TEXAS TECH UNIVERSITY

CS4379: Parallel and Concurrent Programming
CS5379: Parallel Processing

Lecture 8

Guest Lecture by Misha Ahmadian

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Texas Tech University

Course Info

- **Lecture Time**: TR, 12:30-1:50
- **Lecture Location**: ECE 217
- **Sessions**: CS4379-001, CS4379-002, CS5379-001, CS5379-D01
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Outline

- HPCC Resources
- Logging In and Using the Clusters
- Linux Essentials
- Understanding Modules
- Using Compilers on HPCC clusters

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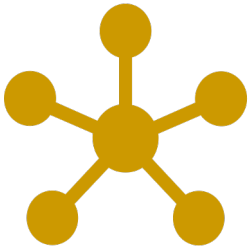
Current Resources

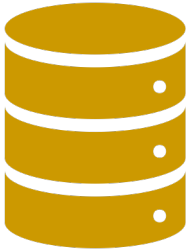


Clusters

Quanah Cluster

Ivy Cluster

Community Clusters



Parallel File System

Lustre File System

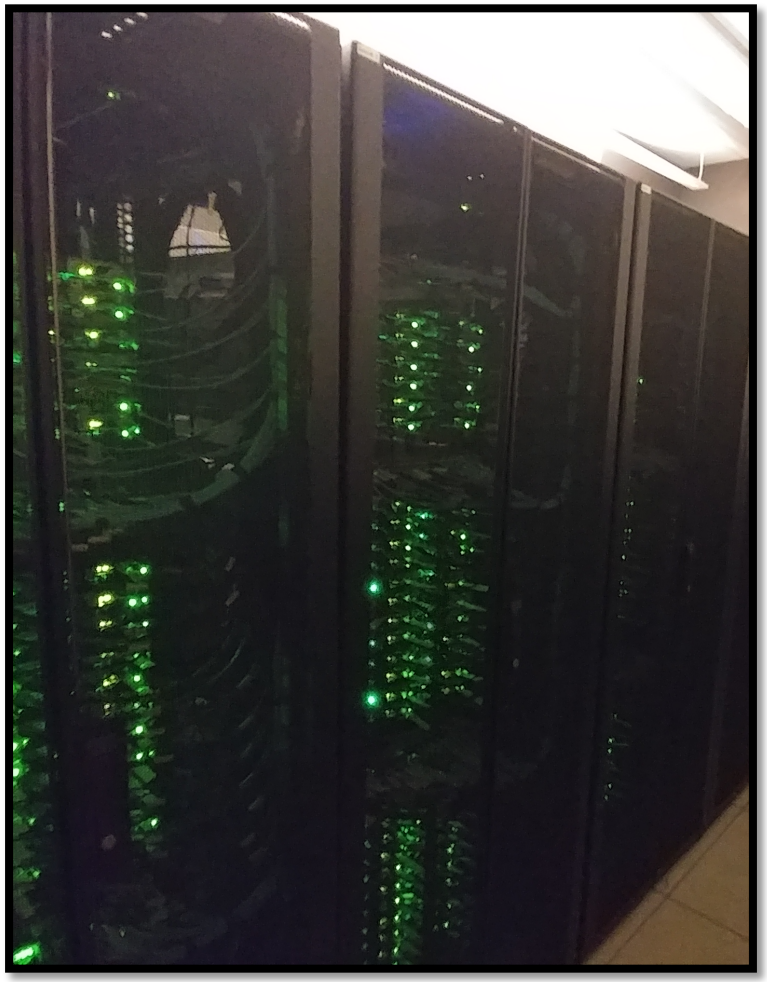
6.9 PB in total space

Ivy Cluster

- Commissioned in 2014
- Running CentOS 7.4
- Currently consists of
  - 100 Nodes
  - 2000 Cores (20 cores/node)
  - 6.25 TB Total RAM (64 GB/node)
  - Xeon E5-2670v2 Ivy Bridge Processors
  - QDR 40 GB/second InfiniBand fabric

Quanah Cluster

- Commissioned in 2017
- Running CentOS 7.4
- Currently consists of
  - 467 Nodes
  - 16,812 Cores (36 cores/node)
  - 87.56 TB Total RAM (192 GB/node)
  - Xeon E5-2695v4 Broadwell Processors
  - Omni-Path (100 Gbps) Fabric
- Benchmarked at 485 Teraflops/sec



Red Raider Cluster

- Arrives Q1 2020
- Commission planned for mid 2020
- Will consist of
  - 240 CPU Nodes
    - 30,720 Cores
    - 120 TB Total RAM (512 GB / node)
    - AMD Rome Processors
  - 20 GPU Nodes
    - 40 NVIDIA Tesla V100 GPUs
      - (2 V100 / node)
    - 10 TB Total RAM (512 GB / node)
  - HDR 200 GB/second Infiniband fabric

Lustre Storage System

- High speed parallel file system
- 6.9 PB of storage space
- Our users may purchase dedicated storage space

Lustre File System

- You have access to three storage areas
  - Home - /home/<eraider>
    - Quota: 300GB
    - Backed up nightly
    - Never purged
  - Work - /lustre/work/<eraider>
    - Quota: 700GB
    - Never backed up nor purged
  - Scratch - /lustre/scratch/<eraider>
    - Quota: None
    - Never backed up
    - Purged

Quota / Backup / Purge per Lustre Area

Area	Quota	Backup	Purged
/home/<eraider>	**300 GB**	Yes	No
/lustre/work/<eraider>	700 GB	No	No
/lustre/scatch/<eraider>	None	No	Monthly

Example Quota Results

```
Current Storage Usage for errees:
                /home - Currently using  19 of 300 GB ( 6%).
          /lustre/work - Currently using   2 of 700 GB ( 0%).
```

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Accessing HPCC Resources

- Host names:
  - `quanah.hpcc.ttu.edu`
  - `ivy.hpcc.ttu.edu`
- Access protocol: SSH (22)
- Log in with your eRaider user ID and your eRaider password with any SSH client software

```
ssh eraidername@quanah.hpcc.ttu.edu

ssh eraidername@ivy.hpcc.ttu.edu
```

Accessing HPCC Resources (cont.)

- **On Linux**
  - Open terminal
  - ssh eraidername@quanah.hpcc.ttu.edu
  - Then provide your eRaider password

Accessing HPCC Resources (cont.)

- **On Mac**
  - Launchpad->utilities->terminal
  - ssh eraidername@quanah.hpcc.ttu.edu
  - Then provide your eRaider password

Accessing HPCC Resources (cont.)

- **On Windows**
  - Download and install MobaXterm
  - https://mobaxterm.mobatek.net
  - Open a new terminal tab and use just like Linux/Mac
  - Or open a new SSH session from the Session tab and provide the Hostname, username, and eRaider password

X Windows

- Interactive GUI using **Linux/Mac**
  - Install X Server (Xquartz) on Mac
  - Add the following options to your normal **ssh** command:
    - -Y
  - Example:
    - ssh –Y <eraider_user>@quanah.hpcc.ttu.edu
  - Run a test command like xclock.

- Interactive GUI using **Window**
  - Install MobaXterm:
    - https://mobaxterm.mobatek.net
  - Log into the cluster.
  - Run a test command like `xclock`.

Access from off-campus

- 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 – Not owned/maintained by HPCC
  - Establish a VPN - https://goo.gl/4LbuWG - **Preferred Method**

Logging In

Upcoming or Current Downtimes
Always good to check this every time you log in.

Upcoming HPCC Training Sessions
Not always just “New User Training”

MoTD Last Updated Date/Time

Current Storage Usage

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Basic Linux/Unix Commands

ls (directory)	list your files	ls src
ls -a (file/dir)	hidden files	ls -a
ls -l (file/dir)	list size/detail	ls -l mpi.c
mkdir (dir)	create a directory	mkdir src
cd (directory)	change to directory	cd src;cd ../bin
cd (blank)	to your home dir	cd
rm (file)	delete a file	rm a.out
rm -r (dir)	delete a directory	rm -r src
vi (file)	terminal text editor	vi mpi.c
mv (file/dir)	move/rename	mv src src1
man command	display help info	man ls

Editing Files

- Create new file
  - $ touch newfile.c
- Edit existing file
  - $ vi newfile.c
  - type **i** to enter the insert mode
  - type **esc** to exit insert mode
  - type **:wq** or **:x** to save&exit
  - type **:q!** to exit without save

Environment Settings

- **User Environments**
  - **.bashrc**
    - Bash script that runs whenever you start an interactive login.
    - Often used to set up user environments.
    - While you may add to your .bashrc file, do not remove any default settings!
  - **Modules**
    - The primary way to change your user environment.
    - Running on Quanah and Ivy

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Modules

- Modules commands:
  - module avail
  - module list
  - module load <module_name>
  - module unload <module_name>
  - module spider <keyword>
  - module purge
  - module swap

```
quanah:$ module avail

------------------------------------------ /opt/apps/nfs/module/modulefiles ------------------------------
   gnu/5.4.0    gurobi/v751    intel/17.3.191    java/1.8.121    matlab/R2017b    perl/5.16.3

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

quanah:$ module spider python

----------------------------------------------------------------------------------------------------------
  python:
----------------------------------------------------------------------------------------------------------
    Description:
      Python-2.7.9 compiled with Intel

     Versions:
        python/2.7.9-gnu
        python/2.7.9-intel

----------------------------------------------------------------------------------------------------------
  For detailed information about a specific "python" module (including how to load the modules) use the
name.
  For example:

     $ module spider python/2.7.9-intel
----------------------------------------------------------------------------------------------------------
```

Modules (cont.)

```
$ module avail
```

```
---------------------------------- /opt/apps/nfs/module/modulefiles ----------------------------------
   ampl/v20180822    gurobi/v751           matlab/R2019a (D)    totalview/2017.3.8
   ansys/v193        gurobi/v801    (D)    orca/4.2.0           totalview/2019.2.18 (D)
   cadence/v171      lumerical/2020a       perl/5.16.3          vasp/5.3
   fsl/6.0.0         matlab/R2018a         picard/2.0.1         vasp/5.4.4          (D)
   grads/2.2.1       matlab/R2018b         rosetta/3.9

------------------------------------ /opt/ohpc/pub/modulefiles ------------------------------------
   eigen/3.2.10    gnu7/7.3.0          java/1.6.0    java/1.8.0 (D)    singularity/3.4.2
   gnu/5.4.0       intel/18.0.3.222    java/1.7.0    prun/1.2
```

```
$ module load java/1.7.0
```

```
$ module list
```

```
quanah:$ module list

Currently Loaded Modules:
  1) java/1.7.0
```

Module Tips & Recommendations

- Try to keep all of your module load commands as part of your job submission scripts.
  - Makes debugging and changing between experiments easier.
  - Prevents collisions or accidently running jobs with the wrong environment.
  - Provides yourself and collaborators with a way of tracking the exact software and versions used in any given experiment.

Module Tips & Recommendations (cont.)

- Always contain the version number of a module in the module load command.
  - Makes version tracking easier.
  - Prevents unanticipated changes in version during an experiment.
  - This will make it easier for you to track which experiments and jobs used which versions of different software, which will in turn make writing your research paper's "methods" section easier.
  - Example: Use **module load nwchem/6.6-intel** instead of just **module load nwchem**

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Supported C/C++ Compilers on HPCC

- **GNU Compiler**
  - Produced by GNU Project (Free & Open Source)
  - Supports various programming languages (C, C++, Fortran, …)
  - Available GNU compiler on HPCC systems:
    - `gnu/5.4.0`
    - `gnu7/7.3.0`
- **Intel Compiler**
  - Introduced by Intel (Commercial & not free)
  - Generates optimized code for IA-32 and Intel 64 architecture
  - Supports C, C++, Fortran programming languages
    - `intel/18.0.3.222`

Using Compilers on HPCC

- **Load Required Modules:**
  - For Intel Compilers:
    - `$ module load intel/18.0.3.222`
  - For GNU Compilers:
    - `$ module load gnu/5.4.0`
    - `$ module load gnu7/7.3.0`

GNU Compilers:	• **gcc** -> C • **g++** -> C++ • **gfortran** -> Fortran
Intel Compilers:	• **icc** -> C • **icpc** -> C++ • **ifort -> Fortran**

Questions?

Questions/Suggestions/Comments are always welcome!

Write me: yong.chen@ttu.edu
Call me: 806-834-0284
See me: ENGCTR 315

If you write me an email for this class, please start the email subject with [CS4379] or [CS5379].