Beginner’s Introduction to Computing at CARC

Matthew Fricke and Nick Porter

Version 0.2

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

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

Use your CARC username and password.

Raise your hand if you have any trouble.

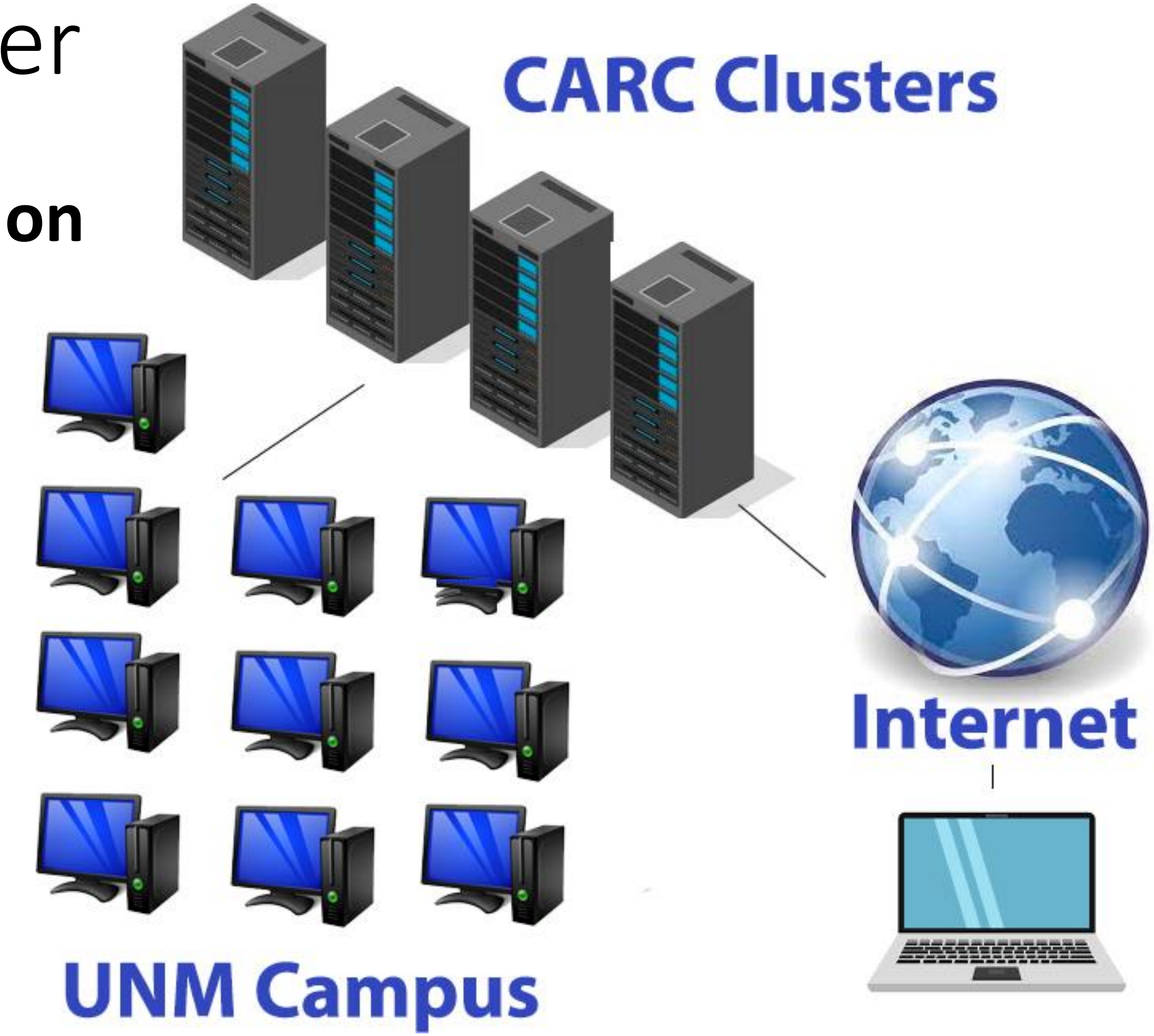
This is an “important step” so don’t let me move on until you have logged in

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.

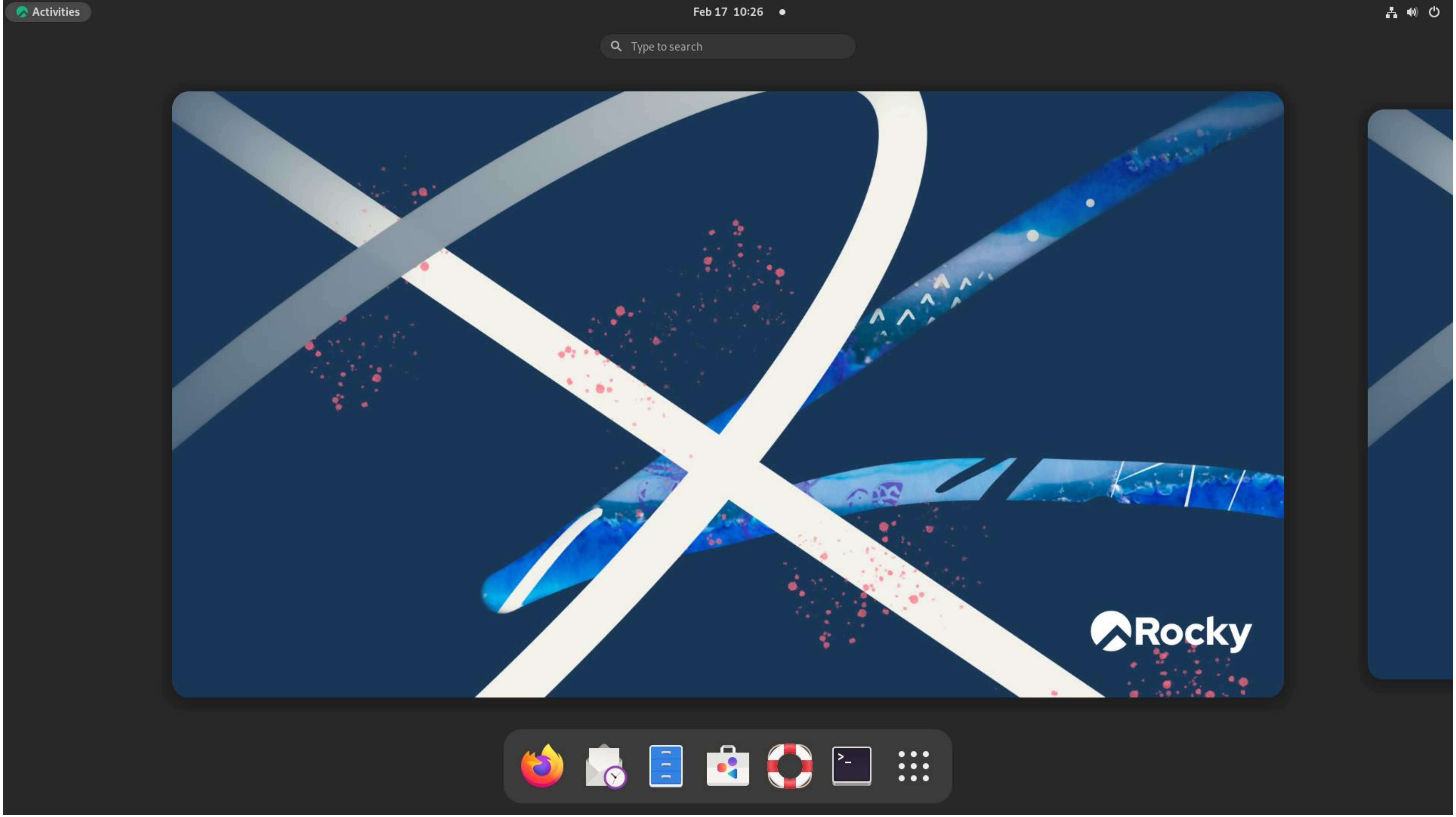


Logging into Wheeler

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.


Activities
Feb 17 10:26
Type to search
Rocky

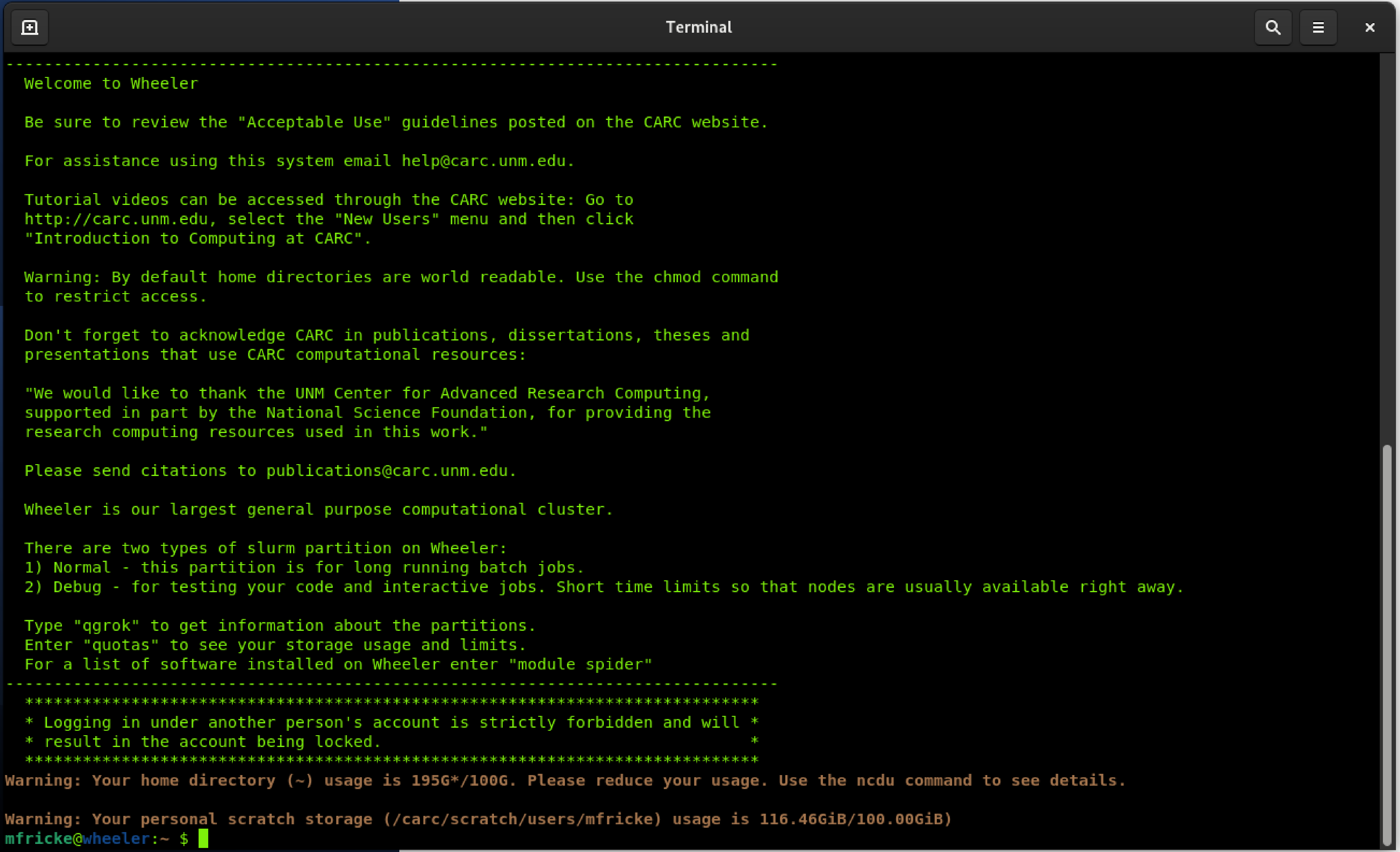
Logging into Wheeler

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

Should prompt you for a password…

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

```
$passwd
```



```
--------------------------------------------------------------------------------
  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.

  Wheeler is our largest general purpose computational cluster.

  There are two types of slurm partition on Wheeler:
  1) Normal - this partition is for long running batch jobs.
  2) Debug - for testing your code and interactive jobs. Short time limits so that nodes are usually available right away.

  Type "qgrok" to get information about the partitions.
  Enter "quotas" to see your storage usage and limits.
  For a list of software installed on Wheeler enter "module spider"
--------------------------------------------------------------------------------
  ****************************************************************************
  * Logging in under another person's account is strictly forbidden and will *
  * result in the account being locked.                                      *
  ****************************************************************************
Warning: Your home directory (~) usage is 195G*/100G. Please reduce your usage. Use the ncdu command to see details.

Warning: Your personal scratch storage (/carc/scratch/users/mfricke) usage is 116.46GiB/100.00GiB)
mfricke@wheeler:~ $
```

Please enter the following command

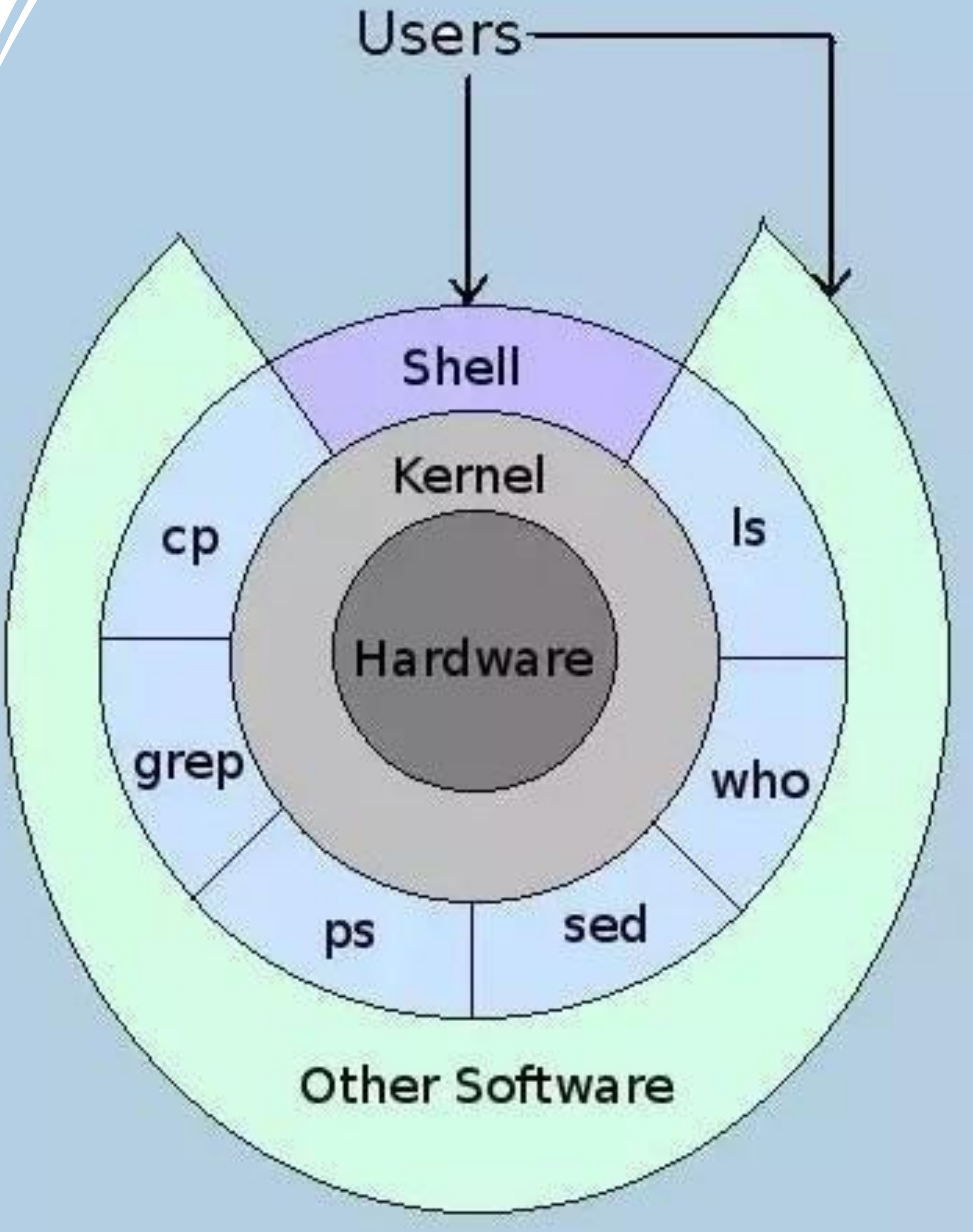
```
cp –r /projects/shared/workshops/beginner/mystuff ~/
```

We will come help you if you have any trouble.

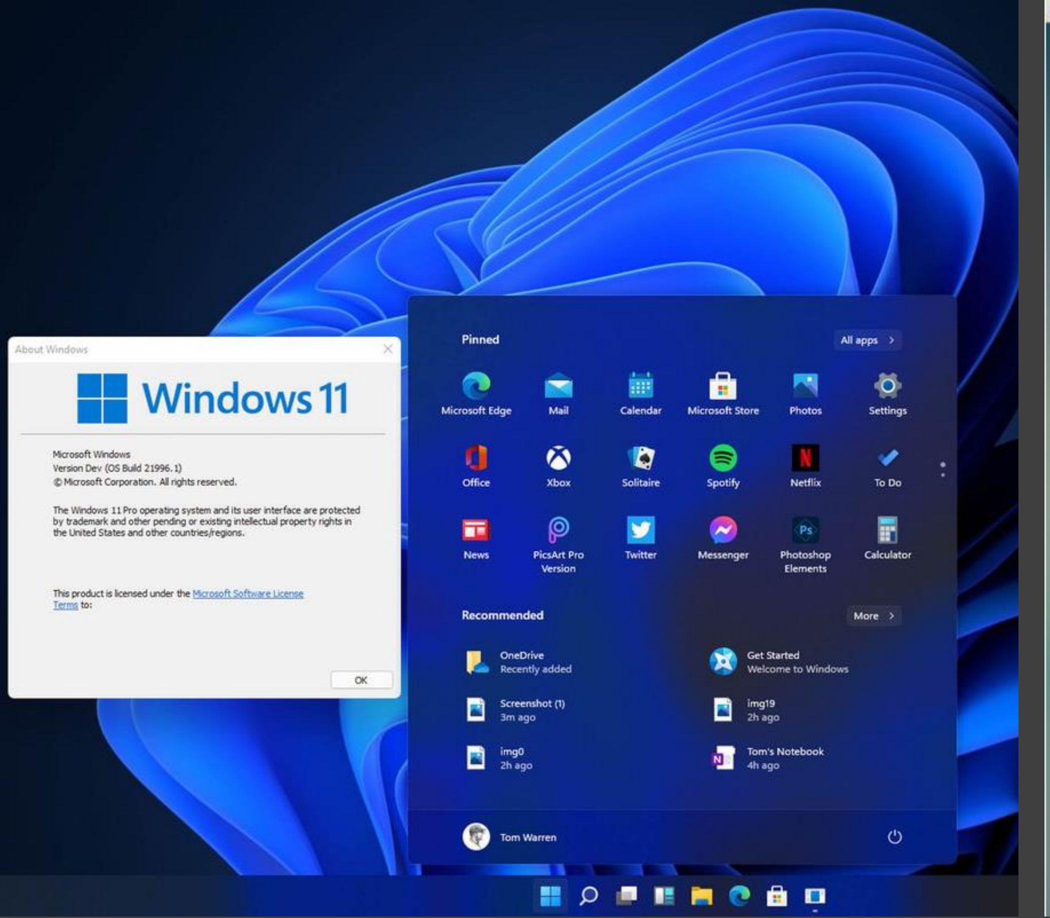
(Later I will go over what this command does)

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.



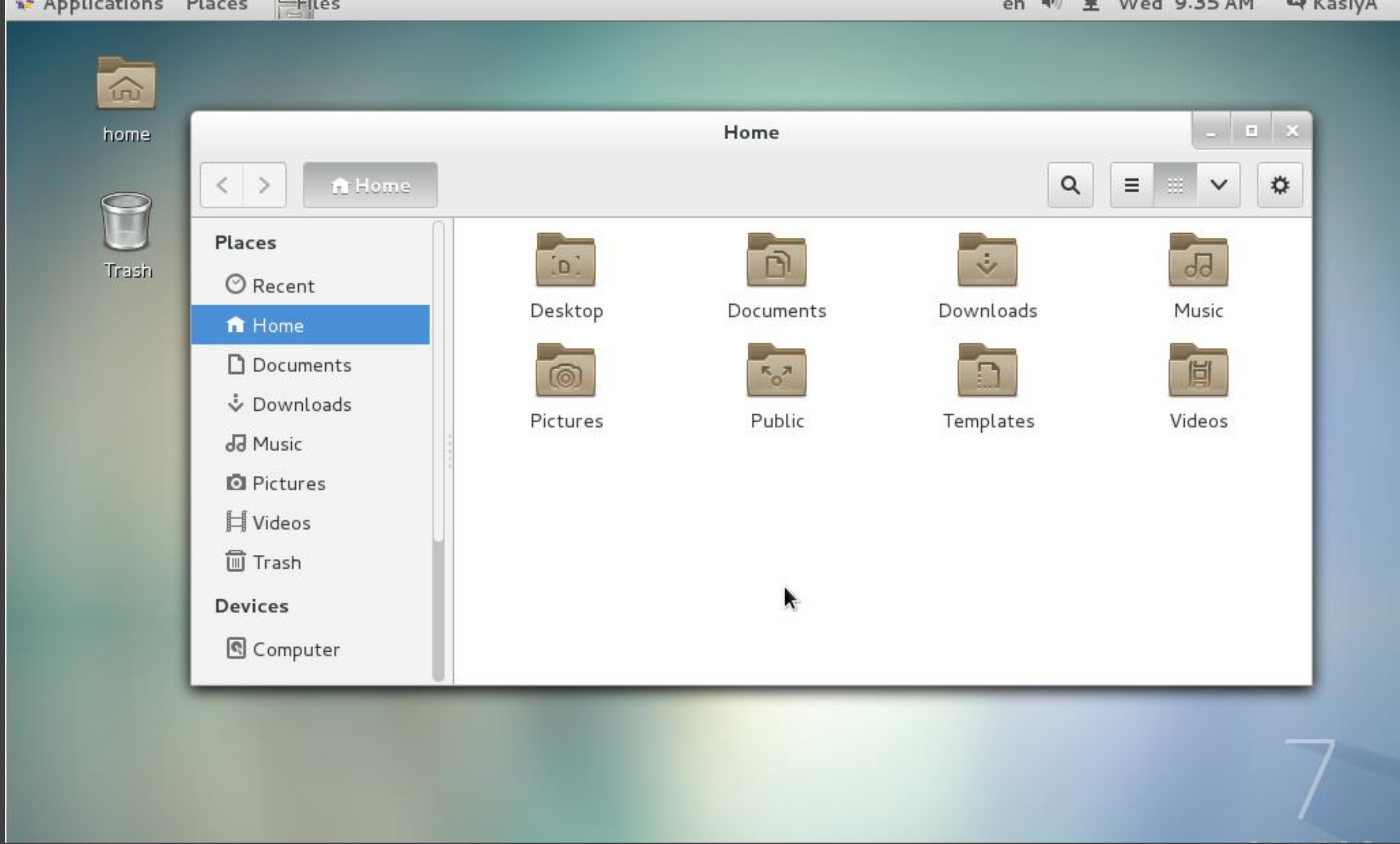
Graphical Shells (GUIs)

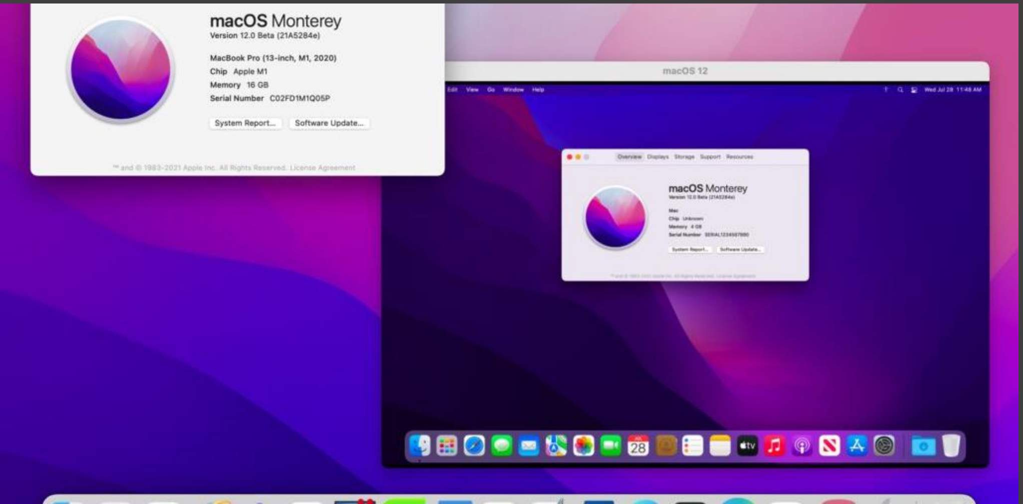

About Windows

Microsoft Windows
Version Dev (OS Build 21996.1)
© Microsoft Corporation. All rights reserved.

The Windows 11 Pro operating system and its user interface are protected by trademark and other pending or existing intellectual property rights in the United States and other countries/regions.

This product is licensed under the Microsoft Software License Terms to:

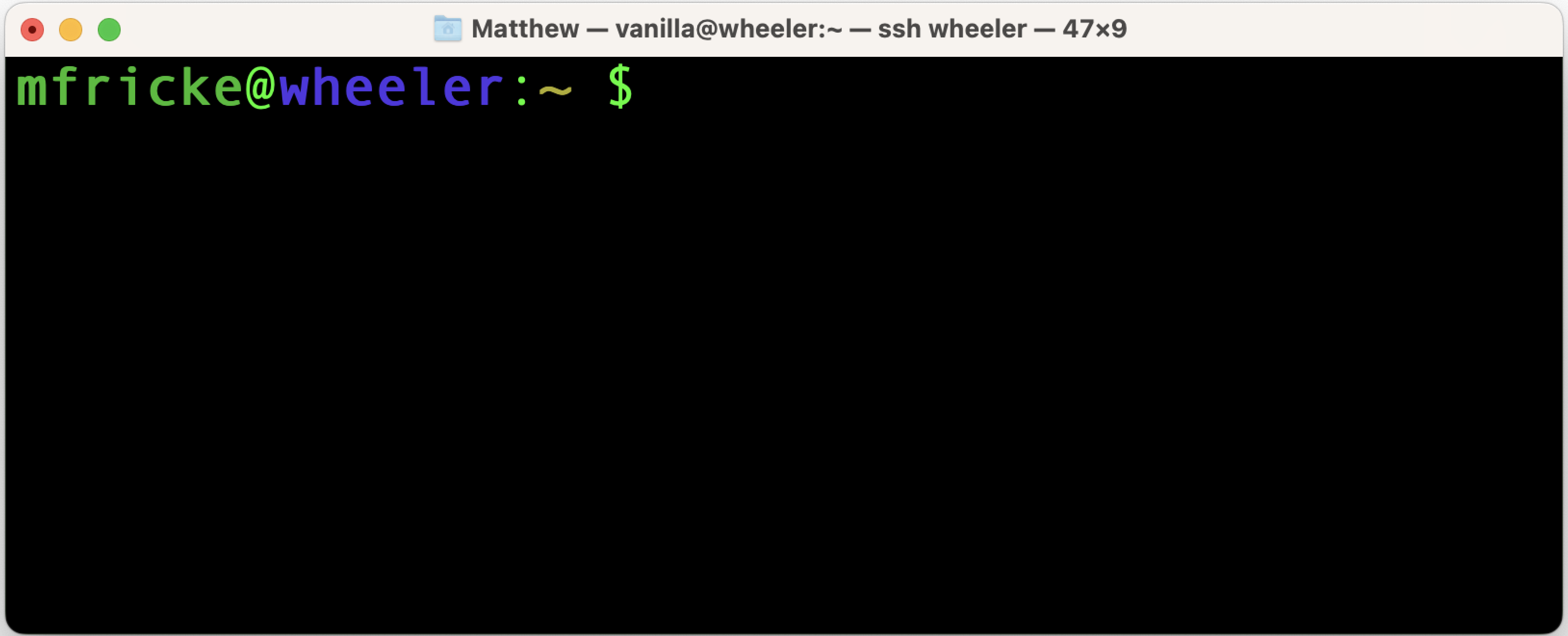



macOS Monterey
Version 12.0 Beta (21A5284e)

MacBook Pro (13-inch, M1, 2020)
Chip Apple M1
Memory 16 GB
Serial Number C02FD1M1Q05P

™ and © 1983-2021 Apple Inc. All Rights Reserved. License Agreement

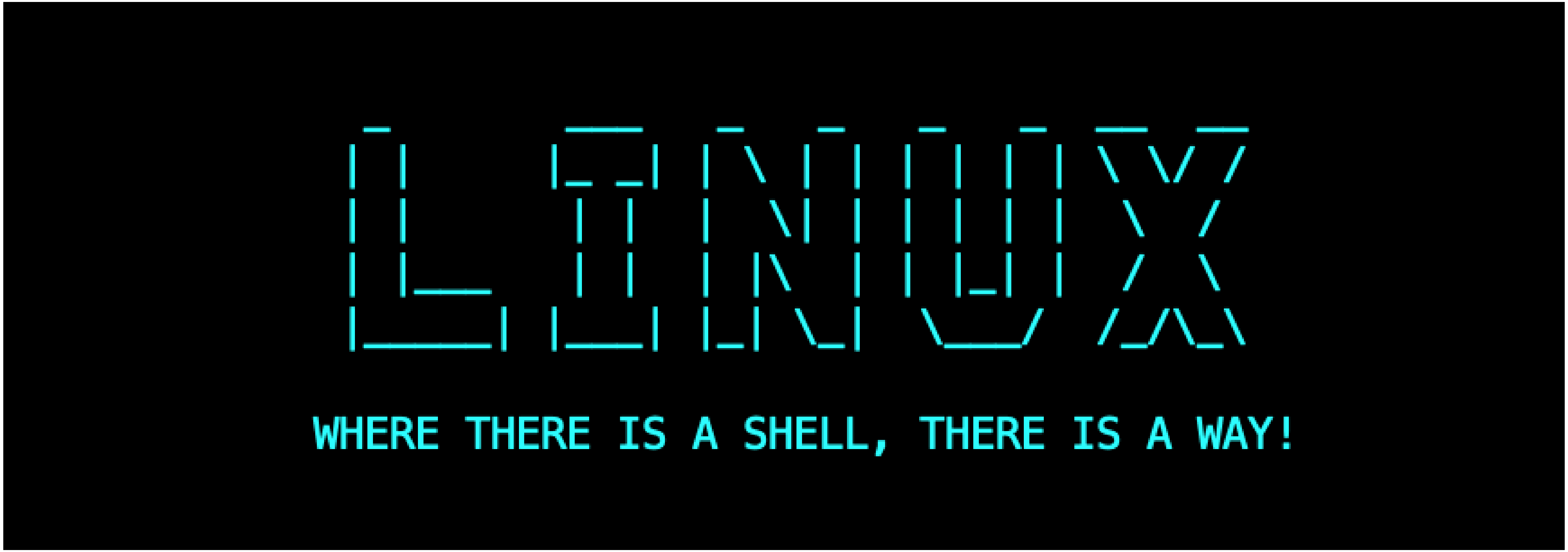
Logging into Wheeler



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

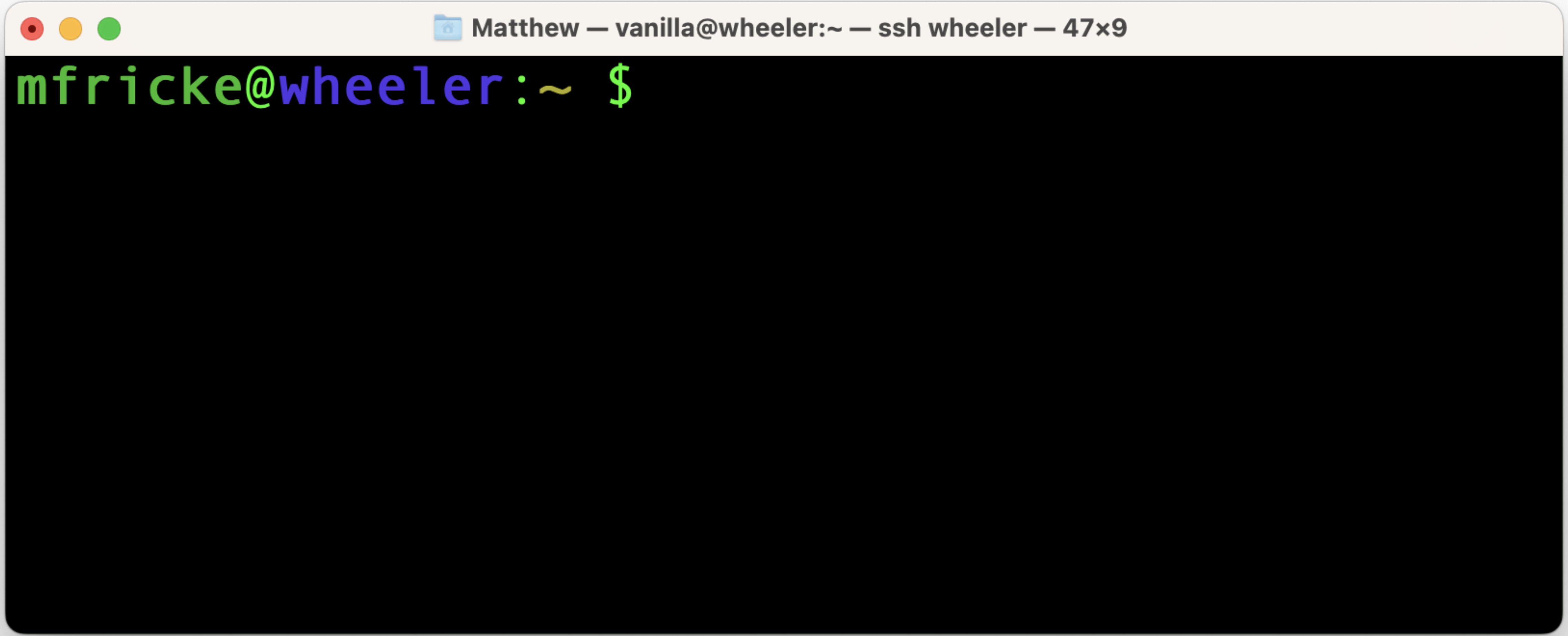
YOU ARE AT THE
RIGHT PLACE

Linux and the BASH Shell

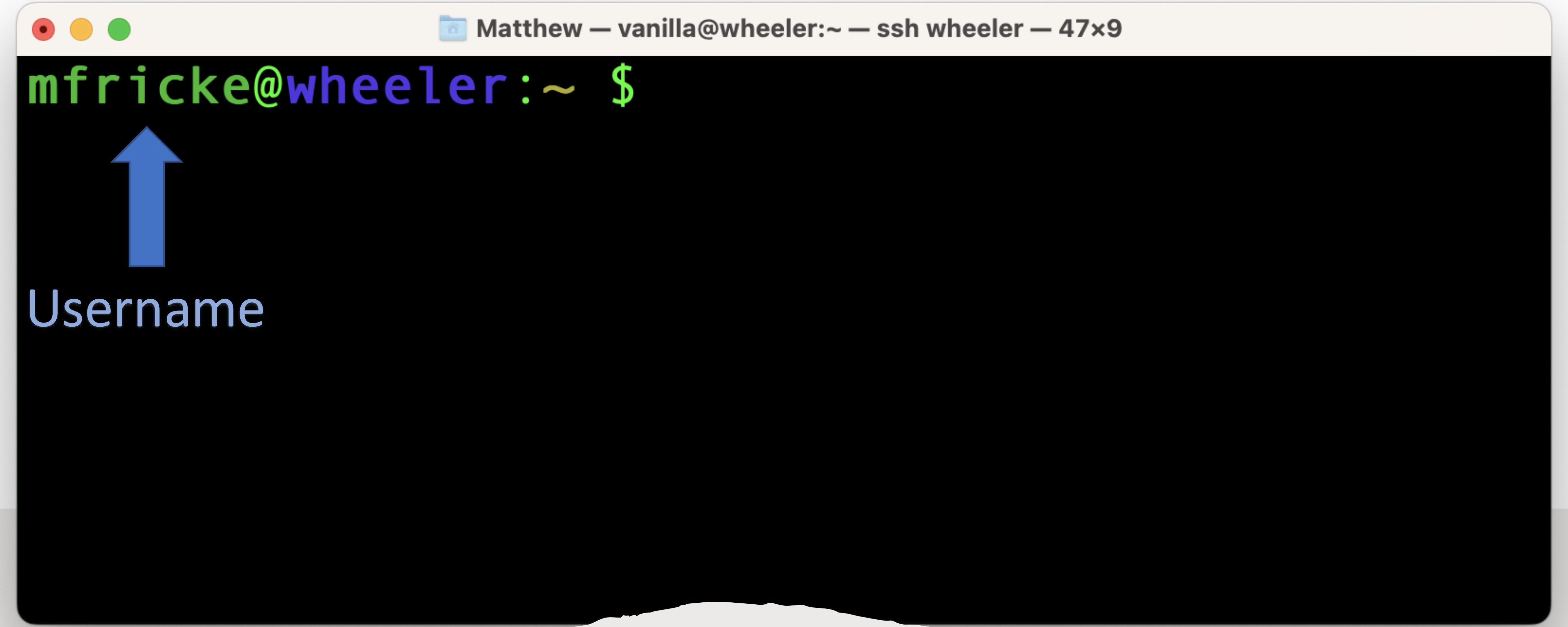


The Borne-Again Shell (BASH)

Written in 1976 by Stephen Bourne for UNIX version 7.



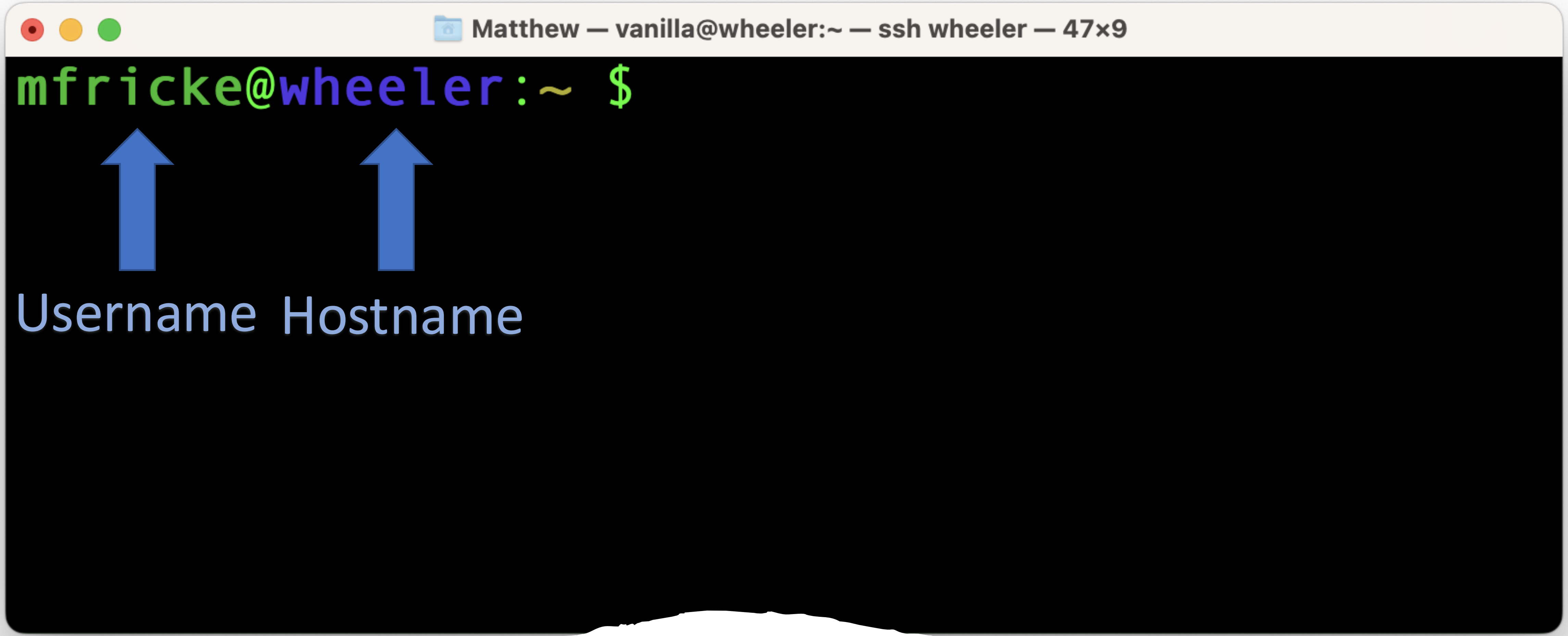
```
mfricke@wheeler:~ $
```



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

Username

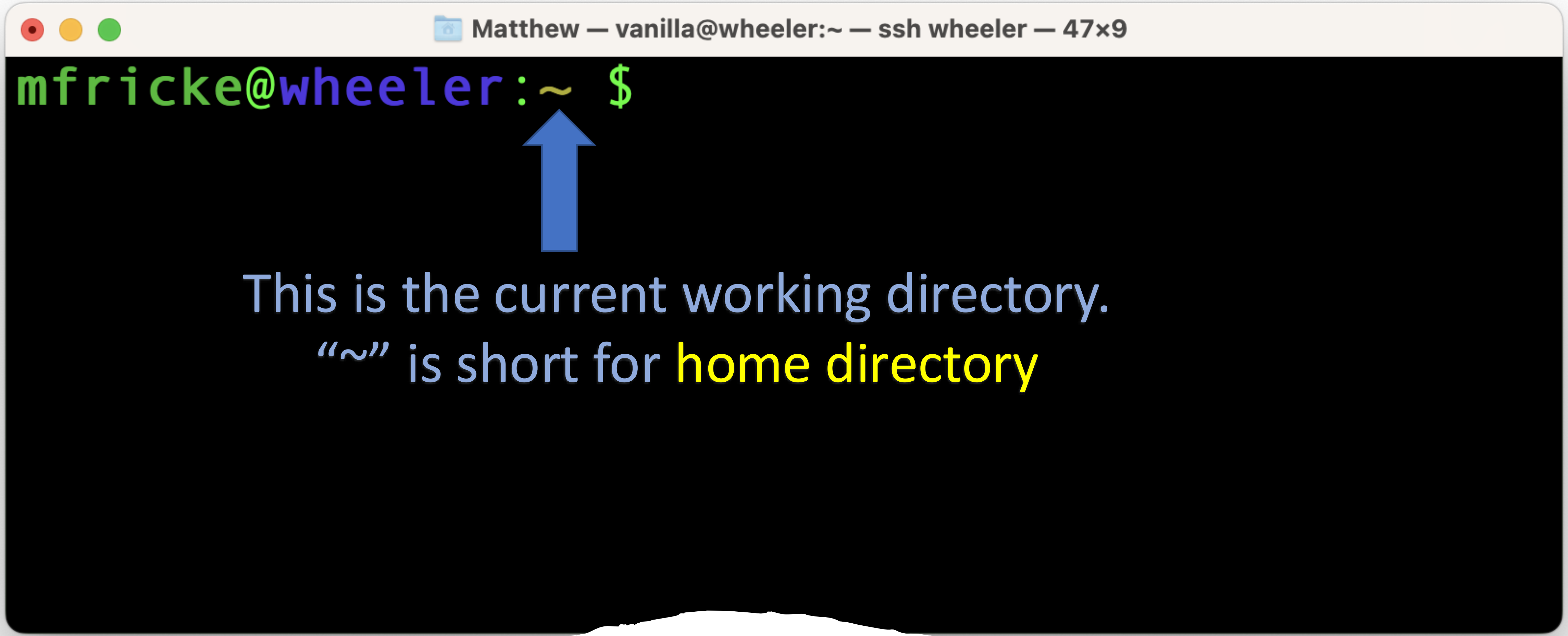
Understanding the BASH prompt...



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

Username Hostname

Understanding the BASH prompt...

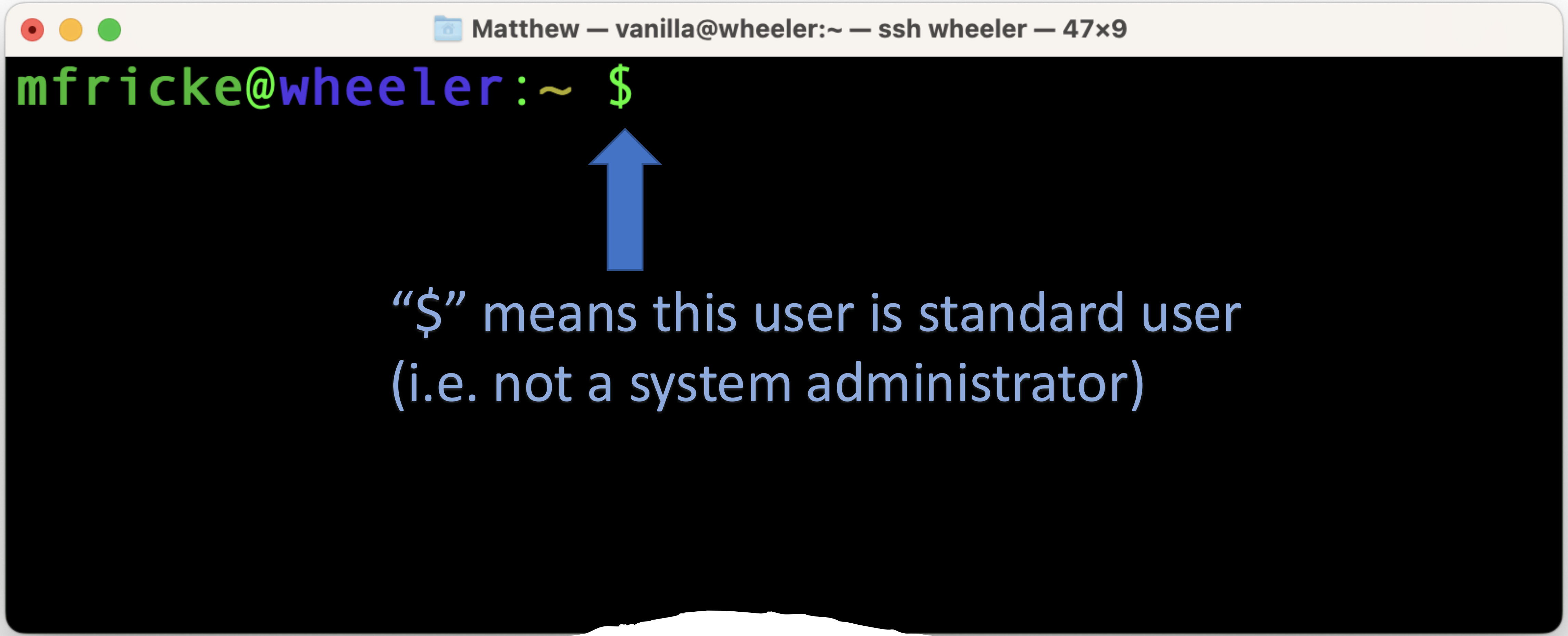


```
mfricke@wheeler:~ $
```

This is the current working directory.

“~” is short for home directory

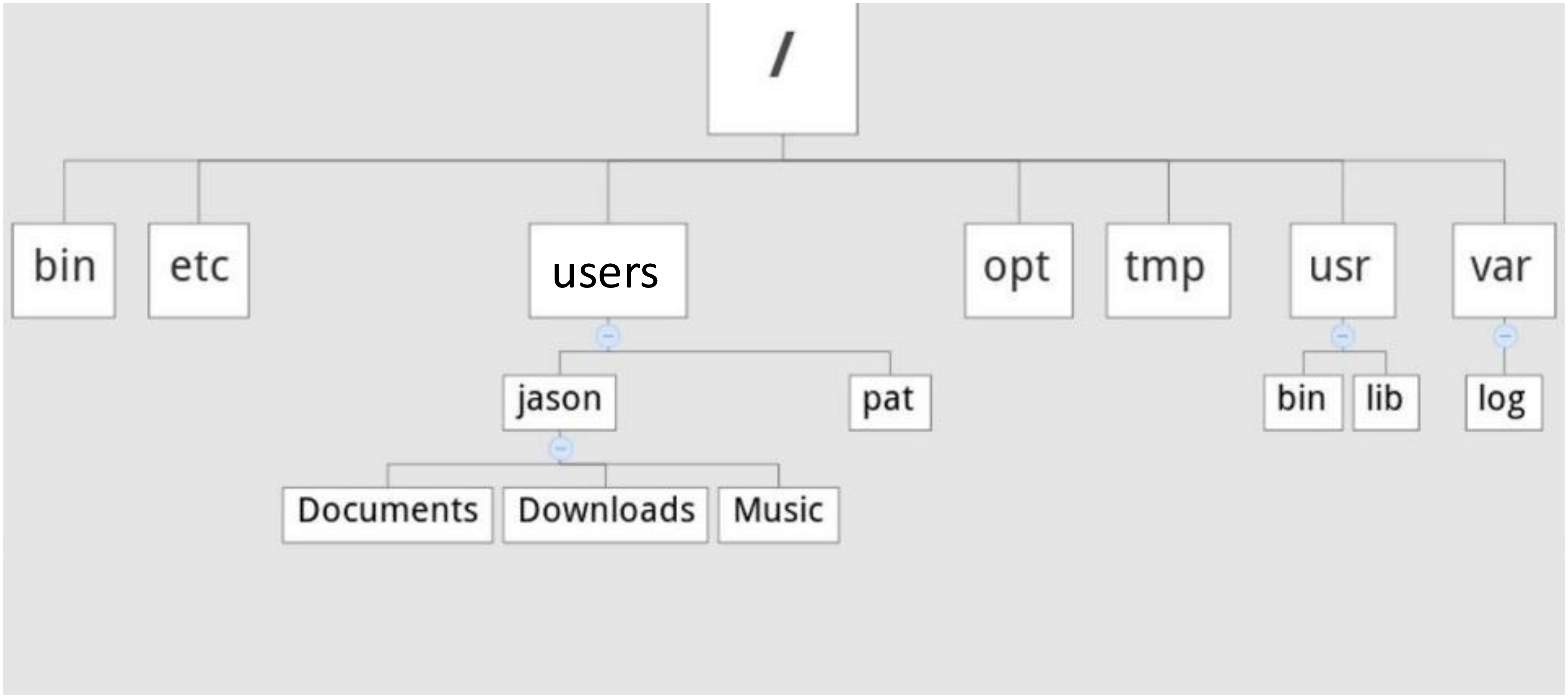
Understanding the BASH prompt…



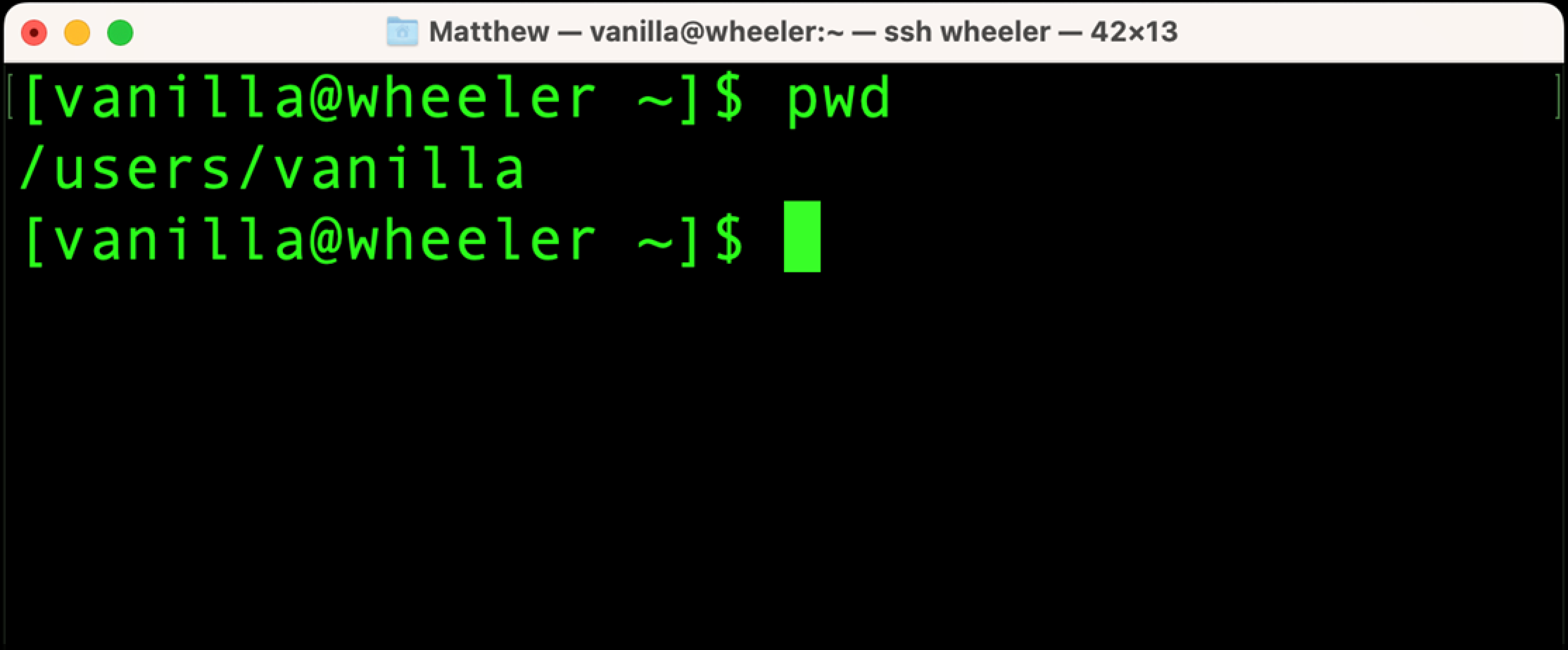
```
mfricke@wheeler:~ $
```

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

Understanding the BASH prompt…

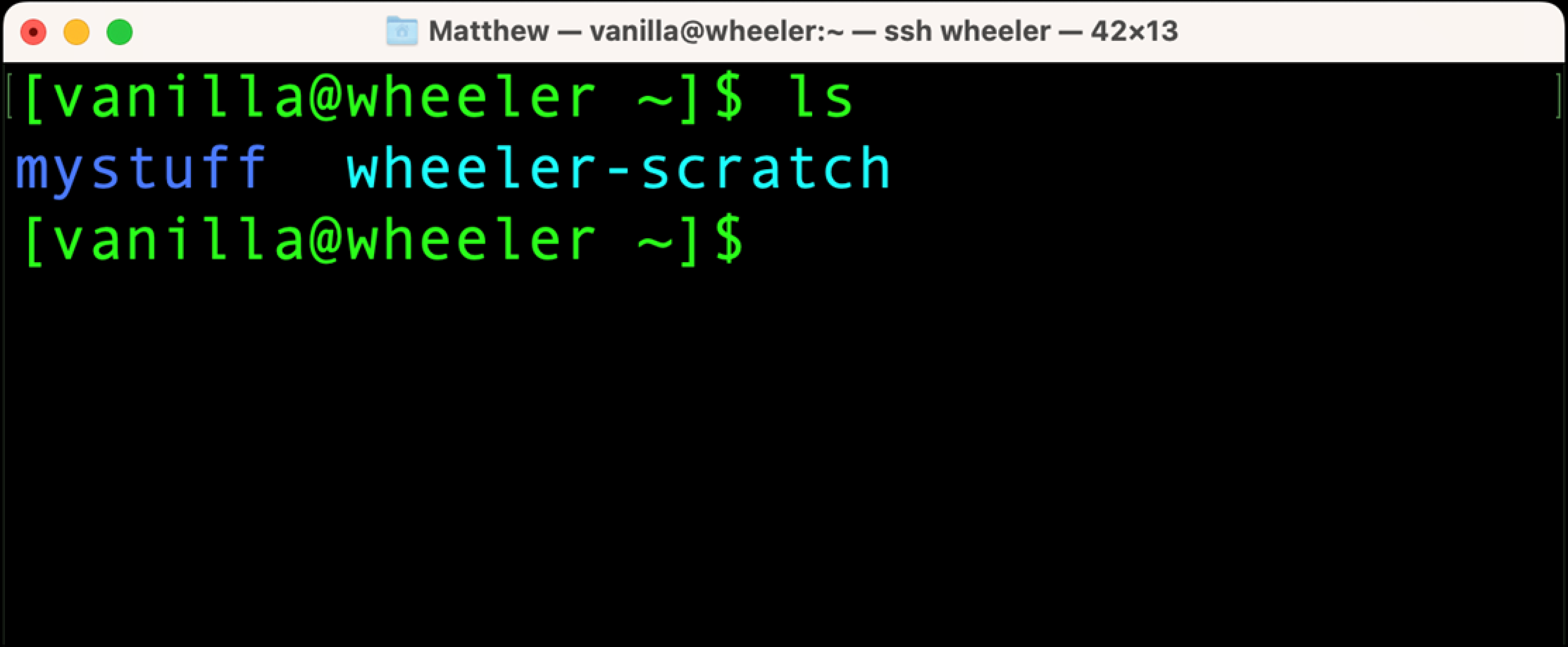


Example Filesystem Tree



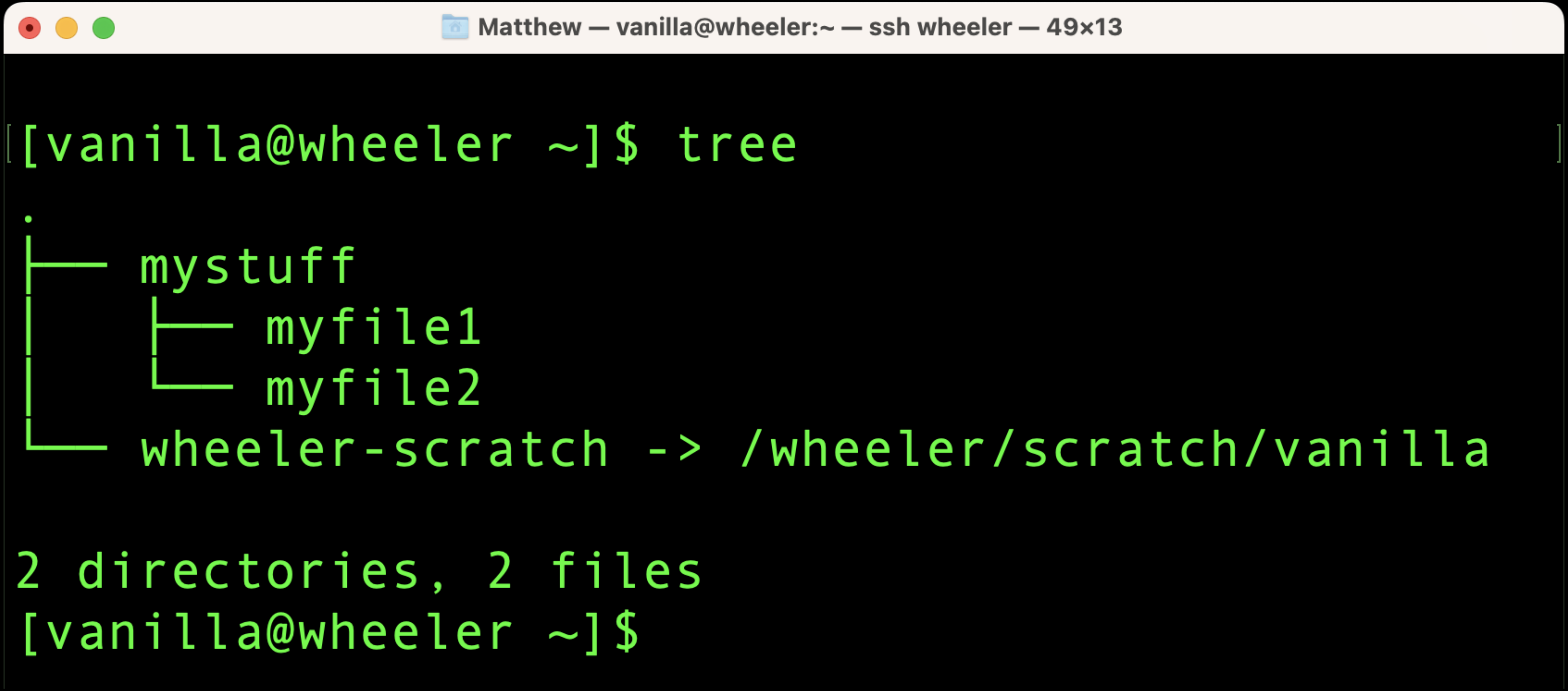
```
[vanilla@wheeler ~]$ pwd
/users/vanilla
[vanilla@wheeler ~]$ 
```

Figuring out where you are in the filesystem...



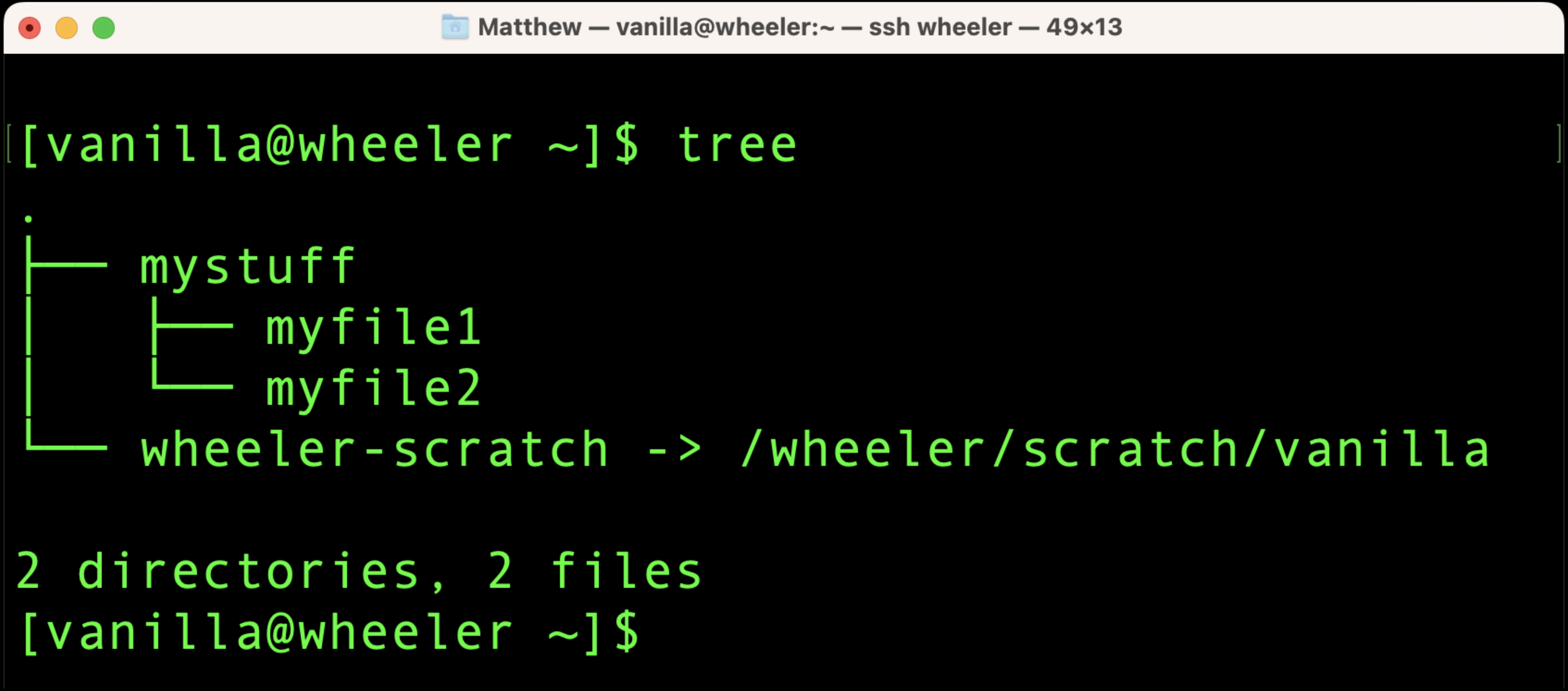
```
[vanilla@wheeler ~]$ ls
mystuff  wheeler-scratch
[vanilla@wheeler ~]$
```

Figuring out where you are in the filesystem…



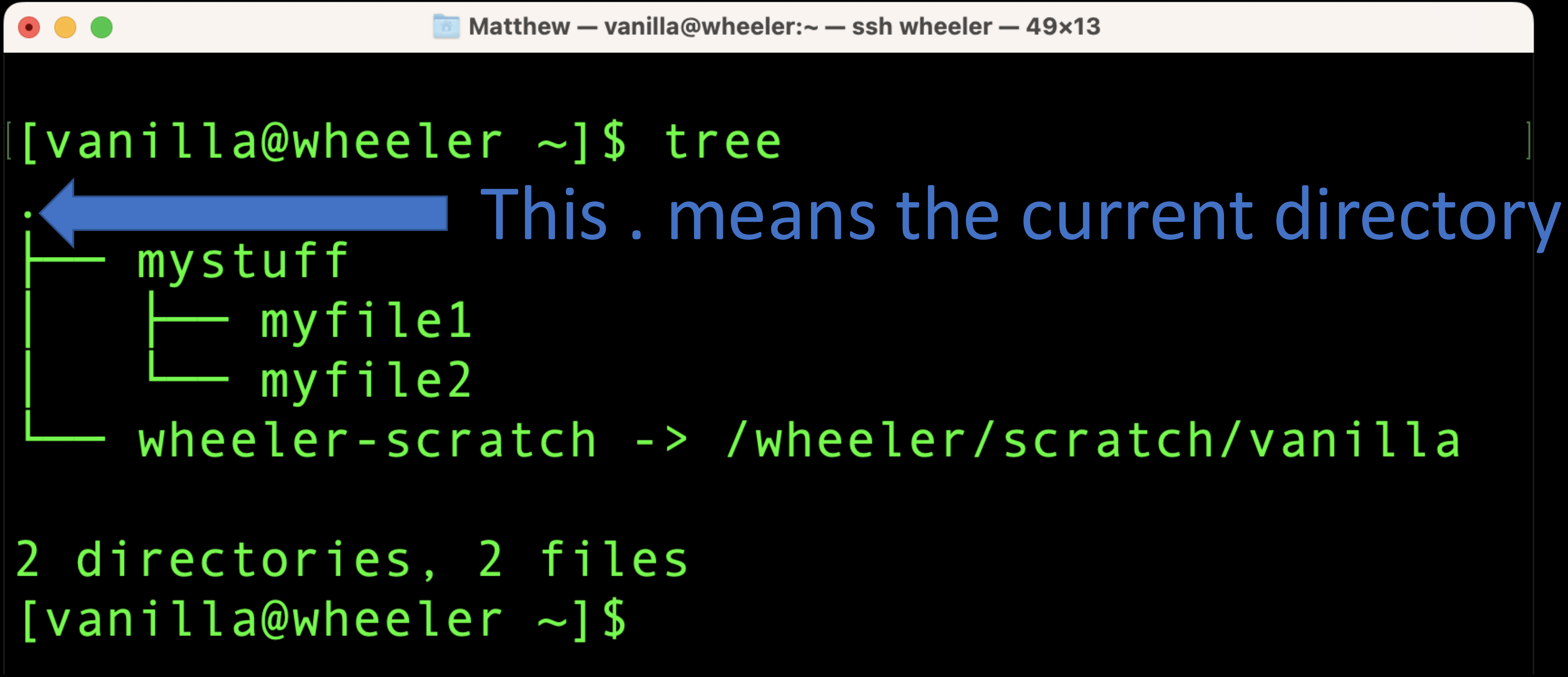
```
[vanilla@wheeler ~]$ tree
.
├── mystuff
│   ├── myfile1
│   └── myfile2
└── wheeler-scratch -> /wheeler/scratch/vanilla

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

2 directories, 2 files
[vanilla@wheeler ~]$
```

This . means the current directory

Figuring out where you are in the filesystem…

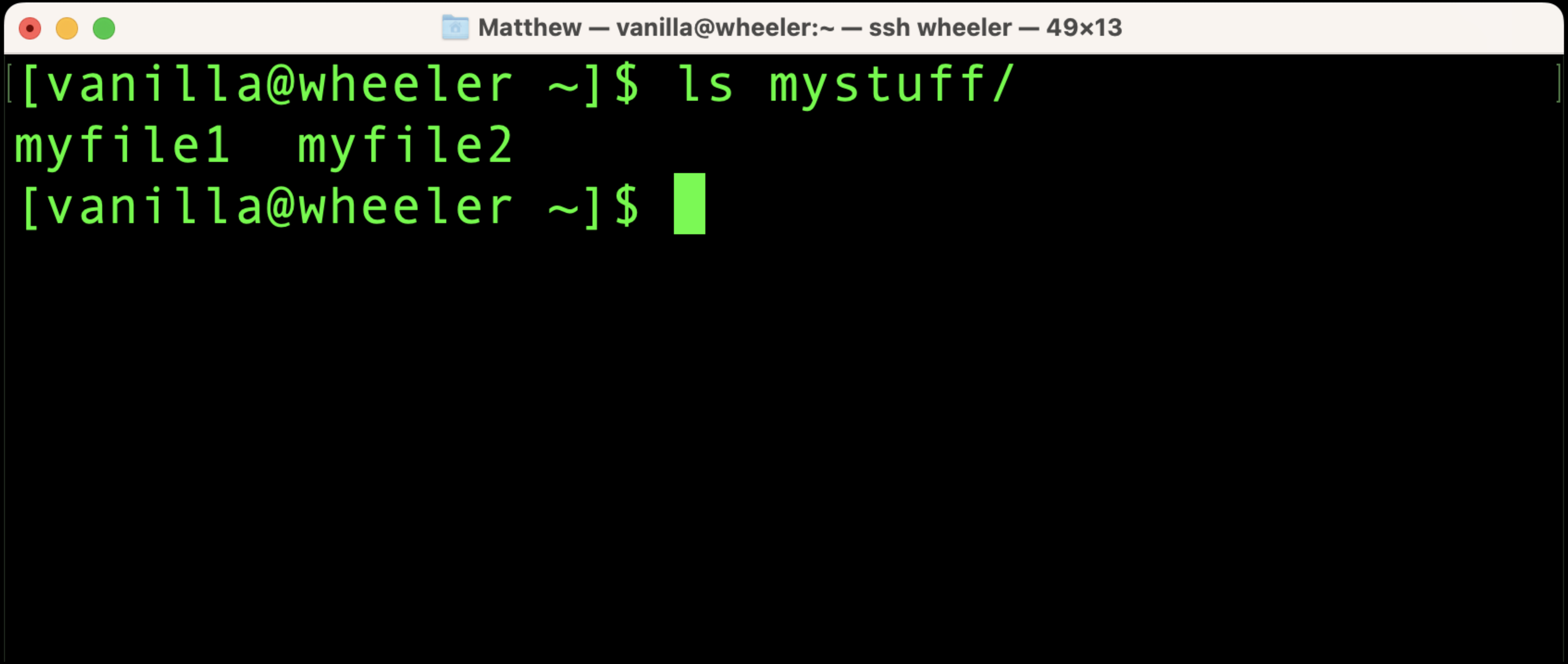
5 Minute Break

“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.

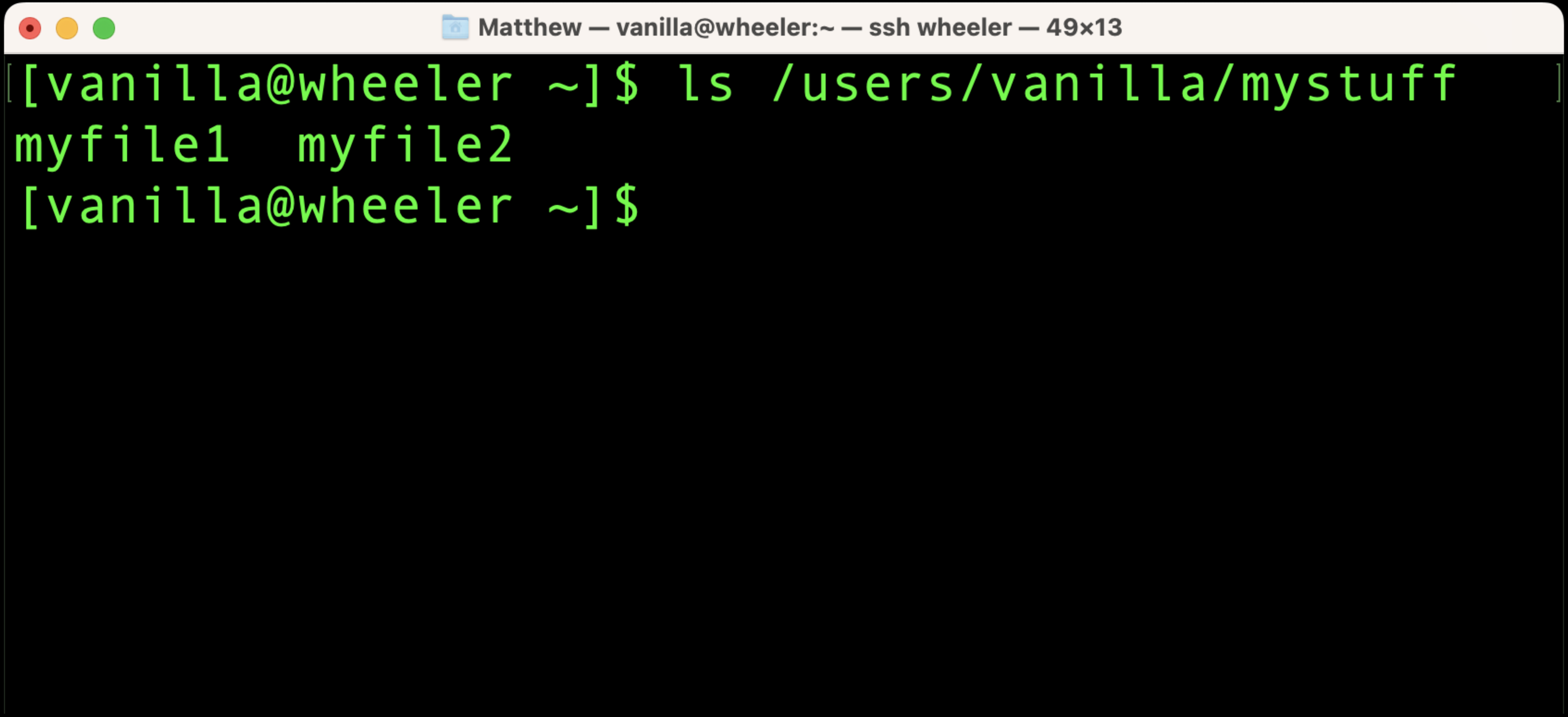
- An absolute path tells one how to get to the destination from starting from the root of the filesystem. E.g “/users/vanilla/mystuff/”

- A relative path specifies how to get there *starting from the current working directory*. E.g vanilla/mystuff/



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

Figuring out where you going…



```
[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.

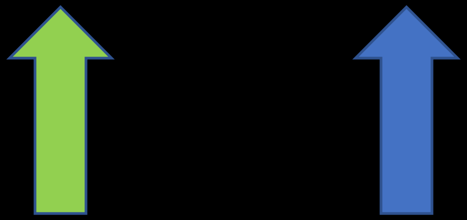
```
[vanilla@wheeler beginner]$ pwd
/projects/shared/workshops/beginner
[vanilla@wheeler beginner]$ cd ~
[vanilla@wheeler ~]$ pwd
/users/vanilla
[vanilla@wheeler ~]$
```

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.

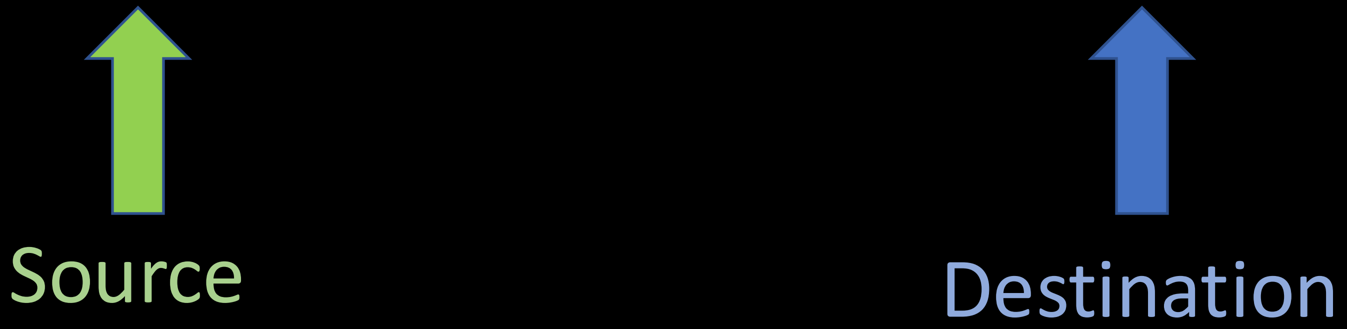
```
[vanilla@wheeler ~]$ cd ~
[vanilla@wheeler ~]$ cp -r mystuff mystuff2
[vanilla@wheeler ~]$
```

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 /tmp/
```



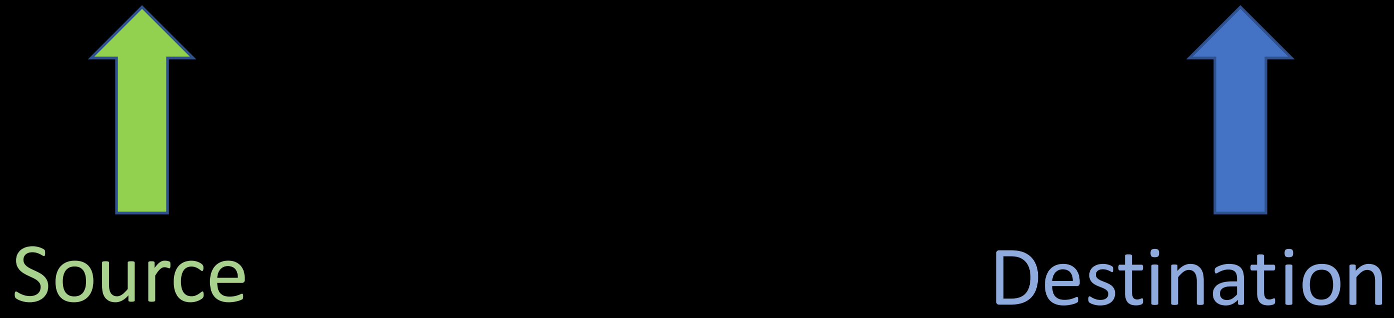
Source

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 /tmp/
```



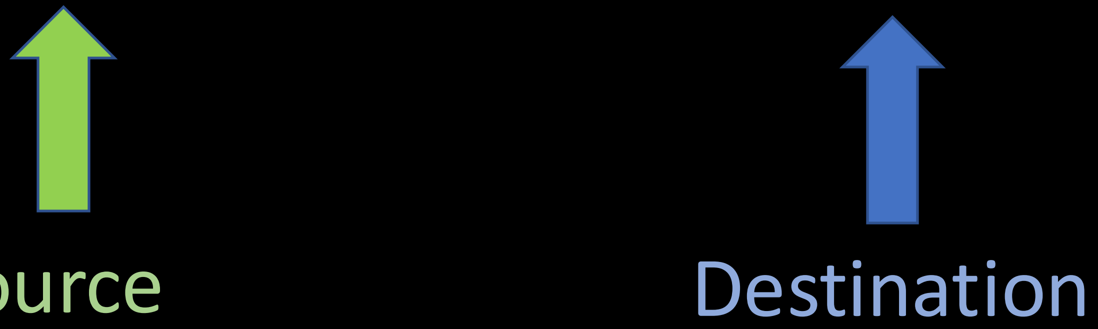
Source

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 /tmp/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…

15 Minute Break

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

Log back into wheeler…

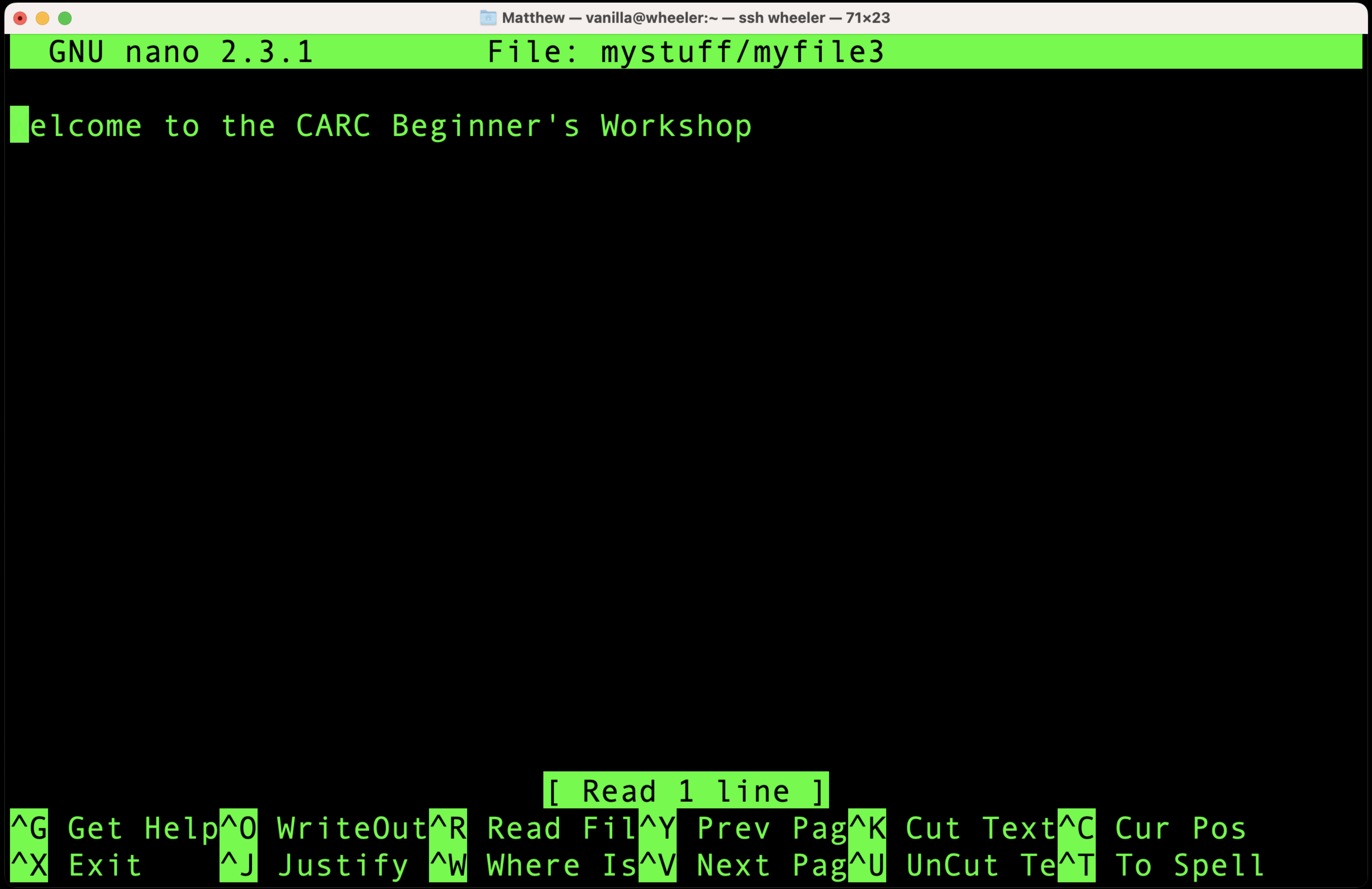
```
[vanilla@wheeler ~]$ file mystuff/myfile0
mystuff/myfile0: data

[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
```

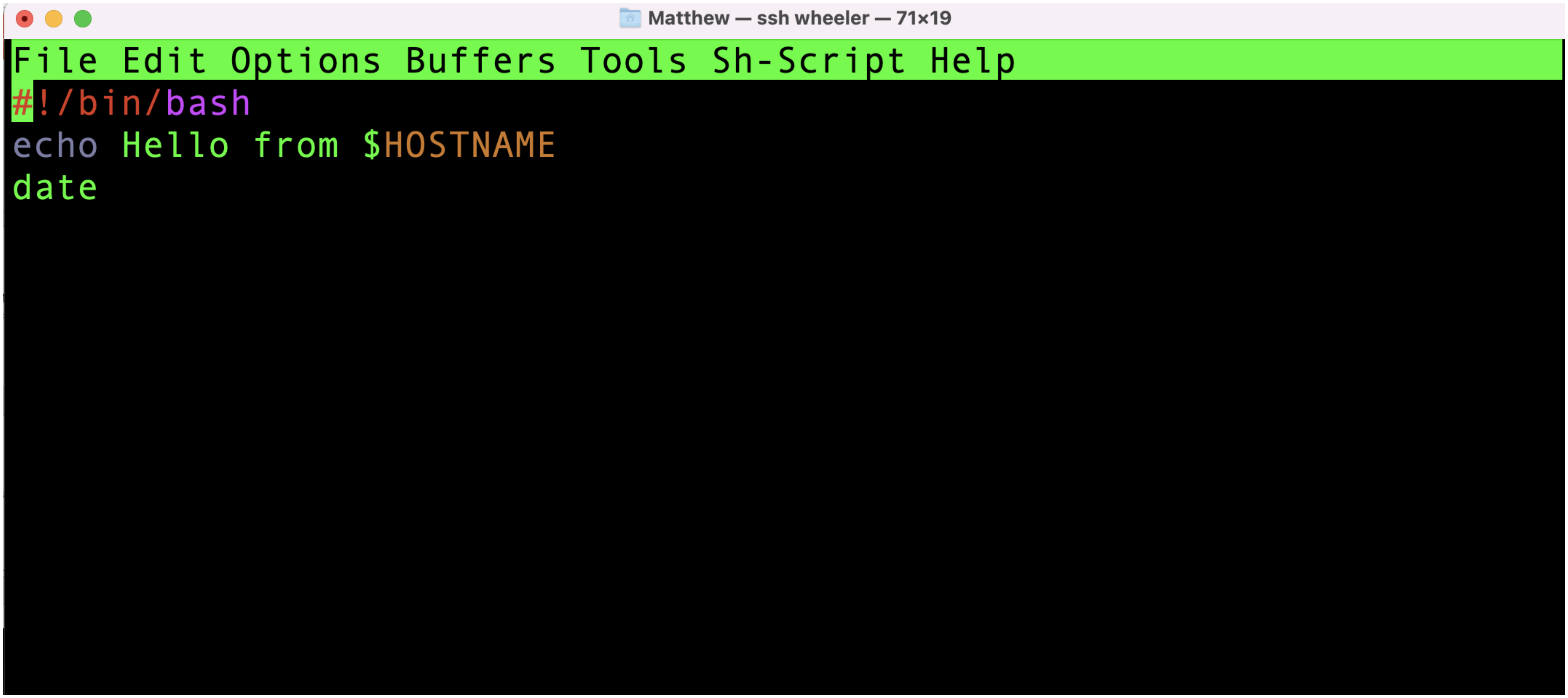


```
  GNU nano 2.3.1           File: mystuff/myfile3

elcome 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…

nano myscript.sh


Matthew — ssh wheeler — 71×19
File Edit Options Buffers Tools Sh-Script Help

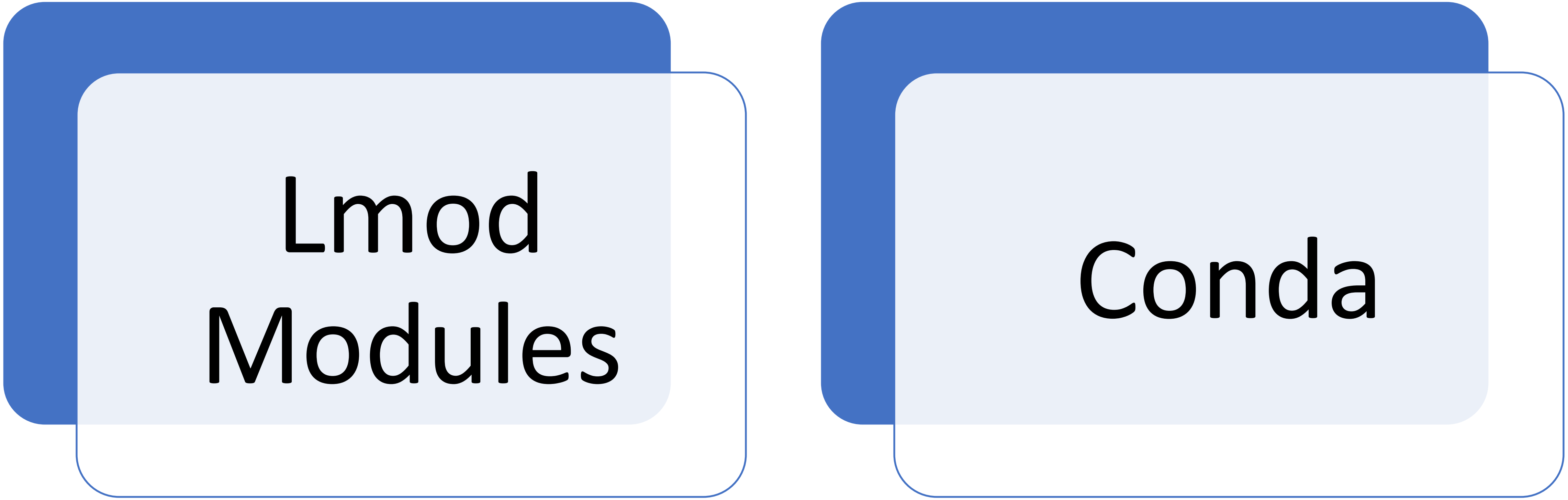
```
#!/bin/bash
echo Hello from $HOSTNAME
date
```

Shell Scripts

```
[vanilla@wheeler ~]$ bash myscript.sh
```

Programs we will use as examples…

Software Access



Lmod Modules

Conda

```
[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
```

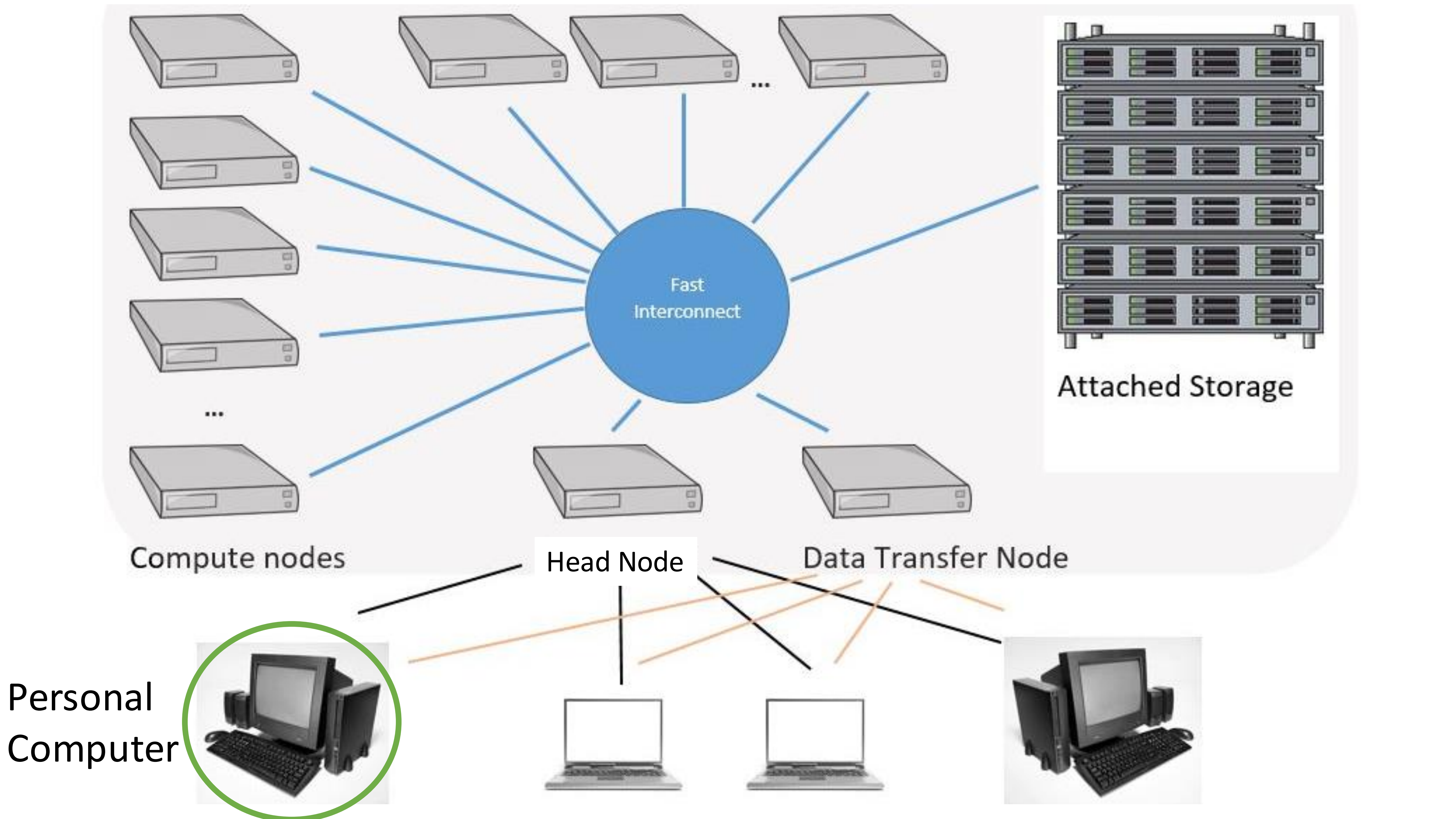
Getting access to software...

```
[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



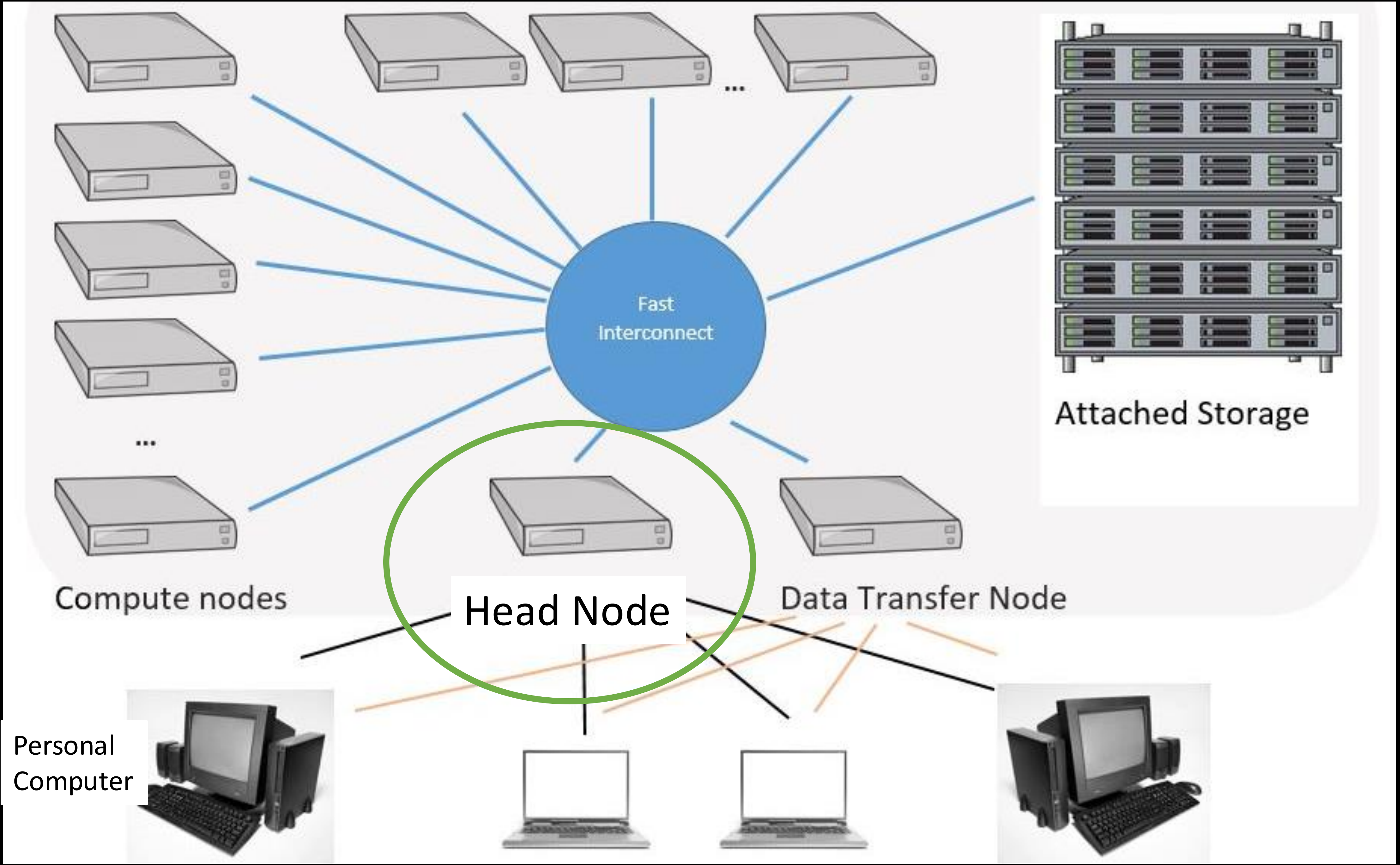
Attached Storage

Compute nodes

Head Node

Data Transfer Node

Personal Computer



Fast Interconnect

...

Attached Storage

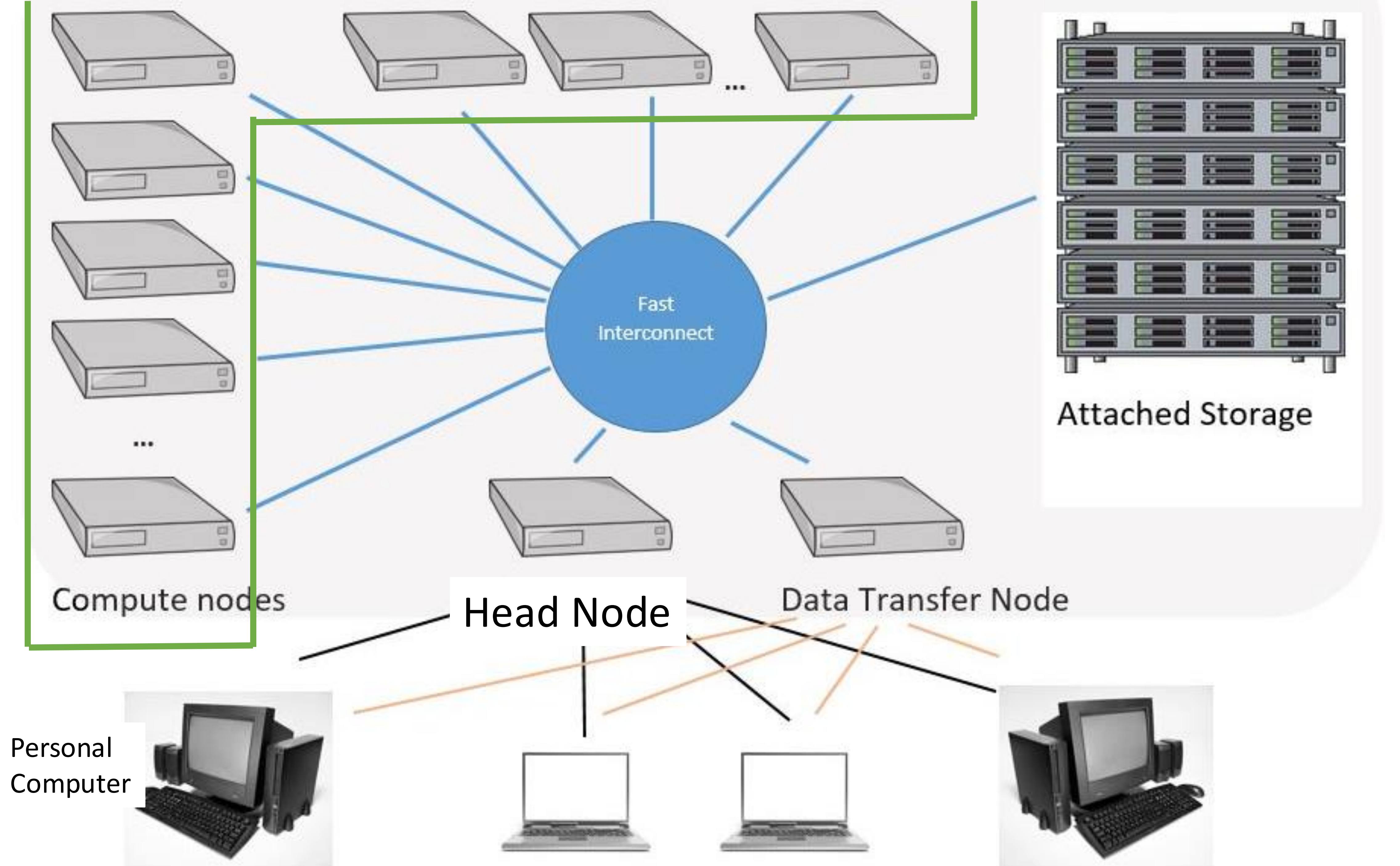
...

Compute nodes

Head Node

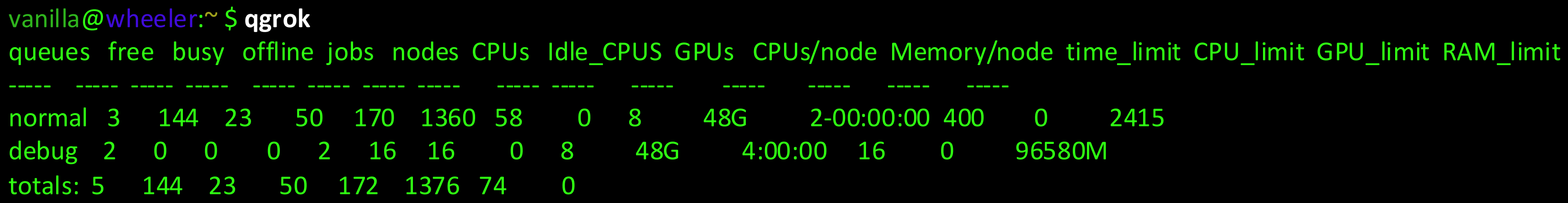
Data Transfer Node

Personal Computer


Fast Interconnect
...
...
Attached Storage
Compute nodes
Head Node
Data Transfer Node
Personal Computer

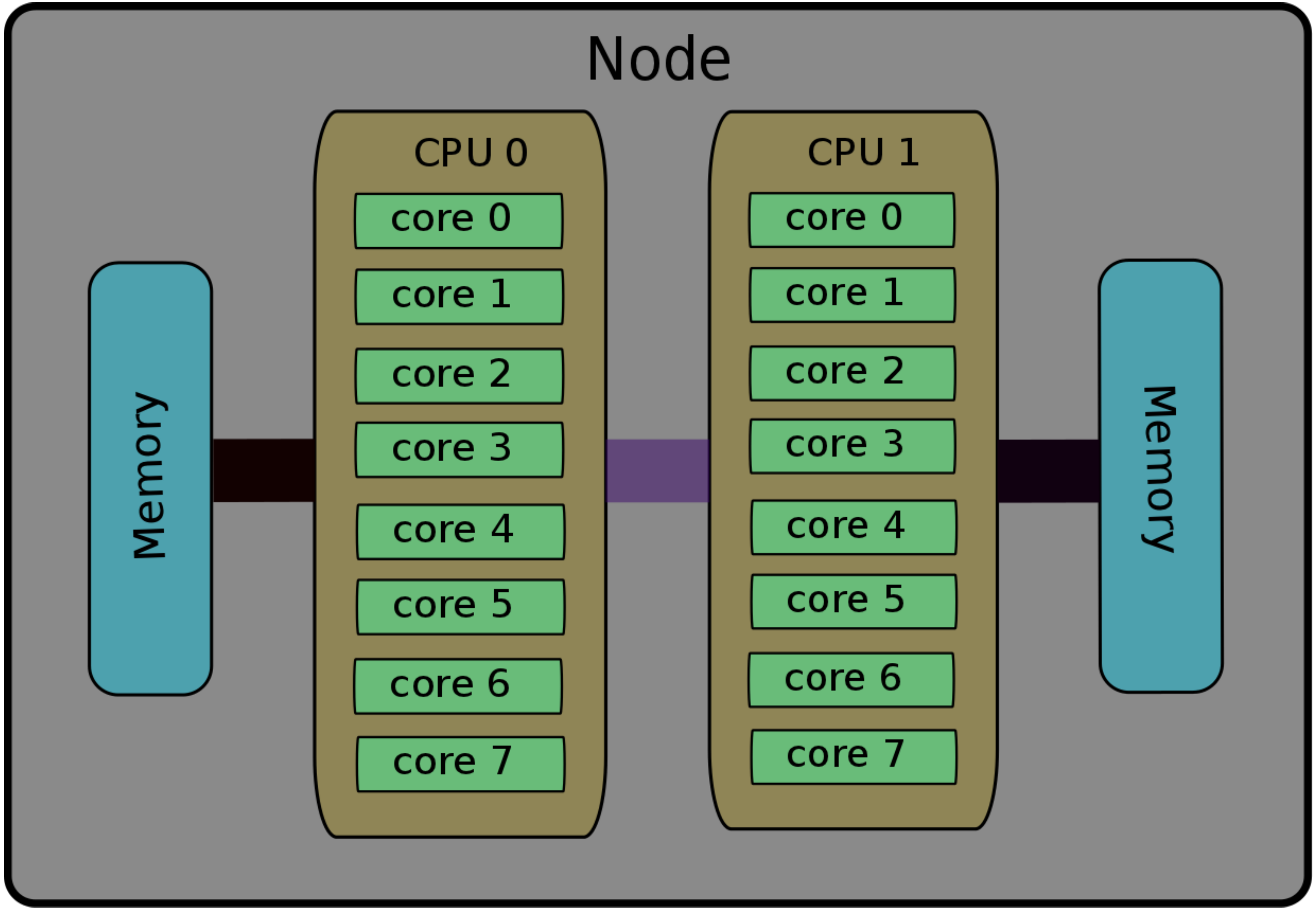
Never run computations on the head node

Always use compute nodes



```
vanilla@wheeler:~ $ qgrok
queues  free  busy  offline  jobs  nodes  CPUs  Idle_CPUS  GPUs  CPUs/node  Memory/node  time_limit  CPU_limit  GPU_limit  RAM_limit
-----   ----- ----- -----    ----- ----- ----- -----      ----- -----     -----        -----       -----      -----
normal  3     144   23       50    170   1360  58         0     8         48G          2-00:00:00  400        0          2415
debug   2     0     0        0     2     16    16         0     8         48G          4:00:00     16         0          96580M
totals: 5     144   23       50    172   1376  74         0
```

Compute nodes and partitions…



Node

Memory

CPU 0

core 0

core 1

core 2

core 3

core 4

core 5

core 6

core 7

CPU 1

core 0

core 1

core 2

core 3

core 4

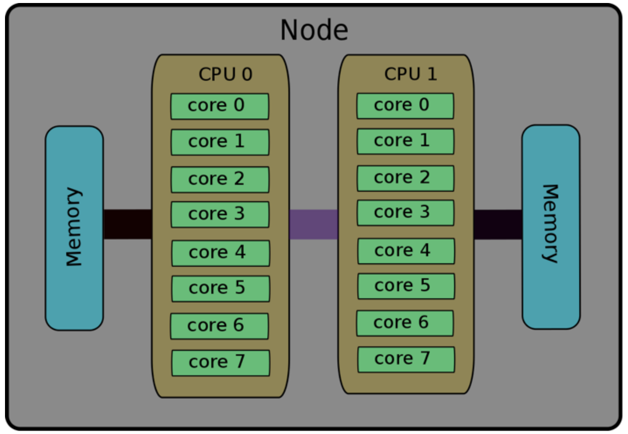
core 5

core 6

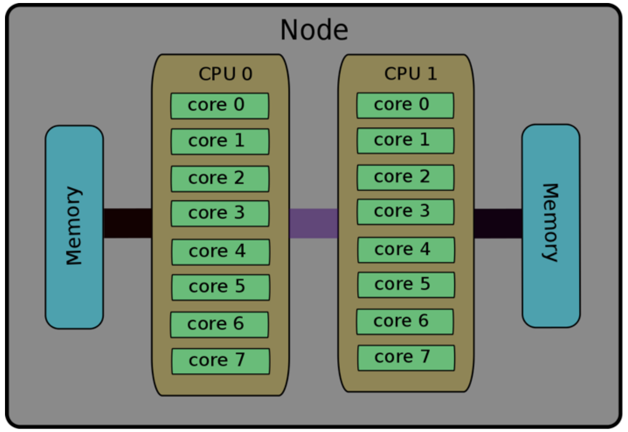
core 7

Memory

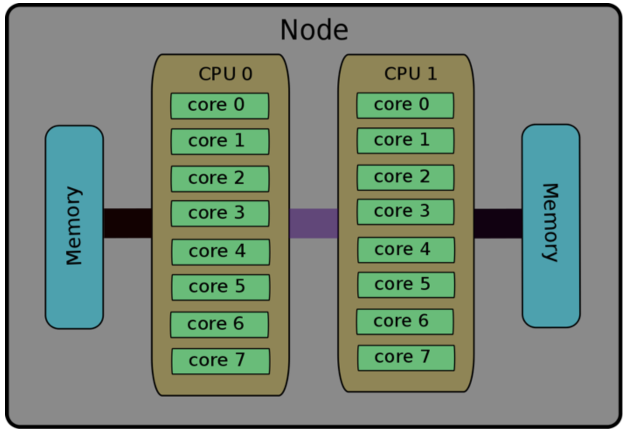
Head Node (wheeler)



Compute Nodes

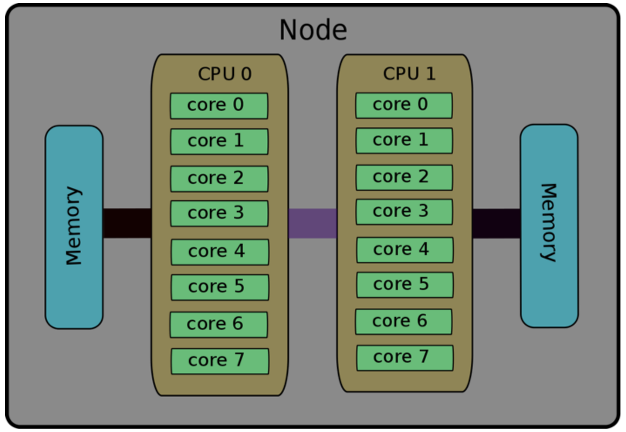


wheeler001



wheeler002

...



wheeler172

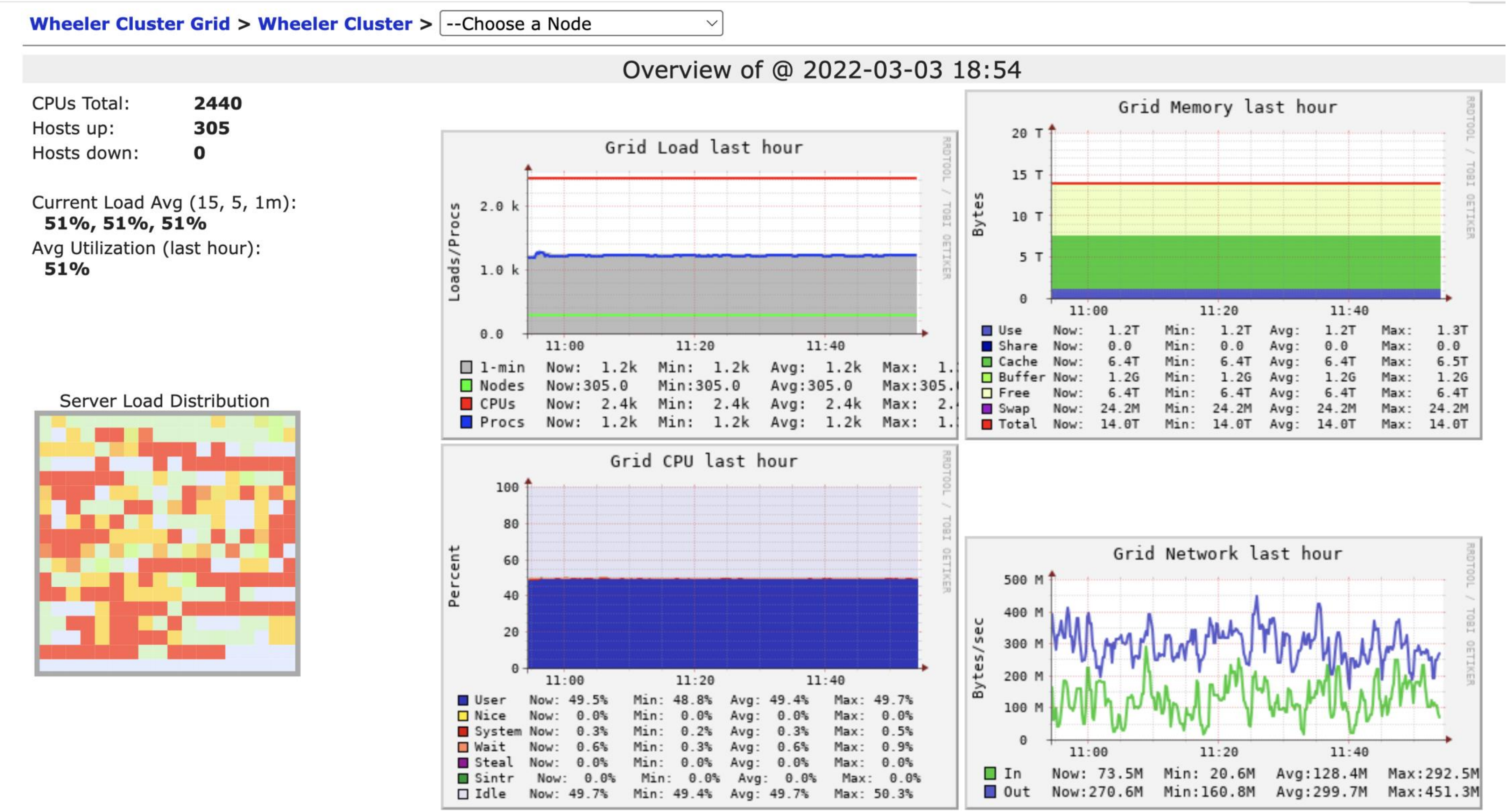
```
[vanilla@wheeler ~]$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                8
On-line CPU(s) list:   0-7
Thread(s) per core:    1
Core(s) per socket:    4
Socket(s):             2
NUMA node(s):          2
Vendor ID:             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** > --Choose a Node

Overview of @ 2022-03-03 18:54

CPUs 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

```
□ 1-min   Now:  1.2k   Min:  1.2k   Avg:  1.2k   Max:  1.
□ Nodes   Now:305.0    Min:305.0    Avg:305.0    Max:305.
□ CPUs    Now:  2.4k   Min:  2.4k   Avg:  2.4k   Max:  2.
□ Procs   Now:  1.2k   Min:  1.2k   Avg:  1.2k   Max:  1.
```

```
□ Use    Now:   1.2T   Min:   1.2T   Avg:   1.2T   Max:   1.3T
□ Share  Now:   0.0    Min:   0.0    Avg:   0.0    Max:   0.0
□ Cache  Now:   6.4T   Min:   6.4T   Avg:   6.4T   Max:   6.5T
□ Buffer Now:   1.2G   Min:   1.2G   Avg:   1.2G   Max:   1.2G
□ Free   Now:   6.4T   Min:   6.4T   Avg:   6.4T   Max:   6.4T
□ Swap   Now:  24.2M   Min:  24.2M   Avg:  24.2M   Max:  24.2M
□ Total  Now:  14.0T   Min:  14.0T   Avg:  14.0T   Max:  14.0T
```

```
□ User   Now: 49.5%   Min: 48.8%   Avg: 49.4%   Max: 49.7%
□ Nice   Now:  0.0%   Min:  0.0%   Avg:  0.0%   Max:  0.0%
□ System Now:  0.3%   Min:  0.2%   Avg:  0.3%   Max:  0.5%
□ Wait   Now:  0.6%   Min:  0.3%   Avg:  0.6%   Max:  0.9%
□ Steal  Now:  0.0%   Min:  0.0%   Avg:  0.0%   Max:  0.0%
□ Sintr   Now:  0.0%   Min:  0.0%   Avg:  0.0%   Max:  0.0%
□ Idle   Now: 49.7%   Min: 49.4%   Avg: 49.7%   Max: 50.3%
```

```
□ In    Now: 73.5M   Min: 20.6M   Avg:128.4M   Max:292.5M
□ Out   Now:270.6M   Min:160.8M   Avg:299.7M   Max:451.3M
```

5 Minute Break

Technology, IT etc.

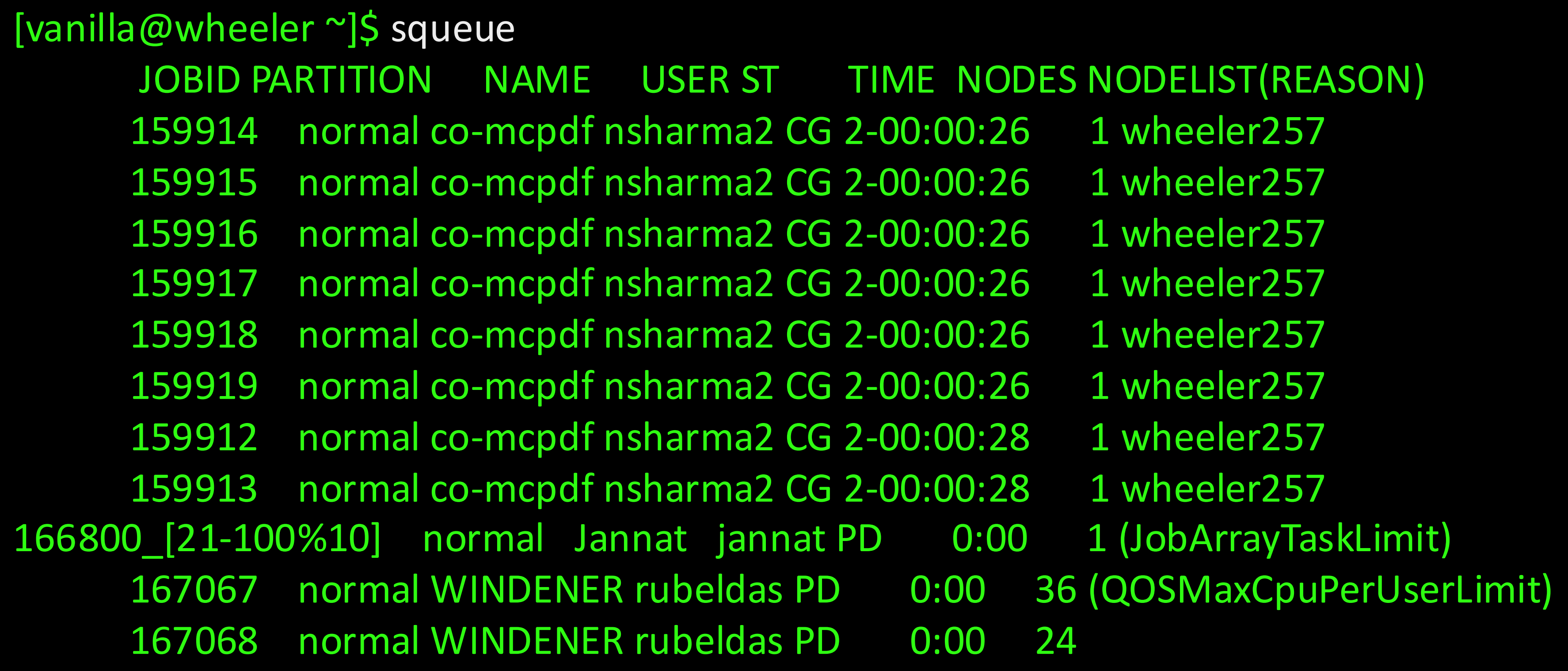
SLURM

means

Simple Linux Utility for Resource Management

by acronymsandslang.com

ENJOY
Slurm
SODA
IT'S HIGHLY ADDICTIVE!
VOTED #1 SOFT DRINK OF THE 31ST CENTURY!
SLURMS MCKENZIE



```
[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?

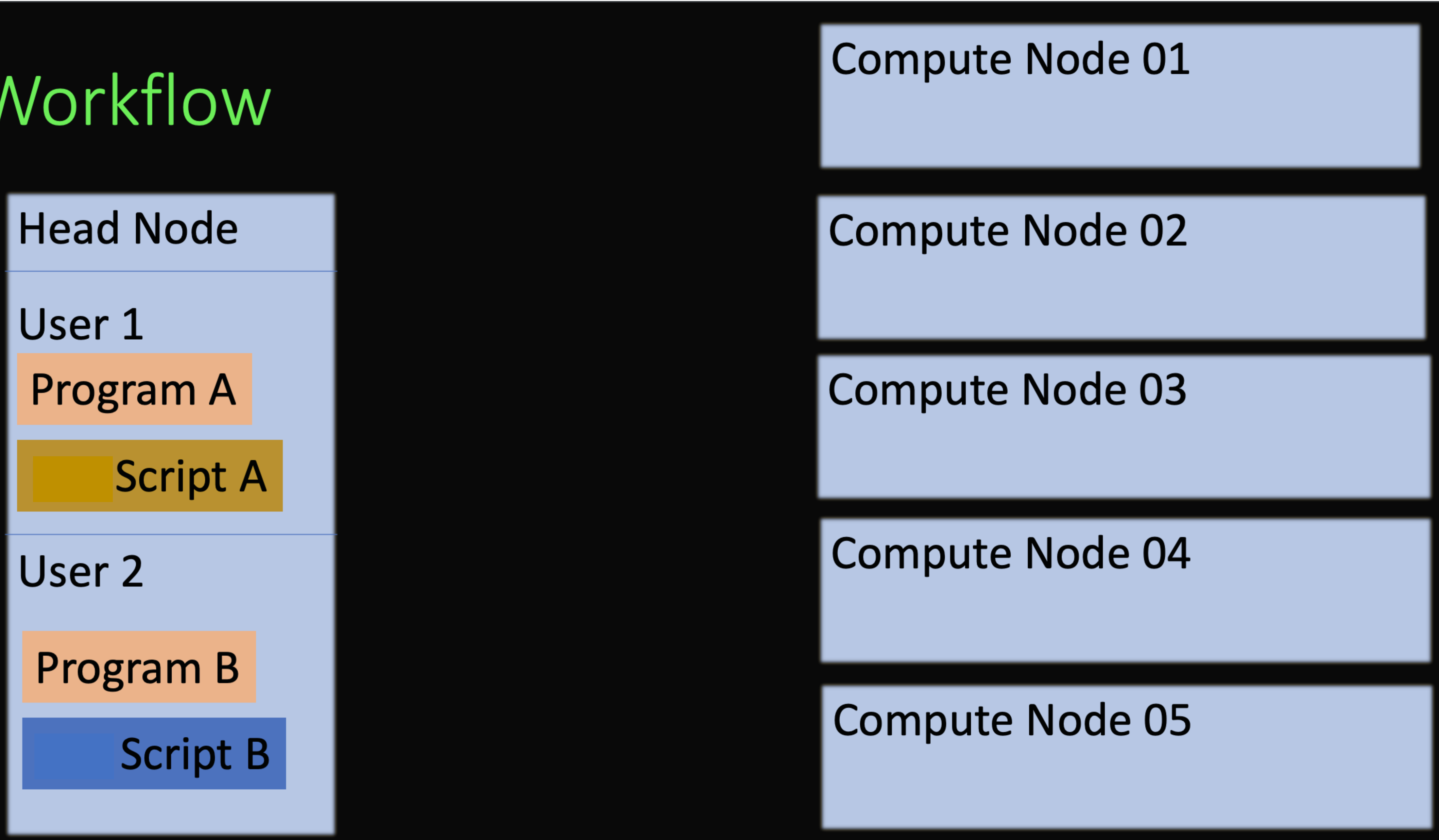
```
[vanilla@wheeler ~/vecadd]$ srun --partition debug --ntasks 4 vecaddmpi
```

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



Head Node

User 1

Program A

Script A

User 2

Program B

Script B

Compute Node 01

Compute Node 02

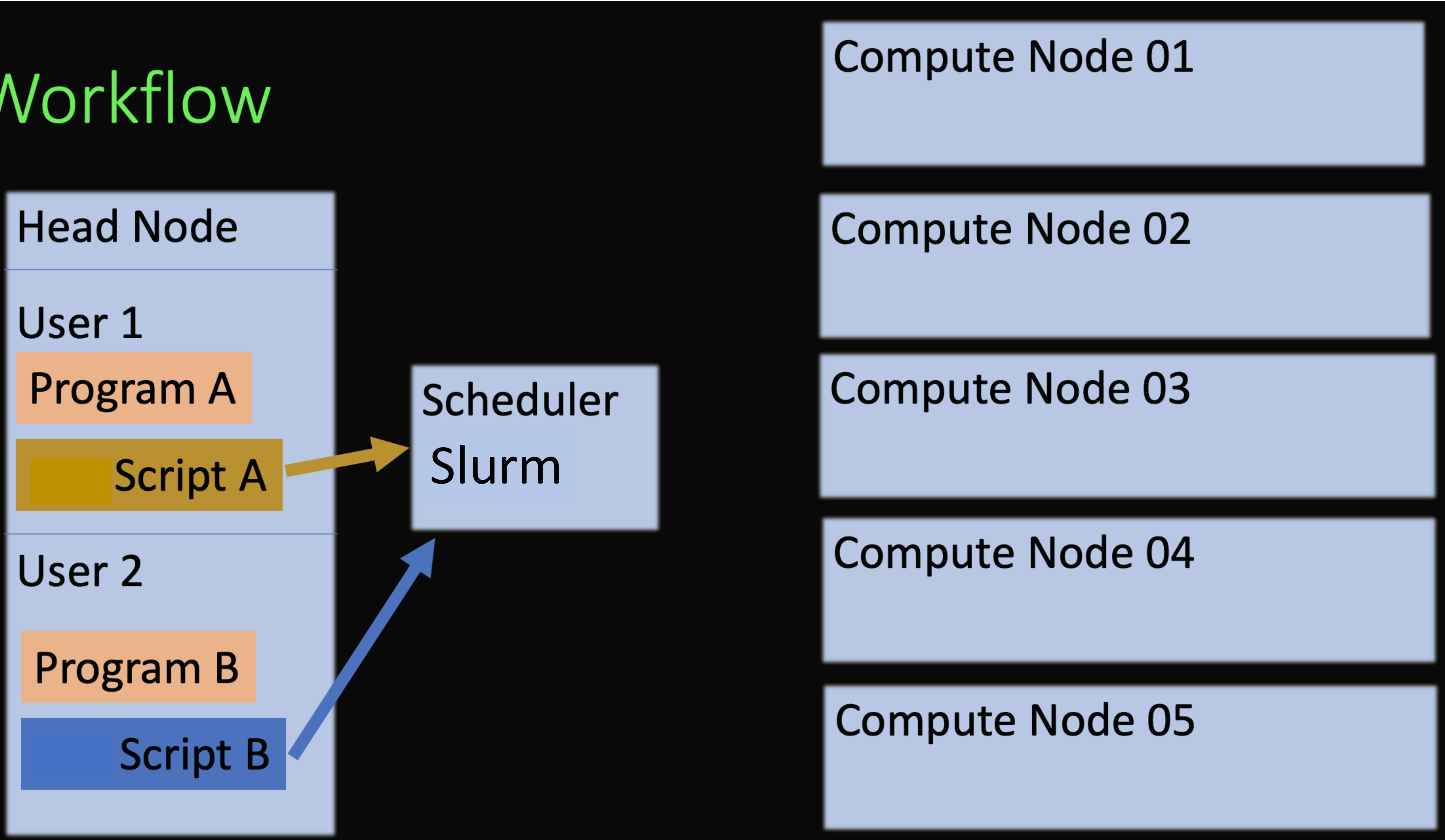
Compute Node 03

Compute Node 04

Compute Node 05

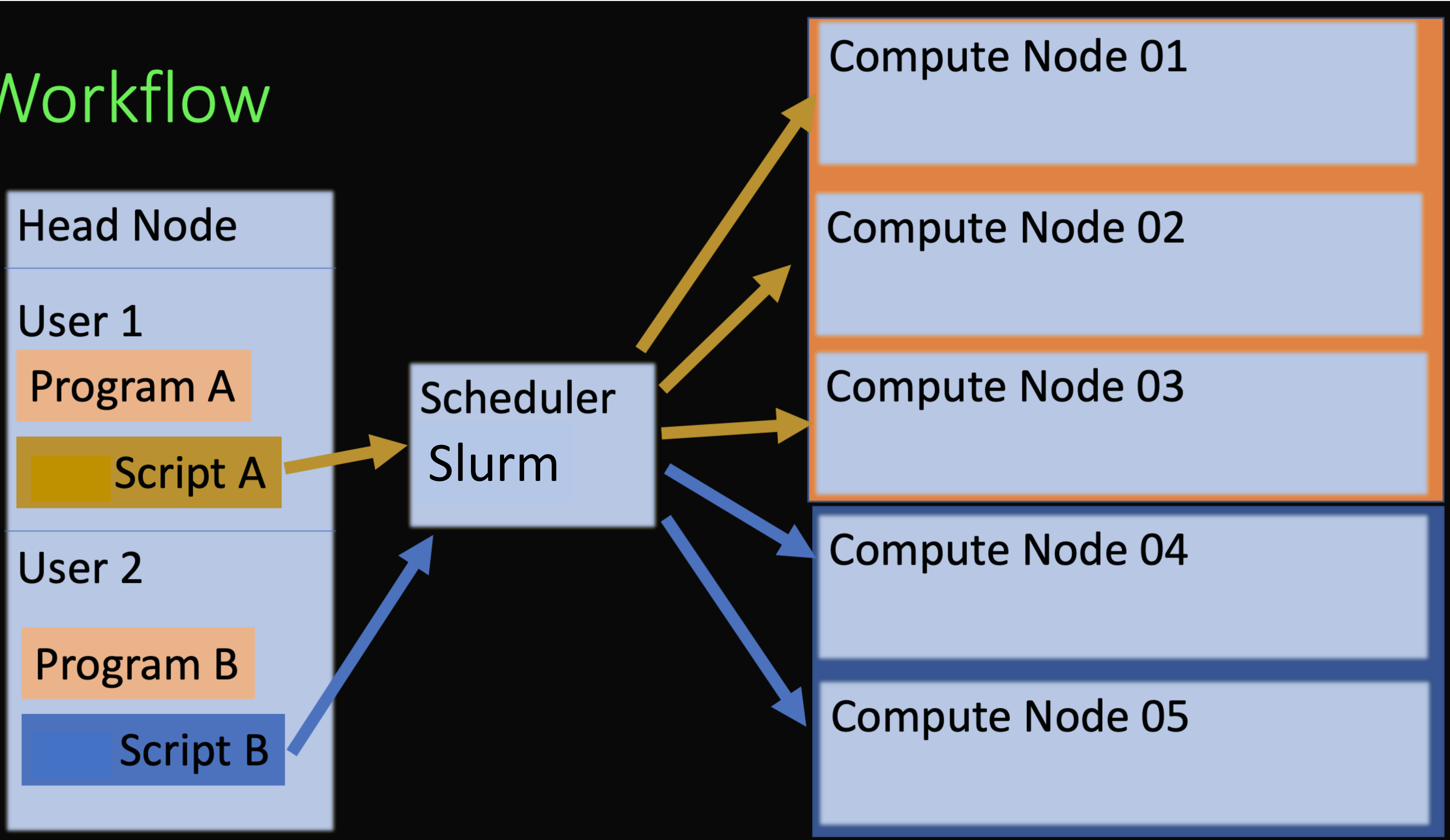
Shared filesystems – All nodes can access the same programs and write output

Workflow



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

Workflow



Head Node

User 1

Program A

Script A

User 2

Program B

Script B

Scheduler

Slurm

Compute Node 01

Compute Node 02

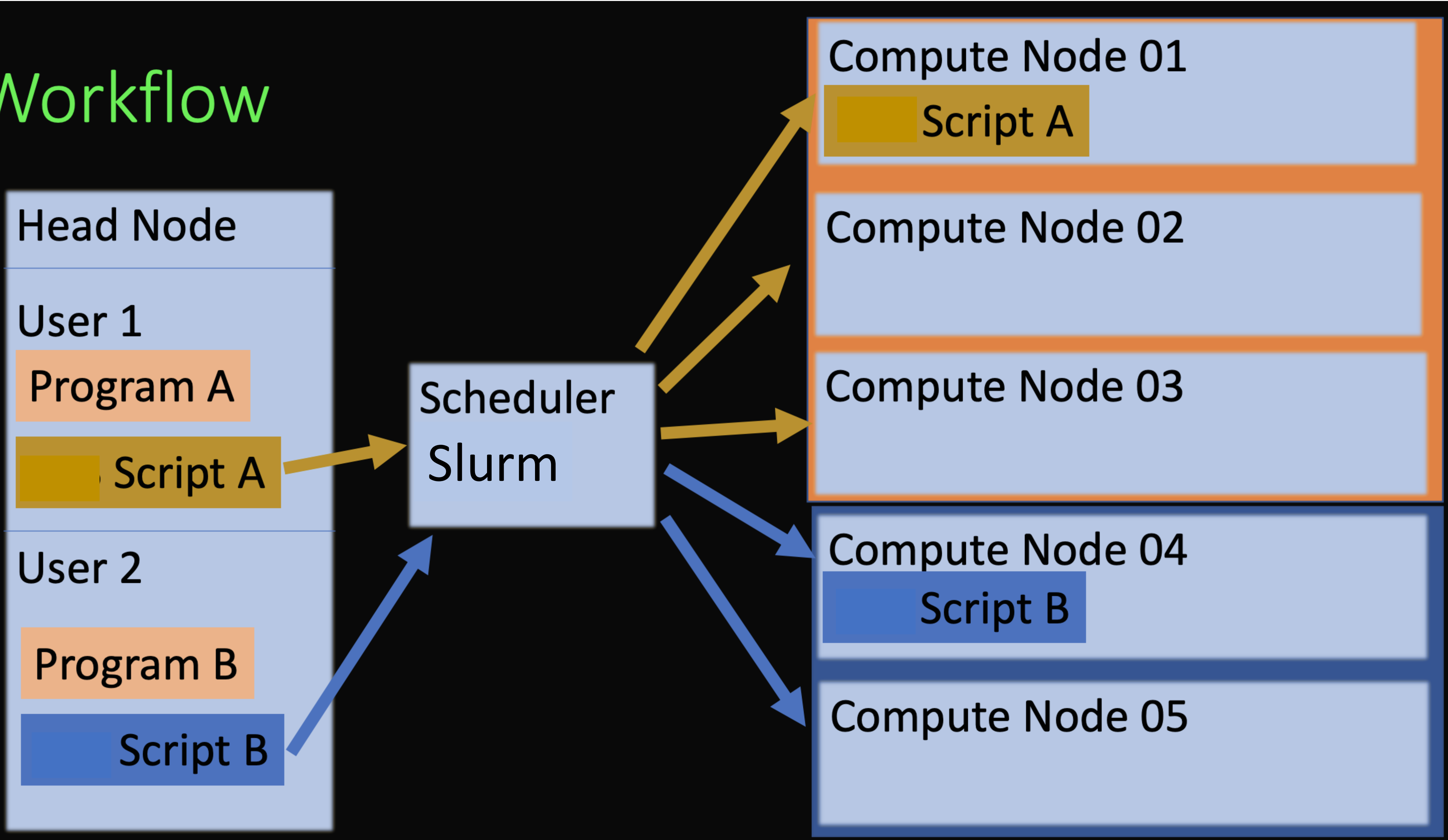
Compute Node 03

Compute Node 04

Compute Node 05

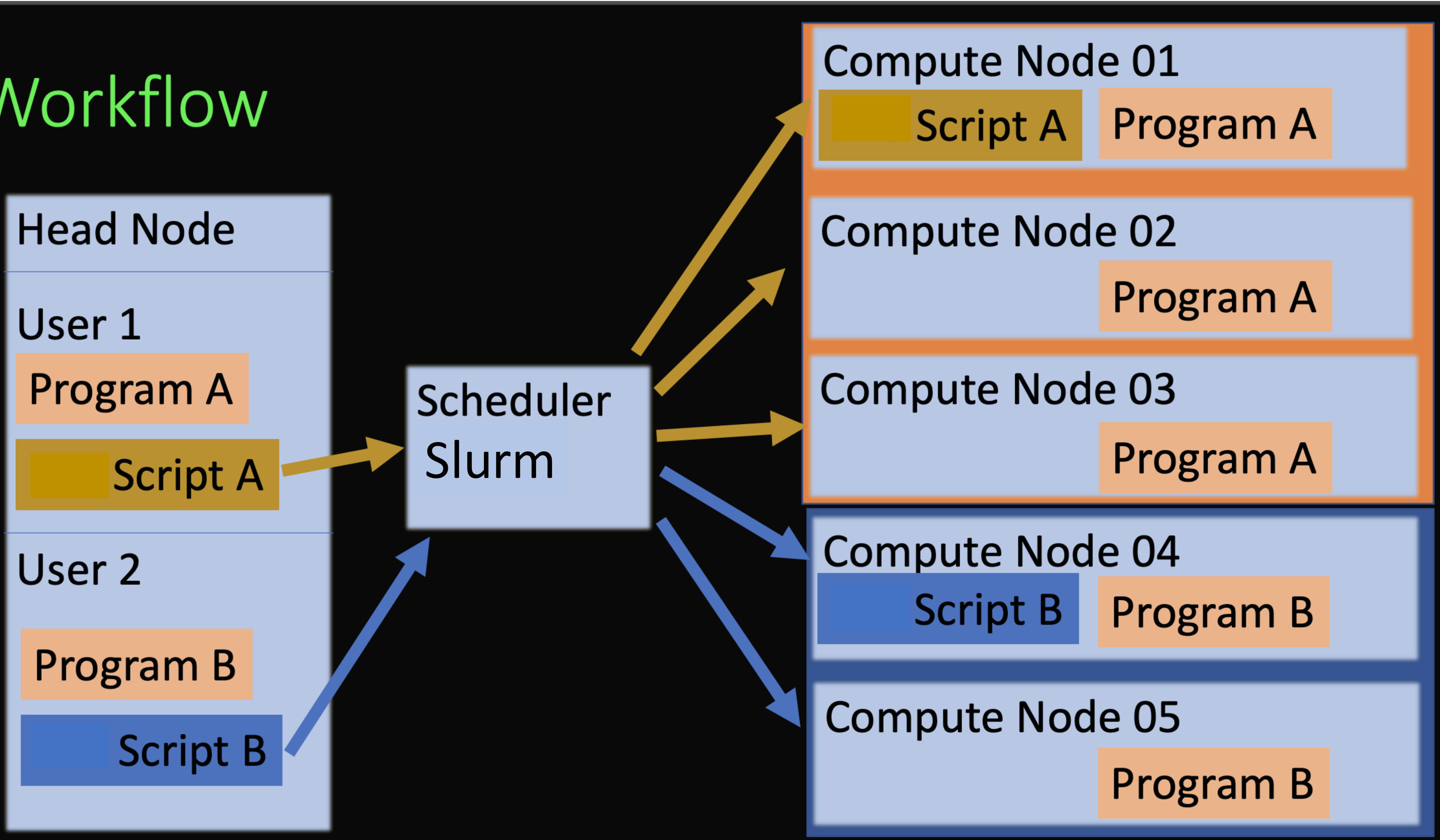
Shared filesystems – All nodes can access the same programs and write output

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

Scheduler

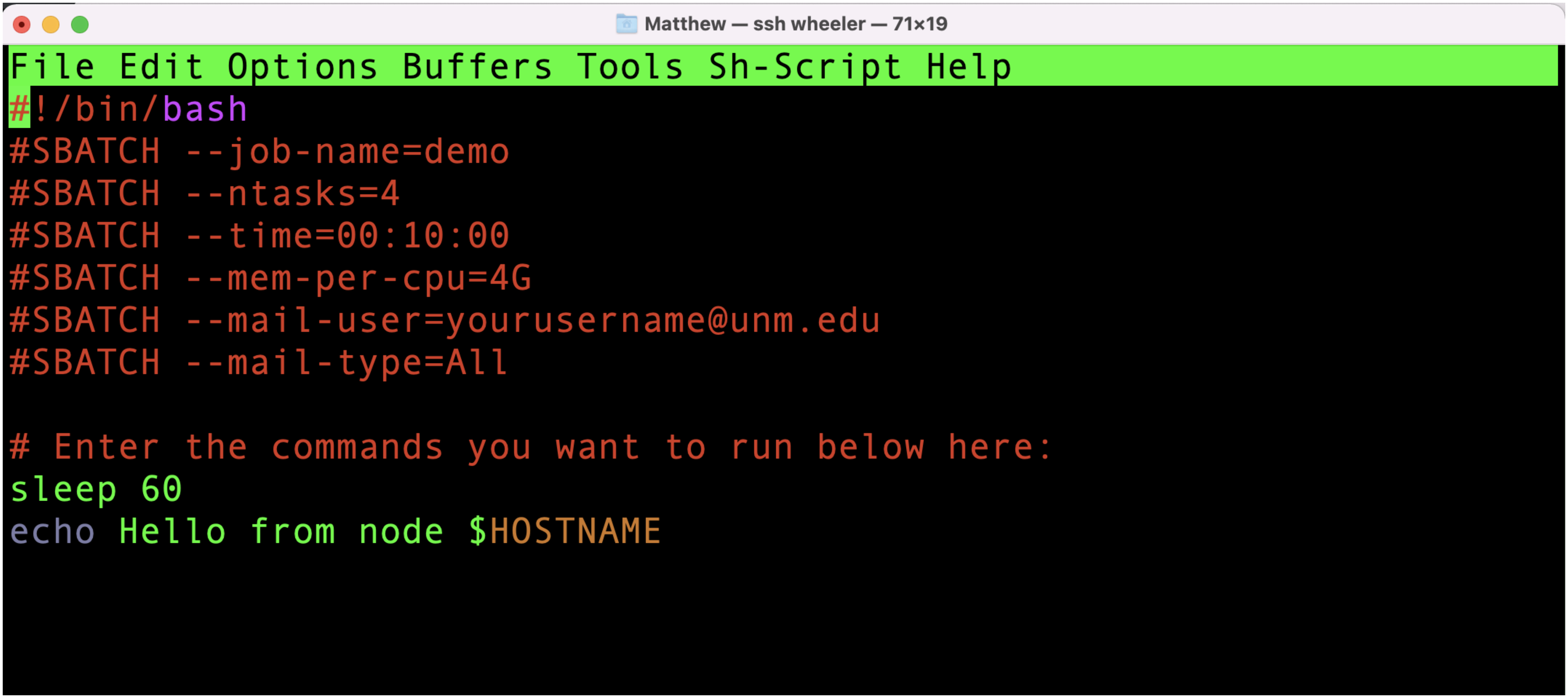
qgrok

sbatch

squeue –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


Matthew — ssh wheeler — 71×19
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

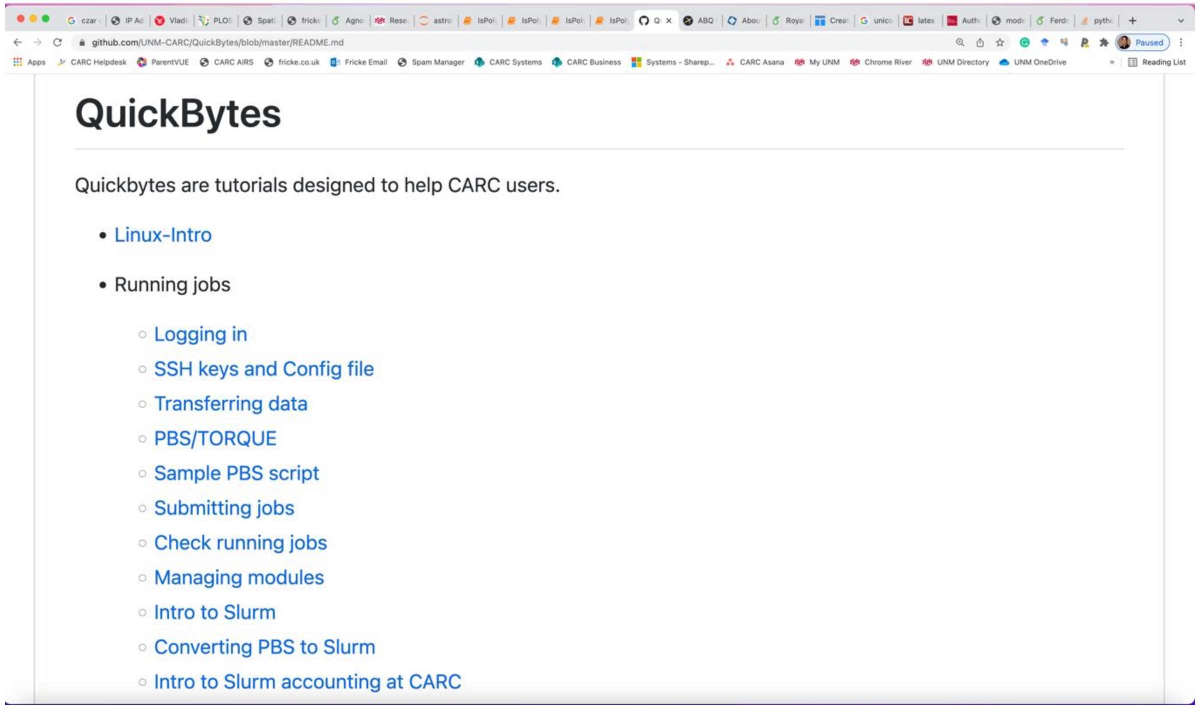
squeue --me --long	shows information about jobs you submitted
squeue --me --start	shows when slurm expects your job to start
scancel jobid	cancels a job
sacct	shows your job history

```
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

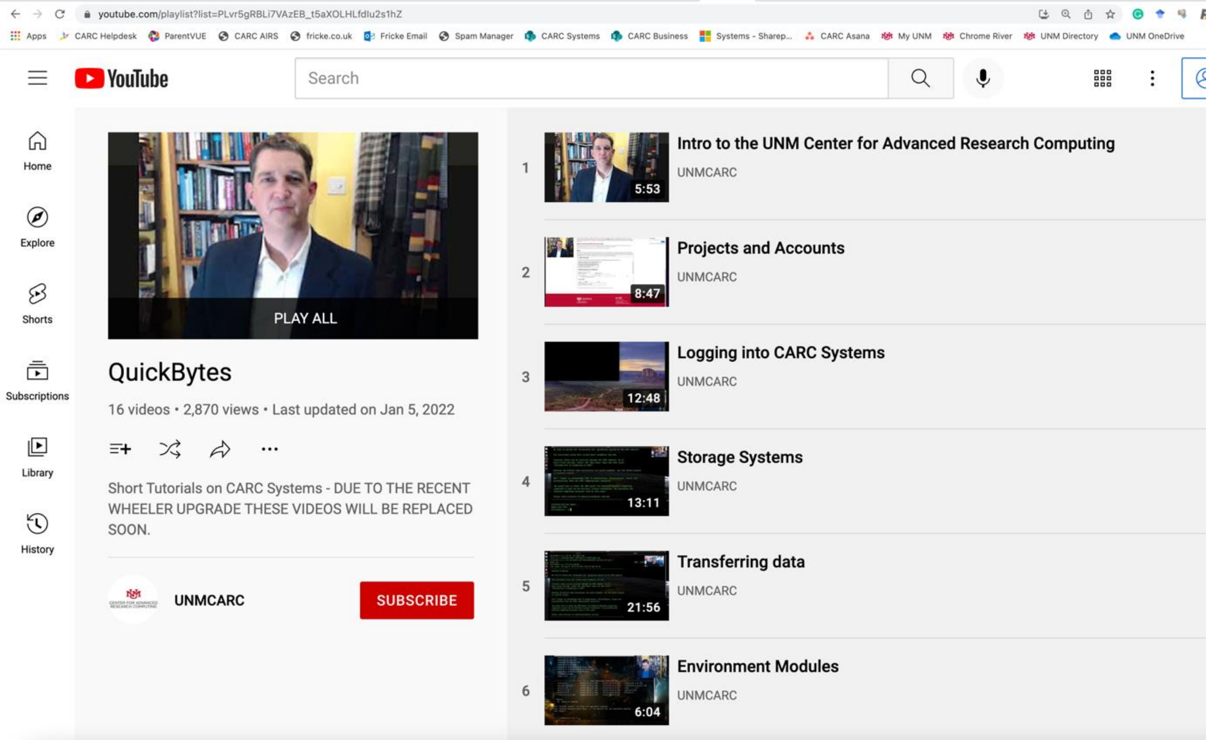
- Tutorial Videos
- Written Tutorials



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



QuickBytes

16 videos • 2,870 views • Last updated on Jan 5, 2022

Short Tutorials on CARC Systems - DUE TO THE RECENT WHEELER UPGRADE THESE VIDEOS WILL BE REPLACED SOON.

UNMCARC

1 Intro to the UNM Center for Advanced Research Computing — UNMCARC — 5:53

2 Projects and Accounts — UNMCARC — 8:47

3 Logging into CARC Systems — UNMCARC — 12:48

4 Storage Systems — UNMCARC — 13:11

5 Transferring data — UNMCARC — 21:56

6 Environment Modules — UNMCARC — 6:04

Getting Help

help@carc.unm.edu

Office hours

Bonus – sview and graphical programs