HPCC New User Training

Getting Started on HPCC Resources

(Part 1/2)

Misha Ahmadian
High Performance Computing Center

Summer 2023

About this Training Workshop?

TEXAS TECH UNIVERSITY
Information Technology Division

Hands-on training that covers all you need to know about HPCC RedRaider Cluster:

- Who are the audiences:
  - ✓ HPCC Users (TTU Students/Faculties/Staff/External Researchers)
  - ✓ None-HPCC users (TTU Students/Faculties/Staff/ External Researchers)
- Is this training sufficient?
  - Could be enough for intermediate to advance users
  - We encourage beginners to review the slides along with the online user guide documents: https://www.depts.ttu.edu/hpcc/userguides/index.php

About this Training Workshop?

TEXAS TECH UNIVERSITY
Information Technology Division

Course Schedule:

- The HPCC New User Training is offered twice per semester.
- Each session will be held for 4 hours per day (10 am – 12 pm) and (1 pm – 3 pm) with a 1-hour lunch break.

Preferred Requirements:

- Attendees are preferred to have their HPCC account ready:
  - If you did not request or receive your new HPCC account, please stay with us!
- Windows/Linux/Mac laptop or desktop

About this Training Workshop?

TEXAS TECH UNIVERSITY
Information Technology Division

How to make the best out of this Training?

- Take your notes during the sessions, but not too many!
- Follow the instructor and try the commands and examples under your HPCC accounts.
- A few exercises will be provided during each session, which will help you to practice and learn.

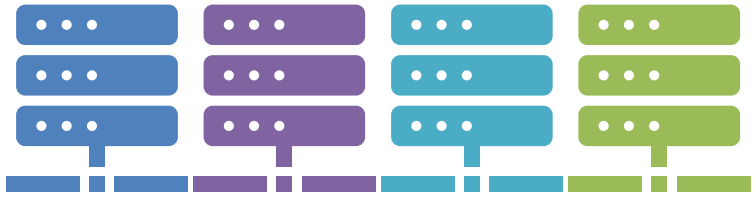
Outline

TEXAS TECH UNIVERSITY
Information Technology Division

Part 1:

- Introduction to High Performance Computing
- HPCC Resources
- Logging and using the Clusters
- Transferring Data

Introduction to High Performance Computing



Simplest Programming Model: Serial Computing

- Software is often written and optimized to run **serially**.
  - Execution occurs on a single computer using a single CPU core.
  - A problem is broken down into a linear series of instructions.
  - Instructions are executed one after another.
  - Only one instruction may execute at any given time.
  - While simple, this model may not make full use of modern multi-core processors.

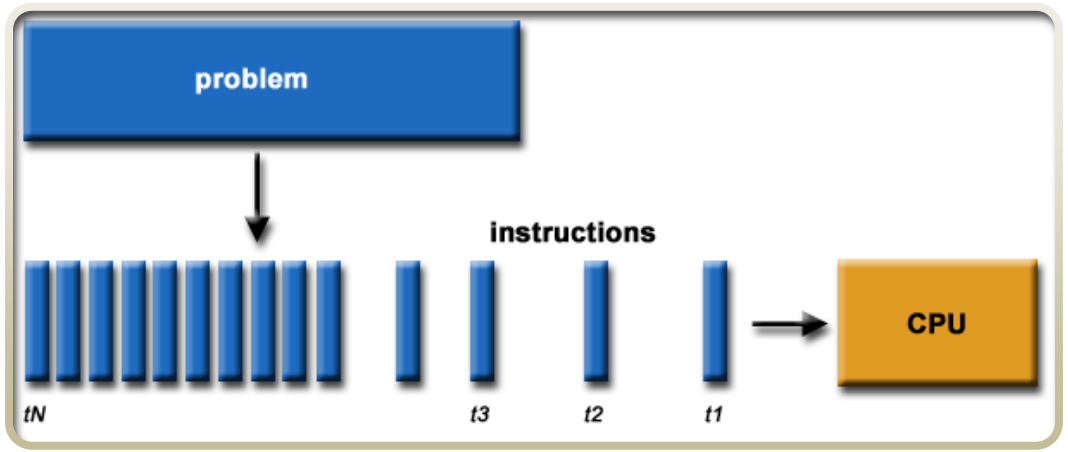


Image provided by Lawrence Livermore National Labs (computing.llnl.gov)

More Advanced Usage: Parallel Computing

- **Parallel Computing** is the simultaneous use of multiple compute resources to solve a computational problem.
  - Execution occurs across multiple CPU cores.
  - A problem is broken into discrete parts that can be solved concurrently.
  - Each part is further broken down into a series of instructions, executed one after another.
  - Instructions from each part execute simultaneously on different CPU cores.

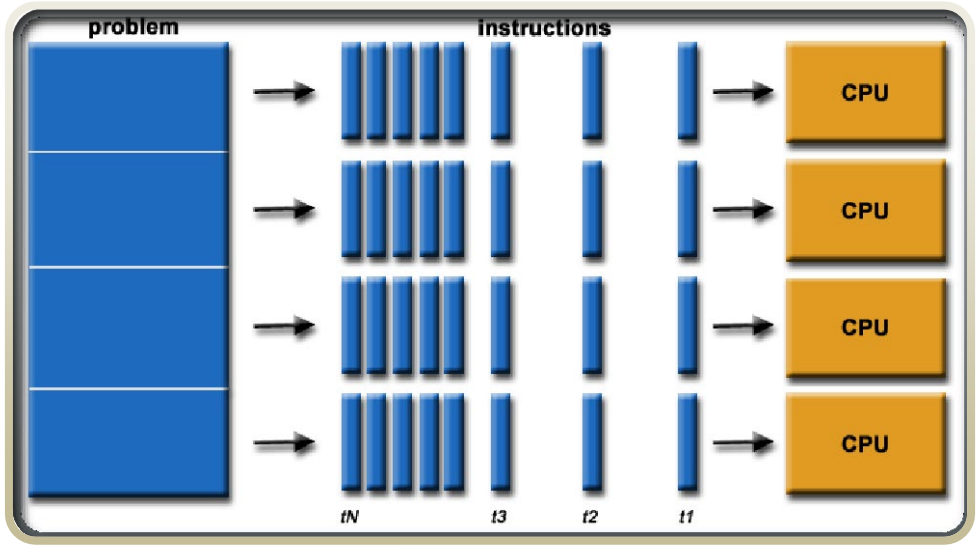
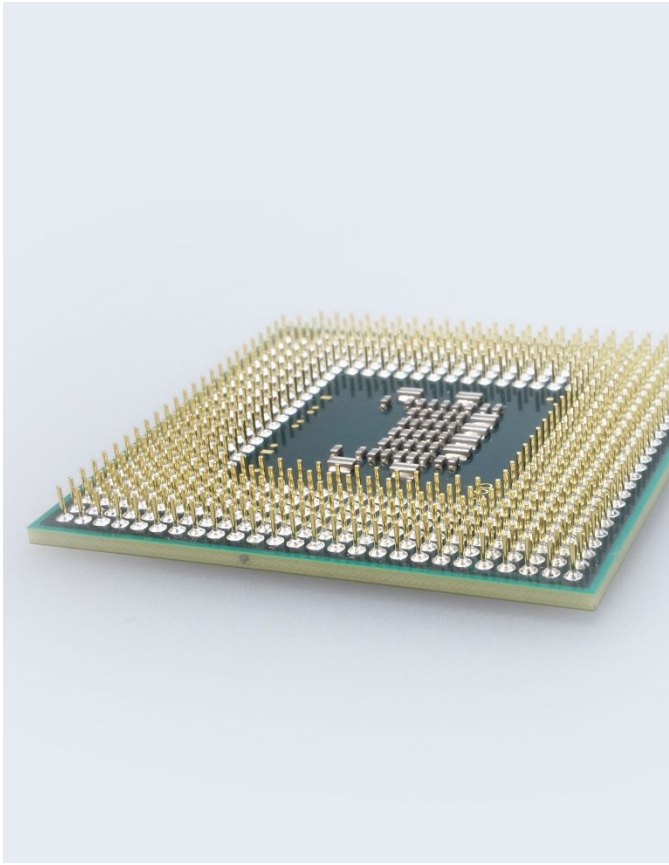


Image provided by Lawrence Livermore National Labs (computing.llnl.gov)

Classes of Parallel Computers

- **Multi-core Computing**:
  - Multi-core processors contain multiple ‘processing units’ (called cores) on a single chip.
  - Allows for parallel execution across cores – each able to reach the same system resources (RAM, Keyboard, Monitor, etc...).



- **Symmetric Multiprocessor (SMP)**:
  - A symmetric multiprocessor is a computer system with multiple identical processors.
  - Each processor likely has multiple cores
  - Allows for parallel execution across cores – each able to reach the same system resources (RAM, Keyboard, Monitor, etc...).

Classes of Parallel Computers

- **Clusters**:
  - Groups of loosely coupled computers working together closely.
  - Processes can be spread across multiple nodes, but processes are unable to reach the same system resources (RAM, Keyboard, Monitor, etc...).

- **Massively Parallel Processors (MPP)**:
  - A group of tightly coupled computers working together closely across a specialized high-speed interconnect.
  - Processes can be spread across multiple nodes, but processes are unable to reach the same system resources (RAM, Keyboard, Monitor, etc...).
  - Common computing paradigm for campus-based HPC centers.

Classes of Parallel Computers

- **National-Scale Supercomputers**:
  - Highly scaled forms of parallel computing run for the National Science Foundation, Department of energy, National Institutes of health, etc.
  - Organized much like larger versions of the TTU HPCC clusters.
  - Awards for time require proposals and are evaluated on a competitive basis.

- **Grid and Cloud Computing**:
  - Highly distributed forms of parallel computing.
  - Clusters or single resources are spread across multiple sites using the Internet for connectivity.
  - Commercial clouds are often more expensive to use than dedicated fully-utilized on-premises clusters for HPC.

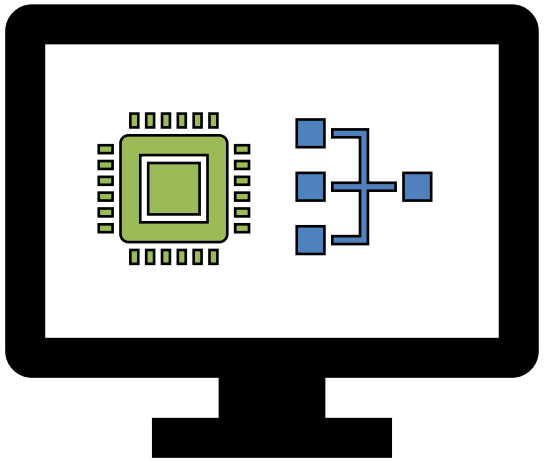
Why does programming style matter?

- Different problems are suited to each of the major programming models.
  - **Serial programming:**
    - Executes serially using a single core/thread
    - *"Single-core machines"*
    - Good for problems that don't require inter-thread or inter-process communication.
  - **Multi-core / Multi-threaded Programming:**
    - Executes in parallel using multiple cores/threads
    - All threads are running on the same machine and access the same RAM
    - *"Multicore & Symmetric Multiprocessing"*
    - Needed for problems that require different threads or processes to share information.
  - **Massively Parallel / Distributed Programming:**
    - Executes in parallel using multiple machines
    - *"Clusters, Massive Parallel Processors, & Grid/Cloud"*
    - Needed for problems that require harnessing multiple large-scale resources.

Match Your Programming Style To The Problem!

- **If your program is not written to use a certain model, it will not necessarily "*just work*" in that model.**
  - Running serial code on a 128-core machine will use 1 core and leave 127 cores sitting idle.
  - Attempting to run multi-threaded code written to be used in just one node across 10 nodes instead without adjustments will result in 1 node being overutilized and 9 nodes sitting idle.
- **Not all multi-threading/MPP is equal!**
  - Try to understand how your program works at a small scale before attempting to "*scale up*".
  - Keep in mind that programming language, developer decisions and even user input data can greatly alter how well an application scales.
  - Many existing codes need to be tuned or configured to run optimally.

TTU HPCC Resources



HPCC Resources: RedRaider Primary Cluster

TEXAS TECH UNIVERSITY
Information Technology Division

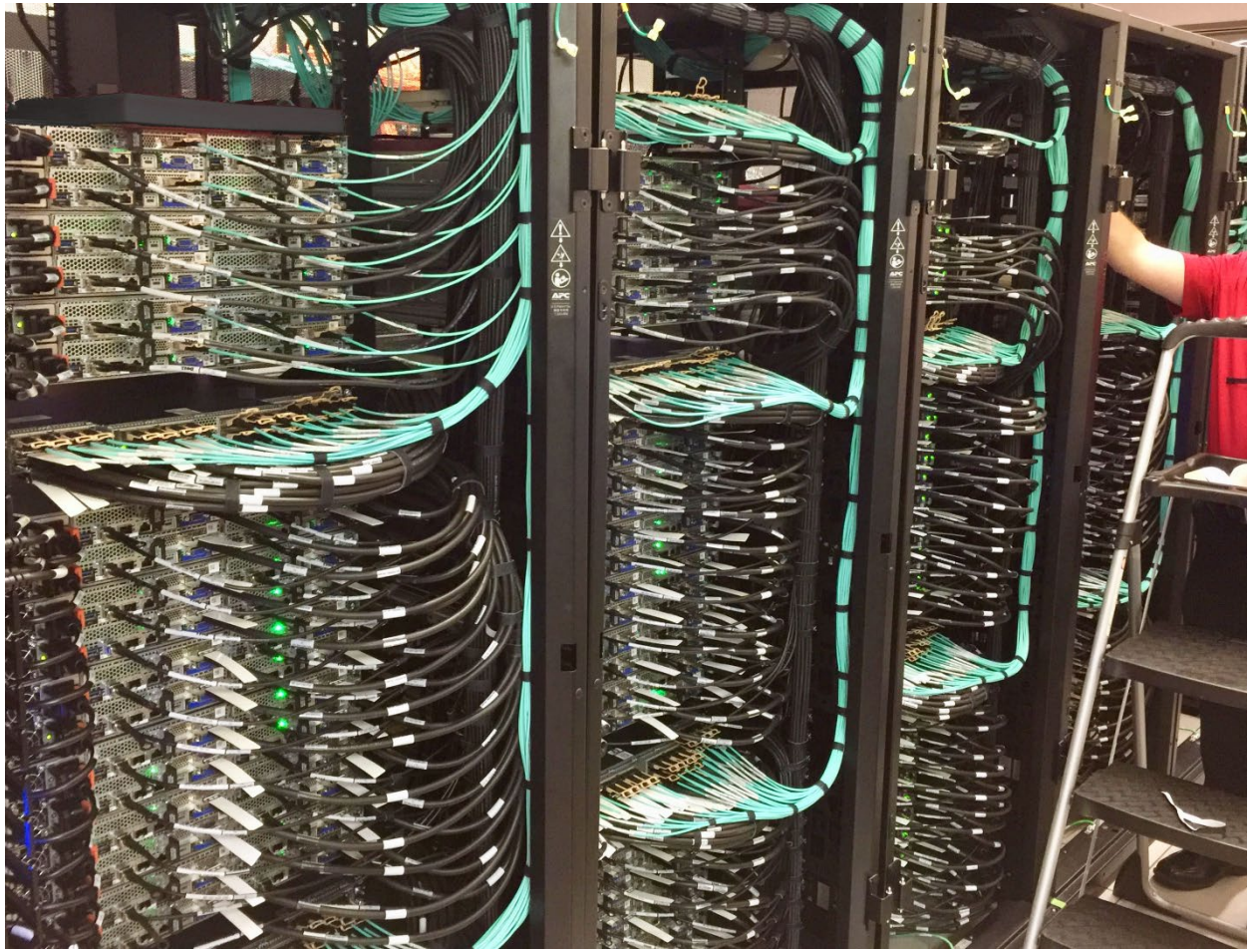
- **RedRaider** Cluster Commissioned in 2021:

  - **Nocona partition** **(240 CPU nodes)**
    - 2x AMD EPYC ROME 7702 processors / node
    - *30,720 Cores* (128 cores/node)
    - 120 TB total RAM (512 GB/node)
    - HDR 200 Gbps InfiniBand fabric
    - 804 Teraflops (81.4% efficiency)

  - **Matador partition** **(20 GPU nodes)**
    - *40 NVIDIA Tesla V100 GPUs* (2 V100 / node)
    - 2x Intel Xeon Cascade lake 6248 processors / node
    - 800 CPU Cores (40 cores/node)
    - 7.5 TB total RAM (384 GB/node)
    - HDR 100 Gbps InfiniBand fabric
    - 226 Teraflops (80.6% Efficiency)

HPCC Resources

- **Quanah partition (467 nodes)**
  - Commissioned in 2017
  - 2x Intel Xeon E5-2695v4 Broadwell Processors/node
  - *16,812 total cores* (36 cores/node)
  - 87.56 TB total RAM (192 GB/node)
  - Non-blocking Omni-Path (100 Gbps) fabric
  - Benchmarked at 485 Teraflops



HPCC Resources: RedRaider Primary Cluster

- **Toreador partition (11 nodes)**
  - *33 NVIDIA Tesla A100 GPUs* (3 A100 / node)
  - 2x AMD EPYC ROAM processors / node
  - 176 CPU Cores (16 cores/node)
  - 2.1 TB total RAM (192 GB/node)
  - HDR 100 Gbps InfiniBand fabric
  - *May expect higher waiting time*

HPCC Resources

TEXAS TECH UNIVERSITY
Information Technology Division

- **XLQuanah partition (16 nodes)**
  - Commissioned in 2022
  - 2x Intel Xeon E5-2695v4 Broadwell Processors/node
  - *512 total cores* (36 cores/node)
  - 4 TB total RAM (256 GB/node)
  - InfiniBand (53 Gbps) fabric
  - *This partition requires a request for special access*

- **Himem-ivy partition (2 nodes)**
  - Commissioned in 2022
  - 2x Xeon E5-2660 **Ivy Bridge** Processors/node
  - *40 total cores* (20 cores/node)
  - 3 TB total RAM (1.5 TB/node)
  - InfiniBand (40 Gbps) fabric

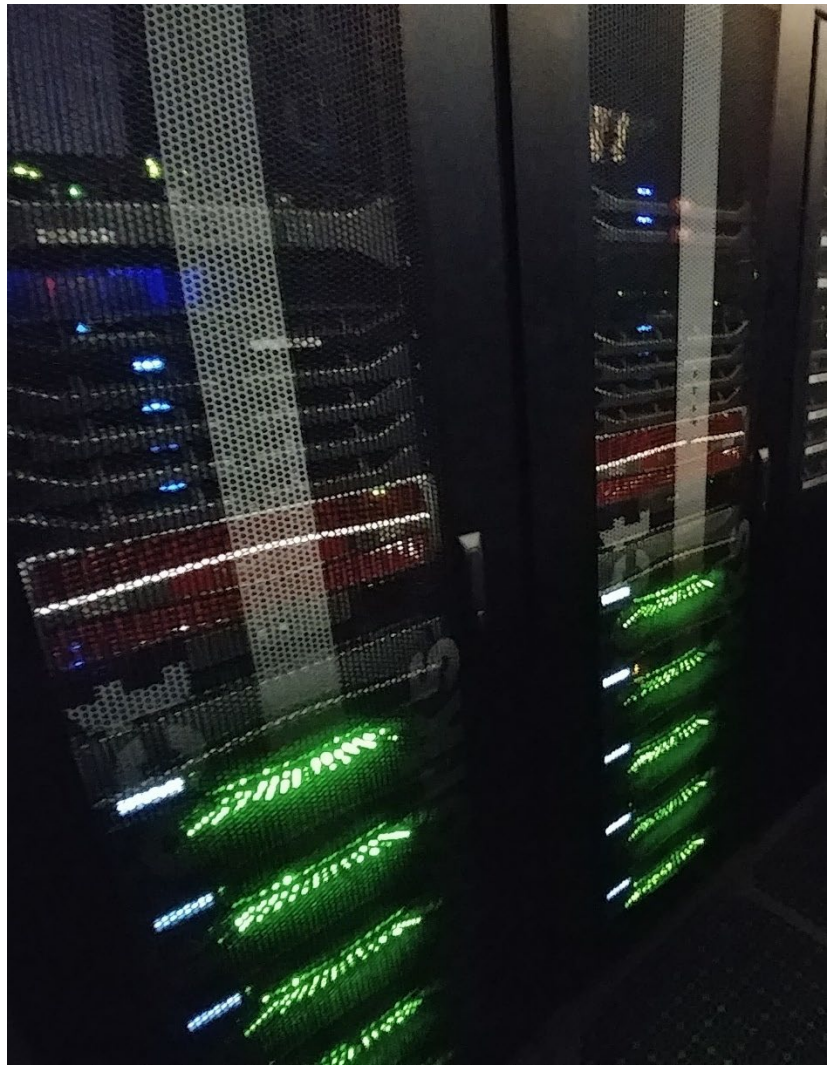
HPCC Resources: Storage

Cluster-Wide Storage System:

- 6.1 PB of total storage space
- 200 Gbps HDR Fabric
- Based on Lustre parallel file system
- Quota/Backup/Purge policies per storage area (free to all accounts):

Area	Quota	File Limit	Backup	Purge
/home/<eraider>	300 GB	1,000,000	**Yes**	No
/lustre/work/<eraider>	700 GB	1,000,000	No	No
/lustre/scratch/<eraider>	None	None	No	**Monthly**

- Researchers/groups may purchase additional dedicated storage space:
  - With Backup: $80/TB/Year
  - Without Backup: $40/TB/Year



RedRaider Cluster Software Environment

TEXAS TECH UNIVERSITY
Information Technology Division

	Quanah	Nocona/Matador/Toreador/XLQuanah/himem-ivy
Operating System	• CentOS 7.4 **	• CentOS 8.1
Job Resource Manager	• Slurm 22.05.8	• Slurm 22.05.8
Package Build Env	• RPM Build	• Spack v0.15
Software Deployment Env	• Lmod 7.7.14	• Lmod 8.2.10
Available C/C++/Fortran /MPI Compilers	• GCC 4.8.5 (Default) • GCC 5.4.0 • GCC 7.3.0 • Intel 18.0.3.222 • impi 2018.3.222 • OpenMPI 1.10.[6-7] • MVAPICH 2.2	• GCC 8.3.1 (Default) • GCC 9.2.0 • GCC 10.1.0 (Recommended) • AOCC/AOCL (Coming Soon) • Intel compiler/MKL/MPI 2019 • OpenMPI 3.1.6, 4.0.4 • MVAPICH (Coming Soon)
GPU Libraries	• N/A	• CUDA 11.0 (default) • Cudnn 8.0.1 (default)

The complete list of available software packages on the RedRaider cluster is available on the HPCC website.

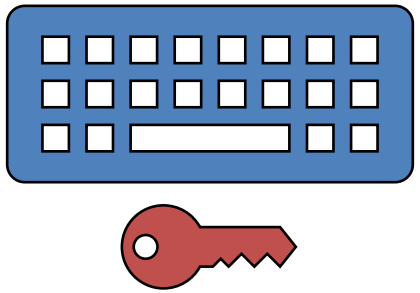
RedRaider Cluster Software Environment

TEXAS TECH UNIVERSITY
Information Technology Division

- List of currently installed software packages on the RedRaider Cluster:

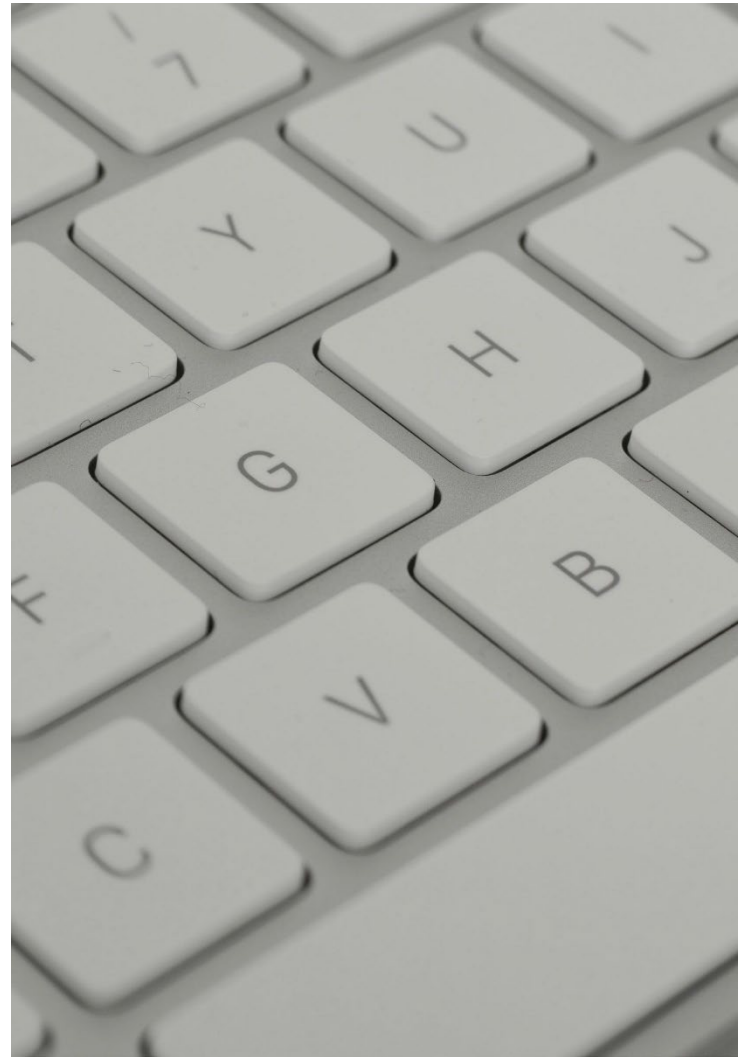
abyss	charm	ete3	git	ImageMagick	libxc	ncbi-rmblastn	ngs	paraview	py-astunparse	py-six	samtools	trinity
ampl	charmpp	exonerate	gnu	impi	libxsmm	ncbi-vdb	nvhpc	pear	py-cython	py-termcolor	scalapack	udunits
ansys	clustalw	fastStructure	gnu7	intel	lumerical	nccl	nwchem	perl	py-gast	python	singularity	vasp
augustus	cmake	fastx-toolkit	gnuplot	intel-mkl	mafft	ncl	octave	phdf5	py-google-pasta	python2	sparsehash	vasp-vtst
bamtools	cuda	fftw	grads	intel-mpi	maftools	nco	openblas	phyluce	py-grpcio	python3	stacks	vcftools
bcftools	cudnn	fftw3	gromacs	intel-tbb	maker	netcdf	openfoam	picard	py-keras-preprocessing	py-wheel	stokes	voro++
bedtools	cufflinks	fmriprep	gromacs-serial	java	matlab	netcdf-c	openjdk	picrust	py-matplotlib	py-wrapt	swig	vsearch
bedtools2	cvmfs	fsl	gsl	kokkos	mkl	netcdf-cxx	openmpi	povray	py-numpy	qiime	tcad	xanim
boost	dos2unix	gatk	gurobi	kokkos-nvcc-wrapper	molden	netcdf-cxx4	openmpi3	presto	py-opt-einsum	R	tcl	xcpEngine
bowtie2	drVM	gcc	hdf5	lammps	mpi4py27	netcdf-fortran	orca	proj	py-protobuf	repeatmasker	tcoffee	zlib
bwa	eigen	gdal	hpl	lapack	mpi4py34	netcdf-serial	osu-micro-benchmarks	protobuf	pyrad	rmblast	tensorflow	zstd
cadence	elpa	geant4	hpx	libgtextutils	mvapich2	netlib-lapack	PAML	prun	py-scipy	root	tensorflow-mpi	
cdo	emboss	geos	htslib	libint	namd	netlib-scalapack	parallel-netcdf	py-absl-py	py-setuptools	rosetta	totalview	

Logging in and Using the Cluster



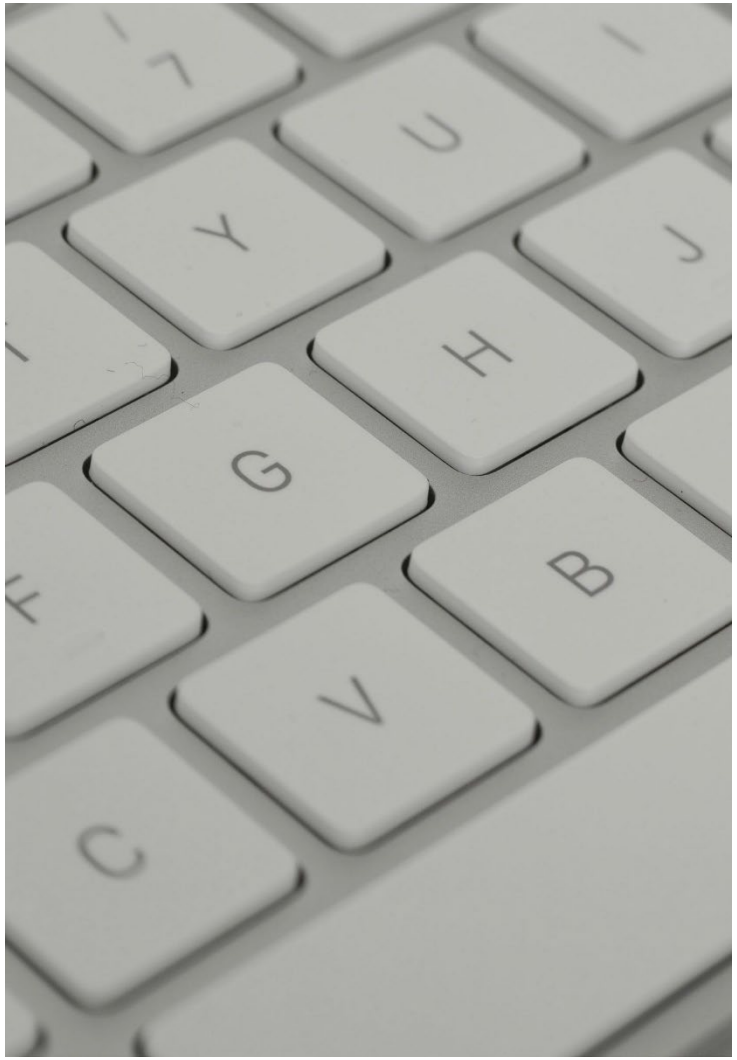
Getting Started

- Account Request:
  - Faculty/Staff account
  - Student account
  - Research Partner account
  - http://www.depts.ttu.edu/hpcc/accounts/index.php
- User Guides:
  - http://www.depts.ttu.edu/hpcc/userguides/index.php
- More details about HPCC equipment:
  - http://www.depts.ttu.edu/hpcc/operations/equipment.php



Getting Started

- Logging to HPCC Resources:
  - http://tinyurl.com/ttu-hpcc-login
- On or Off Campus?
  - On Campus: Wired TTU network & TTUnet wireless network
  - Off Campus: Any other network connection, including
    - TTUHSC networks
    - TTUguest wireless network
- Logging in from Off Campus:
  - Log in via the SSH gateway
  - Establish a VPN - https://goo.gl/4LbuWG
  - Neither system is owned or maintained by HPCC

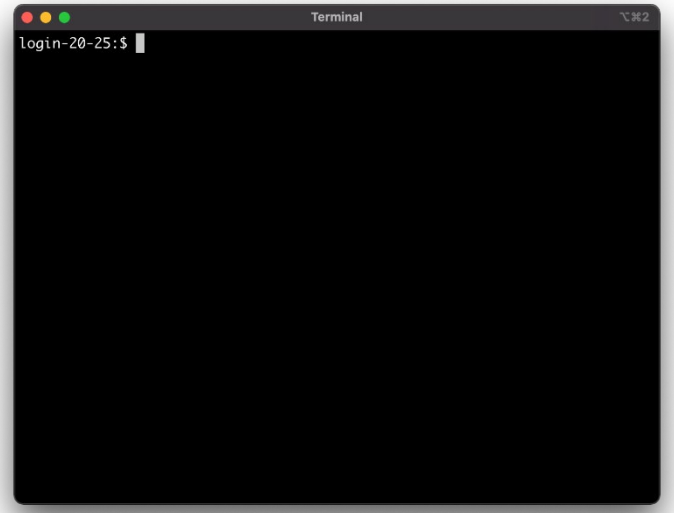


Logging to RedRaider Cluster

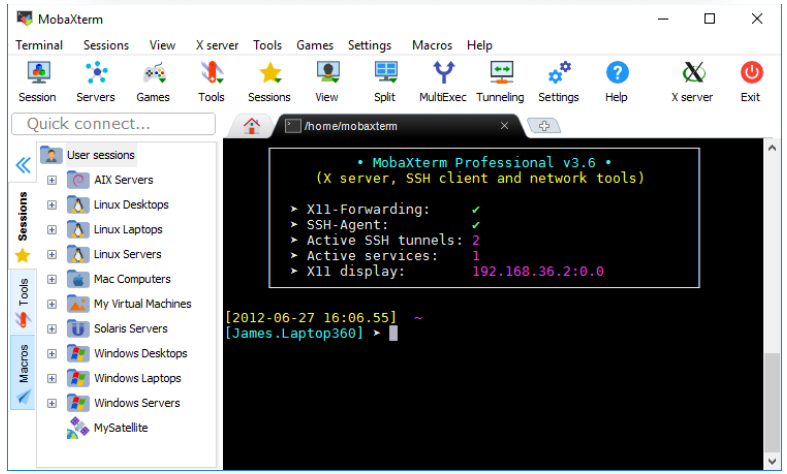
TEXAS TECH UNIVERSITY
Information Technology Division

- Mac/Linux Users:
  - **SSH** (Secure Shell): Freely available on Linux/Unix/MacOS and used via the Terminal.

```
ssh eraider@login.hpcc.ttu.edu
ssh eraider@quanah.hpcc.ttu.edu
```

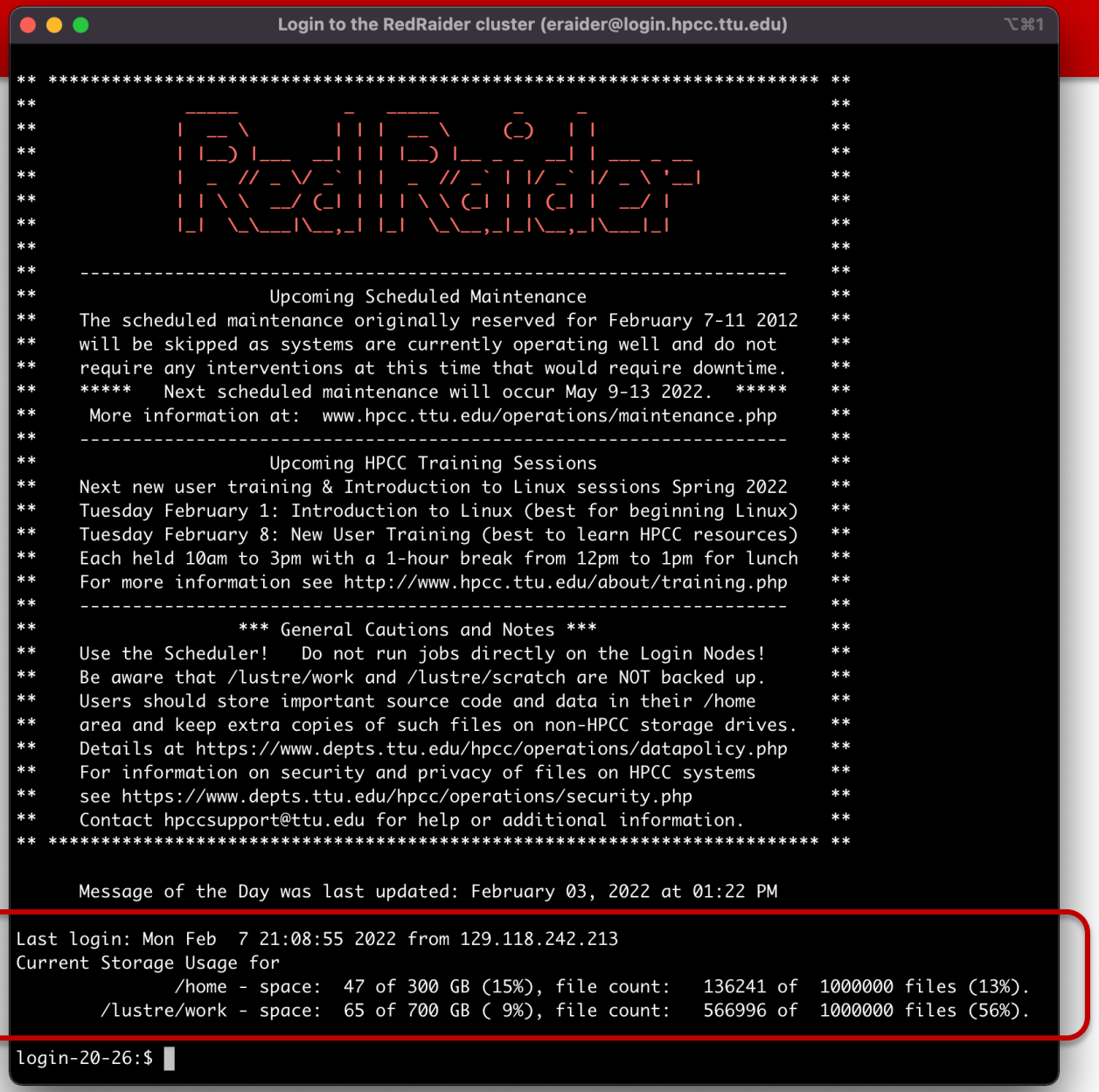


- Windows Users:
  - **MobaXterm** (Recommended): https://mobaxterm.mobatek.net
  - **Putty**: https://www.putty.org



- Once logged in:
  - RedRaider has two login nodes: (**`login-20-25, login-20-26`**)
  - The load-balancer lands your SSH session on one of these nodes.
  - Quanah login node currently still available, login.hpcc.ttu.edu preferred.

Logging In



← Space quota and file limit usage

Environment Settings

- Hostname pattern of the nodes in the RedRaider cluster:
  - Login nodes:
    - **`Login-20-[25-26]`**
    - **`quanah`**
  - CPU worker nodes:
    - **`cpu-<rack#>-<chassis#>`**
    - **E.g., `cpu-23-10`**
  - GPU worker nodes:
    - **`gpu-<rack#>-chassis#>`**
    - **E.g., `gpu-20-7`**

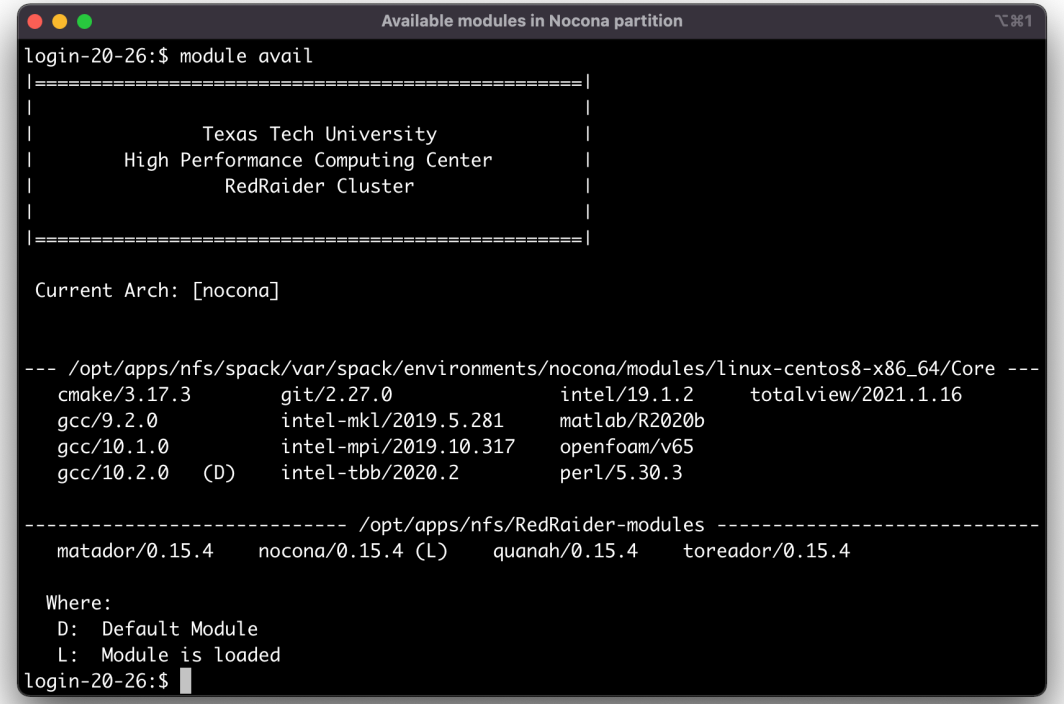
XWindows

- **Interactive GUI using Linux/Mac.**
  - Mac users must install XQuartz. Linux Users can use the Terminal.
  - Logging to the cluster using ”-Y -X” with your normal ssh command:
    - `ssh -Y -X eraider@login.hpcc.ttu.edu`
  - Run a test command like **`xclock`**.

- **Interactive GUI using Windows.**
  - Install MobaXterm. (Consult MobaXTerm web site for details.)
  - Open a new tab in MobaXterm.
  - Logging to the cluster using ”-Y -X” with your normal ssh command:
    - `ssh -Y -X eraider@login.hpcc.ttu.edu`
  - Run a test command like **`xclock`**.

Environment Settings

- Lmod Modules:
  - The primary way to change your user environment.
  - Load/Unload a particular set of cluster-wide installed software packages into your environment or job submissions.
  - Makes life easier by modifying the proper environment variables for you such as PATH, LD_LIBRARY_PATH, etc.
  - User Guide:
    - https://www.depts.ttu.edu/hpcc/userguides/general_guides/software_environment.php



Environment Settings

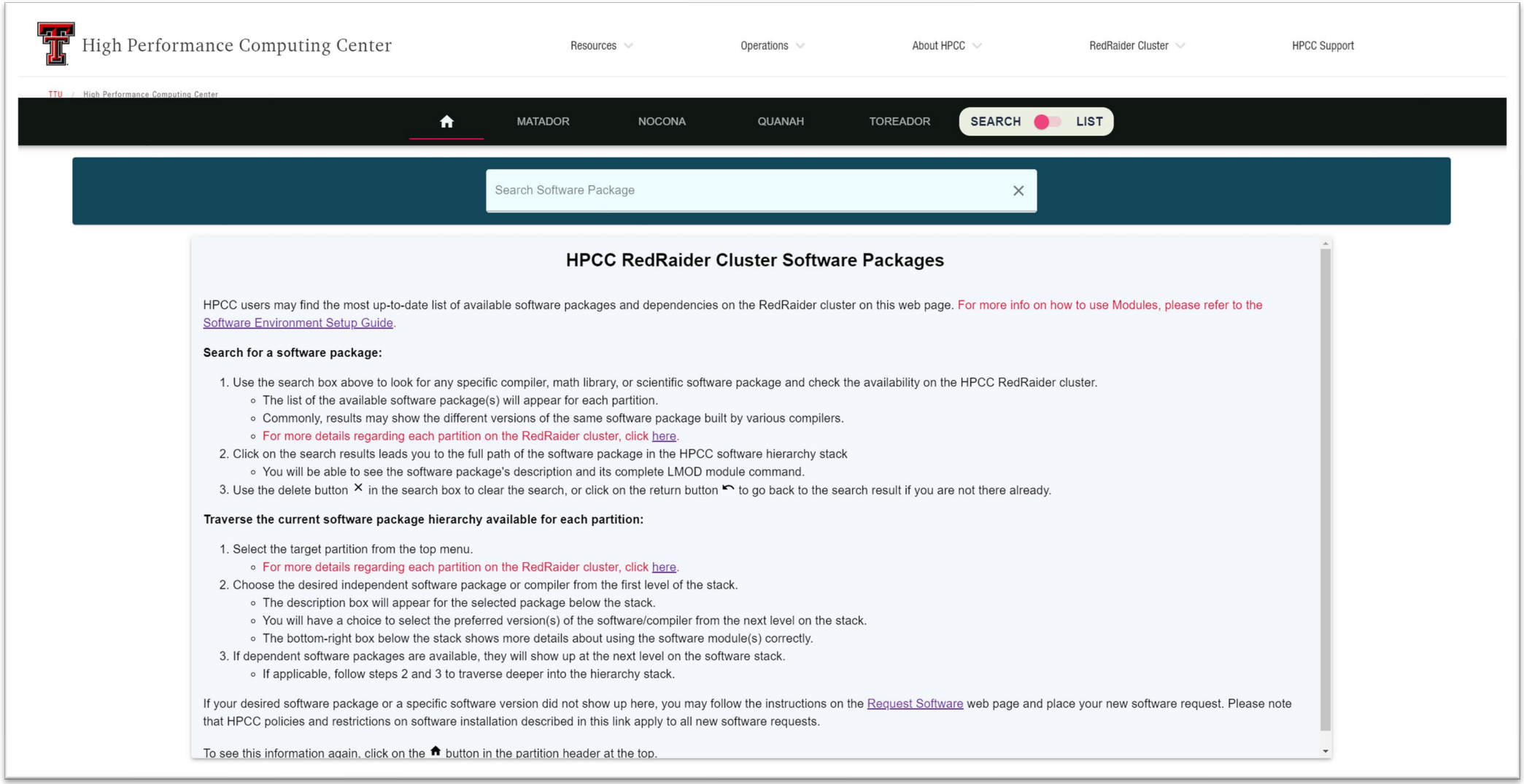
TEXAS TECH UNIVERSITY
Information Technology Division

- Lmod Module Commands:

Command	Description
`module avail`	List all the available modules
`module list`	List all the modules currently loaded
`module load <module_name>`	Load a module in your environment
`module unload <module_name>`	Unload a module from your environment
`module swap <old_module> <new_module>`	Replace the old module with the new one
`module spider <keyword>`	Search for a module in the Lmod hierarchy list
`module purge`	Unload all the modules currently loaded
`module help <module_name>`	Show the description of the module
`module whatis <module_name>`	Show a brief info about the module
`module show <module_name>`	Show a complete info about the module

Search Available Modules on the RedRaider

TEXAS TECH UNIVERSITY
Information Technology Division



[HPCC RedRaider Software Packages]

Modules Tips and Recommendations

- **Try to keep all your module load commands as part of your job submission scripts instead of adding them to your `.bashrc` file.**
  - Makes debugging and changing between experiments and cluster partitions easier.
  - Prevents collisions or accidentally running jobs in the wrong environment.

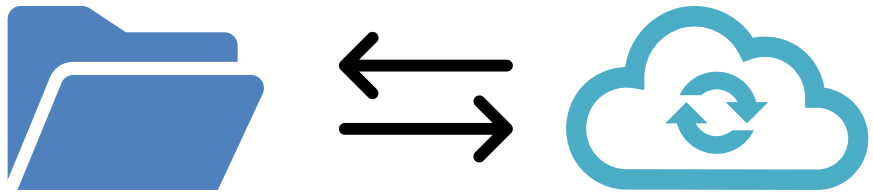
- **Please note that Quanah (Intel nodes), Nocona (AMD nodes), Matador (V100 GPU nodes), and Toreador (A100 GPU nodes) have a different set of modules.**
  - More details about this later in this training.

- **Always include the version number of a module in the module load command.**
  - Makes version tracking easier.
  - Prevents unanticipated changes in version during an experiment.
  - Example: Use **`module load nwchem/6.6-intel`** instead of just **`module load nwchem`**

Exercise #1

1. Log in to the "`login.hpcc.ttu.edu`" using your eraider account.
2. List all the available modules on the cluster:
   - What partition does the Lmod module support?
3. Load the '`gcc/10.1.0`' module
4. Do you see any changes in the list of available modules? Are any new modules on this list?
5. Do you see '`openmpi/4.0.4`' in the updated list? If so, then load it, please.
   - Do you see any changes again?
   - What modules have you loaded so far? Can you get a list of them?
6. Now try to load "`intel/19.1.2`". Is there any problem? What is the solution?
7. Purge all the currently loaded modules. Could you get rid of the partition module?
8. How about modules on "`quanah.hpcc.ttu.edu`"?

Transferring Data

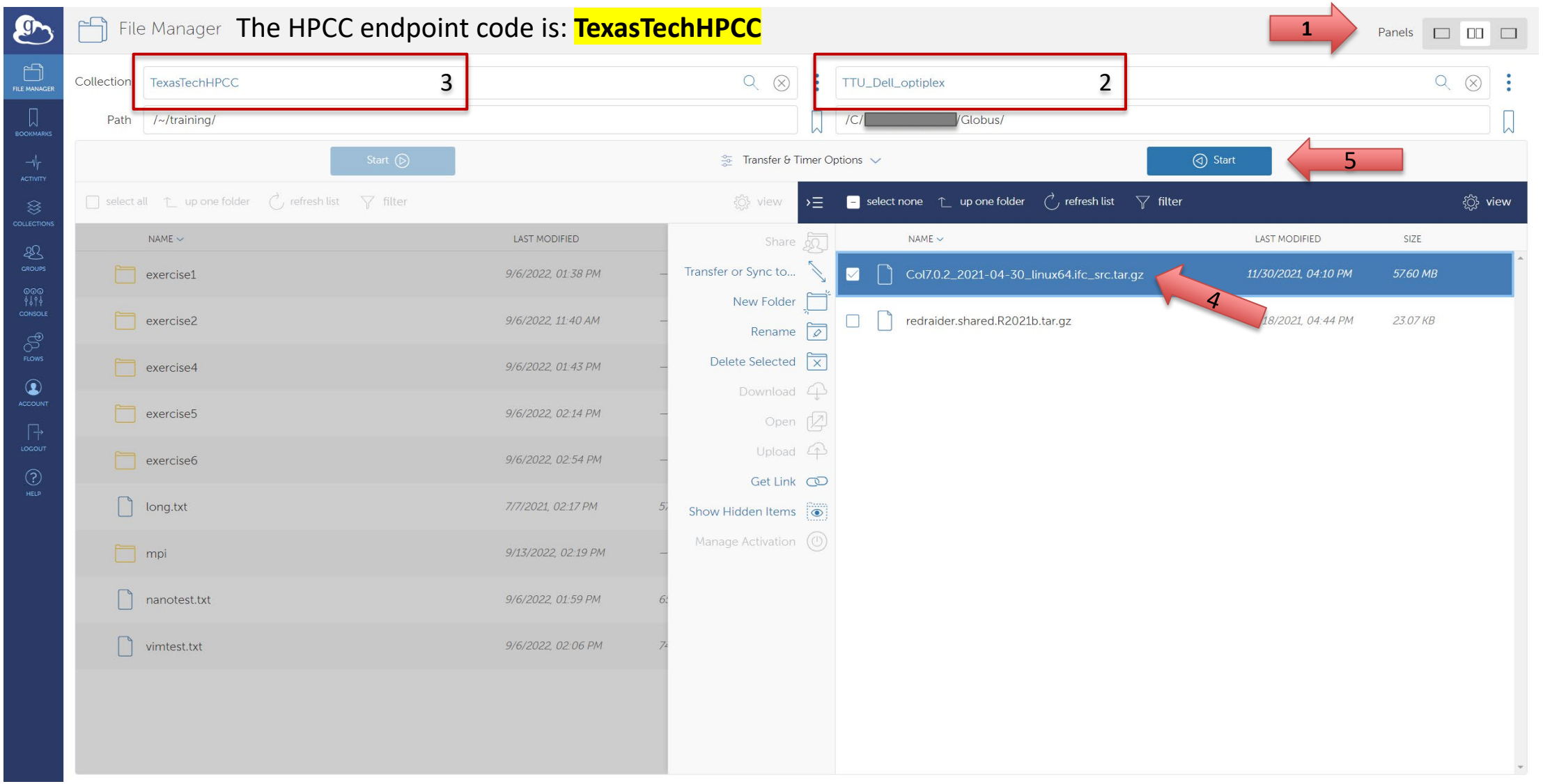


Transferring Data (Using Globus)

- Whenever possible, refrain from using:
  - `scp, sftp, rsync`, or any other data transfer tool
  - Okay for very small transfers, but for large ones, see below.
- Transfer files using Globus Connect personal client:
  - User Guide: http://tinyurl.com/hpcc-data-transfer
  - Globus Connect service is well connected to the campus network.
  - Globus Connect service eliminates the data transfer load from the cluster login nodes.
  - Globus Connect personal client works on **Linux, Mac and Windows** and is easy to control through a simple web GUI.
  - Numerous other sites (including TACC) support Globus Connect data transfers.

Transferring Data (Using Globus)

TEXAS TECH UNIVERSITY
Information Technology Division



Coming in Part 2 of this Training …

TEXAS TECH UNIVERSITY
Information Technology Division

Part 2:

- Resource Allocation and Job Submission with SLURM
- Software builds and installation
- HPCC Policies
- Getting Help

Lunch Break

Let’s get back at 1:00 pm

TEXAS TECH UNIVERSITY

Information Technology Division™