

HPCC New User Training

Getting Started on HPCC Resources

(Part 1/2)

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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: <u>https://www.depts.ttu.edu/hpcc/userguides/index.php</u>



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



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



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



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- 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.

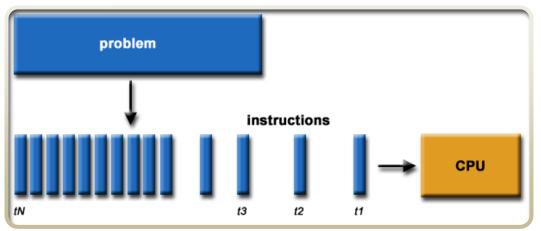


Image provided by Lawrence Livermore National Labs (computing.llnl.gov)

More Advanced Usage: Parallel Computing



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- **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.

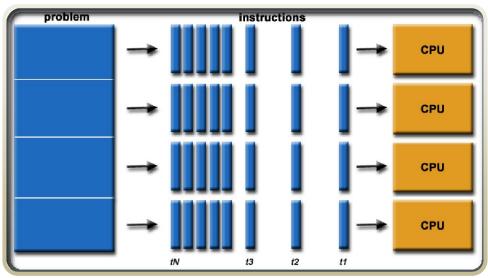


Image provided by Lawrence Livermore National Labs (computing.llnl.gov)

Classes of Parallel Computers

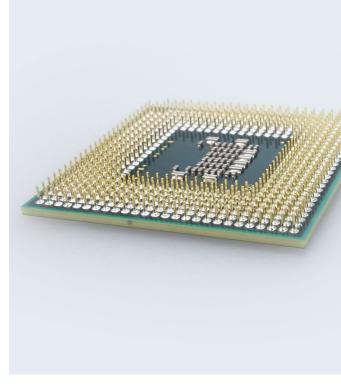


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- Multi-core Computing:
 - Multi-core processors contain multiple 'processing units' (called cores) on a single chip.
 - Allows for parallel execution across cores each able to reach the same system resources (RAM, Keyboard, Monitor, etc...).

• 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



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• 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

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• 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 fullyutilized on-premises clusters for HPC.



Why does programming style matter?



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- 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!

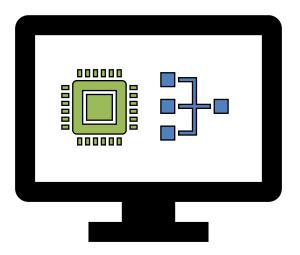
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- If your program is not written to use a certain model, it will not necessarily *"just work"* in that model.
 - Running serial code on a 128-core machine will use 1 core and leave 127 cores sitting idle.
 - Attempting to run multi-threaded code written 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



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- **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



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• **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



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• **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



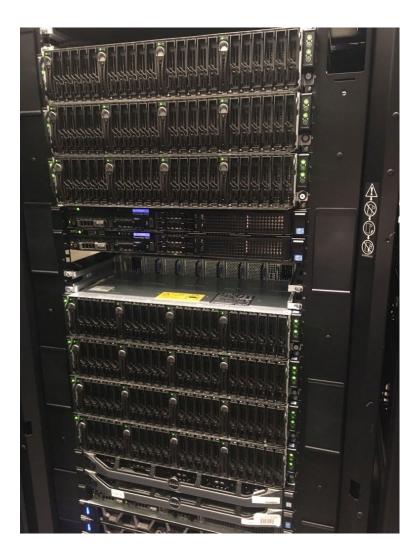
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• XLQuanah partition (16 nodes)

- 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



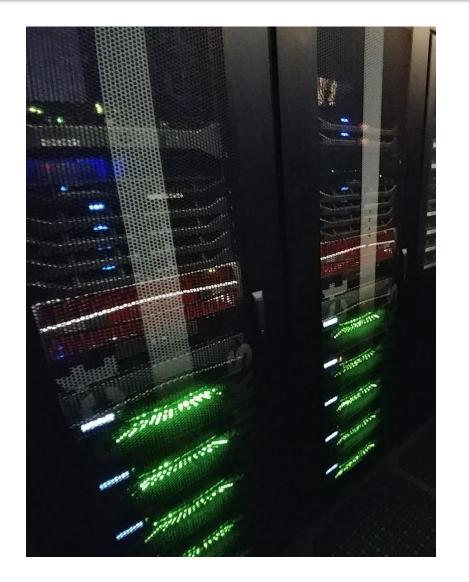
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Cluster-Wide Storage System:

- 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></eraider>	300 GB	1,000,000	Yes	No
/lustre/work/ <eraider></eraider>	700 GB	1,000,000	No	No
/lustre/scratch/ <eraider></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



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	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 <u>HPCC website</u>.

RedRaider Cluster Software Environment



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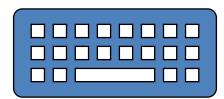
• List of currently installed software packages on the RedRaider Cluster:

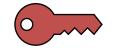
abyss	charm	ete3	git	ImageMagick	libxc	ncbi-rmblastn	ngs	paraview	py-astunparse	py-six	samtools	trinity
ampl	charmpp	exonerate	gnu	impi	libxsmm	ncbi-vdb	nvhpc	pear	py-cython	py-termcolor	scalapack	udunits
ansys	clustalw	fastStructure	gnu7	intel	lumerical	nccl	nwchem	perl	py-gast	python	singularity	vasp
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	



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Logging in and Using the Cluster





Getting Started



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



Getting Started



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- Logging to HPCC Resources:
 - <u>http://tinyurl.com/ttu-hpcc-login</u>
- 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 <u>https://goo.gl/4LbuWG</u>
 - Neither system is owned or maintained by HPCC



Logging to RedRaider Cluster

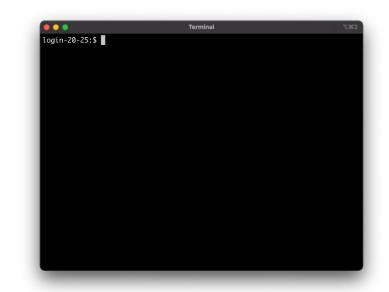


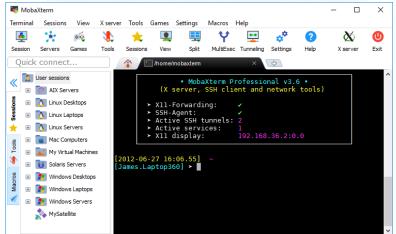
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- Mac/Linux Users:
 - SSH (Secure Shell): Freely available on Linux/Unix/MacOS and used via the Terminal.

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

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









Login to the RedRaider cluster (eraider@login.hpcc.ttu.edu)

** ** ** ** *	
** W ** ro ** *:	Upcoming Scheduled Maintenance he scheduled maintenance originally reserved for February 7-11 2012 ill be skipped as systems are currently operating well and do not equire any interventions at this time that would require downtime. **** Next scheduled maintenance will occur May 9-13 2022. ***** More information at: www.hpcc.ttu.edu/operations/maintenance.php
** ** No ** To ** To ** Eo	Upcoming HPCC Training Sessions ext new user training & Introduction to Linux sessions Spring 2022 uesday February 1: Introduction to Linux (best for beginning Linux) uesday February 8: New User Training (best to learn HPCC resources) ach held 10am to 3pm with a 1-hour break from 12pm to 1pm for lunch or more information see http://www.hpcc.ttu.edu/about/training.php
** U: ** Bi ** U: ** ai ** Di ** Fi ** Si ** Ci	<pre>*** General Cautions and Notes *** se the Scheduler! Do not run jobs directly on the Login Nodes! e aware that /lustre/work and /lustre/scratch are NOT backed up. sers should store important source code and data in their /home rea and keep extra copies of such files on non-HPCC storage drives. etails at https://www.depts.ttu.edu/hpcc/operations/datapolicy.php or information on security and privacy of files on HPCC systems ee https://www.depts.ttu.edu/hpcc/operations/security.php ontact hpccsupport@ttu.edu for help or additional information.</pre>
Last lo	essage of the Day was last updated: February 03, 2022 at 01:22 PM gin: Mon Feb 7 21:08:55 2022 from 129.118.242.213 Storage Usage for

/home - space: 47 of 300 GB (15%), file count: 136241 of 1000000 files (13%).
/lustre/work - space: 65 of 700 GB (9%), file count: 566996 of 1000000 files (56%).

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Space quota and file limit usage

login-20-26:\$

Environment Settings



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- Hostname pattern of the nodes in the RedRaider cluster:
 - Login nodes:
 - Login-20-[25-26]
 - quanah
 - CPU worker nodes:
 - style="font-size: large; color: blue;">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 <u>XQuartz</u>. 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



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- 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.

<pre>ogin-20-26:\$ module avail</pre>	•••	Available modules i	n Nocona partition		∿%1
High Performance Computing Center I RedRaider Cluster I	login-20-26:\$ module	avail			
High Performance Computing Center I RedRaider Cluster I	=====================================		====		
High Performance Computing Center I RedRaider Cluster I		Tech University			
RedRaider Cluster I Image: Current Arch: [nocona] Current Arch: [nocona] Image: Current Arch: [nocona] <td></td> <td>-</td> <td></td> <td></td> <td></td>		-			
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ogin-20-26:\$					
	login-20-26:\$				

- User Guide:
 - <u>https://www.depts.ttu.edu/hpcc/userguides/general_guides/software_environment.php</u>

Environment Settings



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• Lmod Module Commands:

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

Search Available Modules on the RedRaider



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High Performance Computing Center	Resources 🗸	Operations 🗸	About HPCC 🗸	RedRaider Cluster 🗸	HPCC Support
TTU / High Performance Computing Center					
	MATADOR NOCONA	QUANAH	TOREADOR	LIST	
	Search Software Package		×		
	HPCC RedRaide	r Cluster Softwa	re Packages		Â
HPCC users may find the most up-to-date list of availa Software Environment Setup Guide.	ble software packages and dependenci	ies on the RedRaider clus	ter on this web page. For more info o	n how to use Modules, please refer to) the
Search for a software package:					
 Use the search box above to look for any specifies The list of the available software package(s Commonly, results may show the different of For more details regarding each partition of Click on the search results leads you to the full p You will be able to see the software package Use the delete button × in the search box to cle) will appear for each partition. rersions of the same software package h the RedRaider cluster , click <u>here</u> . ath of the software package in the HPC e's description and its complete LMOD	built by various compilers C software hierarchy stac module command.			
Traverse the current software package hierarchy a	vailable for each partition:				
 Select the target partition from the top menu. For more details regarding each partition of Choose the desired independent software packa The description box will appear for the sele You will have a choice to select the preferre The bottom-right box below the stack show If dependent software packages are available, the or If applicable, follow steps 2 and 3 to traverse 	ge or compiler from the first level of the cted package below the stack. d version(s) of the software/compiler fr s more details about using the software ey will show up at the next level on the	om the next level on the s module(s) correctly.	tack.		
If your desired software package or a specific software			the <u>Request Software</u> web page and	place your new software request. Ple	ease note
that HPCC policies and restrictions on software install.	Generalde, kennederske besterner i Birgerie verstaat en ∎et te tek	ew soltware requests.			÷

HPCC RedRaider Software Packages

Modules Tips and Recommendations



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- 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

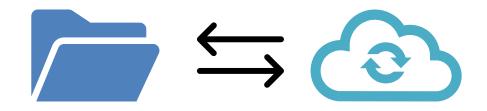




- 1. Log in to the "login.hpcc.ttu.edu" using your eraider account.
- 2. List all the available modules on the cluster:
 - What partition does the Lmod module support?
- 3. Load the 'gcc/10.1.0' module
- 4. Do you see any changes in the list of available modules? Are any new modules on this list?
- 5. 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)



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- Whenever possible, <u>refrain from using</u>:
 - 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: <u>http://tinyurl.com/hpcc-data-transfer</u>
 - 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

Path /~/training/		<<	TTU_Dell_optiplex 2	Q (8)
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exercise2	9/6/2022, 11:40 AM	New Folder	redraider.shared.R2021b.tar.gz	4 18/2021, 04:44 PM 23.07 KB
exercise4	9/6/2022, 01:43 PM	_ Delete Selected]	
exercise5	9/6/2022, 02:14 PM	Download 4		
exercise6	9/6/2022, 02:54 PM	Upload 🏼 🏳 Get Link 👁		
long.txt	7/7/2021, 02:17 PM	5) Show Hidden Items		
mpi mpi	9/13/2022, 02:19 PM	Manage Activation		
nanotest.txt	9/6/2022, 01:59 PM	6:		
vimtest.txt	9/6/2022, 02:06 PM	7-		





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



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