

Beginner's Introduction to Computing at CARC

Matthew Fricke

Version 0.1

Goals

- 1) Basic Linux Literacy
- 2) Ability to run programs on CARC compute nodes

I hope to spend about an hour on each with a 15 minute break.

Outline

- High Performance Computing Overview
- Logging in
- The BASH Shell and Scripts
- The Slurm Job Scheduler
- Storage at CARC
- Transferring data to and from CARC
- Accessing software and the module system
- Parallelization

High Performance Computing

- What is high performance computing?
 - Really just means something that is a lot more powerful than your desktop or laptop.
 - Hardware:
 - That might mean more and faster processors to do the calculations more quickly (eg 400 CPUs instead of 4)
 - More RAM so you can work on bigger problems (3,000 GB instead of 8)
 - Bigger file systems so you can process larger datasets
 - More and bigger GPUs to accelerate your computations (12 GPUs at a time instead of 1)
 - People:
 - Someone else to manage the systems and keep them running and secure
 - Someone to answer your questions and help with problems

Logging into Wheeler



First login to the Linux **workstation** in front of you.

Use your CARC username and password.

Keven, Tannor, and Jose can help you login if you have trouble.

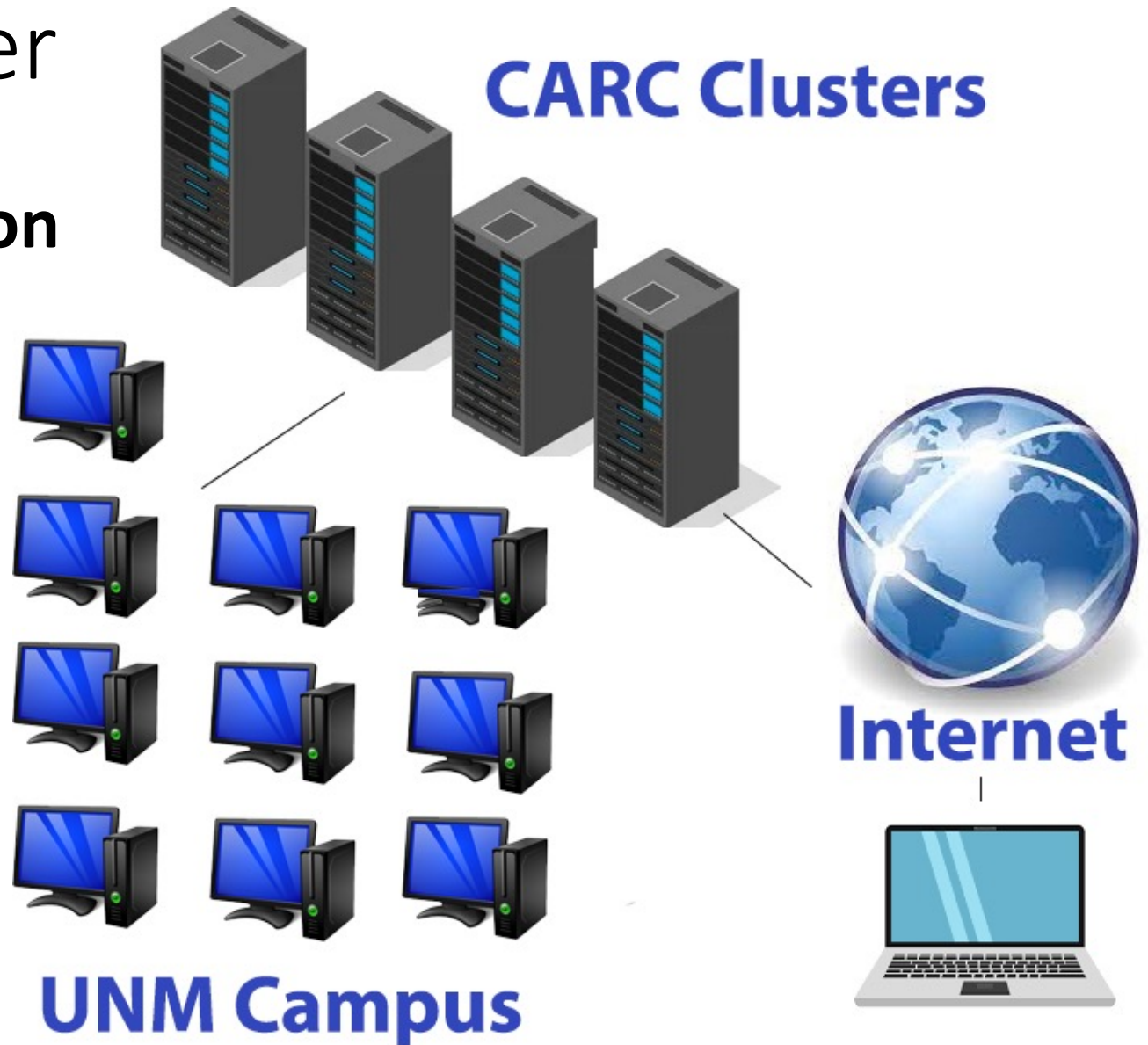
This is an “important step” so don’t let me move on until you have logged in

Logging into Wheeler

First login to the **workstation**
in front of you.

You will always login to
CARC cluster remotely.

These clusters don't even
have monitors.



Logging into Wheeler

We are going to use a program called **secure shell**.

Secure shell (ssh) is now built into every major operating system (Windows, OSX, and Linux).

You don't need third party programs like putty anymore.

Logging into Wheeler



```
ssh mfricke@wheeler.alliance.unm.edu
```

Should prompt you for a password...

Don't let me move on until you are able to login.

Logging into Wheeler

```
Matthew — ssh wheeler — 82x27
last login: Tue Jun 14 14:47:24 2022 from fricke.co.uk
-----
Welcome to Wheeler

Be sure to review the "Acceptable Use" guidelines posted on the CARC website

For assistance using this system email help@carc.unm.edu.

Tutorial videos can be accessed through the CARC website: Go to
http://carc.unm.edu, select the "New Users" menu and then click
"Introduction to Computing at CARC".

Warning: By default home directories are world readable. Use the chmod command
to restrict access.

Don't forget to acknowledge CARC in publications, dissertations, theses and
presentations that use CARC computational resources:

"We would like to thank the UNM Center for Advanced Research Computing,
supported in part by the National Science Foundation, for providing the
research computing resources used in this work."

Please send citations to publications@carc.unm.edu.
-----
Starting SSH Key Agent...
agent pid 19486
fricke@wheeler:~ $
```

Please enter the following command



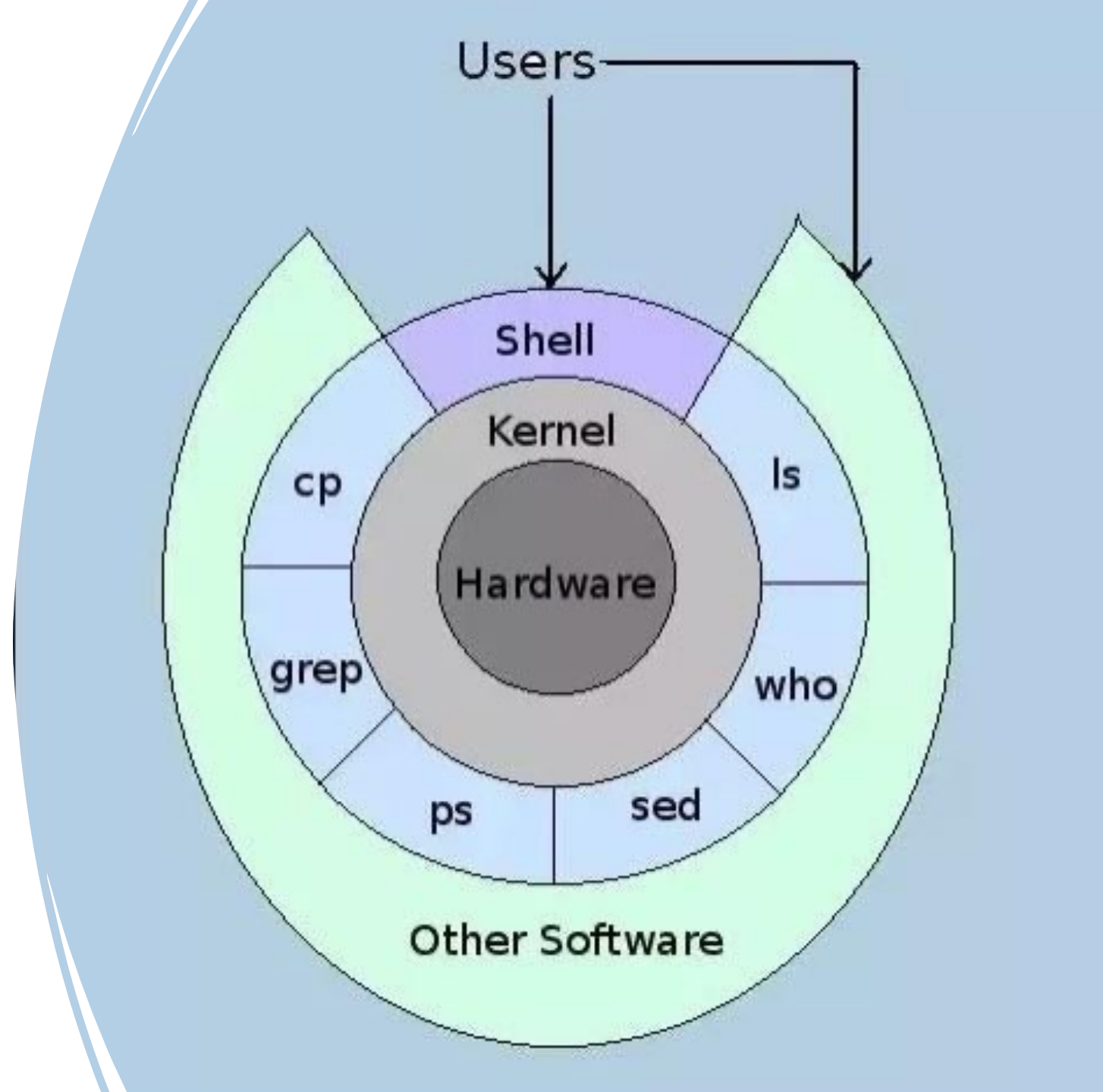
```
cp -r /projects/shared/workshops/beginner/mystuff ~/
```

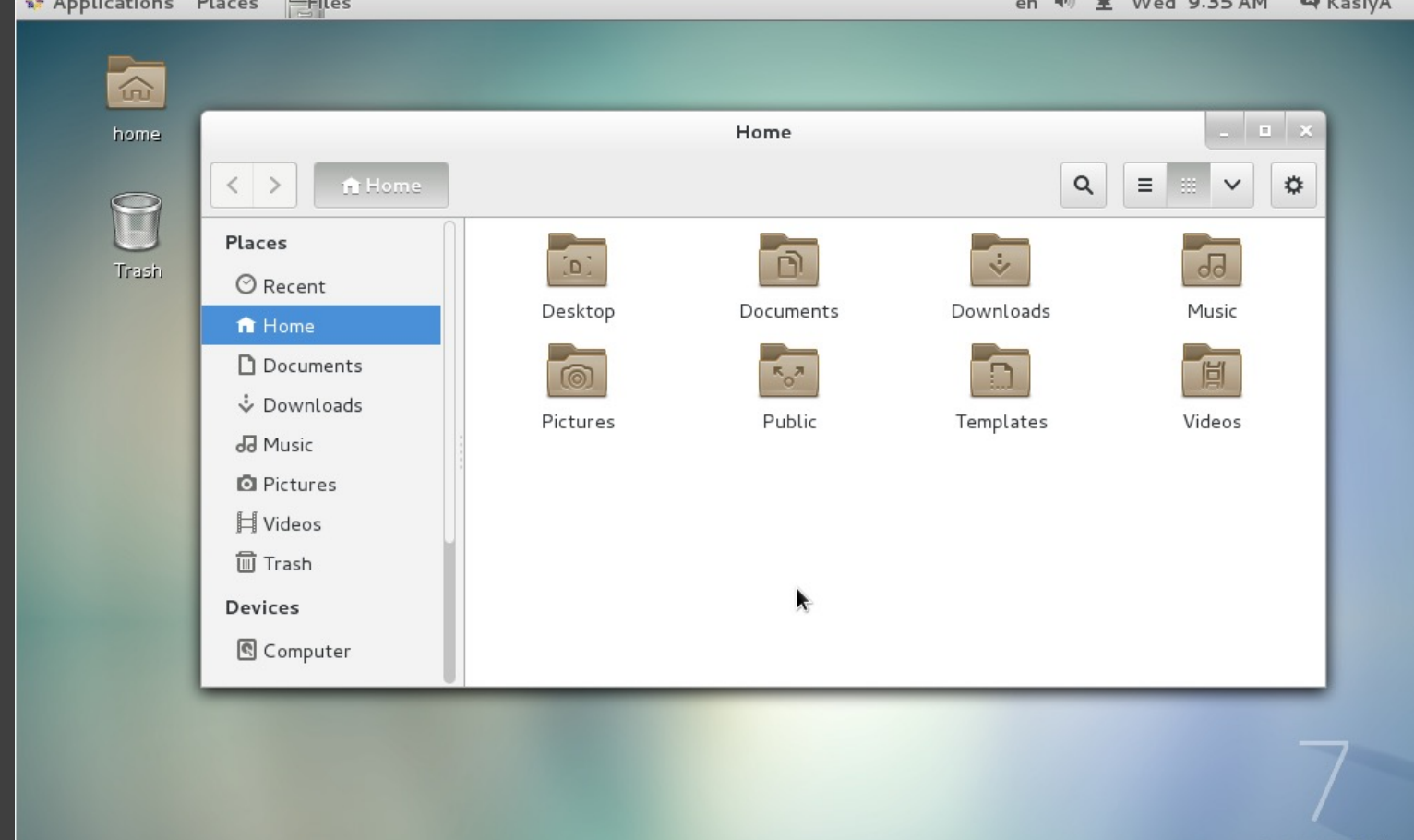
We will come help you if you have any trouble.

(Later I will go over what this command does)

Linux and the BASH Shell

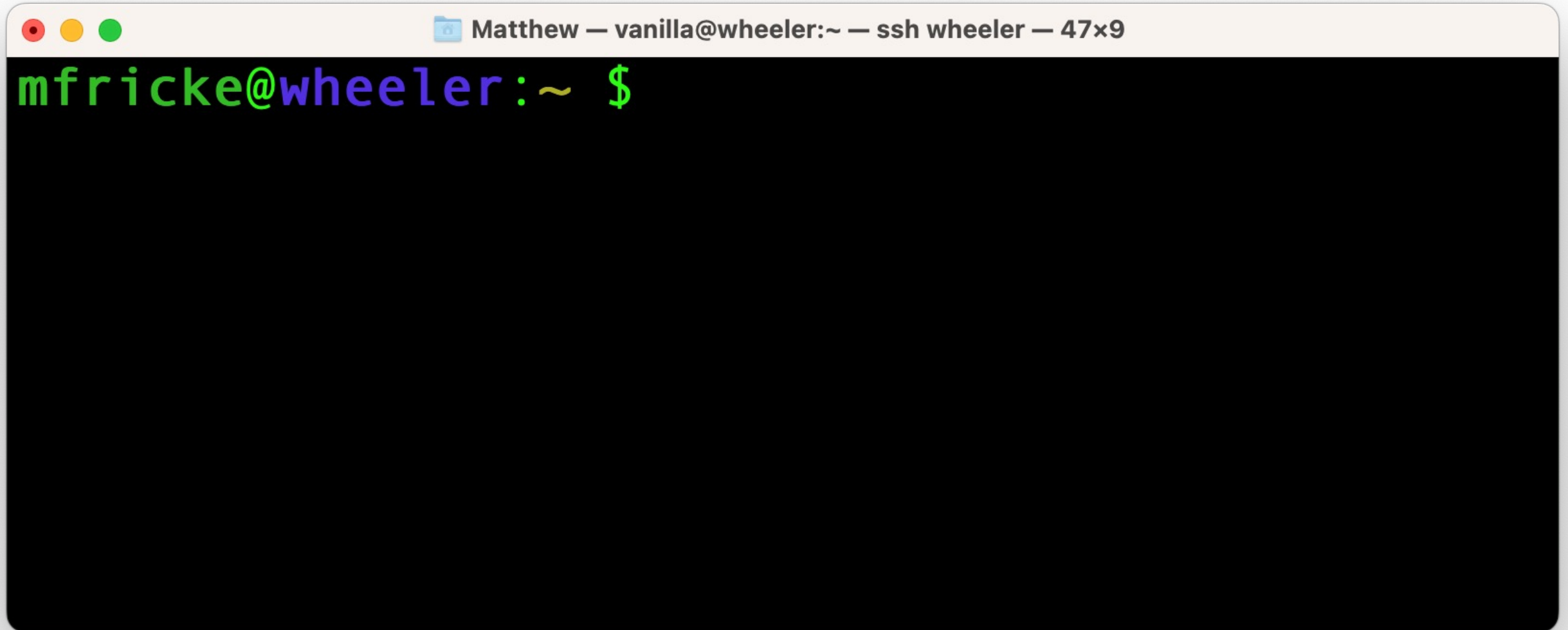
- The Kernel manages access to the hardware in a computer.
- An Operating System (OS) is the Kernel plus useful programs provided by the OS.
- The “shell” is the outermost layer of the OS.
- It is where the user interacts with the OS.





Graphical Shells (GUIs)

Logging into Wheeler





**YOU ARE AT THE
RIGHT PLACE**

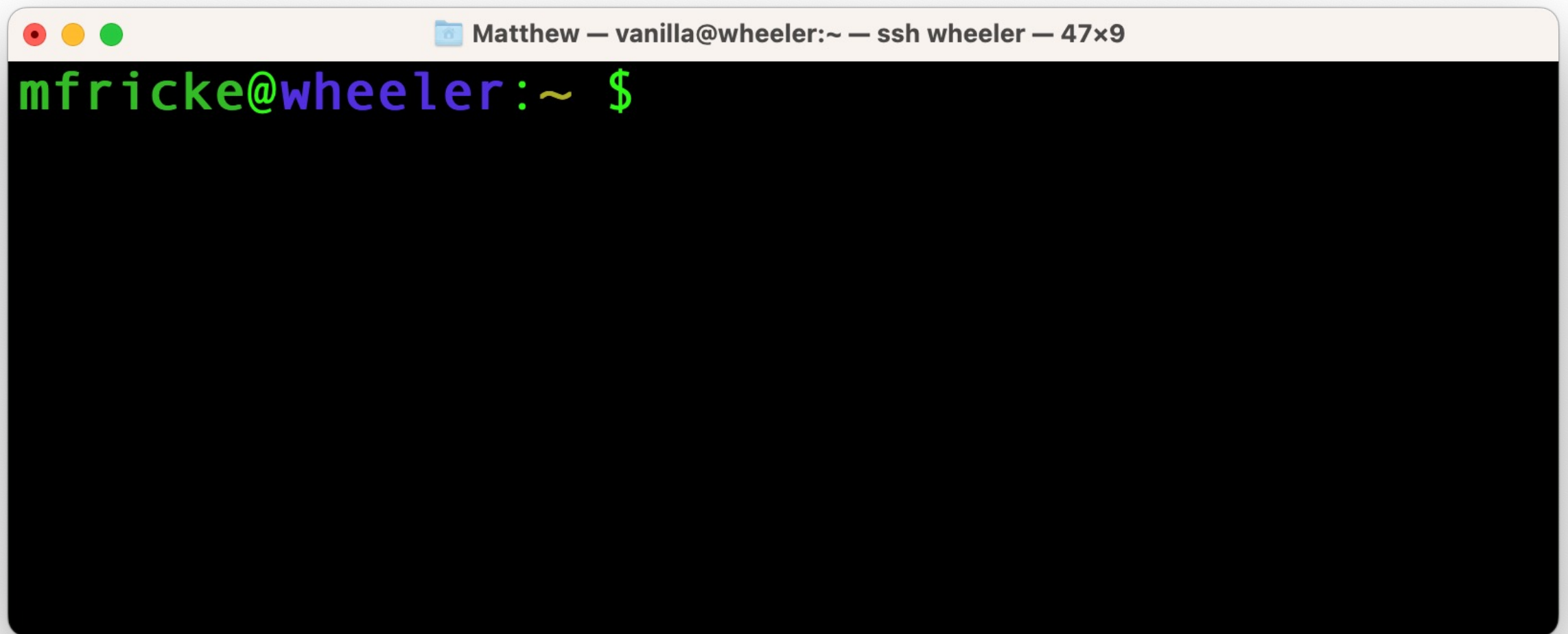
Linux and the BASH Shell

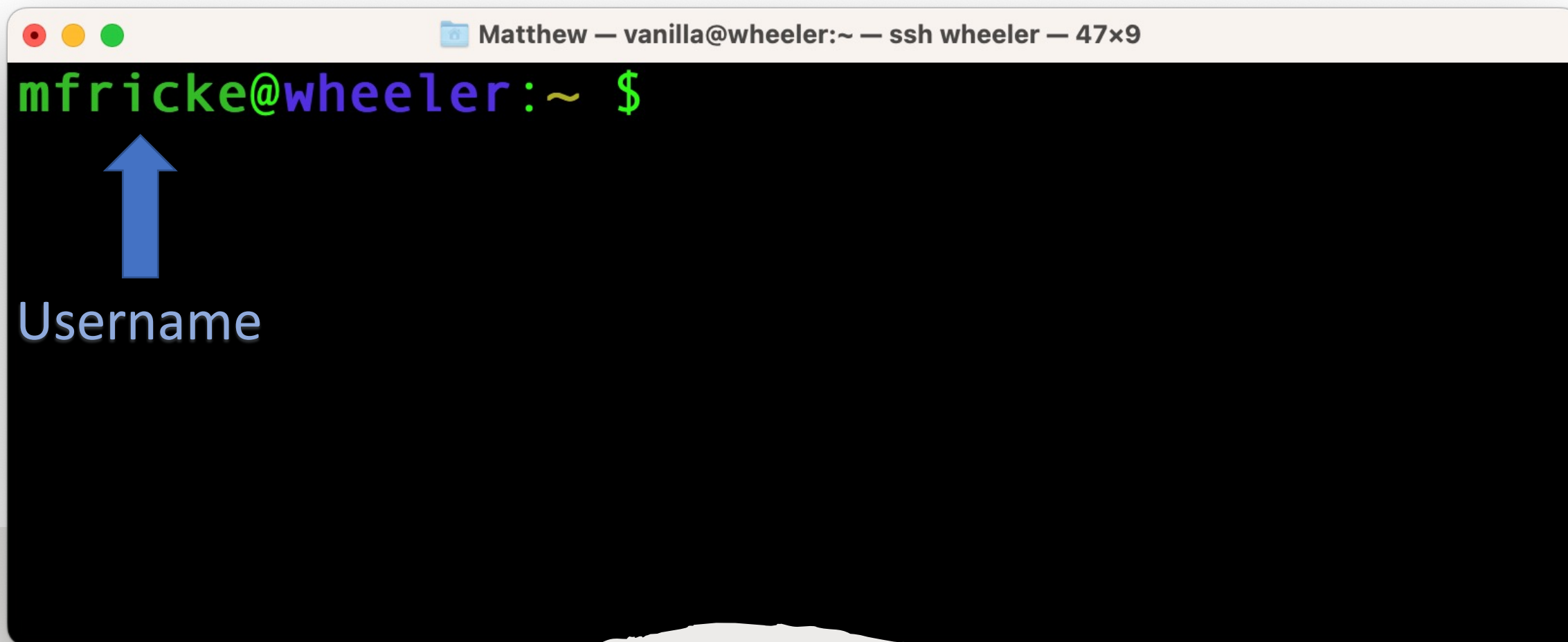
The word "LINUX" is rendered in a stylized, blocky font using only vertical and horizontal lines, resembling a digital or ASCII art style. Each letter is composed of multiple parallel lines, giving it a three-dimensional or shadowed appearance. The letters are white and stand out against a solid black background.

WHERE THERE IS A SHELL, THERE IS A WAY!

The Borne-Again Shell (BASH)

Written in 1976 by Stephen Bourne for UNIX version 7.





A terminal window with a title bar that reads "Matthew — vanilla@wheeler:~ — ssh wheeler — 47x9". The terminal content shows a BASH prompt "mfricke@wheeler:~ \$" where "mfricke" is green, "@wheeler" is blue, ":", "~" are yellow, and "\$" is green. A blue arrow points from the word "Username" below to the "mfricke" part of the prompt.

```
Matthew — vanilla@wheeler:~ — ssh wheeler — 47x9  
mfricke@wheeler:~ $  
↑  
Username
```

Understanding the BASH prompt...

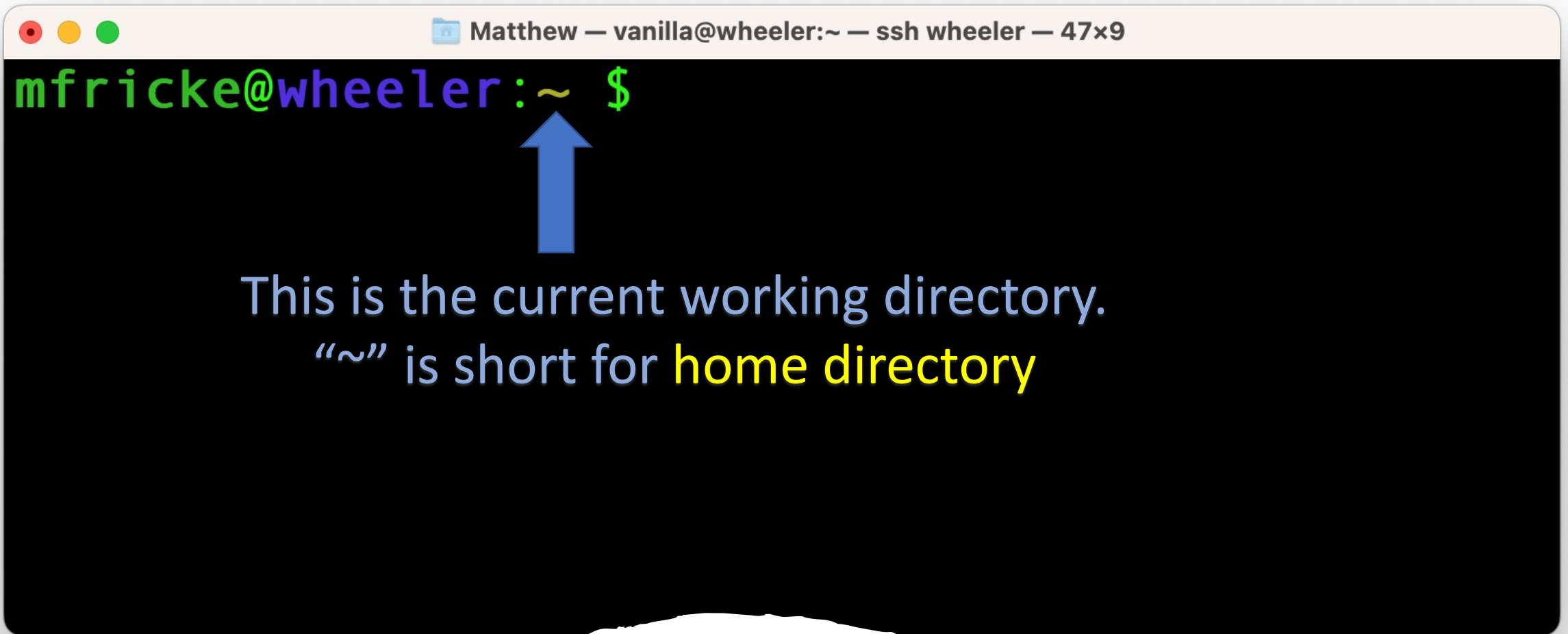


A terminal window titled "Matthew — vanilla@wheeler:~ — ssh wheeler — 47x9". The prompt is "mfricke@wheeler:~ \$". Two blue arrows point from the labels "Username" and "Hostname" below to the parts of the prompt. The arrow from "Username" points to "mfricke", and the arrow from "Hostname" points to "wheeler".

```
mfricke@wheeler:~ $
```

Username Hostname

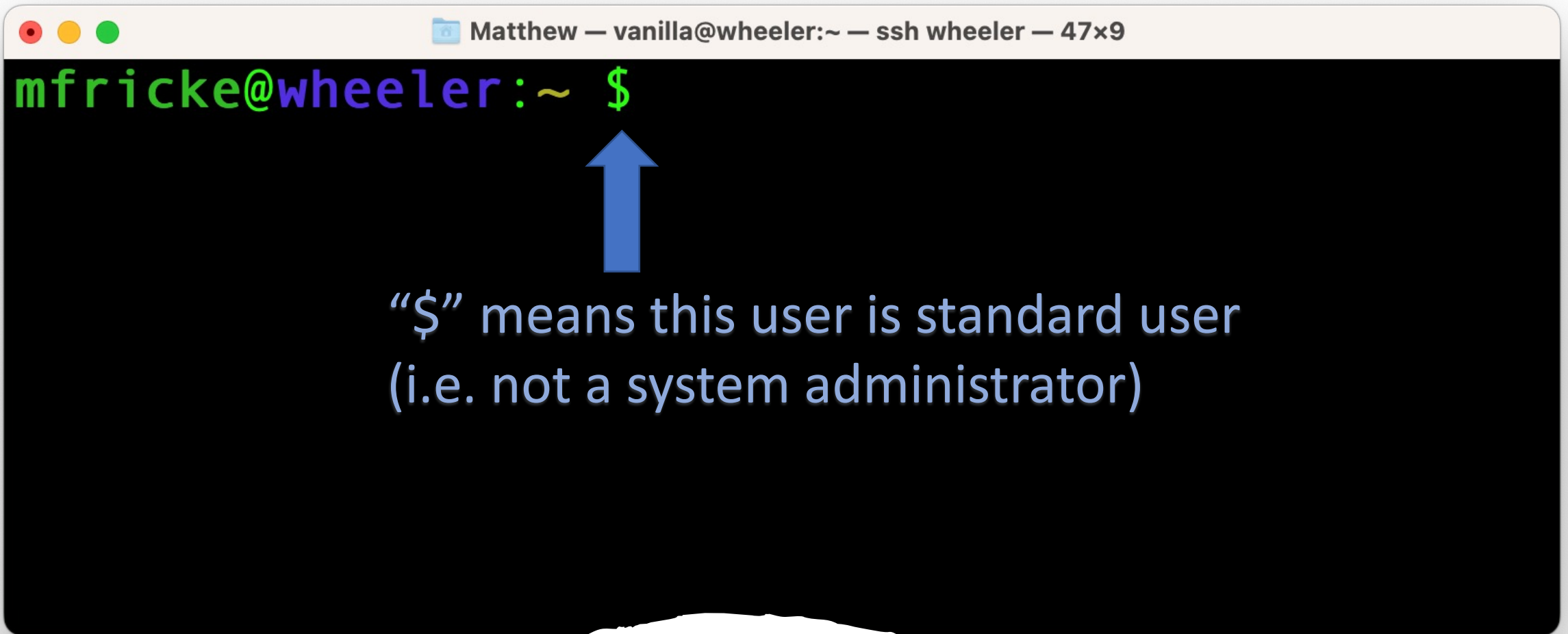
Understanding the BASH prompt...

A terminal window with a title bar that reads "Matthew — vanilla@wheeler:~ — ssh wheeler — 47x9". The terminal content shows the prompt "mfricke@wheeler:~ \$" in green and blue. A blue arrow points from the tilde character (~) to the text "This is the current working directory. '~' is short for home directory" which is displayed in light blue and yellow. The terminal background is black.

```
mfricke@wheeler:~ $
```

This is the current working directory.
“~” is short for **home directory**

Understanding the BASH prompt...

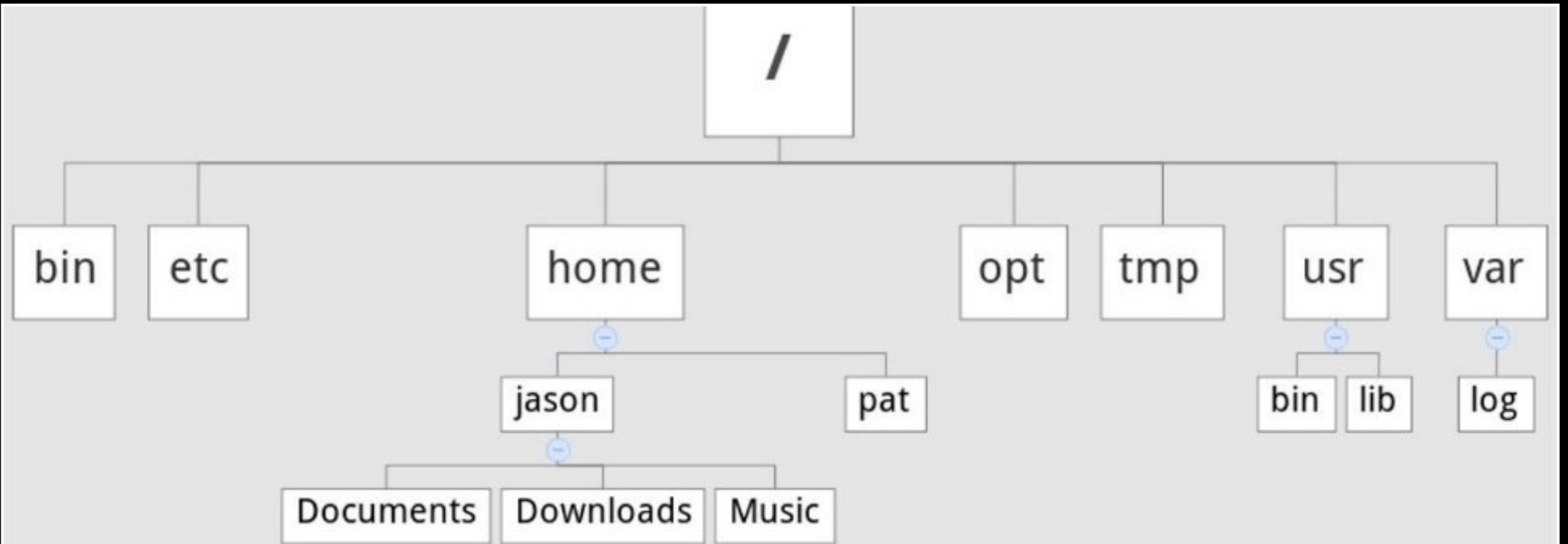


A terminal window with a title bar that reads "Matthew — vanilla@wheeler:~ — ssh wheeler — 47x9". The terminal content shows a BASH prompt "mfricke@wheeler:~ \$" where "mfricke@" is green, "wheeler:" is blue, "~" is yellow, and "\$" is green. A blue arrow points from the text below to the "\$" character. The text below the arrow reads: "\$" means this user is standard user (i.e. not a system administrator).

```
mfricke@wheeler:~ $
```

“\$” means this user is standard user
(i.e. not a system administrator)

Understanding the BASH prompt...



Example Filesystem Tree

```
[vanilla@wheeler ~]$ pwd  
/users/vanilla  
[vanilla@wheeler ~]$
```

Figuring out where you are in the
filesystem...

```
[vanilla@wheeler ~]$ ls  
mystuff  wheeler-scratch  
[vanilla@wheeler ~]$
```

Figuring out where you are in the
filesystem...

```
[vanilla@wheeler ~]$ tree
```

```
.
├── mystuff
│   ├── myfile1
│   └── myfile2
└── wheeler-scratch -> /wheeler/scratch/vanilla
```

```
2 directories, 2 files
```

```
[vanilla@wheeler ~]$
```

Figuring out where you are in
the filesystem...

```
[vanilla@wheeler ~]$ tree
```

```
.
├── mystuff
│   ├── myfile1
│   └── myfile2
└── wheeler-scratch -> /wheeler/scratch/vanilla
```

```
2 directories, 2 files
```

```
[vanilla@wheeler ~]$
```

Figuring out where you are in
the filesystem...

```
[vanilla@wheeler ~]$ tree
```



```
.  
├── mystuff  
│   ├── myfile1  
│   └── myfile2  
└── wheeler-scratch -> /wheeler/scratch/vanilla
```

This . means the current directory

```
2 directories, 2 files
```

```
[vanilla@wheeler ~]$
```

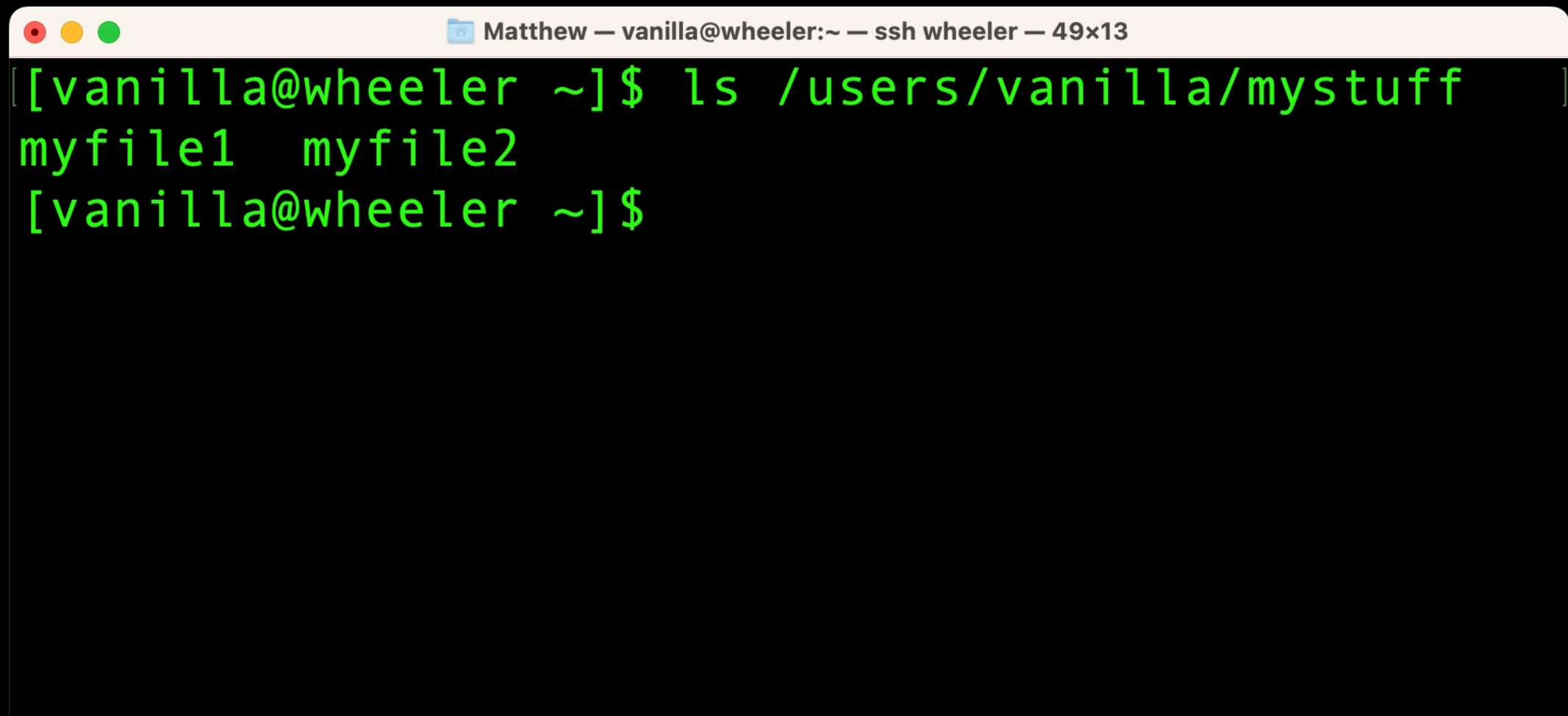
Figuring out where you are in
the filesystem...

“Absolute” paths vs “relative” paths

- A path is a list of directories and/or files. It is a path through the directory tree that tells one how to get somewhere in the filesystem.
- An absolute path tells one how to get to the destination from starting from the root of the filesystem. E.g “/users/vanilla/mystuff/”
- A relative path specifies how to get there *starting from the current working directory*. E.g vanilla/mystuff/

```
Matthew — vanilla@wheeler:~ — ssh wheeler — 49x13  
[vanilla@wheeler ~]$ ls mystuff/  
myfile1  myfile2  
[vanilla@wheeler ~]$
```

Figuring out where you going...

A terminal window with a title bar containing three colored circles (red, yellow, green) on the left and the text "Matthew — vanilla@wheeler:~ — ssh wheeler — 49x13" on the right. The terminal content shows a command prompt "[vanilla@wheeler ~]\$", followed by the command "ls /users/vanilla/mystuff", and then the output "myfile1 myfile2". The prompt "[vanilla@wheeler ~]\$" appears again on the next line.

```
[vanilla@wheeler ~]$ ls /users/vanilla/mystuff
myfile1  myfile2
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ ls ./mystuff/  
myfile1  myfile2  
[vanilla@wheeler ~]$ ls ~/mystuff/  
myfile1  myfile2  
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ ls -a
.          .modulesbeginenv
..         mystuff
.addressbook .oracle_jre_usage
.addressbook.lu .pinerc
.bashrc      .pki
.cache      .rhosts
.comsol     .shosts
.config     .spack
.flexlmrc   .ssh
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ ls -l
total 4
drwxr-xr-x 2 vanilla users 4096 Jun 14 22:05 mystuff
lrwxrwxrwx 1 vanilla users 24 Jun 14 21:20 wheeler-scratch ->
/wheeler/scratch/vanilla
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ ls -l mystuff/  
total 473704  
-rw-r--r-- 1 vanilla users 483165473 Jun 14 23:20 myfile1  
-rw-r--r-- 1 vanilla users          0 Jun 14 22:05 myfile2  
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ ls -lh mystuff/  
total 463M  
-rw-r--r-- 1 vanilla users 461M Jun 14 23:20 myfile1  
-rw-r--r-- 1 vanilla users    0 Jun 14 22:05 myfile2  
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ du -s
```

```
499704 .
```

```
[vanilla@wheeler ~]$ du -sh
```

```
488M .
```

```
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ df -h
```

Filesystem	Size	Used	Avail	Use%	Mounted on
devtmpfs	24G	0	24G	0%	/dev
tmpfs	24G	64K	24G	1%	/dev/shm
tmpfs	24G	968M	23G	5%	/run
tmpfs	24G	0	24G	0%	/sys/fs/cgroup
/dev/mapper/centos-root	930G	567G	363G	61%	/
/dev/sdc2	836G	72G	764G	9%	/tmp
/dev/md126p1	2.0G	333M	1.7G	17%	/boot
172.17.2.254:/mnt/wheeler-scratch	37T	28T	8.7T	77%	/wheeler/scratch
172.17.2.255:/mnt/wheeler-scratch2	37T	28T	9.0T	76%	/wheeler/scratch2
beegfs_nodev	110T	51T	60T	46%	/carc/scratch
chama:/home/homes	65T	36T	30T	55%	/users
chama:/home/carc_projects	65T	36T	30T	55%	/projects

Figuring out where you going...

```
[vanilla@wheeler ~]$ quota -s
Disk quotas for user vanilla (uid 659):
    Filesystem    space   quota   limit   grace   files   quota   limit   grace
chama:/home/homes
                488M    100G    200G           315    4295m    4295m
[vanilla@wheeler ~]$
```

Figuring out where you going...

```
[vanilla@wheeler ~]$ stat mystuff/myfile1
  File: 'mystuff/myfile1'
  Size: 483165473  Blocks: 947408      IO Block: 65536   regular file
Device: 28h/40d Inode: 9232782834205560540  Links: 1
Access: (0644/-rw-r--r--)  Uid: (  659/  vanilla)   Gid: (  100/   users)
Access: 2022-06-14 22:05:27.503289000 -0600
Modify: 2022-06-14 23:20:26.945918000 -0600
Change: 2022-06-14 23:20:48.754917000 -0600
 Birth: -
```

Figuring out what you've got...

```
[vanilla@wheeler ~]$ find -name myfile2  
./mystuff/myfile2
```

```
[vanilla@wheeler ~]$ find -name "myfile*"  
./mystuff/myfile1  
./mystuff/myfile2  
./mystuff/myfile3  
./mystuff/myfile0
```



Wildcard

Figuring out what you've got...

```
[vanilla@wheeler ~]$ cd mystuff/  
[vanilla@wheeler ~/mystuff]$
```

Use the tab key to autocomplete

Going somewhere new...

Now it is your turn...



- For this path:
`/projects/shared/workshops/beginner/vecadd`

- What are the names of the files in that directory?
- When were they last modified?
- How large are the files?

You can find this information with the `ls` command.

Now it is your turn...



- For this path:
`/projects/shared/workshops/beginner/vecadd`

Now “cd” into that directory using <tab> autocomplete.

- Now you know how to find your way around filesystems using bash
- Let's see how to modify the filesystem.
- In bash to move a file we use the `mv` command.
- To copy a file it is `cp`.
- To copy files from CARC to a personal computer use `scp` or `rsync`.

```
[vanilla@wheeler beginner]$ pwd  
/projects/shared/workshops/beginner  
[vanilla@wheeler beginner]$ cd ~  
[vanilla@wheeler ~]$ pwd  
/users/vanilla  
[vanilla@wheeler ~]$
```

First return to your home
directory...

```
[vanilla@wheeler ~]$ cd mystuff  
[vanilla@wheeler ~/mystuff]$ mv myfile1 myfile0  
[vanilla@wheeler ~/mystuff]$ ls  
myfile0  myfile2  myfile3  
[vanilla@wheeler ~/mystuff]
```

Modifying the filesystem...
moving a file.

```
[vanilla@wheeler ~/mystuff]$ cp myfile0 myfile1  
[vanilla@wheeler ~/mystuff]$
```



Source



Destination

```
[vanilla@wheeler ~/mystuff]$ ls  
myfile0  myfile1  myfile2  myfile3  
[vanilla@wheeler ~/mystuff]$
```

Modifying the filesystem...
copying a file.

```
[vanilla@wheeler ~/mystuff]$ mkdir mynewdir  
[vanilla@wheeler ~/mystuff]$
```



New directory name

Modifying the filesystem...
create a new directory.

```
[vanilla@wheeler ~]$ cp -r mystuff mystuff2  
[vanilla@wheeler ~]$
```



Source



Destination

```
[vanilla@wheeler ~]$ ls  
mystuff    mystuff2    wheeler-scratch
```

Copying a whole directory tree...

```
[vanilla@wheeler ~]$ exit
```

```
Lycaon:~ matthew$ scp vanilla@wheeler.alliance.unm.edu:~/mystuff/myfile3 Desktop/
```



Source



Destination

```
(vanilla@wheeler.alliance.unm.edu) Password:
```

```
myfile3          100%  40    2.0KB/s   00:00
```

Copying data to a personal
computer from CARC...

```
Lycaon:~ matthew$ scp -r vanilla@wheeler.alliance.unm.edu:~/mystuff Desktop/
```



Source



Destination

```
(vanilla@wheeler.alliance.unm.edu) Password:
```

myfile1	100%	1024KB	6.5MB/s	00:00
myfile2	100%	2048KB	382.5KB/s	00:05
myfile3	100%	40	3.2KB/s	00:00
myfile0	100%	1024KB	8.8MB/s	00:00

Copying data to a personal
computer from CARC...

```
Lycaon:~ matthew$ scp -r Desktop/mystuff vanilla@wheeler.alliance.unm.edu:~/
```



Source



Destination

```
(vanilla@wheeler.alliance.unm.edu) Password:
```

myfile1	100%	1024KB	591.5KB/s	00:01
myfile0	100%	1024KB	2.0MB/s	00:00
myfile2	100%	2048KB	2.1MB/s	00:00
myfile3	100%	40	2.1KB/s	00:00

To copy from a personal
computer to CARC...

```
ssh vanilla@wheeler.alliance.unm.edu
```

Log back into wheeler...

```
[vanilla@wheeler ~]$ file mystuff/myfile0  
mystuff/myfile0: data
```

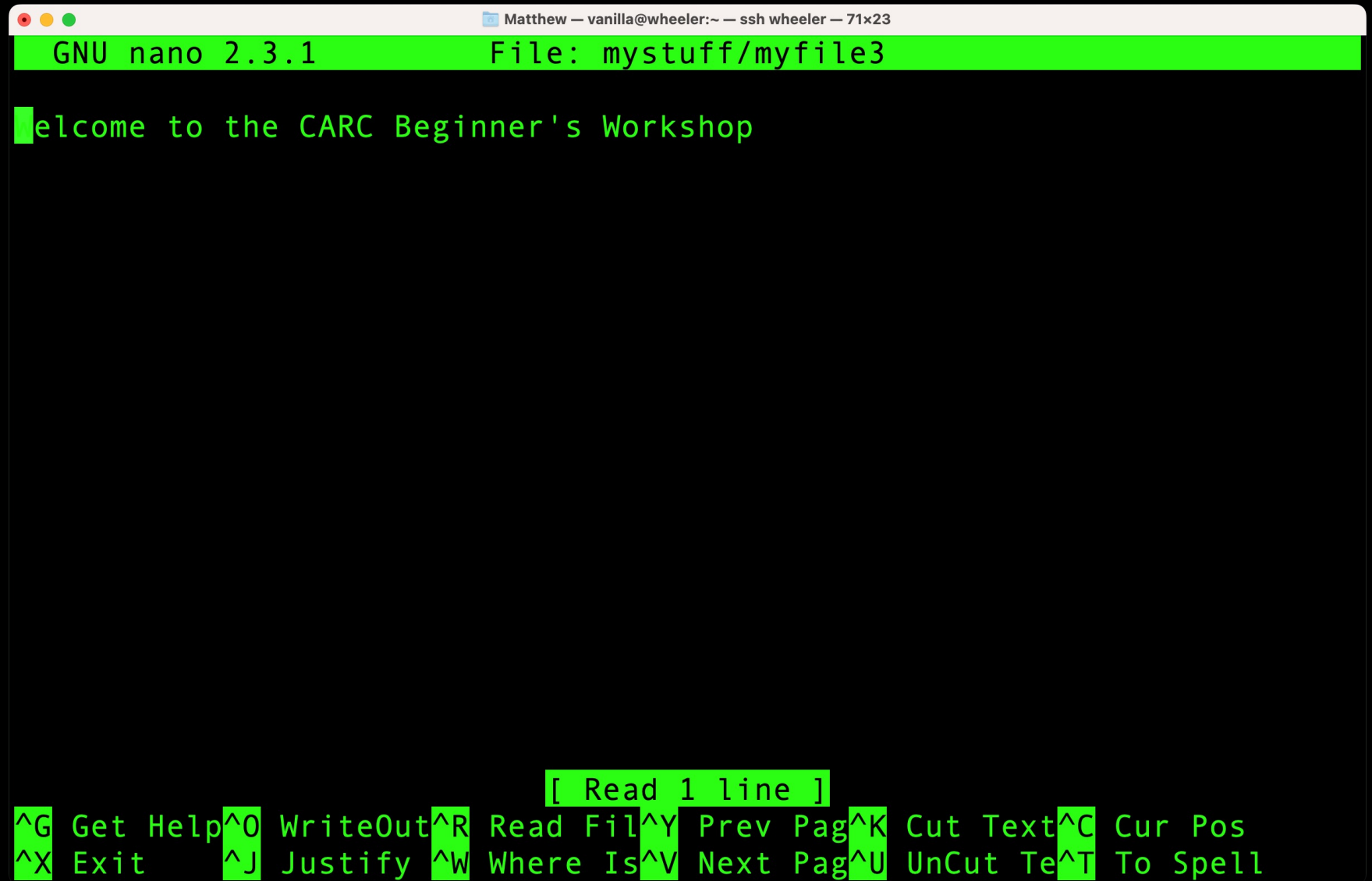
```
[vanilla@wheeler ~]$ file mystuff/myfile3  
mystuff/myfile3: ASCII text
```

Figuring out file types ...

```
[vanilla@wheeler ~]$ cat mystuff/myfile3  
Welcome to the CARC Beginner's Workshop
```

Text files ...

```
[vanilla@wheeler ~]$ nano mystuff/myfile3
```



```
Matthew — vanilla@wheeler:~ — ssh wheeler — 71x23
GNU nano 2.3.1 File: mystuff/myfile3

Welcome to the CARC Beginner's Workshop

[ Read 1 line ]
^G Get Help ^O WriteOut ^R Read Fil ^Y Prev Pag ^K Cut Text ^C Cur Pos
^X Exit ^J Justify ^W Where Is ^V Next Pag ^U UnCut Te ^T To Spell
```

```
[vanilla@wheeler ~]$ date  
Wed Jun 15 03:08:15 MDT 2022
```

```
[vanilla@wheeler ~]$ echo Hello from $HOSTNAME  
Hello from wheeler
```

```
[vanilla@wheeler ~]$ hostname  
wheeler
```

Programs we will use as
examples...

File Edit Options Buffers Tools Sh-Script Help

```
#!/bin/bash
```

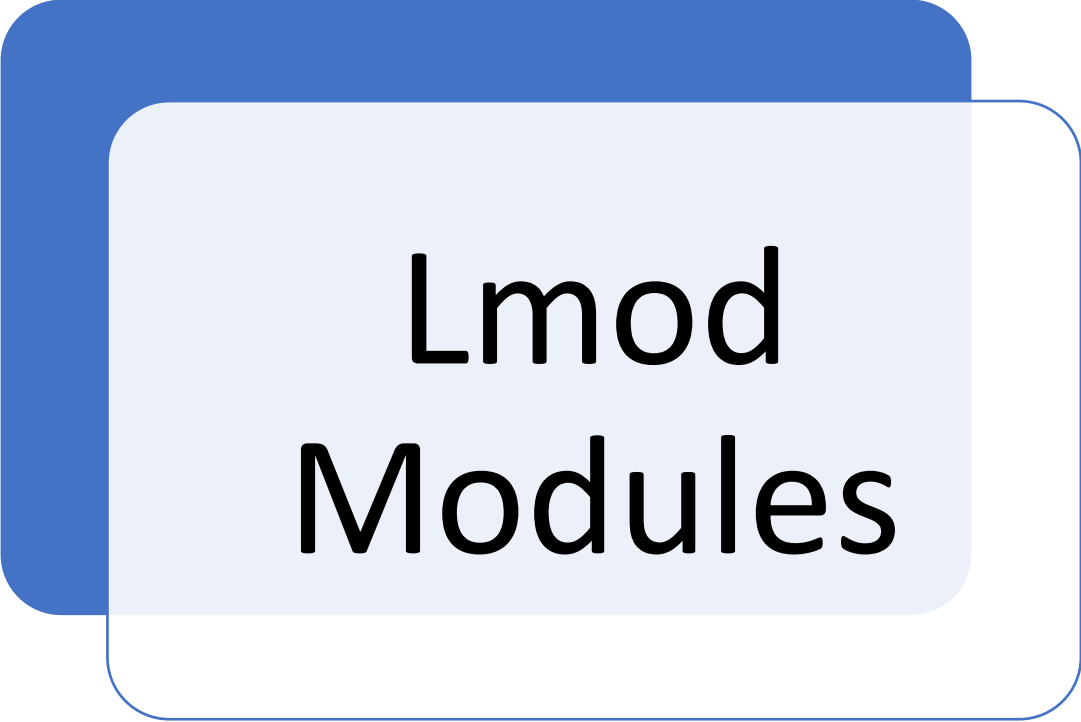
```
echo Hello from $HOSTNAME
```

```
date
```

Shell Scripts

15 Minute Break

Software Access



Lmod
Modules

The diagram consists of a dark blue rounded rectangle with a light blue rounded rectangle nested inside it. The text "Lmod Modules" is centered within the light blue rectangle.



Conda

The diagram consists of a dark blue rounded rectangle with a light blue rounded rectangle nested inside it. The text "Conda" is centered within the light blue rectangle.

```
[vanilla@wheeler ~]$ module spider matlab
```

```
-----
```

```
-
```

```
  matlab:
```

```
-----
```

```
-
```

```
  Versions:
```

```
    matlab/R2017a
```

```
    matlab/R2018b
```

```
    matlab/R2019a
```

```
    matlab/R2020a
```

```
    matlab/R2021a
```

Getting access to software...

```
[vanilla@wheeler ~]$ module load matlab/R2021a
Lmod has detected the following error: Matlab may only be run on compute
nodes. wheeler is not a compute node. Exiting...
While processing the following module(s):
  Module fullname  Module Filename
  -----
matlab/R2021a      /opt/local/modules/matlab/R2021a.lua
```

Getting access to software...

```
[vanilla@wheeler ~]$ module load matlab/R2021a
Lmod has detected the following error: Matlab may only be run on compute
nodes. wheeler is not a compute node. Exiting...
While processing the following module(s):
  Module fullname  Module Filename
  -----
matlab/R2021a      /opt/local/modules/matlab/R2021a.lua
```

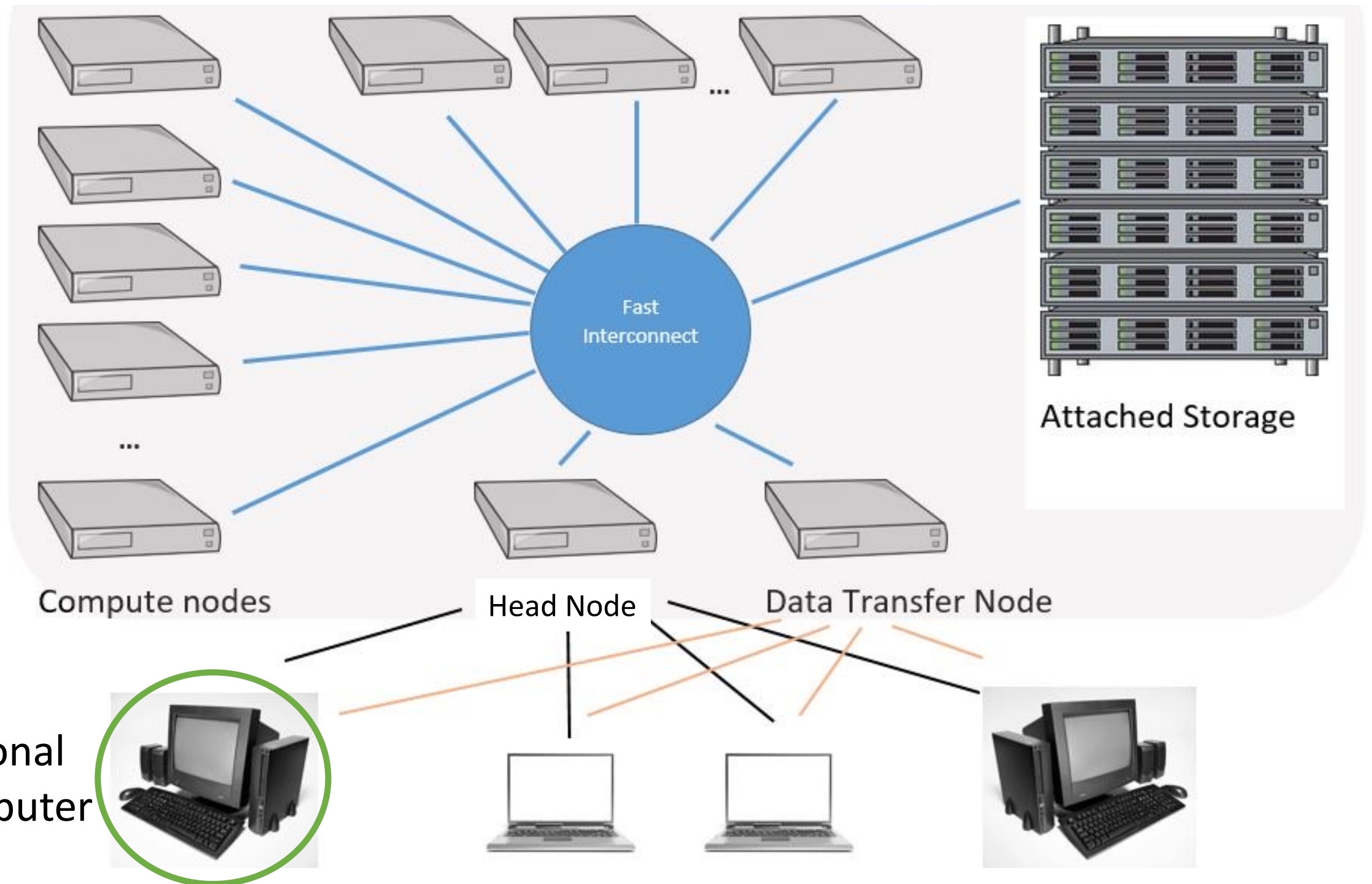
What is a compute node?

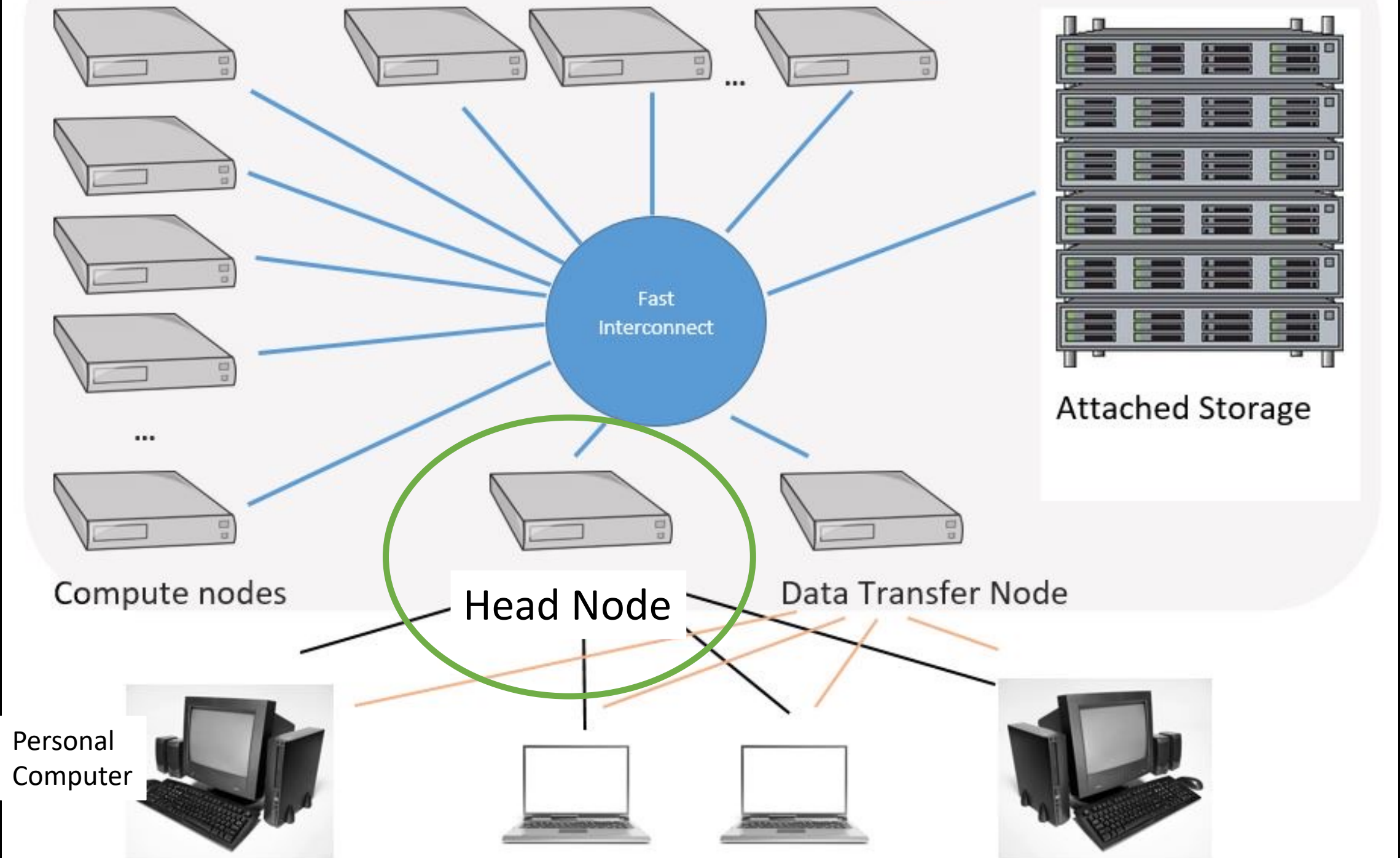
Getting access to software...

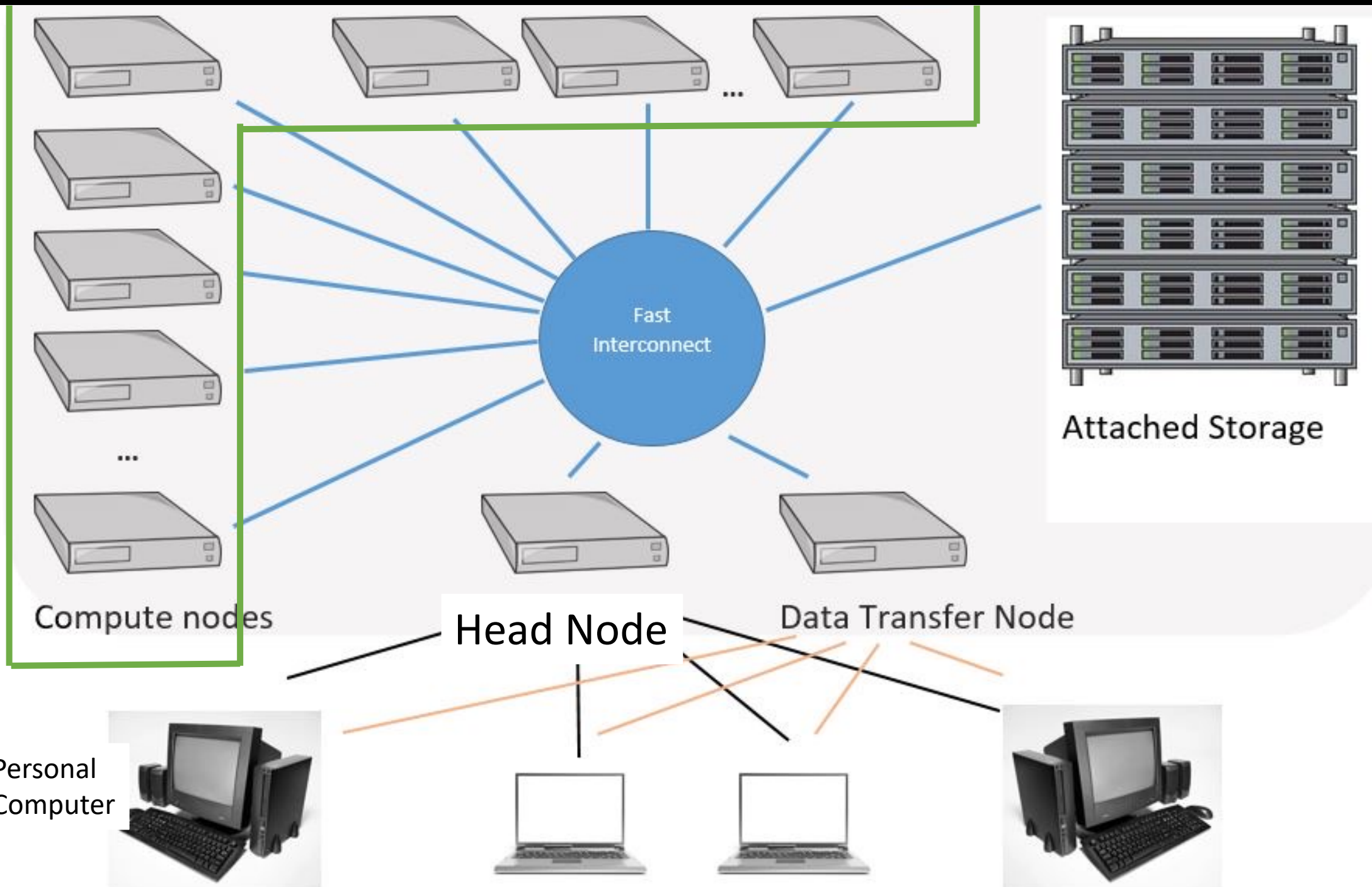
HPC Cluster



Personal
Computer









Never run computations on the head node

Always use compute nodes

```
[vanilla@wheeler ~]$ qgrok
```

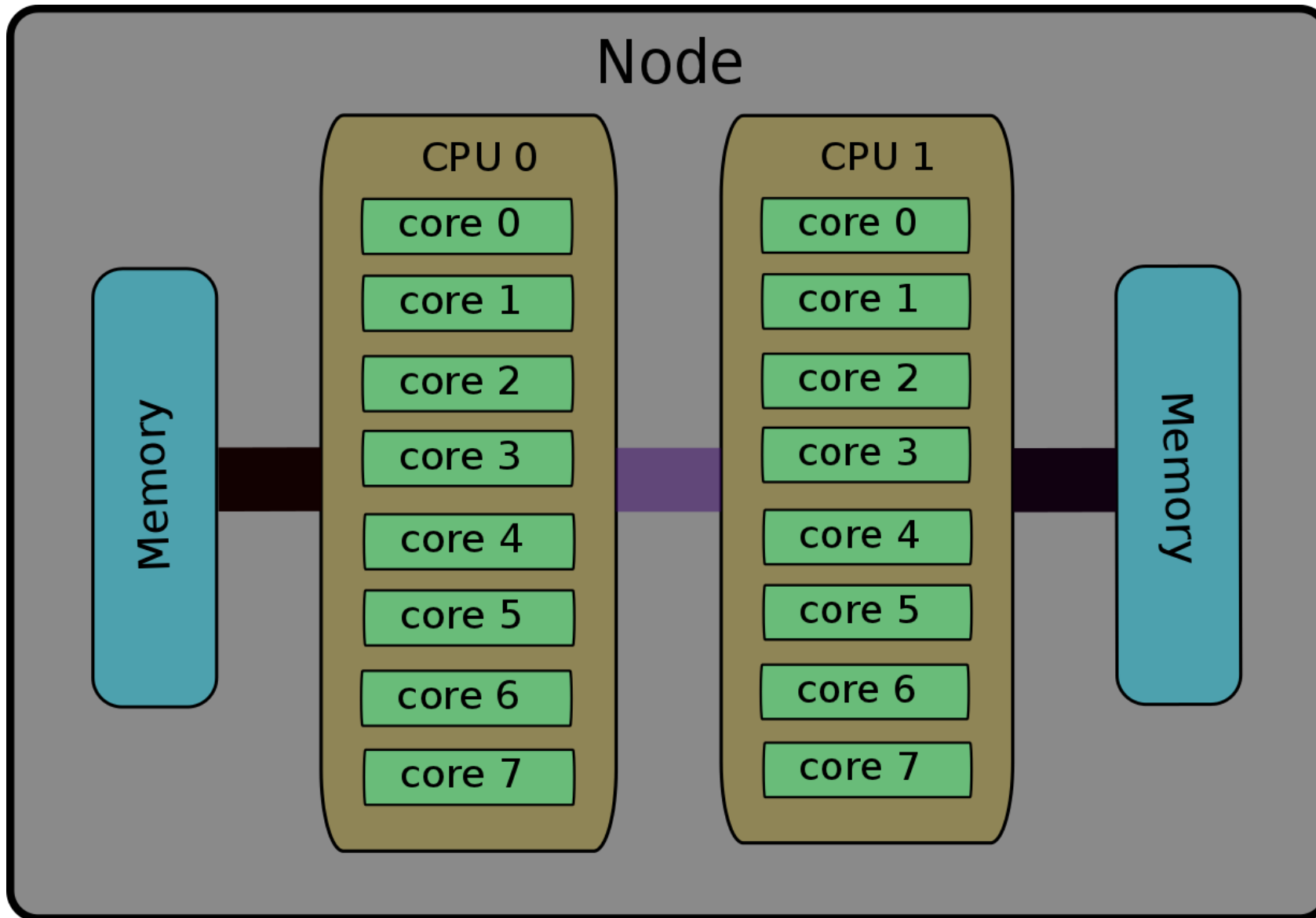
queues	free	busy	offline	jobs	nodes	CPUs
-----	-----	-----	-----	-----	-----	-----
normal	0	299	1	97	300	2400
debug	4	0	0	0	4	32
totals:	4	299	1	97	304	2432

Compute nodes and partitions...

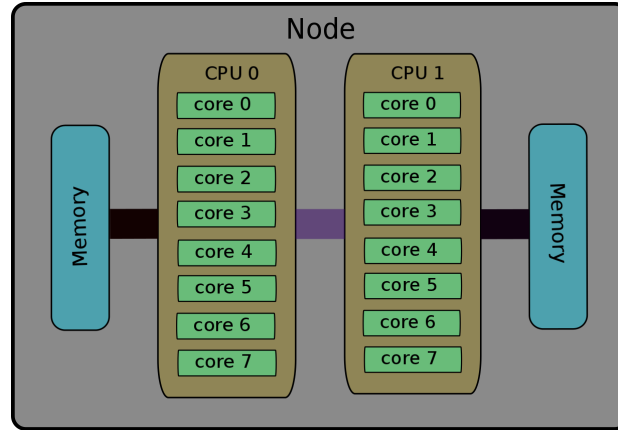
```
qmfricke@hopper:~ $ qgrok
```

queues	free	busy	offline	jobs	nodes	CPUs
-----	-----	-----	-----	-----	-----	-----
general	12	0	0	0	12	384
condo	29	1	7	0	37	1184
bugs	2	0	0	0	2	64
pcnc	2	0	0	0	2	64
pathogen	0	1	0	1	1	32
tc	7	0	3	0	10	320
gold	2	0	0	0	2	64
fishgen	1	0	0	0	1	32
neuro-hsc	13	0	1	0	14	448
cup-ecs	2	0	0	0	2	64
tid	0	0	1	0	1	32
biocomp	0	0	1	0	1	32
chakra	0	0	1	0	1	32
totals:	70	2	14	1	86	2752

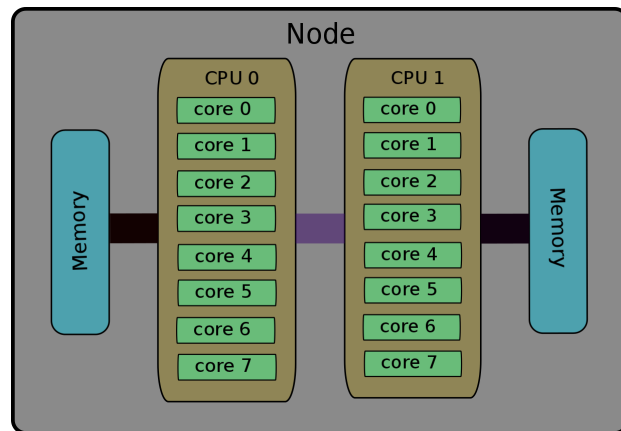
Compute nodes and partitions...



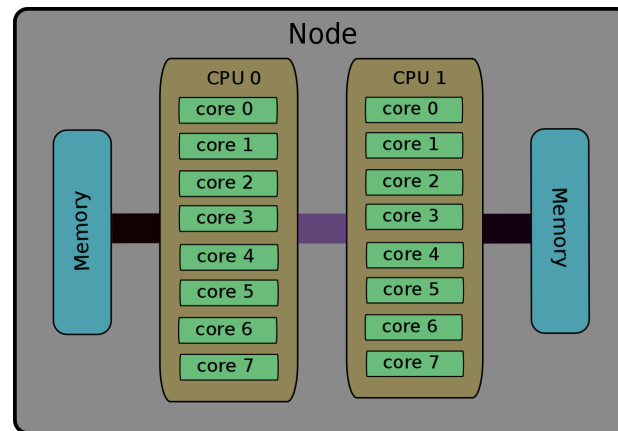
Head Node (wheeler)



Compute Nodes

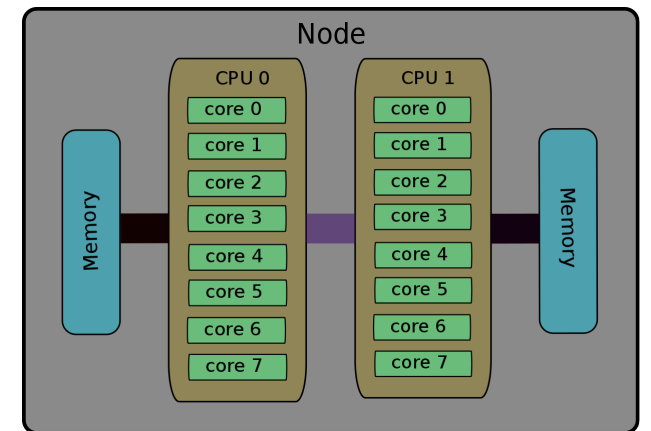


wheeler001



wheeler002

...



wheeler304

```
[vanilla@wheeler ~]$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                8
On-line CPU(s) list:   0-7
Thread(s) per core:    1
Core(s) per socket:    4
Socket(s):             2
NUMA node(s):         2
Vendor ID:             GenuineIntel
CPU family:            6
Model:                 26
Model name:            Intel(R) Xeon(R) CPU X5550  @ 2.67GHz
```

Wheeler has 8 cores per node....

```
mfricke@hopper:~ $ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                64
On-line CPU(s) list:   0-63
Thread(s) per core:    2
Core(s) per socket:    16
Socket(s):             2
NUMA node(s):         2
Vendor ID:             GenuineIntel
CPU family:            6
Model:                85
Model name:            Intel(R) Xeon(R) Gold 6226R CPU @ 2.90GHz
```

Hopper has 32 real cores (64
virtual cores) per node....

Architecture

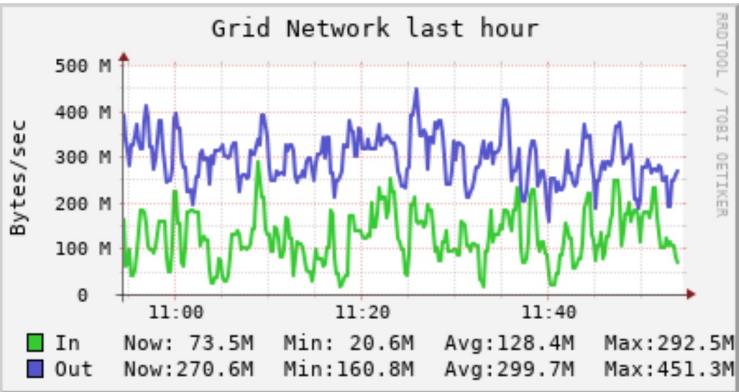
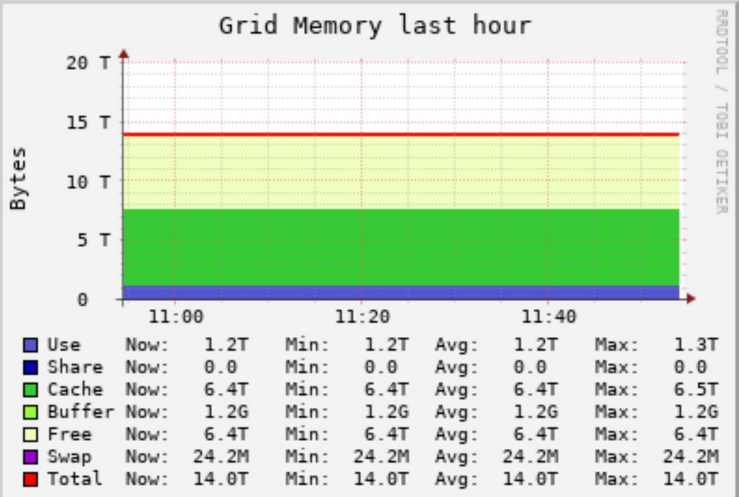
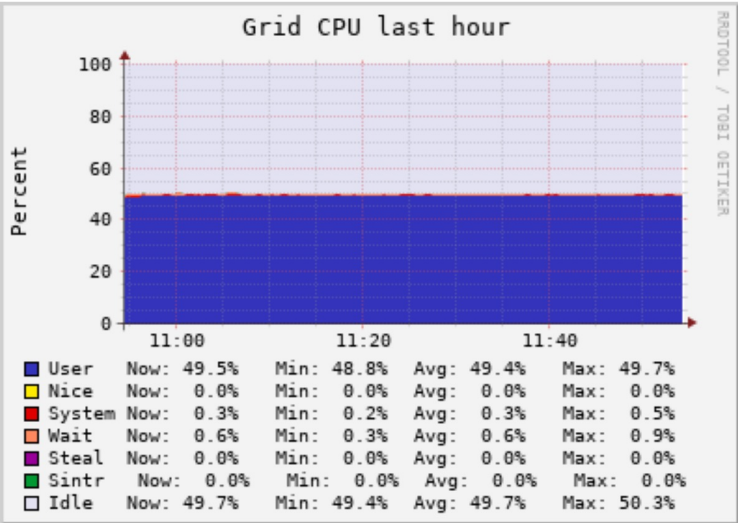
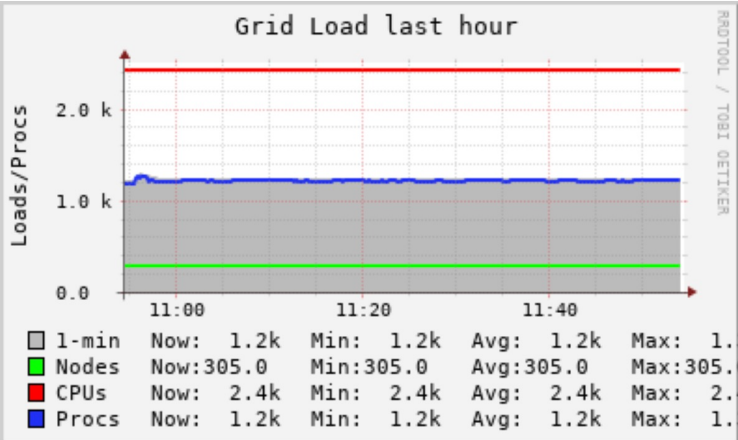
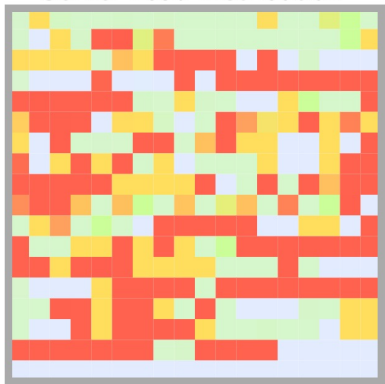
Wheeler Cluster Grid > Wheeler Cluster >

Overview of @ 2022-03-03 18:54

CPU's Total: 2440
Hosts up: 305
Hosts down: 0

Current Load Avg (15, 5, 1m):
51%, 51%, 51%
Avg Utilization (last hour):
51%

Server Load Distribution





Technology, IT etc.

SLURM

means

Simple Linux Utility for Resource
Management

by acronymsandslang.com



VOTED **#1** SOFT DRINK OF THE 31ST CENTURY!



SLURP'S MCKEATHE

```

[vanilla@wheeler ~]$ squeue
      JOBID PARTITION      NAME      USER  ST      TIME  NODES NODELIST(REASON)
    159914    normal co-mcpdf nsharma2 CG 2-00:00:26      1 wheeler257
    159915    normal co-mcpdf nsharma2 CG 2-00:00:26      1 wheeler257
    159916    normal co-mcpdf nsharma2 CG 2-00:00:26      1 wheeler257
    159917    normal co-mcpdf nsharma2 CG 2-00:00:26      1 wheeler257
    159918    normal co-mcpdf nsharma2 CG 2-00:00:26      1 wheeler257
    159919    normal co-mcpdf nsharma2 CG 2-00:00:26      1 wheeler257
    159912    normal co-mcpdf nsharma2 CG 2-00:00:28      1 wheeler257
    159913    normal co-mcpdf nsharma2 CG 2-00:00:28      1 wheeler257
166800_[21-100%10]    normal    Jannat    jannat PD      0:00      1 (JobArrayTaskLimit)
    167067    normal WINDENER rubeldas PD      0:00     36
(QOSMaxCpuPerUserLimit)
    167068    normal WINDENER rubeldas PD      0:00     24

```

Slurm....

```
[vanilla@wheeler ~]$ srun --partition debug --nodes 2 hostname  
srun: Account not specified in script or  
~/.default_slurm_account, using latest project  
wheeler302.alliance.unm.edu  
You have not been allocated GPUs. To request GPUs, use the -G  
option in your submission script.  
wheeler301.alliance.unm.edu  
[vanilla@wheeler ~]$ srun --partition debug --nodes 2 hostname
```

The srun command...

We finally used the HPC Cluster!



```
[vanilla@wheeler ~]$ srun --partition debug --nodes 2 hostname  
srun: Account not specified in script or  
~/.default_slurm_account, using latest project  
wheeler302.alliance.unm.edu  
You have not been allocated GPUs. To request GPUs, use the -G  
option in your submission script.  
wheeler301.alliance.unm.edu  
[vanilla@wheeler ~]$ srun --partition debug --nodes 2 hostname
```

The srun command...

```
[vanilla@wheeler ~]$ srun --partition debug --ntasks 8 hostname  
srun: Account not specified in script or ~/.default_slurm_account, using  
latest project  
wheeler302.alliance.unm.edu  
wheeler302.alliance.unm.edu  
wheeler302.alliance.unm.edu  
wheeler302.alliance.unm.edu  
wheeler302.alliance.unm.edu  
wheeler302.alliance.unm.edu  
You have not been allocated GPUs. To request GPUs, use the -G option in your  
submission script.  
wheeler302.alliance.unm.edu  
wheeler302.alliance.unm.edu
```

The srun command...

```
[vanilla@wheeler ~]$ cp -r /projects/shared/workshops/beginner/vecadd ~  
[vanilla@wheeler ~]$
```

Review, what does this
command do?

```
[vanilla@wheeler ~]$ cd vecadd/  
[vanilla@wheeler ~/vecadd]$ module load openmpi/4.1.2-q2zi
```

What do these commands do?

```
[vanilla@wheeler ~/vecadd]$ srun --partition debug --ntasks 4 vecaddmpi
```

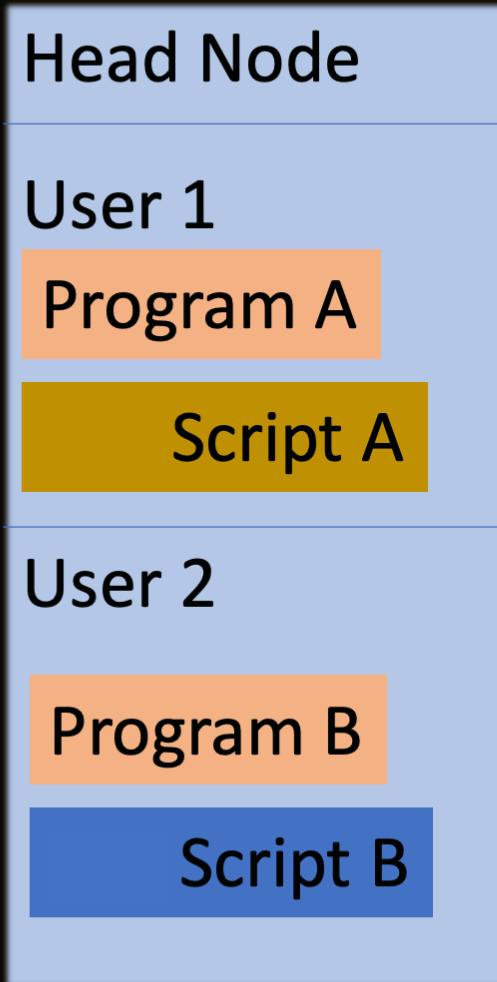
Now run the program with
“srun” ...

```
[vanilla@wheeler ~]$ qgrok
```

queues	free	busy	offline	jobs	nodes	CPUs
-----	-----	-----	-----	-----	-----	-----
normal	0	299	1	97	300	2400
debug	4	0	0	0	4	32
totals:	4	299	1	97	304	2432

srun is good but HPC centers are
busy!

Workflow



Compute Node 01

Compute Node 02

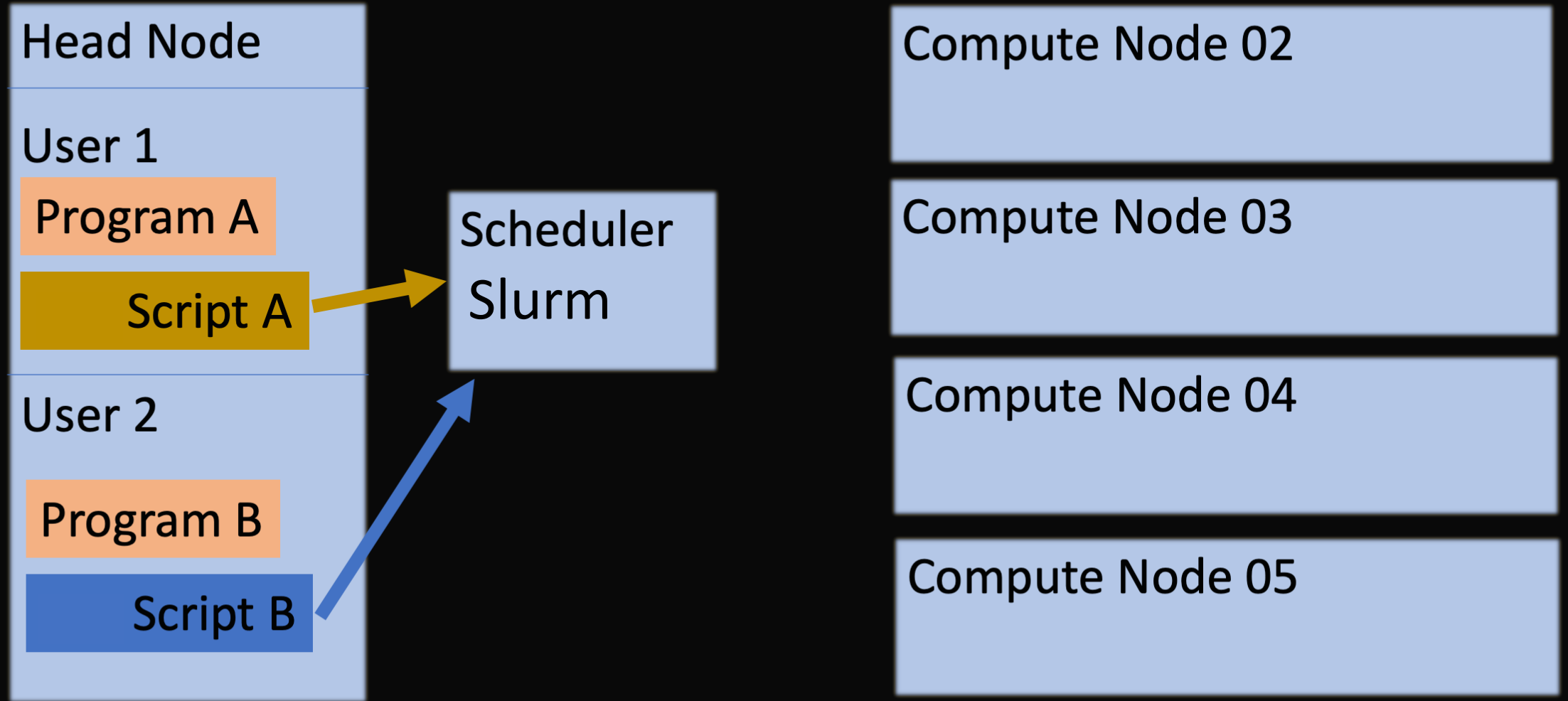
Compute Node 03

Compute Node 04

Compute Node 05

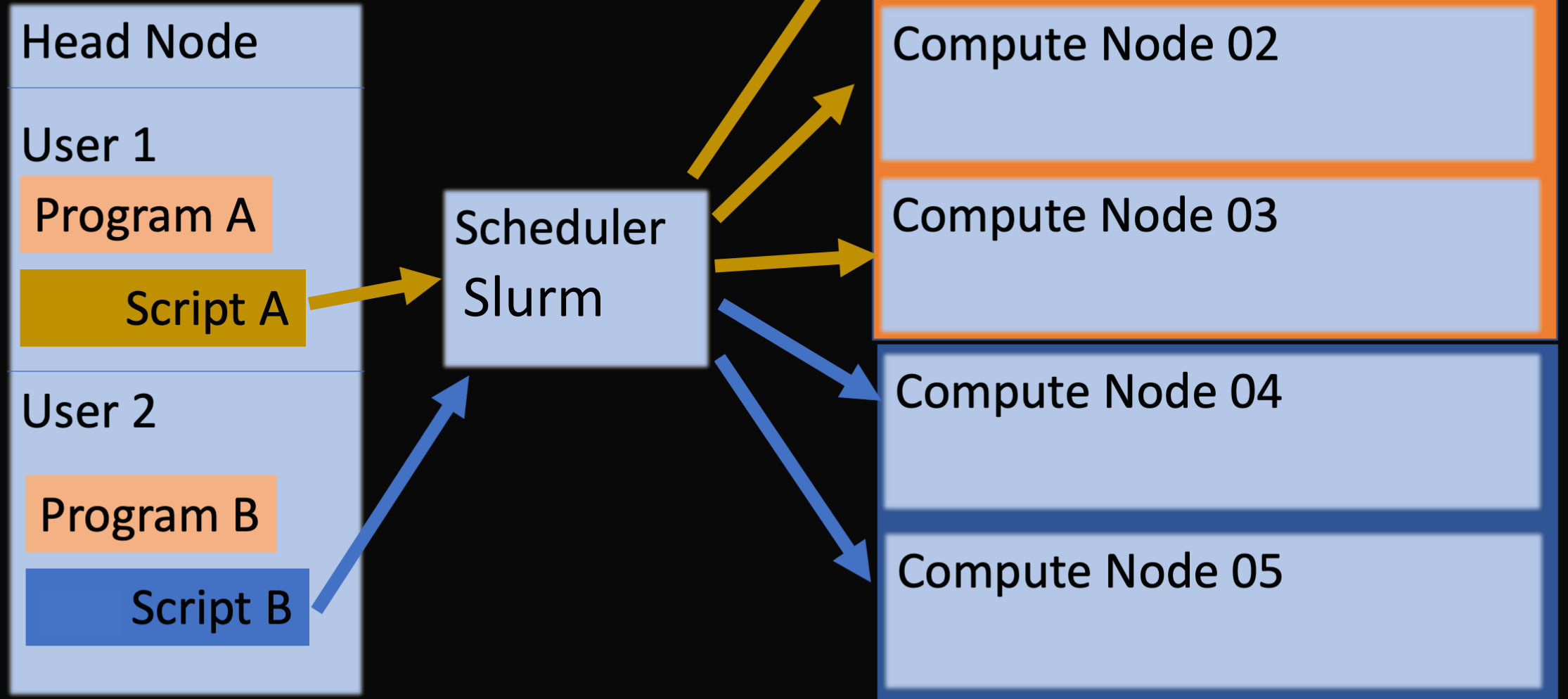
Shared filesystems – All nodes can access the same programs and write output

Workflow



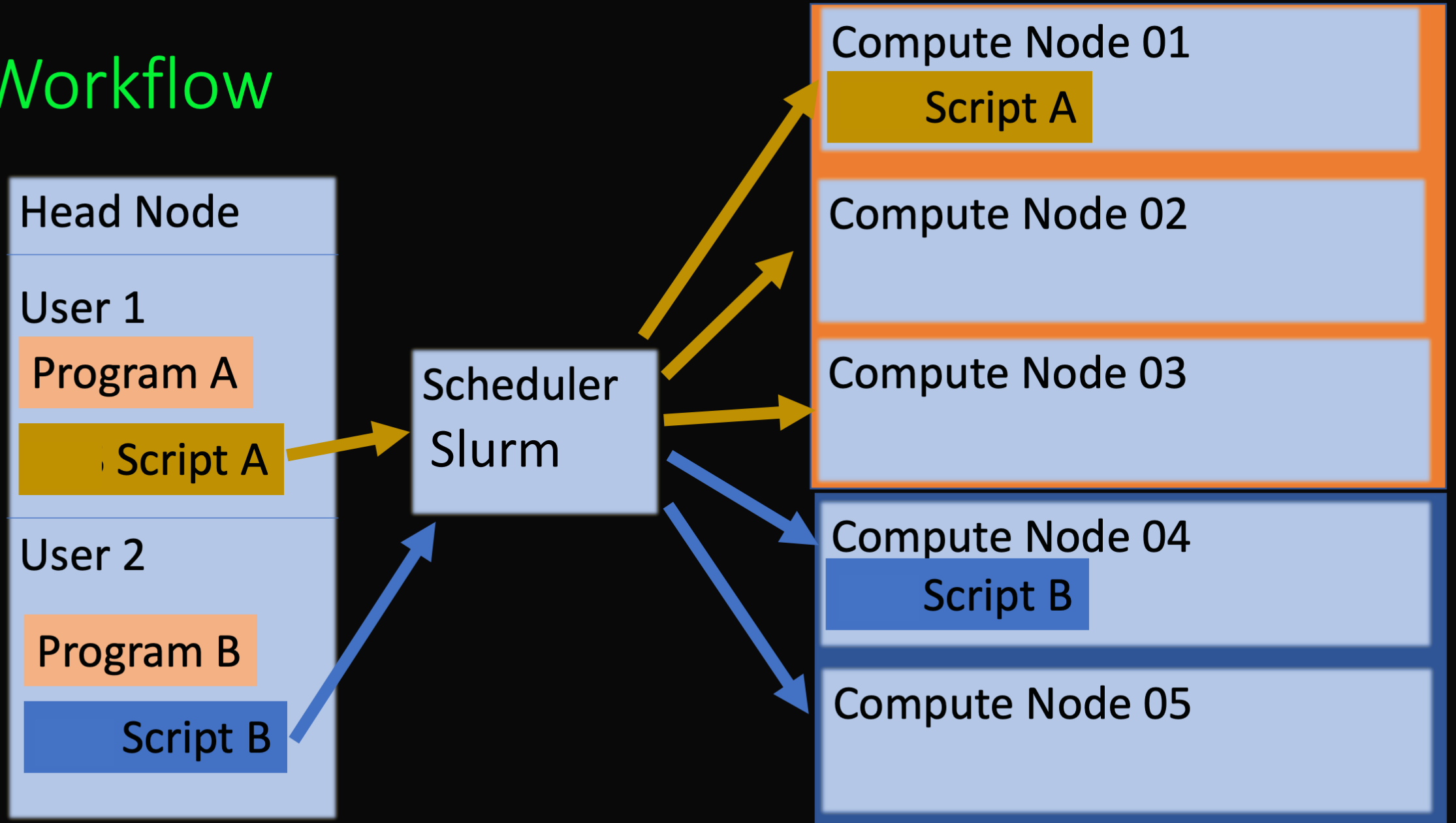
Shared filesystems – All nodes can access the same programs and write output

Workflow



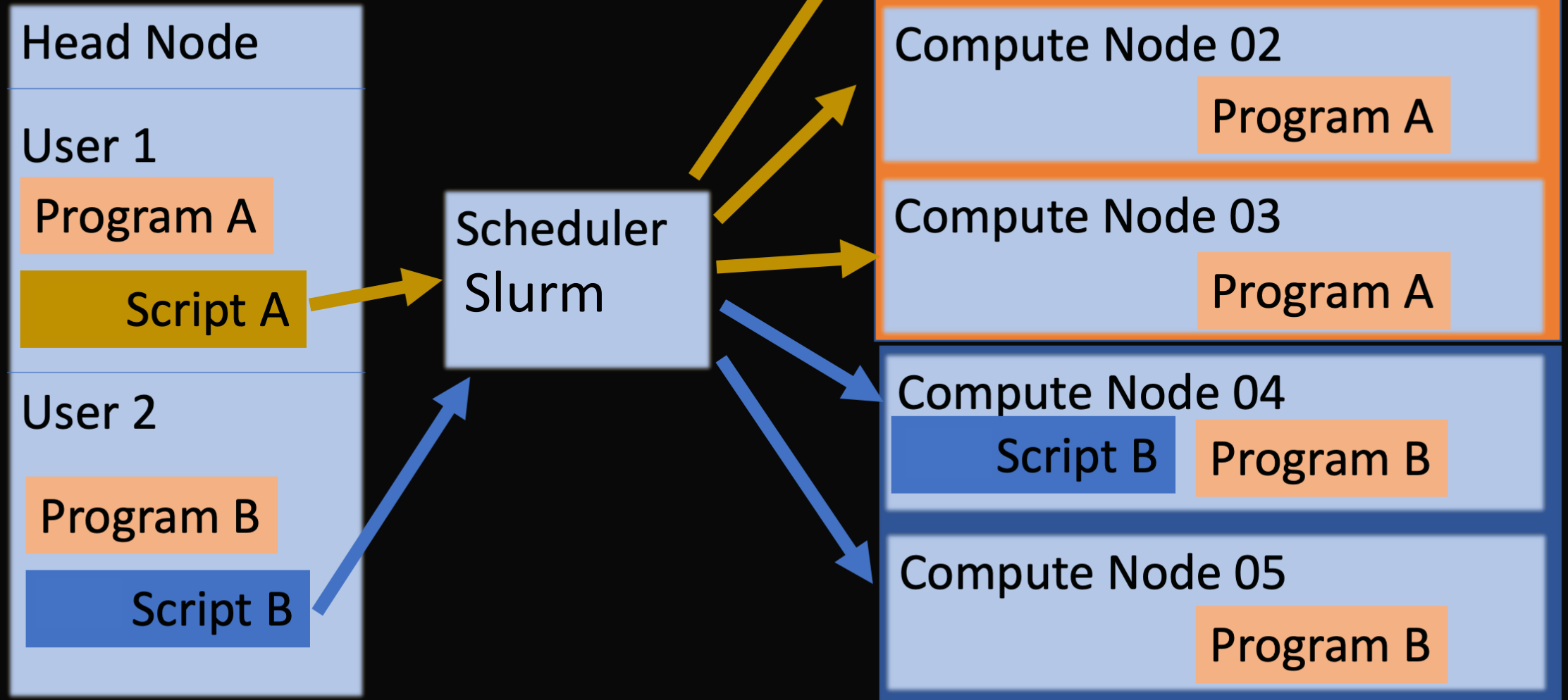
Shared filesystems – All nodes can access the same programs and write output

Workflow



Shared filesystems – All nodes can access the same programs and write output

Workflow



Shared filesystems – All nodes can access the same programs and write output

Scheduler

qgrok

sbatch

queue -u USERNAME

Running Programs on Compute Nodes

- qgrok
- Intro to the Slurm Scheduler
- The srun command
- sbatch
- sinfo
- squeue
- squeue -u username --start
- <https://www.cism.ucl.ac.be/Services/Formations/slurm/2016/slurm.pdf>
- <https://www.nrel.gov/hpc/assets/pdfs/slurm-advanced-topics.pdf>

File Edit Options Buffers Tools Sh-Script Help

```
#!/bin/bash
```

```
#SBATCH --job-name=demo
```

```
#SBATCH --ntasks=4
```

```
#SBATCH --time=00:10:00
```

```
#SBATCH --mem-per-cpu=4G
```

```
#SBATCH --mail-user=yourusername@unm.edu
```

```
#SBATCH --mail-type=All
```

```
# Enter the commands you want to run below here:
```

```
sleep 60
```

```
echo Hello from node $HOSTNAME
```

Slurm Script

```
[vanilla@wheeler ~/vecadd]$ cat vecaddmpi.sh
```

```
#!/bin/bash
```

```
#SBATCH --job-name=vecaddmpi
```

```
#SBATCH --ntasks=4
```

```
#SBATCH --time=00:10:00
```

```
#SBATCH --mem-per-cpu=4G
```

```
#SBATCH --mail-user=mfricke@unm.edu
```

```
#SBATCH --mail-type=All
```

```
#SBATCH --output=vecaddmpi.out
```

```
module load openmpi/4.1.2-q2zi
```

```
srun ./vecaddmpi
```

Slurm Script

```
vanilla@wheeler:~/vecadd $ sbatch vecaddmpi.sh
sbatch: Using account 2016199 from ~/.default_slurm_account
Submitted batch job 167571
```

```
vanilla@wheeler:~/vecadd $ squeue --me
```

	JOBID	PARTITION	NAME	USER	ST	TIME	NODES
NODELIST(REASON)							
	167571	normal	vecaddmp	vanilla	R	0:07	1 wheeler145

Slurm Script

```
vanilla@wheeler:~/vecadd $ tail -f vecaddmpi.out
You have not been allocated GPUs. To request GPUs, use the -G option in your
submission script.
Assigning compute node to rank 1.
ComputeNode: Starting with rank 1.
ComputeNode (1): Waiting for vectors from dataserver with rank 3...
Assigning compute node to rank 2.
ComputeNode: Starting with rank 2.
ComputeNode (2): Waiting for vectors from dataserver with rank 3...
Will try to allocate a vector of size 1 GB.
```

Slurm Script

```
vanilla@wheeler:~/vecadd $ tail -f vecaddmpi.out
You have not been allocated GPUs. To request GPUs, use the -G option in your
submission script.
Assigning compute node to rank 1.
ComputeNode: Starting with rank 1.
ComputeNode (1): Waiting for vectors from dataserver with rank 3...
Assigning compute node to rank 2.
ComputeNode: Starting with rank 2.
ComputeNode (2): Waiting for vectors from dataserver with rank 3...
Will try to allocate a vector of size 1 GB.
```

Slurm Script

Useful Slurm Commands

queue --me --long

shows information about jobs you submitted

queue --me --start

shows when slurm expects your job to start

scancel jobid

Cancels a job

sacct

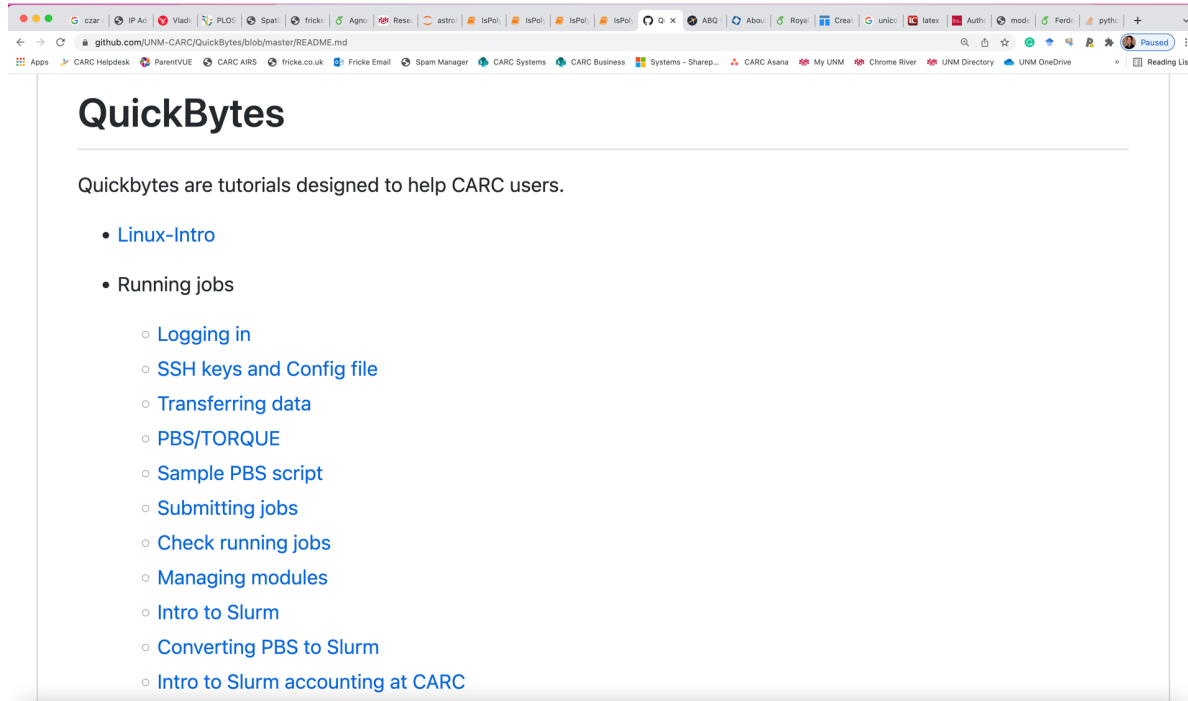
shows your job history

```
vanilla@wheeler:~/vecadd $ seff 167573
Job ID: 167573
Cluster: wheeler
User/Group: mfricke/users
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 4
CPU Utilized: 00:01:03
CPU Efficiency: 78.75% of 00:01:20 core-walltime
Job Wall-clock time: 00:00:20
Memory Utilized: 39.55 MB (estimated maximum)
Memory Efficiency: 0.24% of 16.00 GB (4.00 GB/core)
```

Slurm Script

CARC Resources

- Tutorial Videos
- Written Tutorials

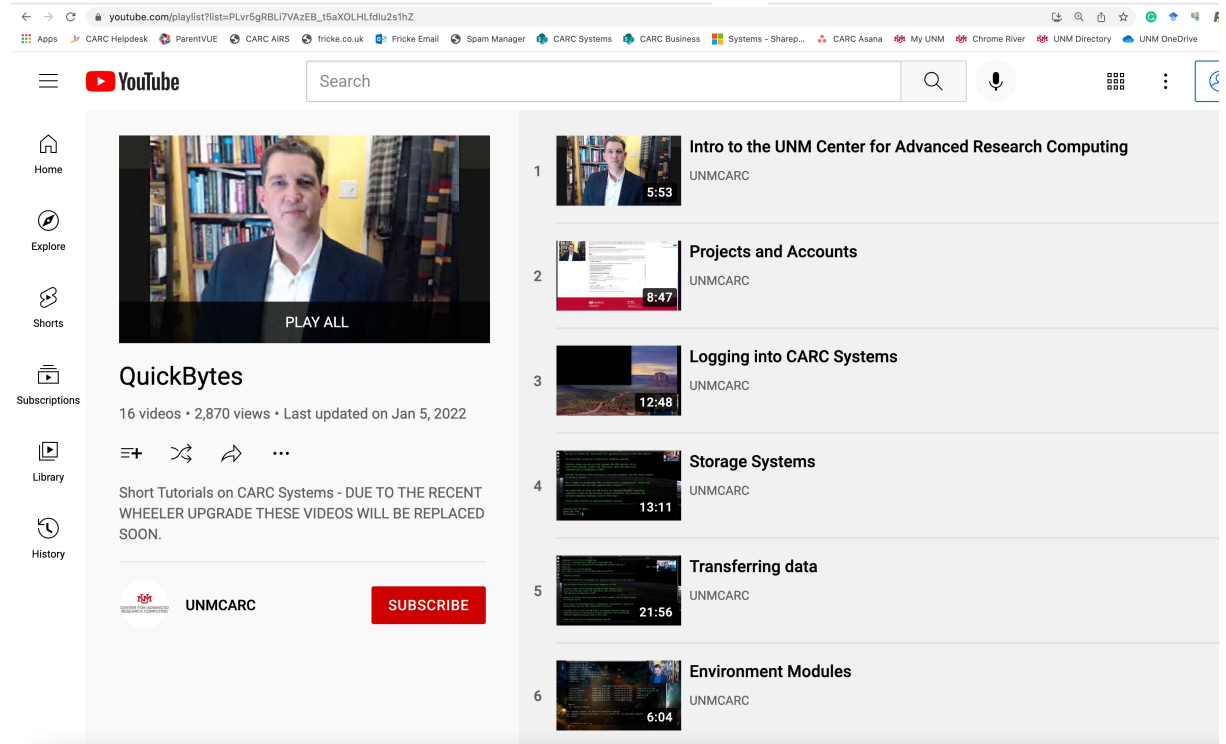


The screenshot shows a web browser window displaying the GitHub repository for UNMC-CARC/QuickBytes. The browser's address bar shows the URL `github.com/UNMC-CARC/QuickBytes/blob/master/README.md`. The repository name "QuickBytes" is prominently displayed at the top. Below the title, a brief description states: "Quickbytes are tutorials designed to help CARC users." A list of tutorial topics is provided, including "Linux-Intro" and "Running jobs", with the latter having a sub-list of specific topics like "Logging in", "SSH keys and Config file", "Transferring data", "PBS/TORQUE", "Sample PBS script", "Submitting jobs", "Check running jobs", "Managing modules", "Intro to Slurm", "Converting PBS to Slurm", and "Intro to Slurm accounting at CARC".

QuickBytes

Quickbytes are tutorials designed to help CARC users.

- [Linux-Intro](#)
- Running jobs
 - [Logging in](#)
 - [SSH keys and Config file](#)
 - [Transferring data](#)
 - [PBS/TORQUE](#)
 - [Sample PBS script](#)
 - [Submitting jobs](#)
 - [Check running jobs](#)
 - [Managing modules](#)
 - [Intro to Slurm](#)
 - [Converting PBS to Slurm](#)
 - [Intro to Slurm accounting at CARC](#)



The screenshot shows a YouTube playlist page for "QuickBytes" by the channel "UNMC-CARC". The playlist contains 16 videos with a total of 2,870 views, last updated on Jan 5, 2022. A note indicates that due to a recent WHEELER UPGRADE, these videos will be replaced soon. A "SUBSCRIBE" button is visible. The video list on the right includes:

1. **Intro to the UNM Center for Advanced Research Computing** (5:53)
2. **Projects and Accounts** (8:47)
3. **Logging into CARC Systems** (12:48)
4. **Storage Systems** (13:11)
5. **Transferring data** (21:56)
6. **Environment Modules** (6:04)

Getting Help

help@carc.unm.edu

Office hours

Bonus – sview and graphical programs