HPCC New User Training

Getting Started on HPCC Resources

(Part 2/2)

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Outline

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Information Technology Division

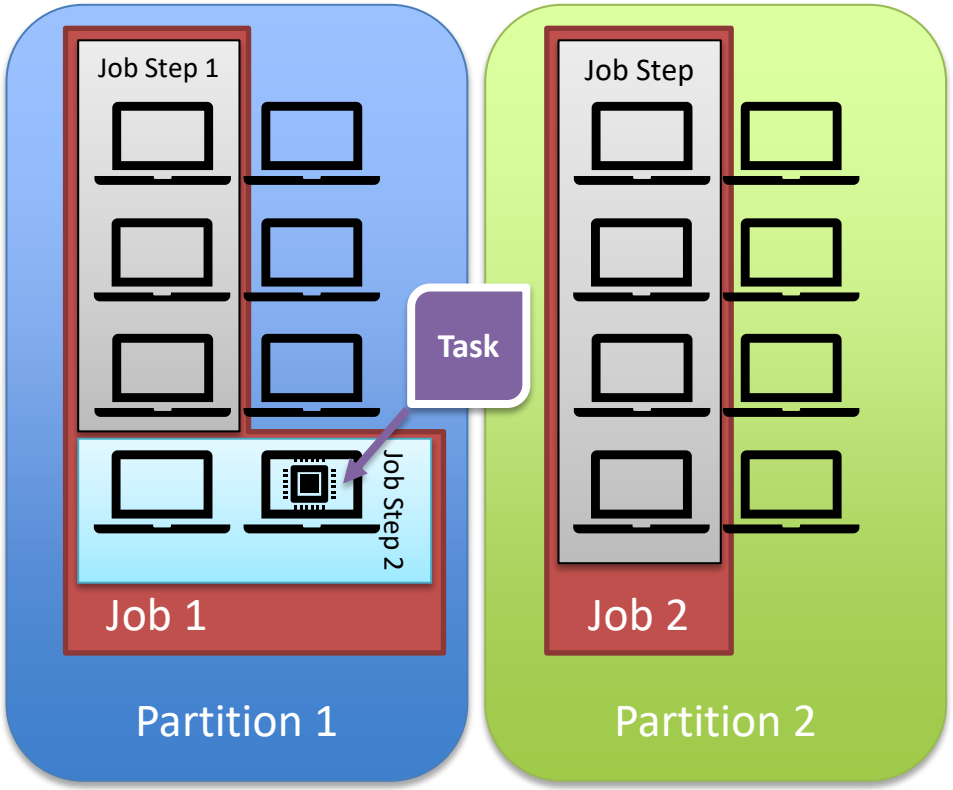
Part 2:

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

Resource Allocation and Job Submission with

Introduction to Slurm

- Simple Linux Utility for Resource Management (SLURM):
  - Primary HPCC scheduler used in RedRaider
  - **Main entities:**
    1. **Nodes:** Physical computing resources
    2. **Partition:** A logical set of nodes
    3. **Jobs:** Allocations of resources assigned to a user for a specified amount of time
    4. **Job Steps:** sets of (possibly parallel) tasks within a job
    5. **Tasks:** Implies the requested/allocated computing resources to process(es) per job or job step
       (By default, each task refers to 1 CPU core)



Slurm Commands

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- **Useful Slurm Commands**:
  - **`sinfo:`**
    - View information about nodes and partitions.
  - **`squeue:`**
    - View information about jobs located in partitions.
    - Useful options to filter the output:
      - **`-u <user>, --user=<user>:`** Shows the list of jobs or job steps that belong to a specific user
      - **`--me:`** Shows the list of jobs or job steps that belong to you (owner)
      - **`-p <partition>, --partition=<partition>:`** Filters the jobs within a partition.
  - **`srun:`**
    - submits a job for execution or initiates job steps in real-time.
    - `srun` has the same options as `sbatch` with a few more. (Please see the man page)
    - `srun` works similar to the "`mpirun`" and it can be replaced with "`mpirun`" as well.

Job Submission in Slurm

- **`sbatch`**:
  - submits a job script for later execution.
    - The submitted job stays in the queue until the requested resources become available.
    - The job submission script is a text file that contains "`#SBATCH`" hints with `sbatch` command line options.

```
#!/bin/bash
#SBATCH -J MPI_test
#SBATCH -N 2
#SBATCH -ntasks-per-node=128
#SBATCH -o %x.%j.out
#SBATCH -e %x.%j.err
#SBATCH -p nocona

module load gcc/10.1.0 openmpi/3.1.6
mpirun ./my_mpi
```

Job Submission in Slurm

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- Job Submission Script Layout:

Description	SLURM
Set the name for job	-J , --job-name=<jobname>
The name of the standard output file	-o, --output=<filename pattern>
The name of the standard error file	-e, --error=<filename pattern>
Define the queue (partition) name	-p, --partition=<partition_names>
Type of parallel env for job/task allocation	-N, --nodes=<# of nodes> --ntasks-per-node=<ntasks>
Reserve memory per slot	--mem-per-cpu=<size[K|M|G|T]>
Set the maximum job run time	-t, --time=<HH:MM:SS>
Specify the cluster policy for this job	-A, --account=<account> | -q, --qos

Job Submission in Slurm

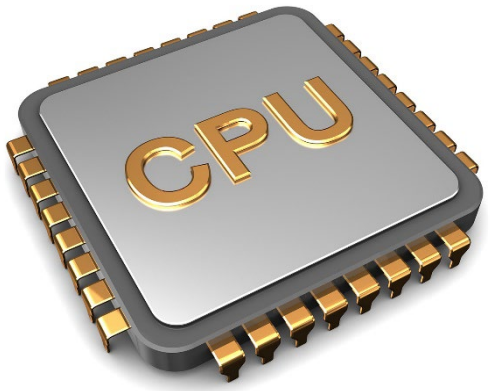
- Select a partition:
  - Partition in Slurm groups physical nodes into a logical set and allows jobs to request for nodes' resources from that partitions.
    - `-p, --partition=<partition_name>`

Name	# of Nodes	Type	Nodes	#Core/Node	#Mem/Node	#Mem/Core	#GPU/node
nocona	240	AMD ROME CPU	cpu-[23-26]-[1-60]	128	503 GB	3.9 GB	N/A
matador	20	Intel/Nvidia V100 GPU	gpu-[20-21]-[1-10]	40	376 GB	9.4 GB	2
gpu-build	1	Intel/Nvidia V100 GPU	gpu-20-11	32	187 GB	5.9 GB	1
toreador	11	AMD/Nvidia A100	gpu-20-[12-15],gpu-21-[11-17]	16	188 GB	11.8 GB	3
quanah	467	Intel Xeon Broadwell	cpu-[1-10]-[*]	36	188 GB	5.3 GB	N/A
xlquanah	16	Intel Xeon Broadwell	cpu-19-[1-16]	36	251GB	6.9 GB	N/A
himem-ivy	2	Intel Xeon Ivy Bridge	cpu-19-[23-24]	20	1.47TB	75.6 GB	N/A

Job Submission in Slurm

- Requesting CPU:
  - In Slurm, users must define the following options in their job submissions in order to request for CPU resources:
    1. Number of nodes: How many total nodes for the job?
       - **`-N, --nodes=<number of nodes>`**
    2. Number of tasks per node: (*Recommended*)
       (By default, each task consumes **1x** CPU core)
       - **`--ntasks-per-nodes=<number of task per node>`**

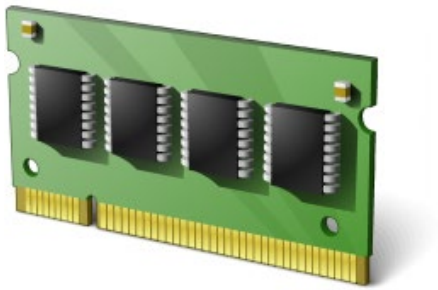
    OR Number of total tasks: How many task across the nodes?
       - **`-n, --ntasks=<number of tasks>`**



  - Requesting the right number of cores is key to optimizing throughput

Job Submission in Slurm

- Requesting Memory:
  - One can specify the size of the consumable Memory in two ways in Slurm:
    1. Memory per core (*Recommended*):
       - **`--mem-per-cpu=<size[M|G]>`**
    2. Memory per node:
       - **`--mem=<size[M|G]>`**



  - If no memory size was specified, Slurm will assign the default memory per core to your job:

Nocona: 4027 MB (3.9 GB) / core	**Matador:** 9639 MB (9.4 GB) / core	**Quanah:** 5370 MB (5.3 GB) / core
Toreador: 12064 MB (11.8 GB) / core	**Xlquanah:** 7162 MB (6.9 GB) / core	**Himem-ivy:** 77406 MB (75.6 G) / core

  - Make sure you won't exceed the total memory per node:
    - `-p nocona -N 1 -n 128 --mem-per-cpu=100G` ✗

Job Submission in Slurm

- Requesting Runtime limits:
  - Recommended that you set the max runtime you expect a job will take.
    - **`-t, --time=<time>`**
    - `<time>` can be:
      - *minute*
      - *minute:seconds*
      - ***hours:minutes:seconds***
      - *days-hours*
      - *days-hours:minutes*
      - *days-hours:minutes:seconds*
    - `E.g., --time=24:00:00`

  - Please note that there is a 48-hour default time limit per job and exceeding this amount will end up with rejecting your job submission.

Job Submission in Slurm

- Requesting GPU:
  - GPUs are available by requesting any node in the matador partition.
    - Number of GPUs per node (*Recommended*):
      - **`--gpus-per-node=[<type>:]<number>`**
    - Total number of GPUs:
      - **`-G, --gpus=<# of gpus>`** (***Currently Unavailable on RedRaider cluster***)
  - There is only one type of GPU in RedRaider Cluster (`v100`) and is optional to be specified.
  - It is required to requesting at least **one GPU per node** when submitting a job to Matador.
  - Make sure you do not exceed more than 2 GPUs per node during the job submission.
    - `--partition=matador --nodes=2 -gpus-per-node=4` ✗
    - `--partition=matador --nodes=2 --gpu-per-node=2` ✓

Job Submission in Slurm

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- Accounts on RedRaider Cluster:
  - Accounts, in Slurm, imposes a set of pre-defined resource limits and assigns the usage/fair-share policies to each job.
    - `-A, --account=<account>`

Account -A, --account	Default Runtime	Maximum Runtime	CPU/Mem Limit per job	Total # Jobs Per User	# Running Jobs / User	Allowed Partitions	Priority	Special Account
default *	**48 hours**	**48 hours**	**No limit**	**2000**	**No limit**	**All Partitions**	**normal**	**No**
xlquanah **	72 hours	14 days	36 cores / 251GB	100	4	xlquanah	normal	Yes
Dedicated resource users	72 hours	No limit	Up to the total available resources	No limit	No limit	Nocona/Quanah	high	Yes

(*) The system will assign the default Account/QoS if the user does not define them in their job submissions.
(**) Request for special access is required. There should be a valid use case to approve the access to the "xlquanah" partition.

Submitting Jobs

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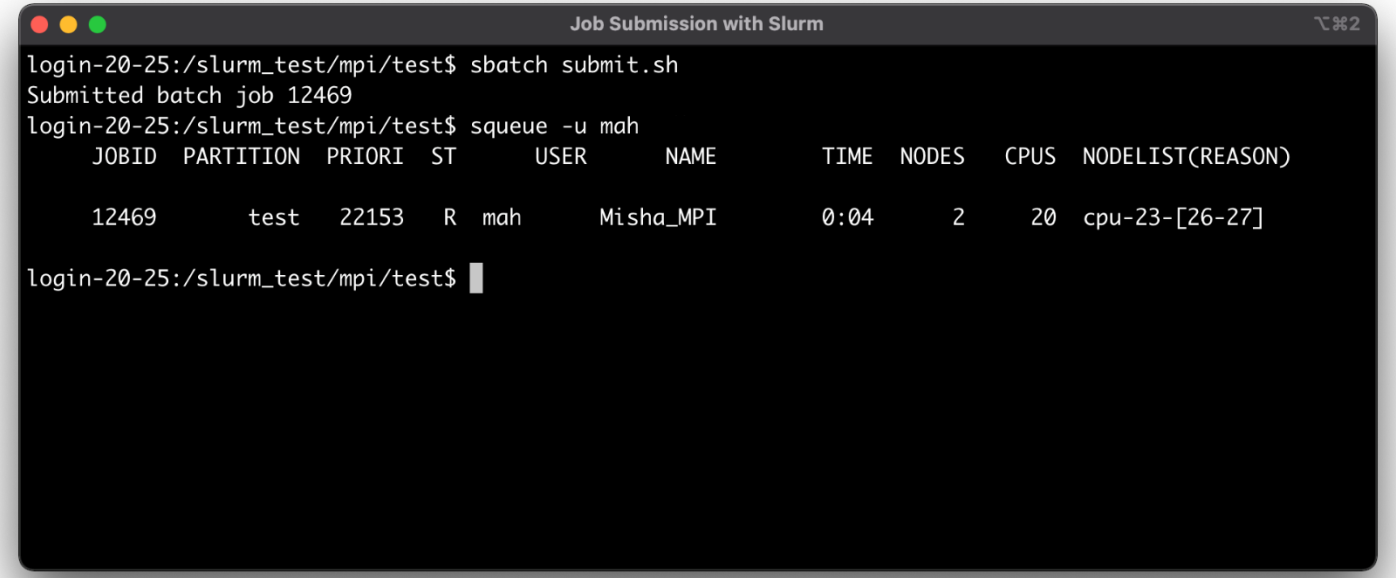
- Example of a simple job to submit an MPI program to Slurm:
  - Create a job submission script file (e.g., submit.sh):

```
#!/bin/bash
#SBATCH -J MPI_test
#SBATCH -N 2
#SBATCH -ntasks-per-node=128
#SBATCH -o %x.%j.out
#SBATCH -e %x.%j.err
#SBATCH -p nocona

module load gcc/10.1.0 openmpi/3.1.6
mpirun ./my_mpi
```

Example: /lustre/work/examples/nocona

  - Submit the job with `sbatch`:
    - **`sbatch submit.sh`**
  - Monitor the job with `squeue`:
    - **`squeue --me`**
    - **`squeue -u <username>`**
  - Cancel the job with `scancel`:
    - **`scancel job_id`**



Exercise #2

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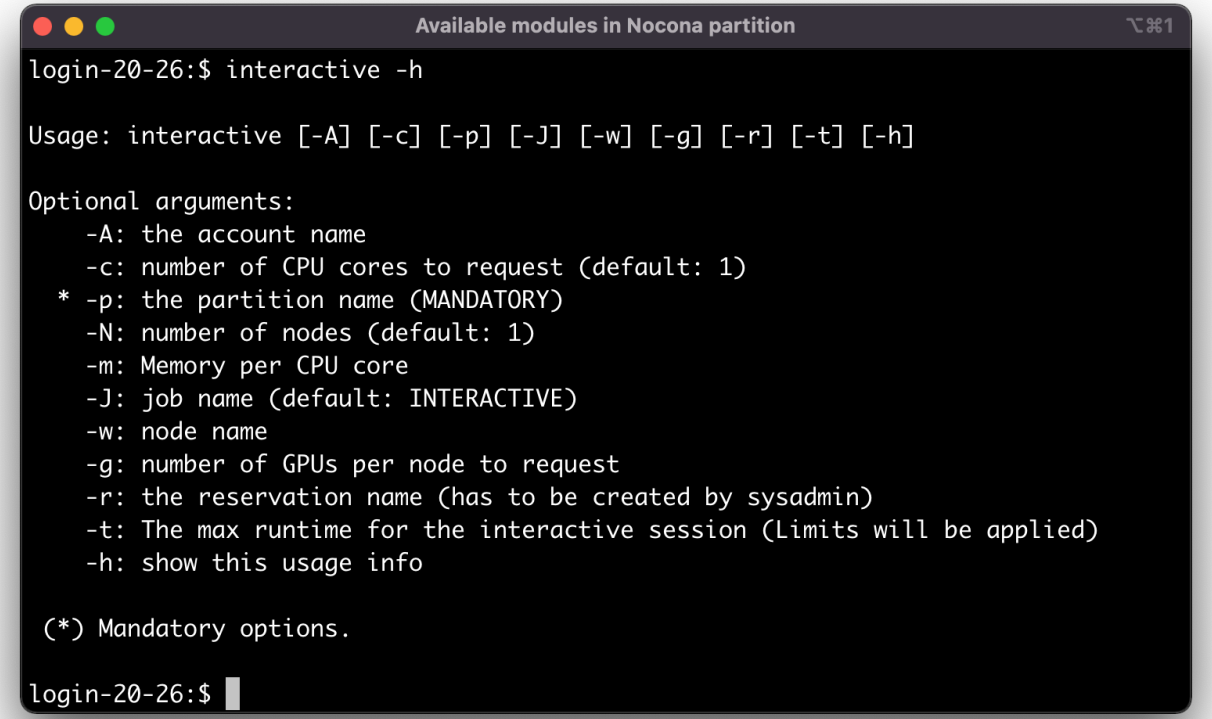
1. Make sure you're already Logged in to the "`login.hpcc.ttu.edu`" using your eraider account.
2. Go to your home directory and copy the following directory into your home directory:

```
$ cp -r /lustre/work/examples/nocona/training/mpi ~/
```

3. Go into the '`mpi`' directory on your home directory:
   a) List the contents of the directory
   b) Print the contents of the '`makefile`' file
   c) Load the proper modules for "GCC 10.1.0" and "OpenMPI 4.0.4"
   d) Run the "`make`" command to compile the "`mpi_hello_world.c`" code
   e) Modify the '`mpi_slurm.sh`' file as follows:
      i. Request 1 node from 'nocona' partition with 2 tasks (CPU cores) per node
      ii. Load the right modules that will work properly with the "`mpi_hello_world`"
   f) Submit the '`mpi_slurm.sh`' job script
   g) Check the current status of your jobs
   h) Check the job's output/error files after it finished.

Interactive Session

- **`interactive`:**
  - Starts an interactive session/job:
    - `interactive -c 2 -p nocona`
    - See the `interactive -h` for all the available options.
  - Make sure the prompt changes to `cpu-#-#`.
  - Make sure you run "exit" when you're finished.
  - Keep in mind resource/runtime limits apply to `interactive` based on the selected account.
  - The `interactive` command will forward the X11 if the SSH session was established with `-X` or `-Y`.
  - Please note that direct SSH to any worker nodes not part of your job is blocked on the RedRaider cluster.



The ‘gpu-build’ Partition

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- Building and Testing GPU applications:
  - The `gpu-build` partition contains one Intel/GPU node with **1x Nvidia V100** GPU device, **32x Intel CPU cores** and **192 GB RAM**, which allows users to:
    - Build their own GPU applications.
    - Test GPU applications and the environment setup before submitting a job to Matador partition.
    - Accessing the Lmod Module environment for GPU compilers/applications.
  - In order to access the ‘gpu-build’ node, you need to establish an `interactive` session:
    - **`$ interactive -p gpu-build -c 2`**
  - Limitations:

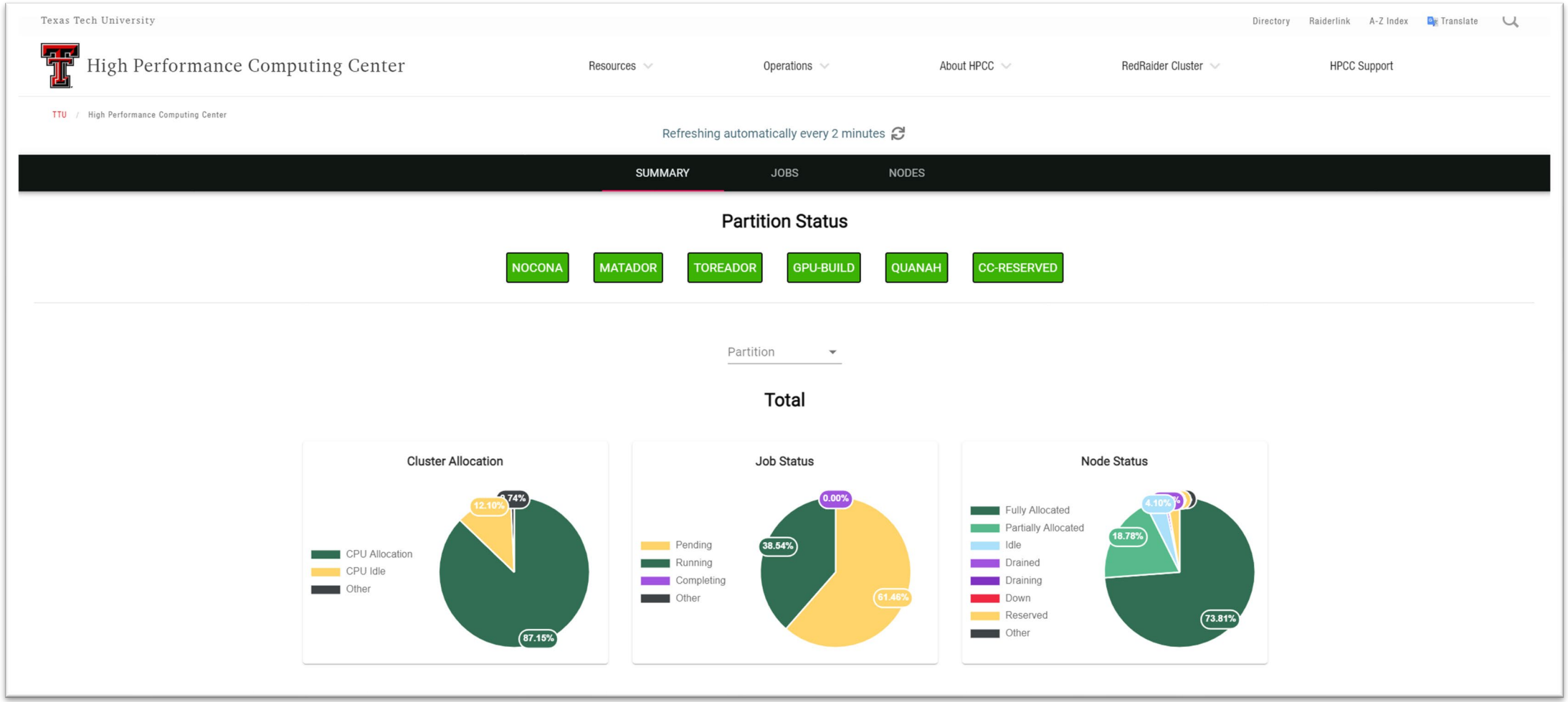
Partition	Max Runtime (per job)	Max CPU per user (in total)	Max Mem per user (in total)	Max interactive session per user
gpu-build	5 hours	6	36006 MB (35 GB)	2

Debugging a Finished Job

- **`sacct`**:
  - reports accounting information about active or completed jobs or job steps.
    - **`sacct -j <jobid>`**
  - More filter options are available by checking the `-e, --helpformat` options of `sacct` command.
    - `sacct -j <jobid> --format=partition,jobid,ntasks,nodelist,maxrss,maxvmsize,exitcode`
  - When debugging:
    - Check the output and error files
    - Check the output of sacct for:
      - ✓ Memory usage
      - ✓ Exit code
      - ✓ Start and end time.

Current Status of the Job Scheduler

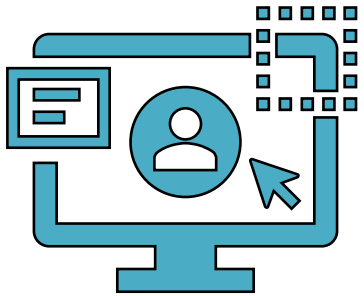
- You can check the current status of the Slurm Job Scheduler at this Link.



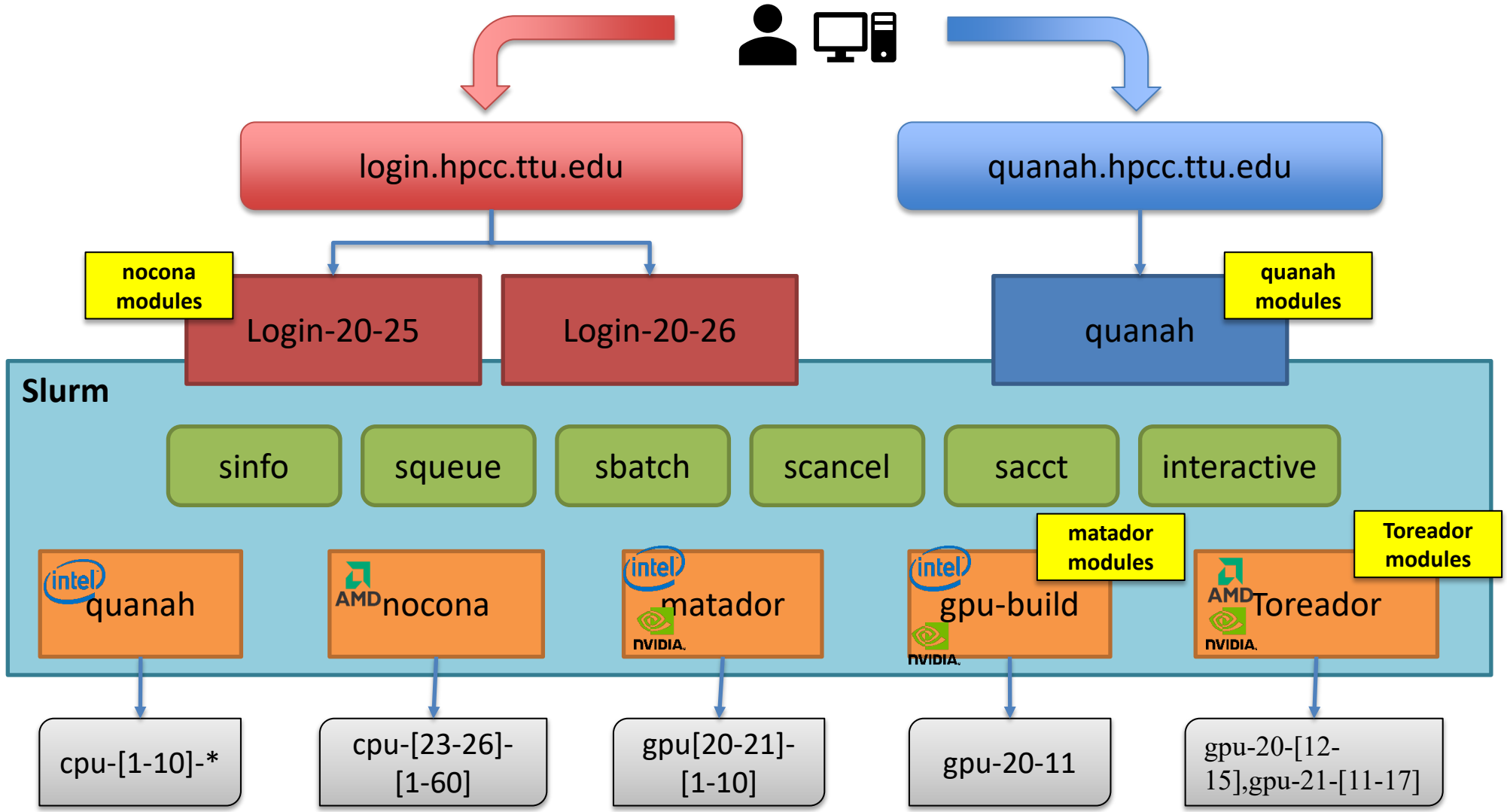
Exercise #3

1. Make sure you're already Logged in to the "login.hpcc.ttu.edu" using your eraider account.
   - For this example, please assure your SSH session has the X11 forwarding enabled!
2. Make an interactive session to one of the Nocona nodes:
   - Use the' `interactive`' command.
   - Request for 1 CPU core from 'nocona' partition.
   - You can use the same temporary reservation as you used in the last exercise.
3. Once the worker node was allocated, locate the "MATLAB" module
4. Try to run the MATLAB graphical user interface (GUI) on the cluster:
   - `cpu-#-#$ matlab`
5. Close the MATLAB window to exit the program.
6. Exit the interactive session.

Software build and installation



HPCC RedRaider Cluster – Overall Look



HPCC RedRaider Cluster - CPU Architectures

- Multiple partitions – Multiple architectures:

Nocona
AMD EPYC ROME

Matador
Intel Xeon Cascade Lake
Nvidia V100

Quanah/XLquanah
Intel Xeon Broadwell

Toreador
AMD EPYC ROME
Nvidia A100

Software builds on HPCC Clusters

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- Modules & compiled code are different on each of the RedRaider partitions!
  - Each CPU architecture may bring a different set of features and instructions.
  - Compiled programs (C/C++/Fortran) need to be re-compiled to match each CPU architecture.
  - E.g., programs that are compiled on **Intel** nodes may not work properly/efficiently on **AMD** nodes.
  - Different Compilers/Math libraries optimize the programs differently on each architecture.

Compiler	AMD ROME	Intel Broadwell	Intel Ivy Bridge	Intel Cascade Lake	Nvidia GPU
GNU/GCC	**GCC 10+**	GCC 4+	GCC 4+	**GCC 10+**	GCC 8+
Intel	May work	**Optimized**	**Optimized**	**Optimized**	Intel 19+
AOCC	**Optimized**	Not Applicable	Not Applicable	Not Applicable	N/A
MKL	May work	Optimized	Optimized	Optimized	MKL 19+
AOCL	**Optimized**	Not Applicable	Not Applicable	Not Applicable	N/A
CUDA	N/A	N/A	N/A	N/A	**CUDA 10+**

Software builds on HPCC Clusters

- Tips and Recommendations:

1. Create a separate directory for each CPU architecture, and make a copy from your code/program and place it under each directory:
   - **`mkdir nocona matador quanah`**
2. Login to the RedRaider login node, and for each CPU architecture make an interactive session to the corresponding worker node:
   - **`interactive -p nocona –c 10`**
3. Go to the directory of you code that has the same name as the current session's partition:
   - **`cd nocona`**
4. Load a proper compiler module and recompile your code:
   - **`module load gcc/10.1.0`**
5. If applicable, add the `-O3` optimization flag to all the `CFLAGS, CPPFLAGS, CXXFLAGS, FFLAGS.`
   - **`CFLAGS=-O3 FFLAGS=-O3 make –j 10 all`**

Software builds on HPCC Clusters

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- Tips and Recommendations:

5. We recommend mapping the MPI jobs to the L3-cache memory on **Nocona (AMD)** nodes:
   - `mpirun -map-by l3cache ./mpi_app`

6. **HPCC will not support Python v2 on Nocona and Matador nodes with CentOS 8. (This rule will be applied to Quanah and Ivy in the near future.)**
   - Users can still get Python v2 from Conda (Anaconda/Miniconda)
   - Python 2 is NOT RECEIVING SECURITY UPDATES and should be retired from your workflows ASAP.

7. Python applications (including the applications from Conda repo) will continue working with different architectures without recompiling them.

8. All the job submissions to **Quanah** partitions must be performed from "**quanah.hpcc.ttu.edu**," and jobs submissions to all other partitions must go through "**login.hpcc.ttu.edu**".

Local Python Package Installation

- Install a Python package into your home folder:

```
$ module load intel python
$ pip install --user <package name>
    • Example: pip install --user matplotlib
```

- Install a local copy of Python using Conda:

```
$ /lustre/work/examples/InstallPython.sh
$ . $HOME/conda/etc/profile.d/conda.sh
$ conda activate
$ conda install <package name>
    • Example: conda install biopython
```

[Installing a local copy of Python | User Guides | High Performance Computing Center | TTU]

Local R Package Installation

- Install an R package into your home folder:
  - Example (On Quanah Node:)

```
$ module load intel R
$ R
$ install.packages('<package name>')
    Example: install.packages('readr')
```

  - Select a mirror
  - The R application will ask if you want to install it locally the first time you do this.

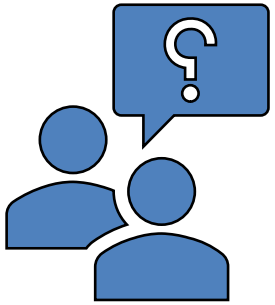
https://www.depts.ttu.edu/hpcc/userguides/HPCC_R_Jobs_User_Guide.pdf

HPCC Policies

HPCC Policies

- Login nodes (login.hpcc.ttu.edu, quanah.hpcc.ttu.edu):
  - No jobs are allowed to run on the login node.
- SSH Access:
  - No direct SSH access allowed to a node(s) if you have no job running on the node(s)
- Software Installation:
  - Software requests are handled on a case-by-case basis
  - Requesting software does not guarantee it will be installed “cluster-wide”.
  - May take two or more weeks to complete your request.
- Scratch Purge Policy:
  - Scratch will be purged monthly by removing of all files not accessed within the past year, or sufficient to bring total scratch space usage across all accounts down to 80% of capacity.

Getting Help



Further Assistance

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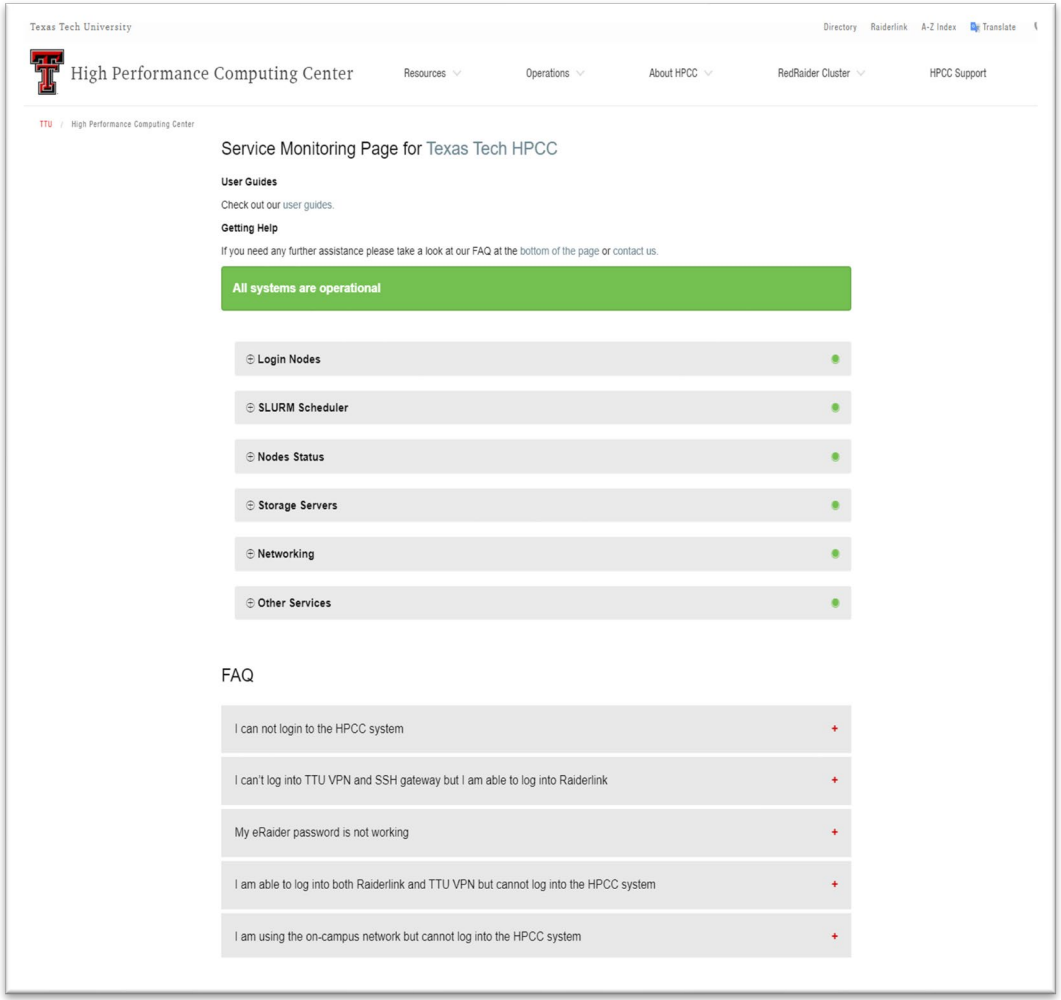
- Visit Our Website:
  - Most up-to-date user guide documents
    - https://www.depts.ttu.edu/hpcc/userguides/index.php
  - Job scheduler and resource allocation status page
    - https://www.depts.ttu.edu/hpcc/status/slurm_web.php
  - Current status of all HPCC services
    - https://www.depts.ttu.edu/hpcc/status/cachet.php
- Read the documentation!
  - https://slurm.schedmd.com/documentation.html
- Submit a support ticket:
  - Send an email to hpccsupport@ttu.edu



Quick Reminder

- HPCC Training Courses
  - Please check the website for upcoming User Training workshops
    - *http://www.depts.ttu.edu/hpcc/about/training.php*
- ShortCourse Survey
  - Looking forward to have your feedback on this Training Workshop
    - *You will receive a survey in your inbox from TTU ShortCourse*
- The PowerPoint slides are available online
    - *http://www.depts.ttu.edu/hpcc/about/training.php*

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