HPCC USER GROUP MEETING

October 16, 2025

HIGH PERFORMANCE COMPUTING CENTER

TEXAS TECH
Information Technology

ALAN SILL

MISHA AHMADIAN

MEETING AGENDA

1) Motivation for the upgrade
(Alan Sill, HPCC Managing Director)

- Security upgrades and requirements
- Operating System and package maintainability

2) Upgrade details (Misha Ahmadian)

- New HPCC Hardware Upgrades
  - Primary Lustre storage
  - Application storage
- New HPCC Software Environment
  - Partition Operating System Updates
  - HPC and AI Software Packages
  - Self-Installed Packages
- New RedRaider Cluster Interactive Web Portal

Motivation

- Security upgrades and requirements
  - In late 2023, the HPCC was alerted by TTUNet Security of the possible involvement of the Quanah partition login node in a campus-wide security incident. Later searches of log files showed no evidence of compromise, but the decision was made to upgrade the operating system to a modern, more maintainable, more secure framework
- Operating System and package maintainability
  - CentOS was changed by Red Hat from a stand-alone distribution to an upstream test and development role for Red Hat Enterprise Linux.
- Both of these requirements were met by switching from CentOS to Rocky Linux with a Long-Term Support (LTS) contract
  - Contract also covers cluster provisioning software (Warewulf) and container framework (Apptainer), greatly saving HPCC staff time

HPCC Staff and Students

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Wyatt Tyson
Jaechang Kim

RedRaider Cluster Primary Storage Upgrade

Lustre-based file system storage

Home, Work, Scratch, and Research areas

Timeline

- **6.1 PB**
- All Spinning Disk Drives (HDD)
- DDN EXA 5.x
- Lustre 2.12.x

DDN 14K (2019)

DDN NVX2 (2025)

- **12 PB**
- 1 PB NVMe + 11 PB HDD
- DDN EXA 6.x LTS
- Lustre 12.14.x

Quota/Backup/Purge Policies

- The space quota for all regular HPCC account holders has been doubled!

Areas	Old Quota	New Quota	File Limit	Grace	Backup	Purge
/home/<eraider>	300 GB	500 GB	1,000,000	1 Day	**Yes**	No
/lustre/work/<eraider>	700 GB	1.5 TB	1,000,000	1 Day	No	No
/lustre/scratch/<eraider>	None	None	100,000,000	1 Day	No	**Yes**

✓ Researchers/groups may also purchase additional dedicated storage space:

- With Backup: $80/TB/Year (recommended for important or non-replaceable data)
- Without Backup: $40/TB/Year (adequate if you also back up data remotely or can replace it)

- Beginning August 2025, a new backup software system (Bacula) has replaced the old software, which was no longer maintained by its vendor. (Transition was done with no downtime.)

1PB NVMe Storage Pool

1) Hotpool

- **Pros:**
  - All write operations go directly to the NVMe pool (Hotpool) before they go to the HDD pool.
  - Instant performance gain upon all writes.
- **Cons:**
  - Creates duplicate inodes, which could lead to excessive inode usage.
  - Performance gain is temporary and does not guarantee similar performance on future reads and writes.

2) PFL Performance Pool ✓

- **Pros:**
  - Seamless performance gain on all read/write IOPs.
  - Ideal for small files.
  - No duplicate inodes.
- **Cons:**
  - Only a small chunk of the files stays on the NVMe pool.
  - Large file IOPs won't gain much performance increase.

** Historically, HPCC researchers have generated far more small files than large ones.

Lustre PFL

- Progressive File Layout (PFL):
  - Lustre PFL stripes each file into a series of components.
  - Then increases the stripe count in a step-wise manner as the file grows.
  - Users can expect reasonable performance for a variety of normal file IO patterns without the need to explicitly understand their IO model.

Storage Pool	Drive type	Capacity	Component length	Stripe Size	Stripe Count
Performance	NVMe	1 PB	256 KiB	256 KiB	1
Capacity	HDD	11 PB	10 GiB	1 MiB	1
Capacity	HDD	11 PB	Infinity	1 MiB	8

Default File Layout of all files under Home, Work, and Research areas

Lustre PFL (Cont.)

- Progressive File Layout (PFL):

Storage Pool	Drive type	Capacity	Component length	Stripe Size	Stripe Count
Capacity	HDD	11 PB	1 GiB	1 MiB	1
Capacity	HDD	11 PB	10 GiB	1 MiB	4
Capacity	HDD	11 PB	Infinity	1 MiB	8

Default File Layout of all files under Scratch area

- NOTE!
  - Access for files smaller than 1MiB wastes bandwidth!
  - Aggregated data structures preferred for large numbers of small files

RedRaider Cluster Application Storage Upgrade

Data storage for the cluster-wide HPC/AI software packages

Application Storage

- Application storage is meant for serving a location for all cluster-wide HPC/AI software packages.
  - Shared with all CPU/GPU worker nodes.
  - Requires high throughput for read-intensive activity.
  - Must be capable of handling millions of open files all at the same time.

- In conjunction with the cluster OS/Software upgrade in 2025, we gradually transitioned application storage to a new system.

NVMesh®

BeeGFS®

Application Storage (New Vs. Old)

- What is new?

Application Storage (Old)	Application Storage (New)
Commodity hardware (3x servers)	Hardware designed for NVMesh® software defined storage (4x Servers)
~40 TB All spinning drives (HDD)	~80 TB all NVMe drives
Up to one server failure tolerance	Up to one server and two disk failure tolerance
GlustreFS distributed file system (has been discontinued)	**BeeGFS** parallel file system
Limited to 1 million open files at once.	No limit
Performance was limited to each server's performance	Read/Write loads are distributed across all four servers in parallel
TCP over Ethernet	RDMA over InfiniBand – TCP over Omni-Path

RedRaider Cluster Operating System Upgrade

Migration from CentOS 7 & 8 to Rocky Linux 8 & 9

Background

- History of previous operating system versions on the RedRaider cluster:

Quanah Partition	All other partitions in RedRaider Cluster (Nocona, Matador, Toreador, …)
Commissioned in 2017	Commissioned in 2021
CentOS 7.4 (2017 – 2025) ~8 years	CentOS 8.1 (2021 – 2025) ~4 years
No essential OS updates since 2017, including security patches	No essential OS updates since 2021, including security patches

  - In December 2020, Red Hat announced that CentOS Linux would be discontinued at the end of 2021 to shift focus to CentOS Stream.
  - CentOS 7 end-of-life (EOL) date was June 30, 2024 (CentOS 7.9 was the last version)
- The HPCC prioritizes operating system and environment stability, but a transition to a new long-term supportable OS and software environment was required.

Software Support Conflicts

- Problems of a cluster with an obsolete operating system:
  - **For researchers:**
    - That's all we want!
    - But we also want everything to always be totally up to date!
  - **For HPCC staff:**
    - SECURITY NIGHTMARE!
    - MAINTAINABILITY NIGHTMARE!
    - VERSION CONFLICT AND SOFTWARE COMPATIBILITY NIGHTMARE!
    - Hard to keep current with the latest software installation requests.
    - Hard to upgrade the critical software components, such as network and GPU drivers (especially important for GPU and AI software)

Challenges

- Why did it take so long to do the 2025 upgrade?
  - We needed to rethink and redesign the way we provision the operating system on all worker nodes in the cluster:
  - We explored new opportunities that helped reshape the previous cluster management methods:
    - Transition from CentOS to a stable and affordable commercial Linux distribution:
      - Rocky Linux with Long Term Support (LTS) and compatibility. Rocky Linux
    - Upgrade the backend cluster management tools to allow future-proof planning:
      - WareWulf 4.x
    - Explore modernized HPC/API software package installation methods. (Spack)
  - We tried out our ideas on the Quanah partition first:
    - which took most of the first half of CY 2025. Based on success there, pursued a much faster upgrade path for the rest of the partitions of the RedRaider cluster.

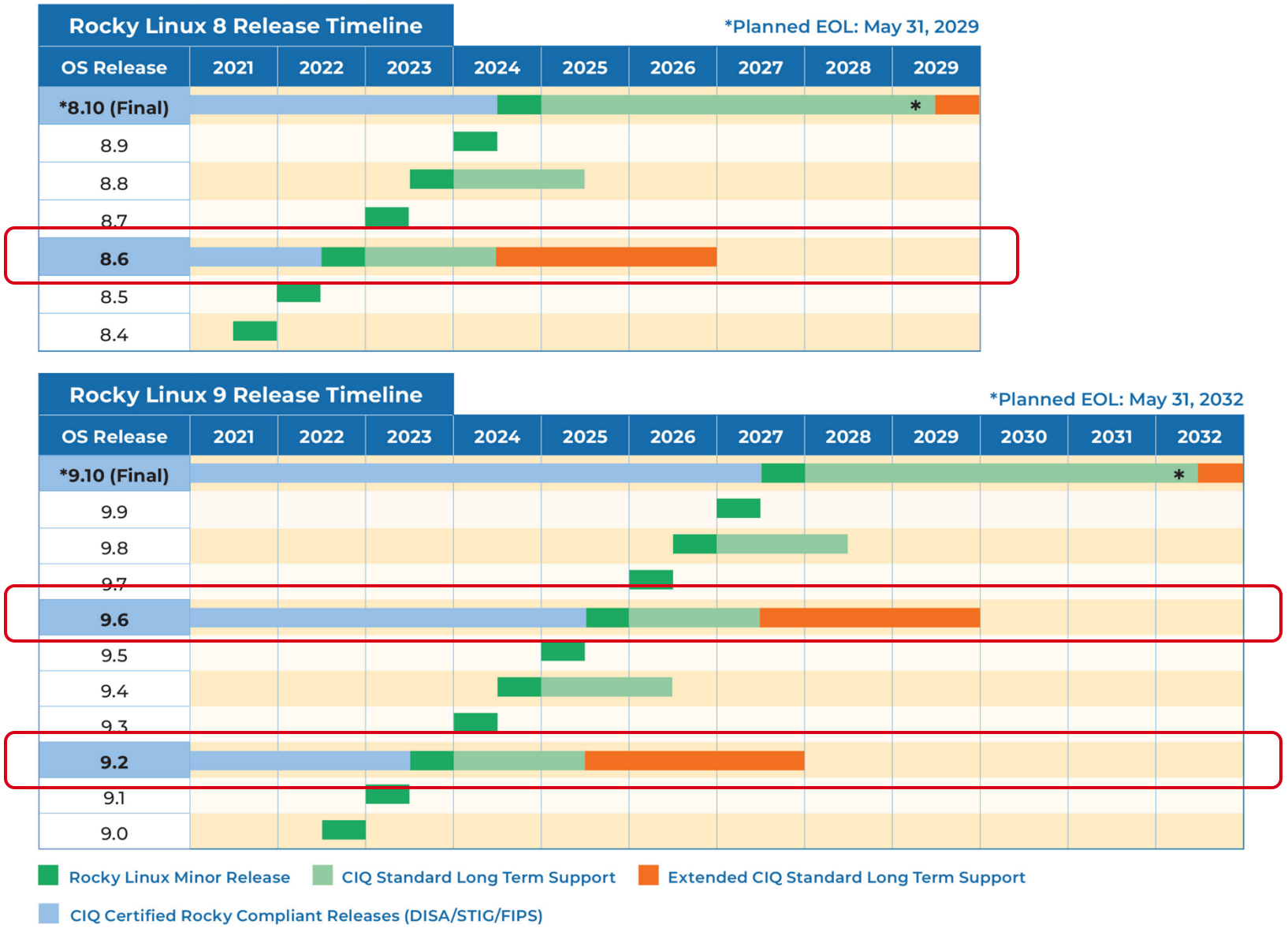
OS Support: CIQ LTS

- CIQ Rocky Linux Long-Term Support model:

Feature	Rocky Linux Community	Rocky Linux LTS from CIQ ***
CVE Remediation	Best-effort timing patches	**Fast, guaranteed patching with SLOs**
Package Repositories	Community-managed with basic signing	**Verified, secure, U.S.-based CIQ repositories**
OS Updates	Variable time to remediation	**Guaranteed updates with service-level objectives**
Accountability	Community-managed processes	**Indemnification and verified package content**

*** TTU HPCC has subscribed to Rocky Linux LTS from CIQ

CIQ LTS Support Timelines



HPCC OS Upgrade Sequence

March 2022	• Started the CIQ commercial support
March 2024	• Started the Long-Term Support (LTS) with CIQ
March 24 – January 25	• Implementing the new OS provisioning system • Installing new HPC software packages
February 2025	• Upgrading Quanah partition to Rocky Linux 9.2
May 2025	• Upgrading XLQuanah, Himem-ivy partitions to Rocky Linux 8.6-LTS
August 2025	• Completed the data transfer from the old Lustre storage to the new one. Brought up the new storage into production. • Upgraded Matador partitions with 100 nodes in Nocona to Rocky Linux 9.6-LTS
October 2025	• Upgraded the remaining nodes in the Nocona and all nodes in Toreador partitions.

Current Status: All Upgrades Complete!

- Current partitions' OS version:

Partition(s):	Current Rocky Linux version	LTS Expiration Date	Comments
XLQuanah, Himem-ivy, interactive-ivy	8.6-LTS	End of 2026	Due to the use of old HW in these partitions, the latest, longest-supported Rocky Linux version has been provisioned on the nodes.
Quanah	9.2-LTS	End of 2027	At the time of the OS update, the latest, longest-supported version of Rocky Linux available was used.
Nocona, Matador, Toreador	9.6-LTS	End of 2029	The latest and longest-supported version of Rocky Linux as of October 2025.

Future Maintenance Updates

- Periodic Software Update Plan:
  - Immediate critical updates:
    - All critical OS software packages will be remediated as soon as possible when needed to apply security patches and other critical updates
    - Should not affect operation of applications or software
  - Quarterly scheduled maintenance:
    - Full OS updates, including all the security and Kernel patches.
    - Currently installed software packages will continue working.
    - The latest version of network and GPU device drivers will be updated as they become available.
  - Upon LTS expiration or for rare OS transition requirements:
    - HPCC will plan to upgrade the OS entirely.
    - All software packages need to be reinstalled or upgraded.

RedRaider Cluster Software Packages Upgrade

Reinstall and/or upgrade all HPC/AI software packages

Application Support Challenges

- Major operating system upgrades can easily break compiled software packages, causing them to fail to run as they did earlier.
- In general, maintaining HPC software packages is not easy!
  - New OS environments are often not compatible with older compilers.
  - Older software packages are not always compatible with new compilers and libraries.
  - Major HPC software packages depend on many other libraries and software packages that must be installed first, which is extremely time-consuming.
  - Essential math libraries and parallel software packages (MPI, OpenMP, etc.) require careful installation to ensure they are well-optimized for the hardware architecture, networking, and storage.

Methods

- Software installation methods we use at HPCC:
  1. Prebuilt RPMs and binaries from the current operating system repositories.
     - Not all software packages are available in OS repos.
     - HPC/AI software packages are definitely missing.
     - Some of the prebuilt binaries have not been optimized for the target hardware.
  2. Manual software compilation:
     - Requires an intermediate to advanced level of knowledge of compiling software packages in Linux.
  3. Spack:
     - Spack is a package manager for supercomputers, Linux, macOS, and Windows. It [is supposed to] make installing scientific software easy.
     - Provides a recipe for over 8,500 software packages.
     - Configuration and package management are not easy.

Spack

Methods (Cont.)

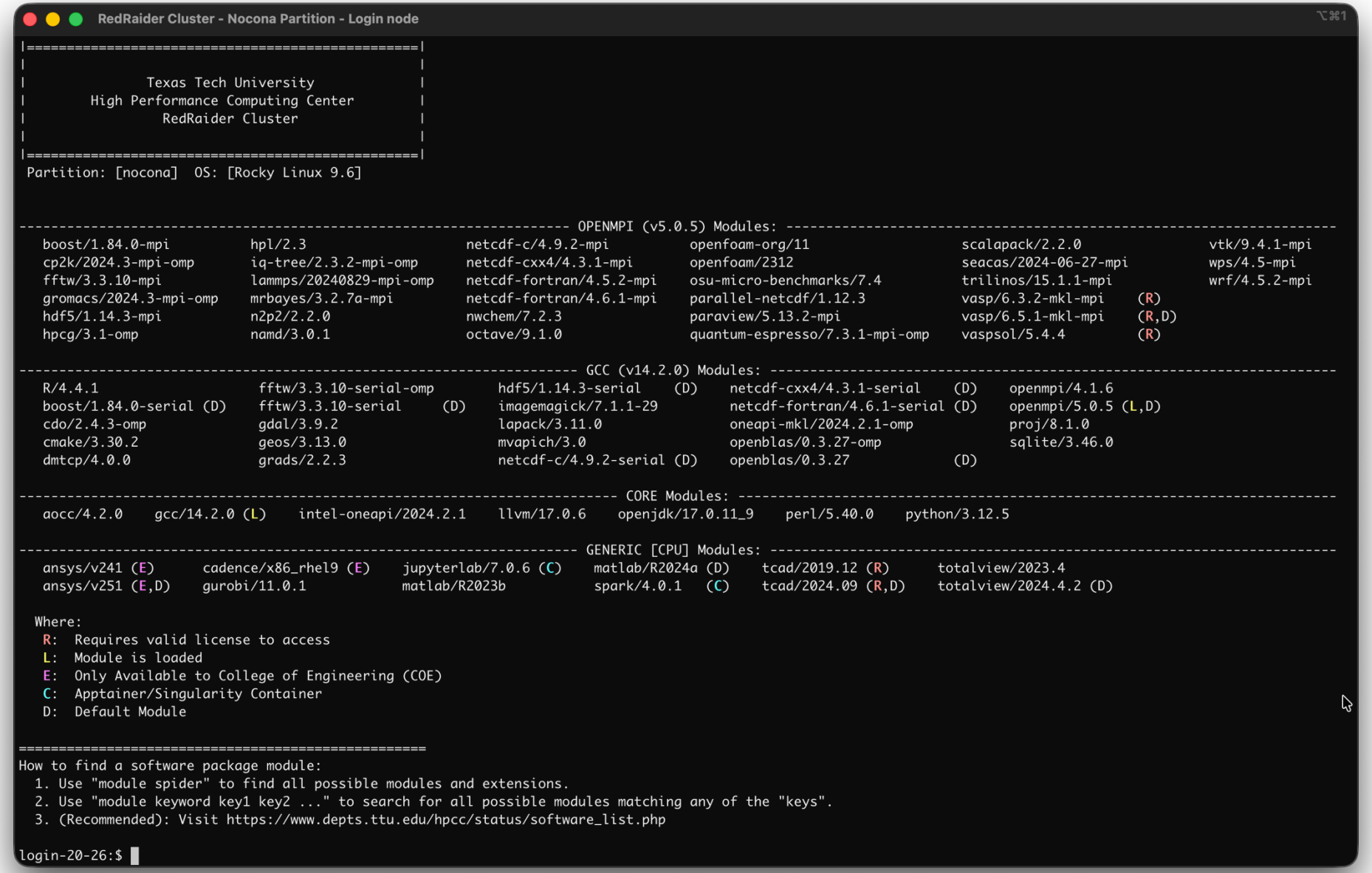
3. Containers:
   - If available, they're easiest to download and use.
   - Requires container management platforms such as Docker, Podman, and Apptainer (formerly known as Singularity).
     - HPCC recommends, provides, and supports Apptainer. No other container management system is supported on the RedRaider Cluster.
   - Can containerize software package(s) on different operating systems.
   - Prebuilt containers may not be fully optimized for the target hardware. (This is not the case with Nvidia GPU Containers running on Nvidia GPU devices!)

4. Anaconda/Miniconda/MiniForge:
   - Package and environment management systems that allow you to install, run, and update software packages and their dependencies.
   - Perfect for Python and R packages.

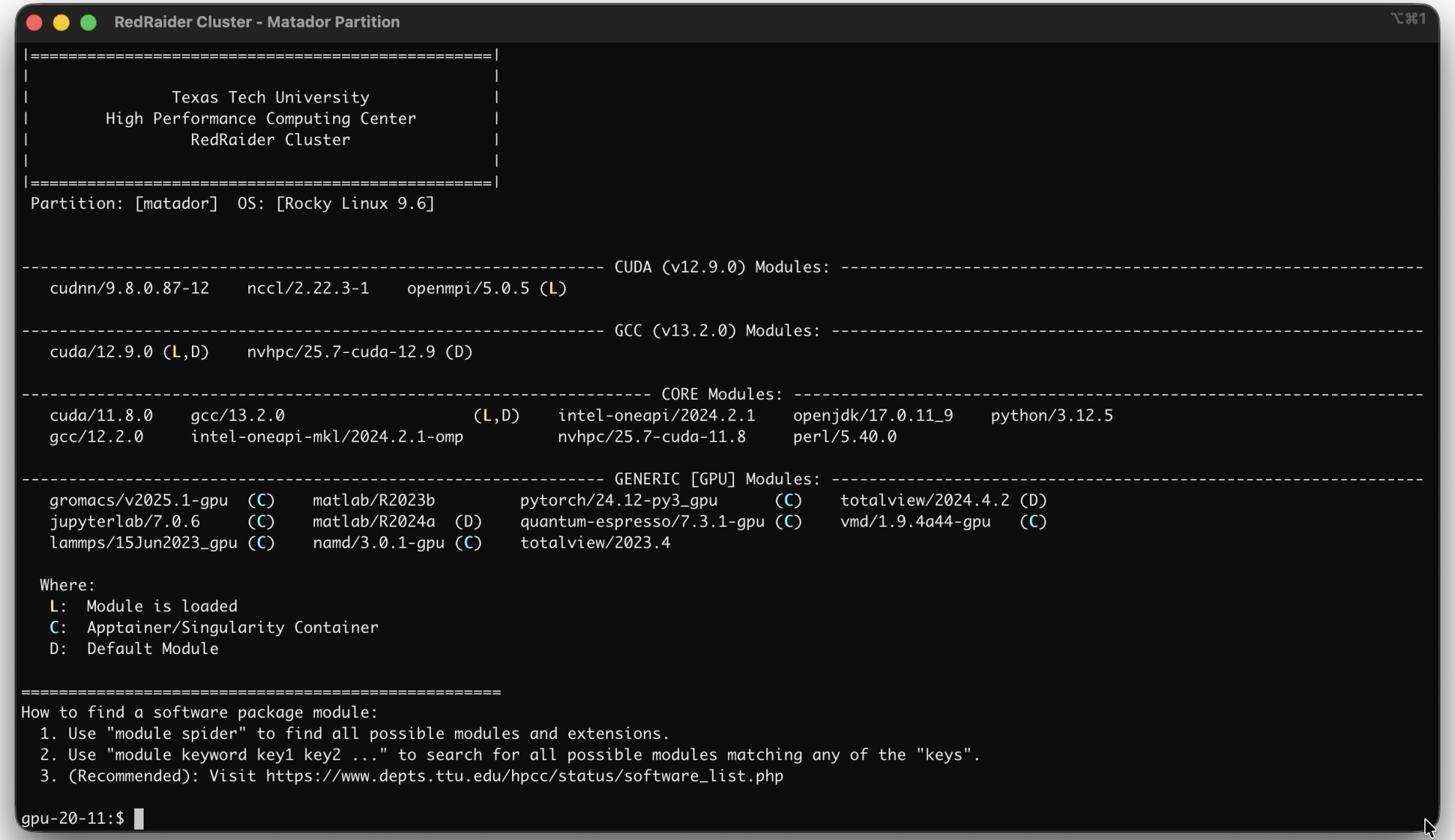
New Partition Software Environment

	Quanah/Nocona	Matador/Toreador	XLQuanah/Himem-Ivy
Operating System	• Rocky Linux 9.2-LTS / 9.6-LTS	• Rocky Linux 9.6-LTS	• Rocky Linux 8.6-LTS
Package Build Env	• Spack 0.23 • Apptainer/Singularity Containers	• Spack 0.23 • Apptainer/Singularity Containers	• Spack v0.23 • Apptainer/Singularity Containers
Software Deployment Env	• Lmod Modules 8.7.55	• Lmod Modules 8.7.55	• Lmod 8.7.55
Available C/C++/Fortran /MPI Compilers	• GCC 11.3.1 / GCC 11.5.0(Default) • GCC 14.2.0 (Recommended) • Intel OneAPI 2024.2.1 • OpenMPI 4.1.6 – 5.0.5 • Intel OneAPI MPI 2021.13.1 • AMD AOCC/AOCL 4.2.0 (Nocona)	• GCC 11.5.0 (Default) – CUDA 11.x • GCC 12.2.0 (CUDA 12.0 – 12.3) • GCC 14.2.0 (CUDA 12.4+) • Intel OneAPI 2024.2.1 • OpenMPI 4.1.6 – 5.0.5 with CUDA	• GCC 8.5.0 (Default) • GCC 14.2.0 (Recommended) • Intel OneAPI 2024.2.1
GPU Libraries	• N/A	• CUDA 11.8.0 • CUDA 12.3.2 • CUDA 12.9 • cudnn/9.8.0.87 • nccl/2.22.3	• N/A

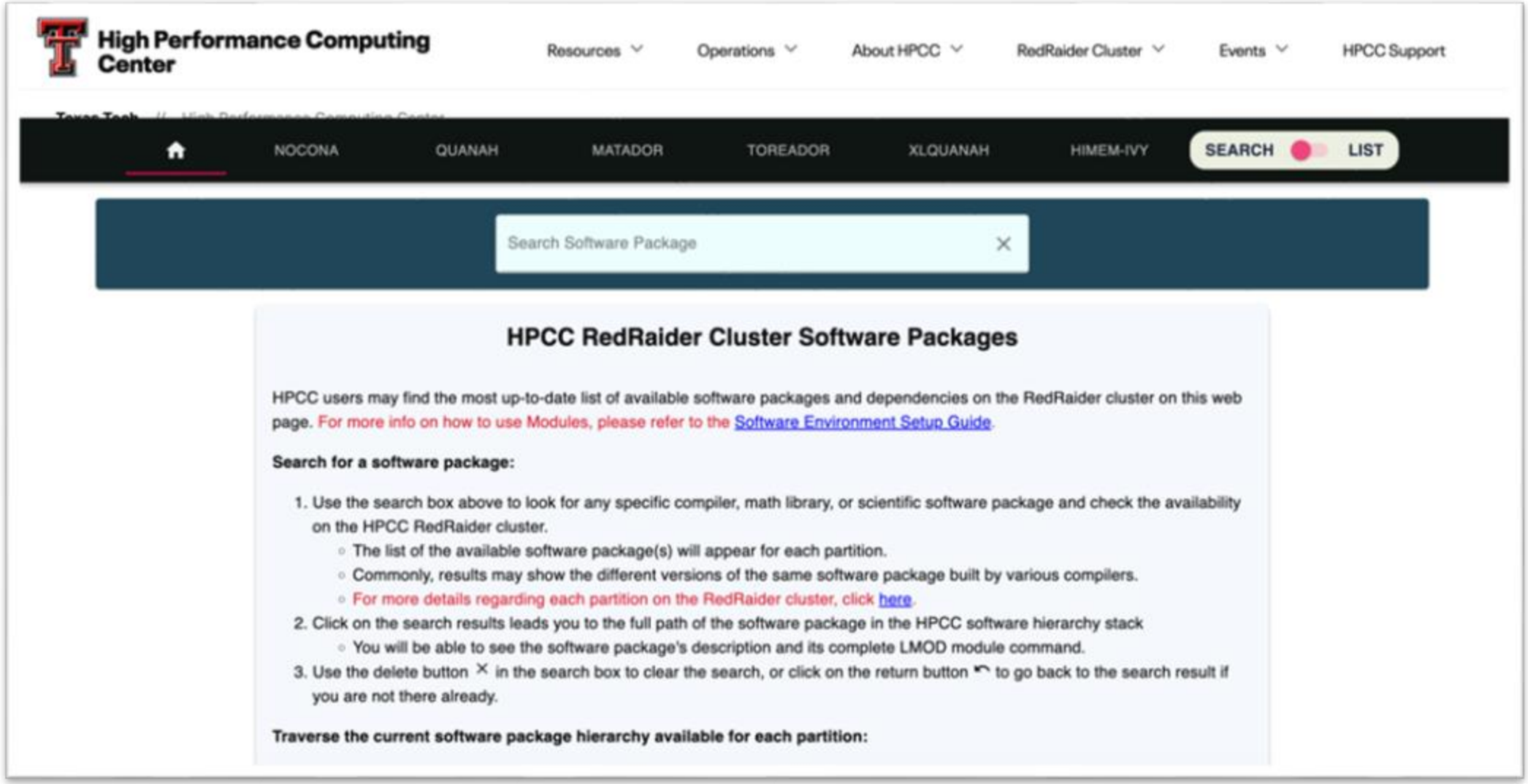
Lmod Modules (CPU Nodes)



Lmod Modules (GPU Nodes)



Search for Available Modules



HPCC RedRaider Software Packages (TTU VPN is required to access the portal when connected from an off-campus network)

Self-Installed Software Preferred

- Wherever possible, use Conda or other methods to install software into your own account if it does not require root access.
- HPCC staff will prioritize assistance with installing software packages that are **not** available in Conda or otherwise self-installable.
- Upon approval, all cluster-wide software package installations will be maintained seamlessly across CPU/GPU partitions.
- On GPU nodes, users can install any version of CUDA that is not installed cluster-wide.
  - The latest supported version of CUDA on the Matador partition is 12.9.
- We appreciate your patience with software installation requests after the OS upgrade, as wait times have increased due to new requests.

(We’re really proud of this one!)

RedRaider Cluster Interactive Web Portal

Introducing HPCC Open OnDemand Interactive Web Portal.

Introduction to Open OnDemand

- HPCC Open OnDemand interactive portal provides a user-friendly, web-based portal that simplifies access to advanced computing resources.

- Using a standard web browser, researchers and students can seamlessly manage files, submit and monitor jobs, and launch interactive applications, all without complex command-line operations.

- The portal is available and open to all HPCC account holders starting today.

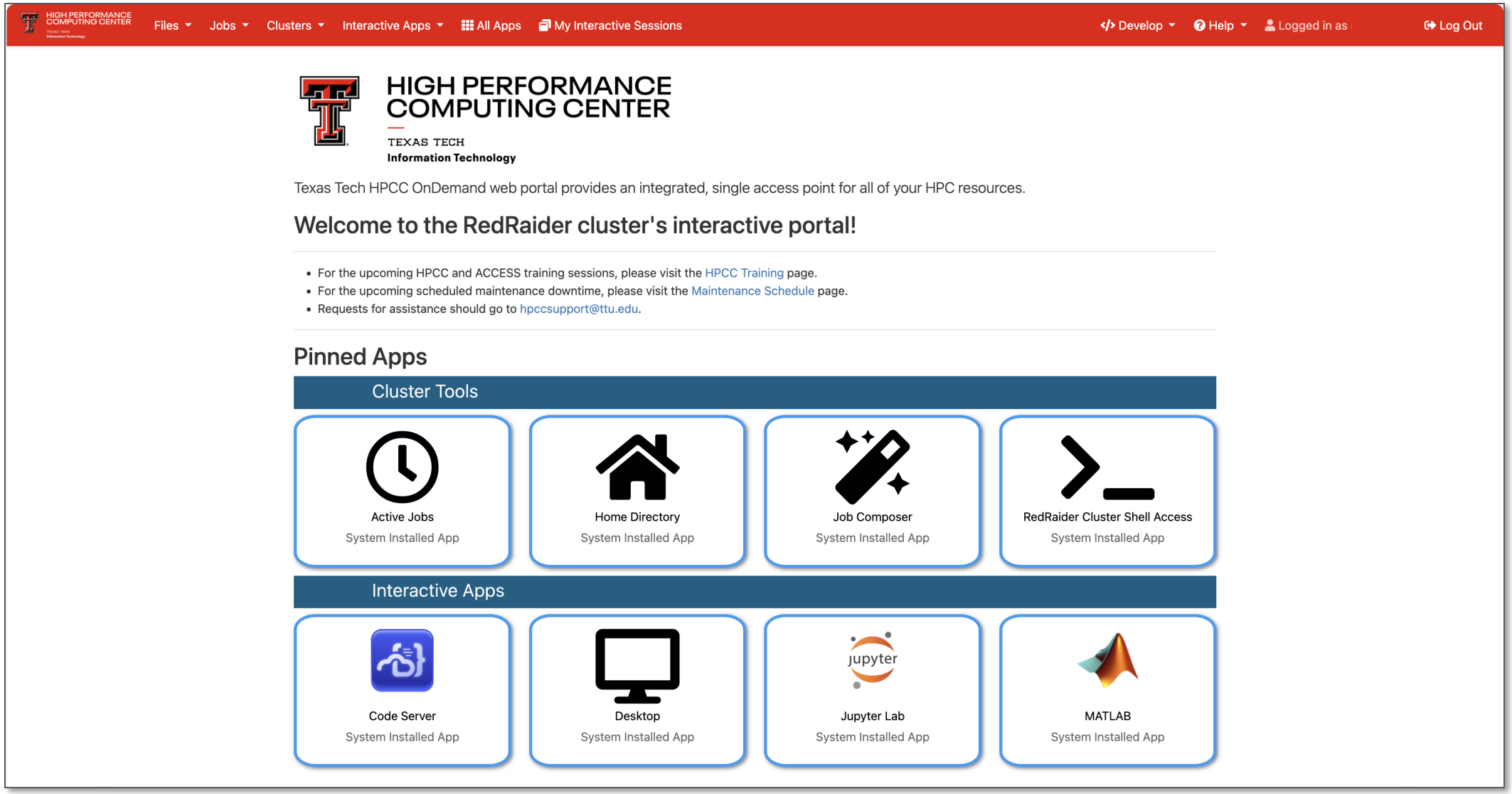
Interactive-ivy Partition

- Along with the OOD portal, we have also launched a new partition, called interactive-ivy, to provide resources for interactive applications:

- Interactive-ivy partition (12 nodes)
  - 2x Intel Xeon E5-2670 Ivy Processors/node
  - 240 total cores (20 cores/node)
  - 1.5 TB total RAM (128 GB/node)
  - InfiniBand (53 Gbps) fabric

  - Jobs are limited to
    - 10 CPU cores per job
    - 12-hour runtime
    - 2 running jobs per user
    - No more than 10 pending/running jobs per user

Let’s explore the portal



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Raise a support ticket:

hpccsupport@ttu.edu