



HIGH PERFORMANCE
COMPUTING CENTER

TEXAS TECH
Information Technology

HPCC USER GROUP MEETING

October 16, 2025

ALAN SILL

MISHA AHMADIAN



FROM HERE, IT'S POSSIBLE.™





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 Quannah 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



Dr. Alan Sill
Managing Director,
HPCC
Adjunct Professor,
Dept. of Physics and
Astronomy

Misha Ahmadian
Senior Research
Associate

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Research Associate

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Enterprise System
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III

Travis Turner
Server Administrator
III

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Tomas Rohatynski

Undergraduate Student Assistants:
Andrew Glore
Rajat Jadhav

Wyatt Tyson
Jaechang Kim

RedRaider Cluster Primary Storage Upgrade

Lustre-based file system storage

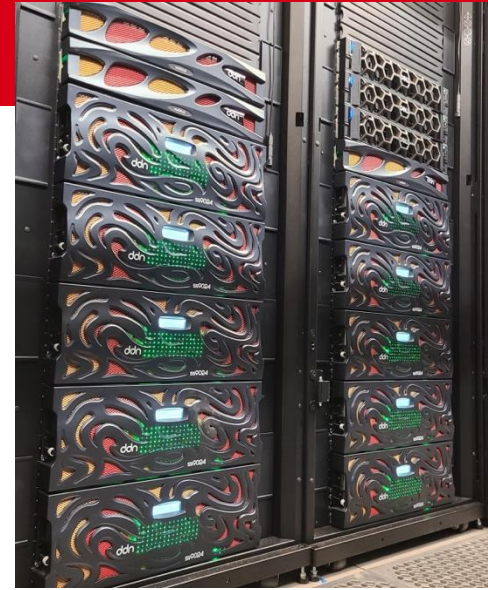
Home, Work, Scratch, and Research areas



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, HPC 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 NVMe [®] 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
GlusterFS 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



Rocky Linux



Background

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

Quannah 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 Quannah 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.

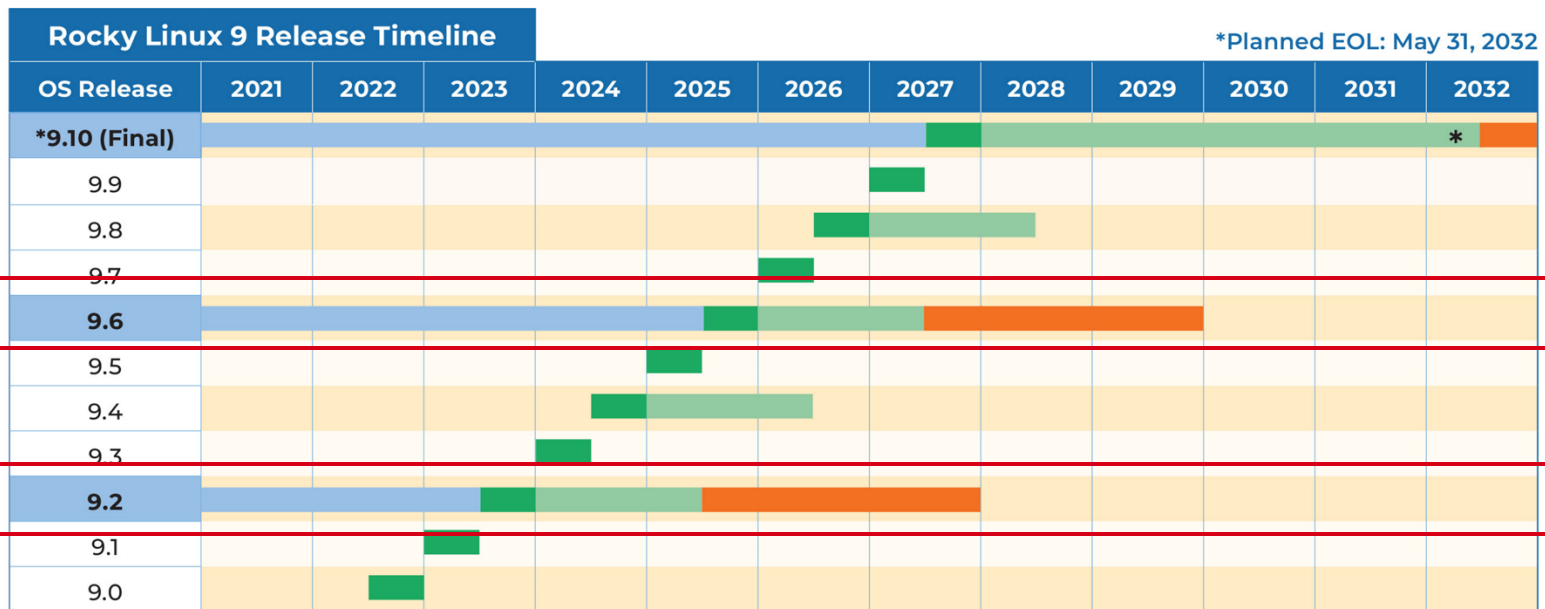
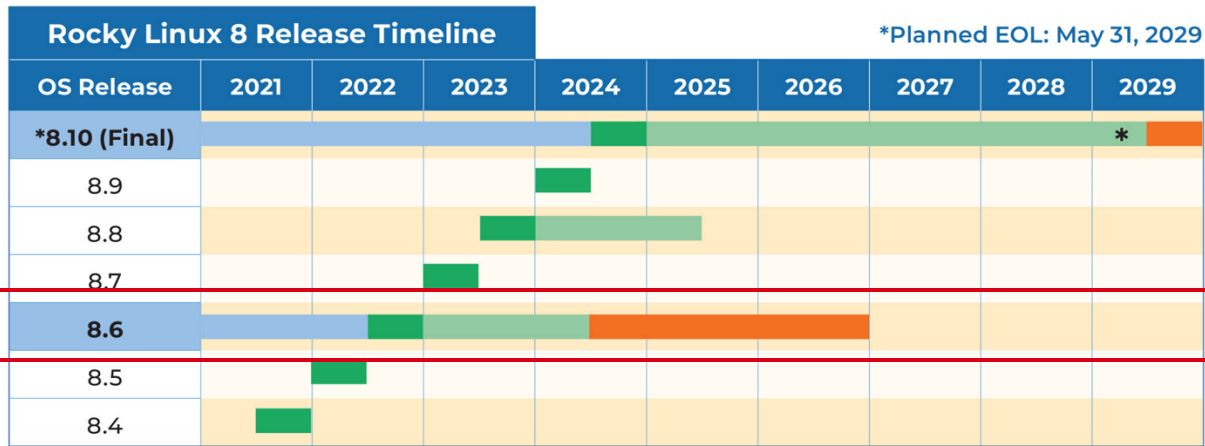
OS Support: CIQ LTS

- 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

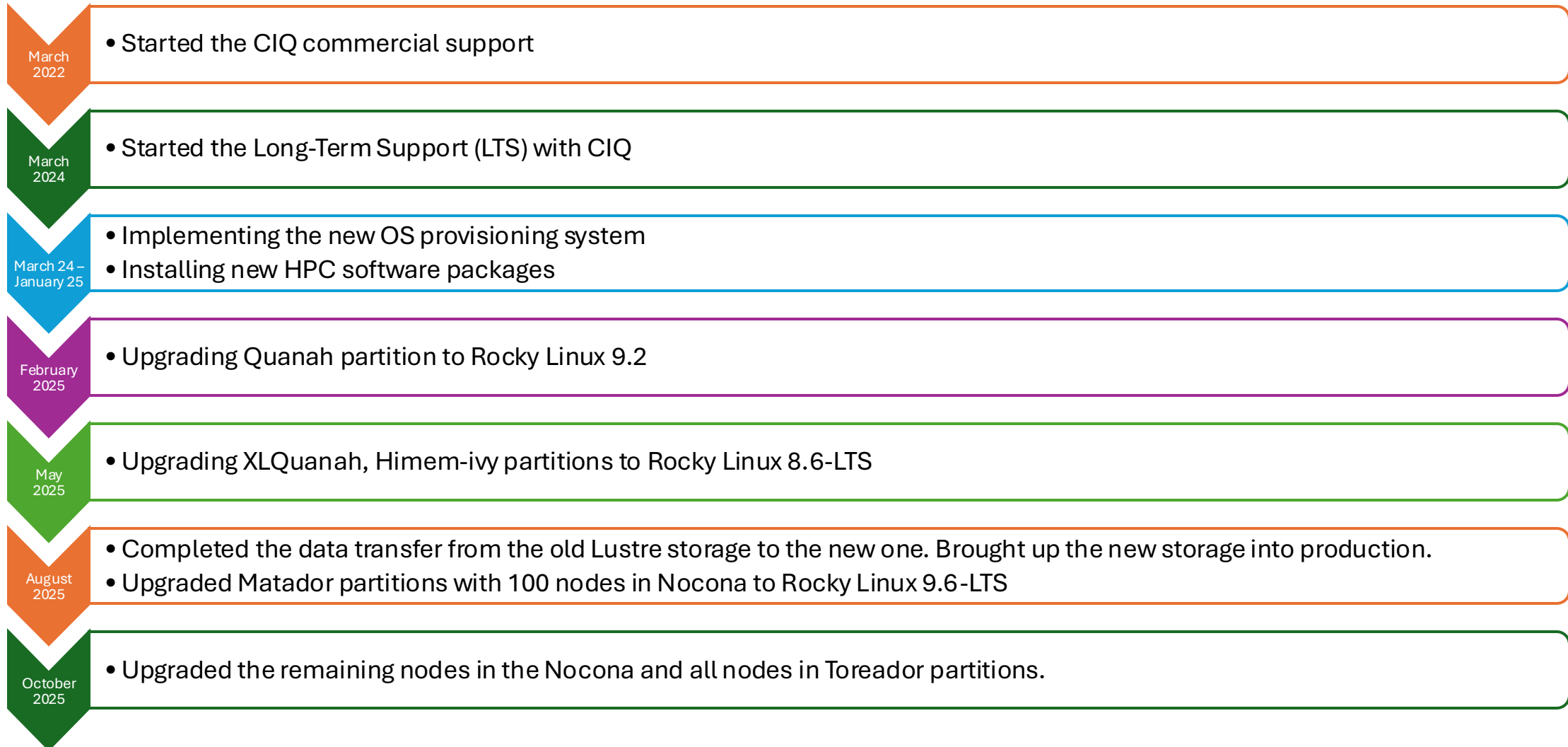
*** TTU HPCC has subscribed to Rocky Linux LTS from CIQ

CIQ LTS Support Timelines



■ Rocky Linux Minor Release
 ■ CIQ Standard Long Term Support
 ■ Extended CIQ Standard Long Term Support
■ CIQ Certified Rocky Compliant Releases (DISA/STIG/FIPS)

HPCC OS Upgrade Sequence



Current Status: All Upgrades Complete!

- Current partitions' OS version:

Partition(s):	Current Rocky Linux version	LTS Expiration Date	Comments
XLQuannah, 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.
Quannah	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.

- Software installation methods we use at HPCCC:
 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.



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).
 - HPCCC 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	<ul style="list-style-type: none"> Rocky Linux 9.2-LTS / 9.6-LTS 	<ul style="list-style-type: none"> Rocky Linux 9.6-LTS 	<ul style="list-style-type: none"> Rocky Linux 8.6-LTS
Package Build Env	<ul style="list-style-type: none"> Spack 0.23 Apptainer/Singularity Containers 	<ul style="list-style-type: none"> Spack 0.23 Apptainer/Singularity Containers 	<ul style="list-style-type: none"> Spack v0.23 Apptainer/Singularity Containers
Software Deployment Env	<ul style="list-style-type: none"> Lmod Modules 8.7.55 	<ul style="list-style-type: none"> Lmod Modules 8.7.55 	<ul style="list-style-type: none"> Lmod 8.7.55
Available C/C++/Fortran /MPI Compilers	<ul style="list-style-type: none"> 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) 	<ul style="list-style-type: none"> 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 	<ul style="list-style-type: none"> GCC 8.5.0 (Default) GCC 14.2.0 (Recommended) Intel OneAPI 2024.2.1
GPU Libraries	<ul style="list-style-type: none"> N/A 	<ul style="list-style-type: none"> CUDA 11.8.0 CUDA 12.3.2 CUDA 12.9 cuda/9.8.0.87 nccl/2.22.3 	<ul style="list-style-type: none"> N/A

Lmod Modules (CPU Nodes)

```
RedRaider Cluster - Nocona Partition - Login node
-----
Texas Tech University
High Performance Computing Center
RedRaider Cluster
-----
Partition: [nocona] OS: [Rocky Linux 9.6]
-----
----- OPENMPI (v5.0.5) Modules: -----
boost/1.84.0-mpi      hpl/2.3      netcdf-c/4.9.2-mpi  openfoam-org/11  scalapack/2.2.0    vtk/9.4.1-mpi
cp2k/2024.3-mpi-omp  iq-tree/2.3.2-mpi-omp  netcdf-cxx4/4.3.1-mpi  openfoam/2312    seacas/2024-06-27-mpi  wps/4.5-mpi
fftw/3.3.10-mpi      lammps/20240829-mpi-omp  netcdf-fortran/4.5.2-mpi  osu-micro-benchmarks/7.4  trilinos/15.1.1-mpi  wrf/4.5.2-mpi
gromacs/2024.3-mpi-omp  mrbayes/3.2.7a-mpi  netcdf-fortran/4.6.1-mpi  parallel-netcdf/1.12.3  vasp/6.3.2-mkl-mpi (R)
 hdf5/1.14.3-mpi      n2p2/2.2.0    nwchem/7.2.3        paraview/5.13.2-mpi  vasp/6.5.1-mkl-mpi (R,D)
 hpcg/3.1-omp         namd/3.0.1    octave/9.1.0        quantum-espresso/7.3.1-mpi-omp  vaspsol/5.4.4 (R)
-----
----- GCC (v14.2.0) Modules: -----
R/4.4.1              fftw/3.3.10-serial-omp  hdf5/1.14.3-serial (D)  netcdf-cxx4/4.3.1-serial (D)  openmpi/4.1.6
boost/1.84.0-serial (D)  fftw/3.3.10-serial (D)  imagemagick/7.1.1-29  netcdf-fortran/4.6.1-serial (D)  openmpi/5.0.5 (L,D)
cdo/2.4.3-omp          gdal/3.9.2            lapack/3.11.0        oneapi-mkl/2024.2.1-omp  proj/8.1.0
cmake/3.30.2          geos/3.13.0          mvapich/3.0          openblas/0.3.27-omp  sqlite/3.46.0
dmtcp/4.0.0           grads/2.2.3          netcdf-c/4.9.2-serial (D)  openblas/0.3.27 (D)
-----
----- CORE Modules: -----
aocc/4.2.0  gcc/14.2.0 (L)  intel-oneapi/2024.2.1  llvm/17.0.6  openjdk/17.0.11_9  perl/5.40.0  python/3.12.5
-----
----- GENERIC [CPU] Modules: -----
ansys/v241 (E)      cadence/x86_rhel9 (E)  jupyterlab/7.0.6 (C)  matlab/R2024a (D)  tcad/2019.12 (R)  totalview/2023.4
ansys/v251 (E,D)  gurobi/11.0.1          matlab/R2023b         spark/4.0.1 (C)  tcad/2024.09 (R,D)  totalview/2024.4.2 (D)

Where:
R: Requires valid license to access
L: Module is loaded
E: Only Available to College of Engineering (COE)
C: Apptainer/Singularity Container
D: Default Module

=====
How to find a software package module:
1. Use "module spider" to find all possible modules and extensions.
2. Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
3. (Recommended): Visit https://www.depts.ttu.edu/hpcc/status/software_list.php

login-20-26: $
```

Lmod Modules (GPU Nodes)

```
RedRaider Cluster - Matador Partition
=====
|
|          Texas Tech University
|      High Performance Computing Center
|          RedRaider Cluster
|
|=====
Partition: [matador] OS: [Rocky Linux 9.6]

----- CUDA (v12.9.0) Modules: -----
cudnn/9.8.0.87-12  nccl/2.22.3-1  openmpi/5.0.5 (L)

----- GCC (v13.2.0) Modules: -----
cuda/12.9.0 (L,D)  nvhpc/25.7-cuda-12.9 (D)

----- CORE Modules: -----
cuda/11.8.0  gcc/13.2.0 (L,D)  intel-oneapi/2024.2.1  openjdk/17.0.11_9  python/3.12.5
gcc/12.2.0  intel-oneapi-mkl/2024.2.1-omp  nvhpc/25.7-cuda-11.8  perl/5.40.0

----- GENERIC [GPU] Modules: -----
gromacs/v2025.1-gpu (C)  matlab/R2023b  pytorch/24.12-py3-gpu (C)  totalview/2024.4.2 (D)
jupyterlab/7.0.6 (C)  matlab/R2024a (D)  quantum-espresso/7.3.1-gpu (C)  vmd/1.9.4a44-gpu (C)
lammps/15Jun2023_gpu (C)  namd/3.0.1-gpu (C)  totalview/2023.4

Where:
L: Module is loaded
C: Apptainer/Singularity Container
D: Default Module

=====
How to find a software package module:
1. Use "module spider" to find all possible modules and extensions.
2. Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
3. (Recommended): Visit https://www.depts.ttu.edu/hpcc/status/software\_list.php

gpu-20-11: $
```

Search for Available Modules

The screenshot shows the HPC RedRaider Cluster Software Packages search page. At the top, there is a navigation bar with the HPC Center logo and links for Resources, Operations, About HPC, RedRaider Cluster, Events, and HPC Support. Below this is a secondary navigation bar with links for home, NOCONA, QUANAHA, MATADOR, TOREADOR, XLQUANAHA, and HIMEM-IVY, along with SEARCH and LIST buttons. A search box is prominently displayed in the center, containing the text "Search Software Package" and a clear button (X). Below the search box, the page title "HPC RedRaider Cluster Software Packages" is shown. The main content area contains a paragraph explaining that users can find the most up-to-date list of available software packages and dependencies on the RedRaider cluster. It also provides instructions on how to use modules and refers to a Software Environment Setup Guide. A section titled "Search for a software package:" lists three steps: 1. Use the search box to look for any specific compiler, math library, or scientific software package and check the availability on the HPC RedRaider cluster. 2. Click on the search results leads you to the full path of the software package in the HPC software hierarchy stack. 3. Use the delete button X in the search box to clear the search, or click on the return button to go back to the search result if you are not there already. Finally, there is a section titled "Traverse the current software package hierarchy available for each partition:".

[HPC 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.
- HPC 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 HPC 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

The screenshot shows the Texas Tech HPCC OnDemand web portal. At the top, there is a navigation bar with links for Files, Jobs, Clusters, Interactive Apps, All Apps, and My Interactive Sessions. On the right side of the navigation bar, there are links for Develop, Help, Logged in as, and Log Out. The main content area features the HPCC logo and the text "HIGH PERFORMANCE COMPUTING CENTER" and "TEXAS TECH Information Technology". Below this, a welcome message states: "Texas Tech HPCC OnDemand web portal provides an integrated, single access point for all of your HPC resources. Welcome to the RedRaider cluster's interactive portal!". A list of links provides information about training sessions, maintenance schedules, and support requests. The "Pinned Apps" section is divided into two categories: "Cluster Tools" and "Interactive Apps". The "Cluster Tools" category includes Active Jobs, Home Directory, Job Composer, and RedRaider Cluster Shell Access. The "Interactive Apps" category includes Code Server, Desktop, Jupyter Lab, and MATLAB. Each app icon is accompanied by its name and the text "System Installed App".

Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ All Apps ▾ My Interactive Sessions ▾ </> Develop ▾ ? Help ▾ Logged in as | Log Out

 **HIGH PERFORMANCE COMPUTING CENTER**
TEXAS TECH
Information Technology





Texas Tech HPCC OnDemand web portal provides an integrated, single access point for all of your HPC resources.

Welcome to the RedRaider cluster's interactive portal!





- For the upcoming HPCC and ACCESS training sessions, please visit the [HPCC Training](#) page.
- For the upcoming scheduled maintenance downtime, please visit the [Maintenance Schedule](#) page.
- Requests for assistance should go to hpccsupport@ttu.edu.

Pinned Apps

Cluster Tools

-  **Active Jobs**
System Installed App
-  **Home Directory**
System Installed App
-  **Job Composer**
System Installed App
-  **RedRaider Cluster Shell Access**
System Installed App

Interactive Apps

-  **Code Server**
System Installed App
-  **Desktop**
System Installed App
-  **Jupyter Lab**
System Installed App
-  **MATLAB**
System Installed App



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—
TEXAS TECH
Information Technology

Raise a support ticket:
hpcsupport@ttu.edu