY-HH-MM</b>	Show information for all of your jobs since YYYY-HH-MM
<b>lnu</b> job_id	Show resource usage for a job
<b>pestat -u \$USER</b>	Show resource usage for a running job
<b>seff</b> 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  
DIVISION OF RESEARCH

# 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)

