Introduction to Linux and Cluster Computing Environments for Bioinformatics

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What you will learn

- Linux Supercomputer overview
- Basics of a Linux shell, including moving/editing/creating/deleting files, how to launch/terminate programs, check progress
- Basic shell scripting, parallel execution
- Fundamentals of cluster supercomputer use
- Example of scaling things up

The rice.rcac.purdue.edu cluster

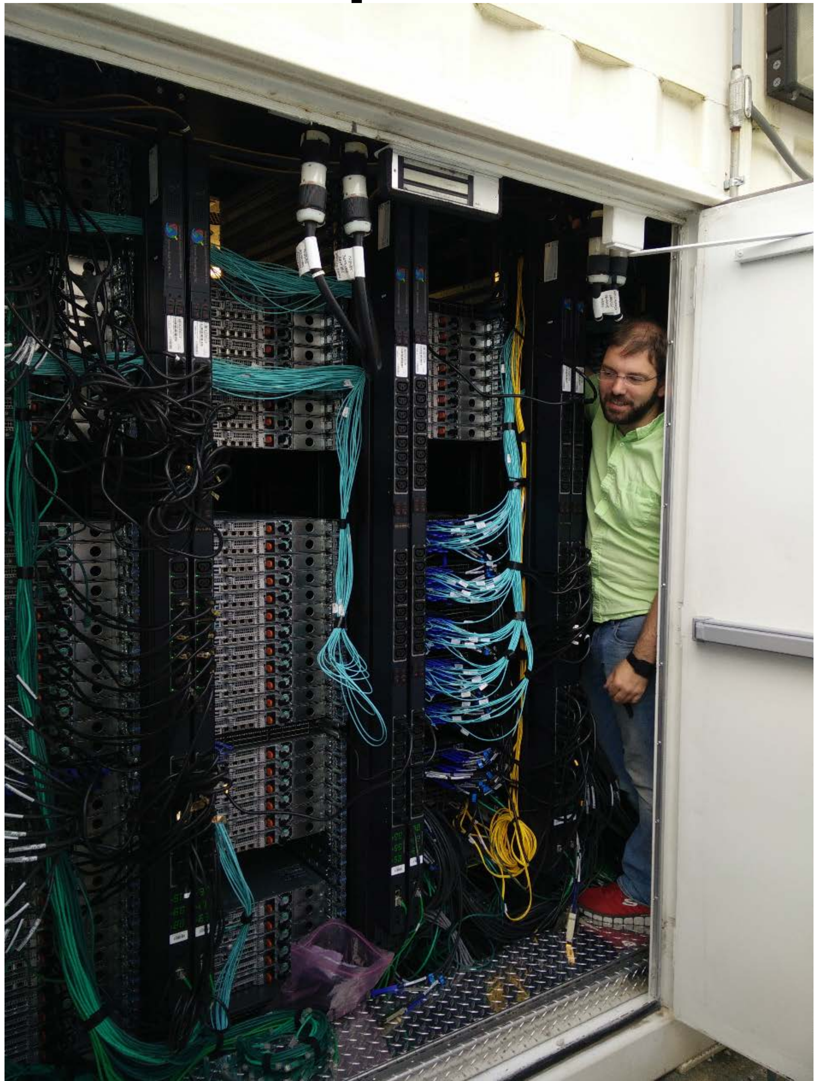
The rice.rcac.purdue.edu cluster

An individual node

The brown.rcac.purdue.edu cluster

The brown.rcac.purdue.edu cluster

The brown.rcac.purdue.edu cluster



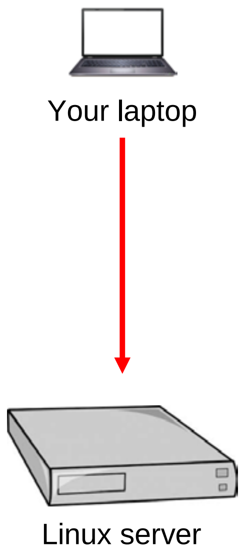
Brown supercomputer stats

- 550 Nodes, 13,200 total CPU cores
- Each nodes has 24 CPU cores, 96GB RAM
- 3.4 Petabytes of scratch space for this cluster alone
- 4.5 Petabytes of long term storage shared among all clusters
- Currently #302 on top500.org, Conte is #190.

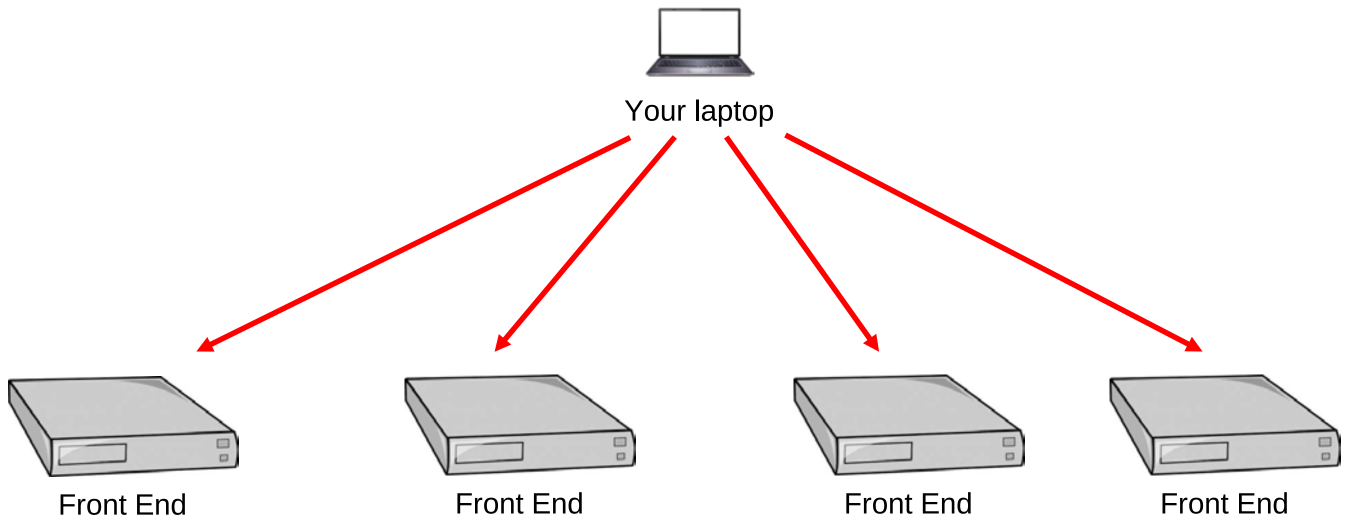
Anecdote time!

- A colleague was working on a game theory problem…

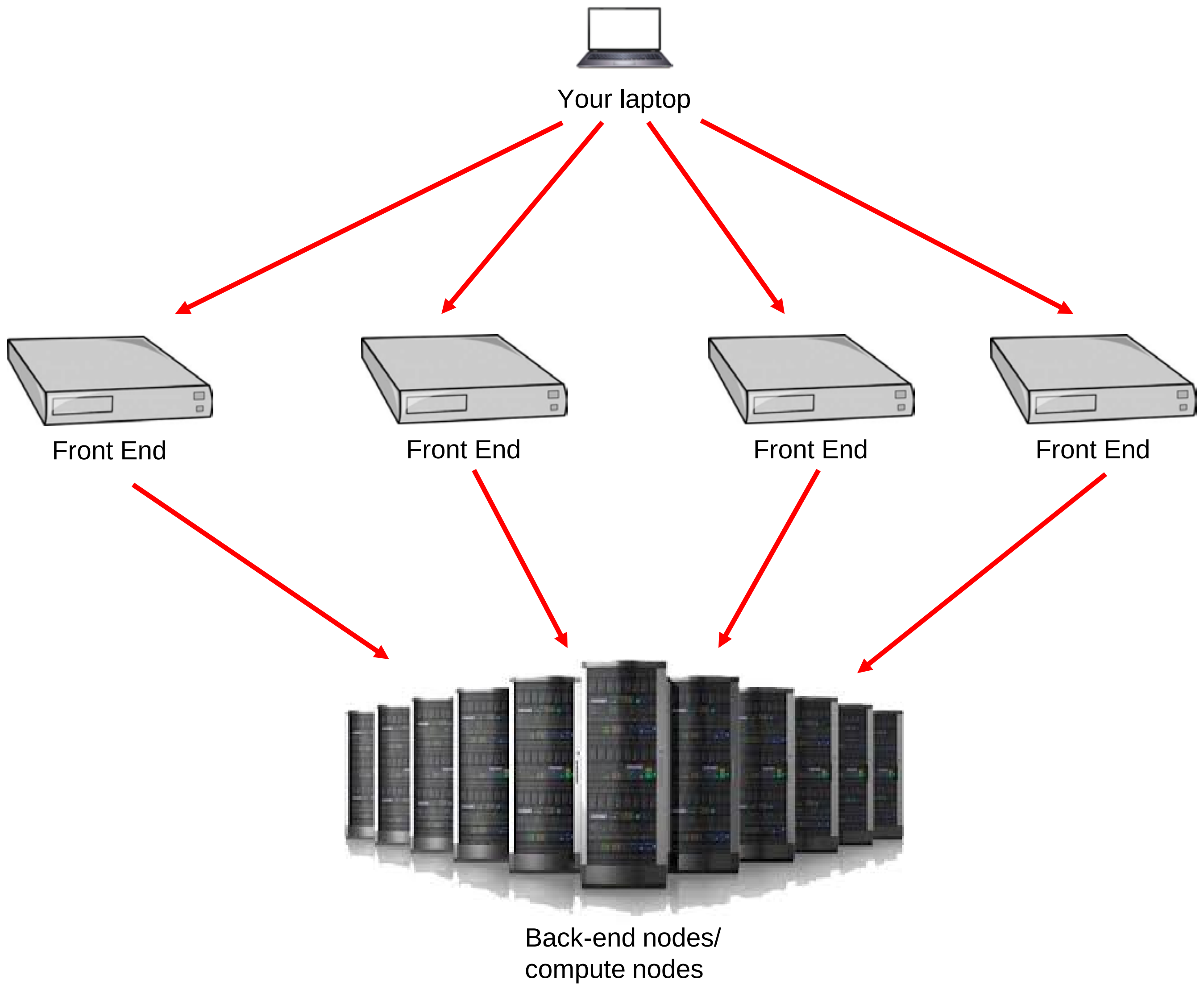
Linux and Cluster Computing Environments



Linux and Cluster Computing Environments



Linux and Cluster Computing Environments



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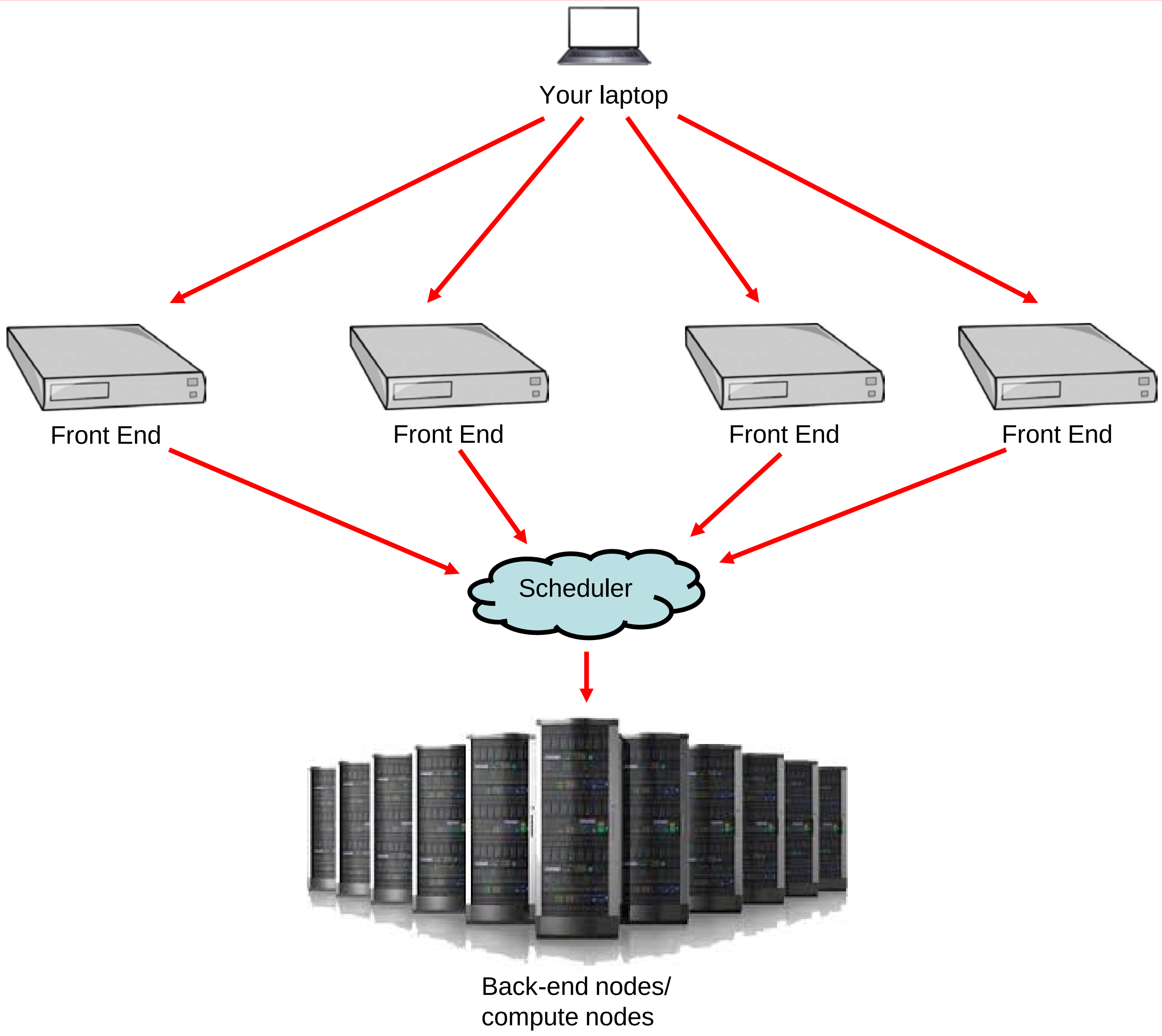
Linux and Cluster Computing Environments



Why Linux?

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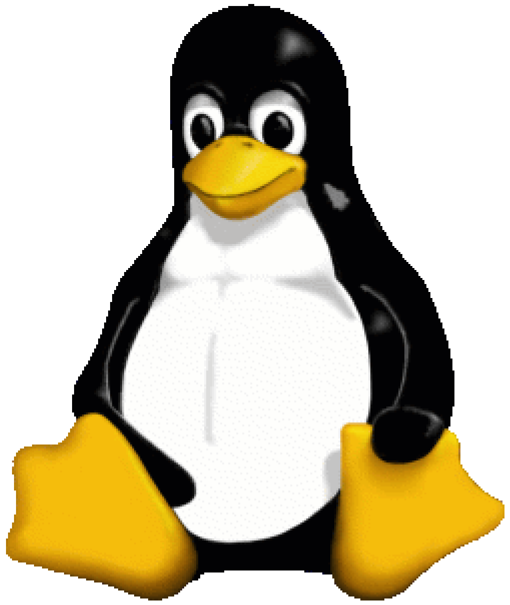

Why Linux?

- Can be desktops, but tend to be larger servers in some remote, environmentally controlled data center (or pod!)
- Multiple CPU cores per server (~8-44)
- Large amounts of RAM (64GB – 1TB is common)
- Multiple users can use the same computer simultaneously

Why Linux? (cont.)

- Can interact with a graphical interface
- More common to interact with a text based interface
- Servers tend to stay up for a long time between reboots (months)
- Commonly launch programs and walk away for days, weeks, or months as they run
- Computations can scale up as servers added

But where are the keyboards, mice, and monitors?

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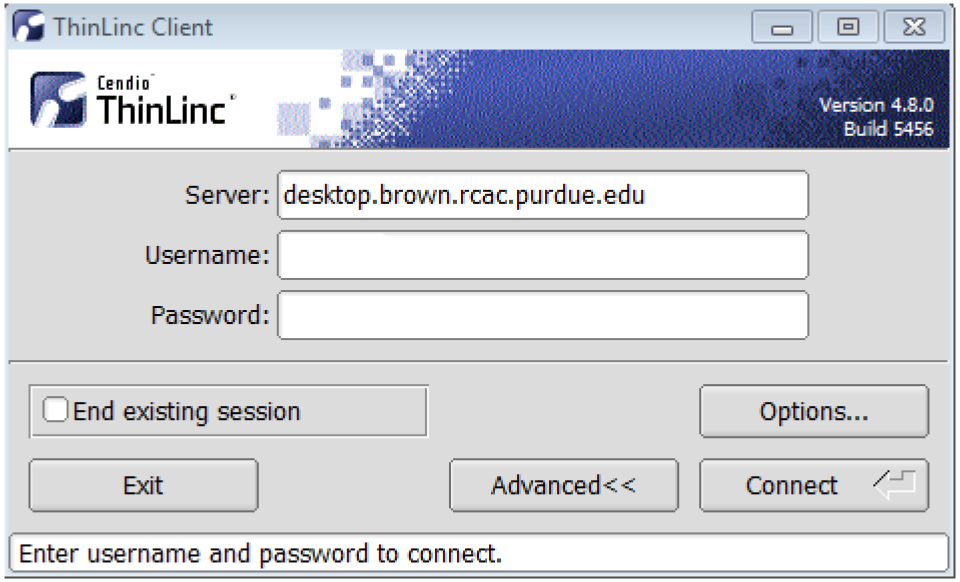
ThinLinc Linux graphical interface

- We will use ThinLinc to provide a graphical user interface on a Brown front-end
- From the front-end we'll connect to a Brown node, aka back-end node, aka compute node, where we will do the real computing
- The ThinLinc client is free (and better), but you can actually use a web browser instead

Logging in via ThinLinc Client



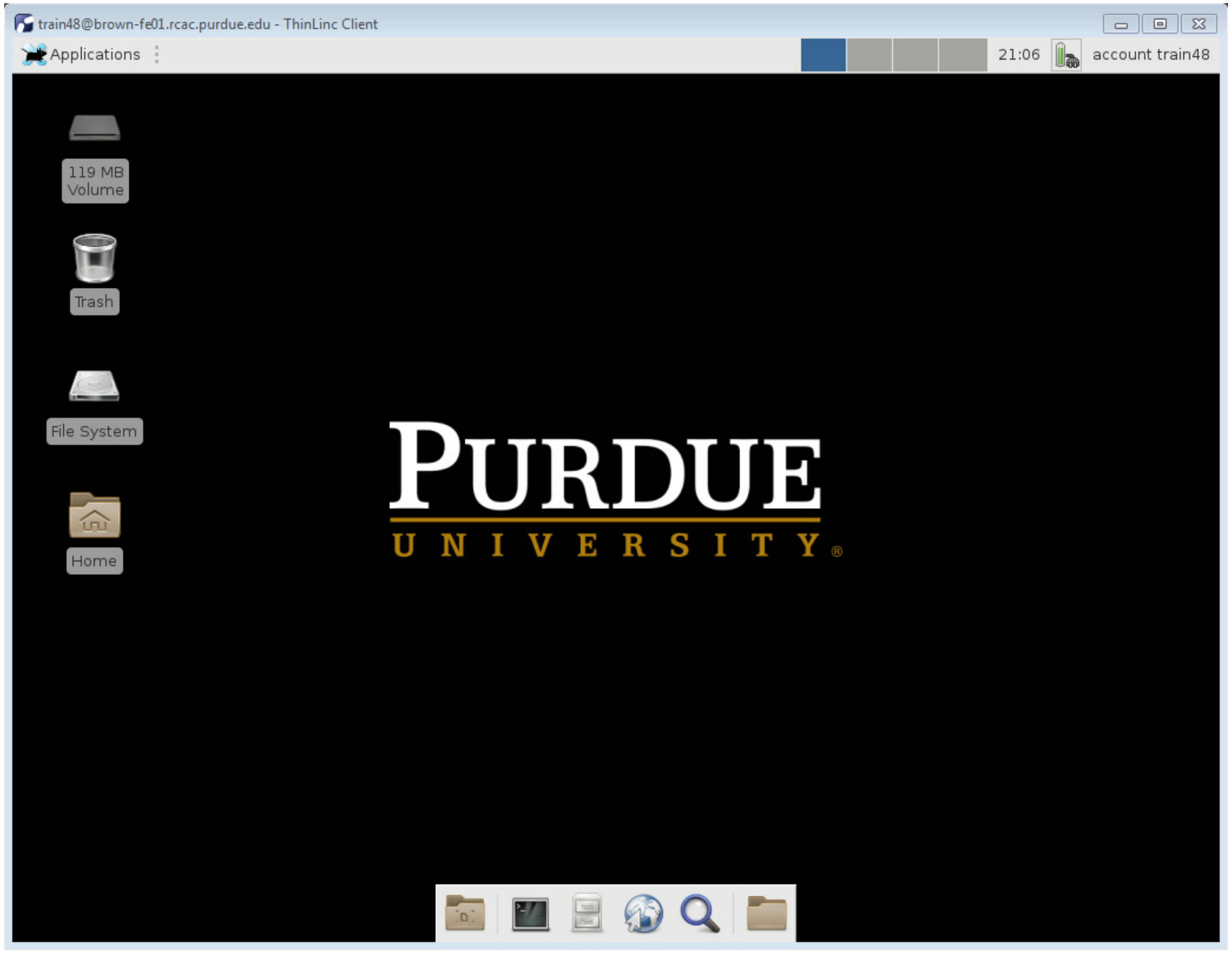
Server: desktop.brown.rcac.purdue.edu

Username:

Password:

Enter username and password to connect.

Connected!!!


train48@brown-fe01.rcac.purdue.edu - ThinLinc Client
Applications
21:06
account train48
119 MB Volume
Trash
File System
Home
PURDUE
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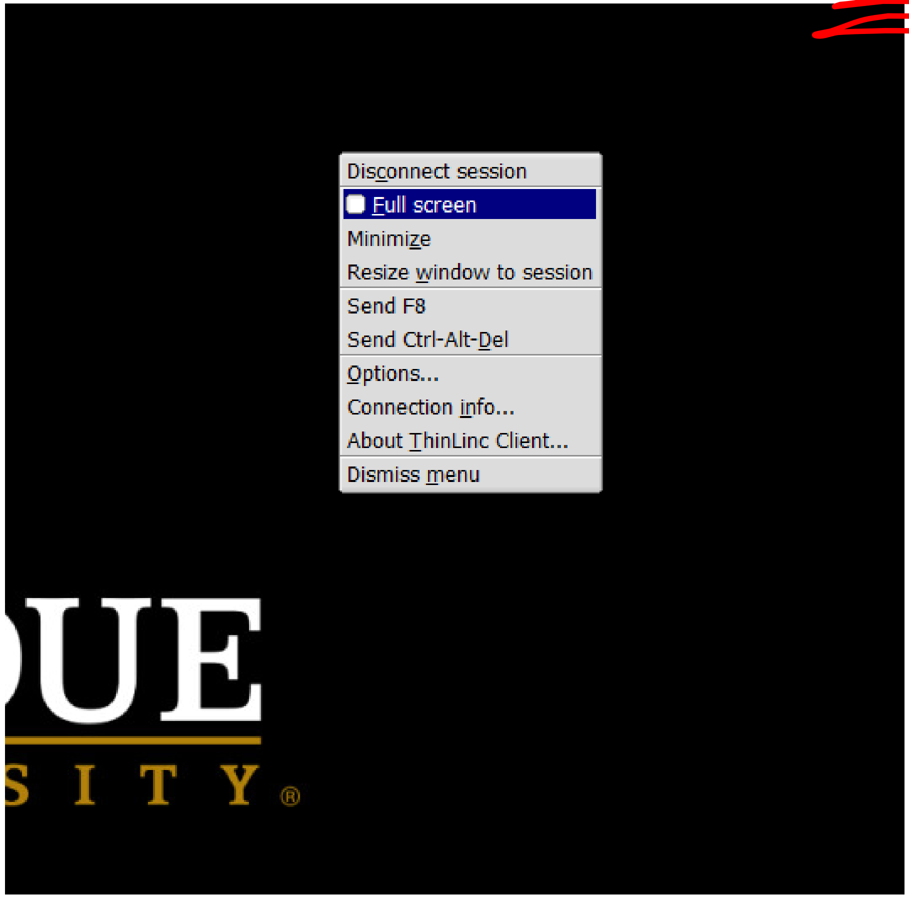
Toggle full screen on ThinLinc client by pressing the F8 key



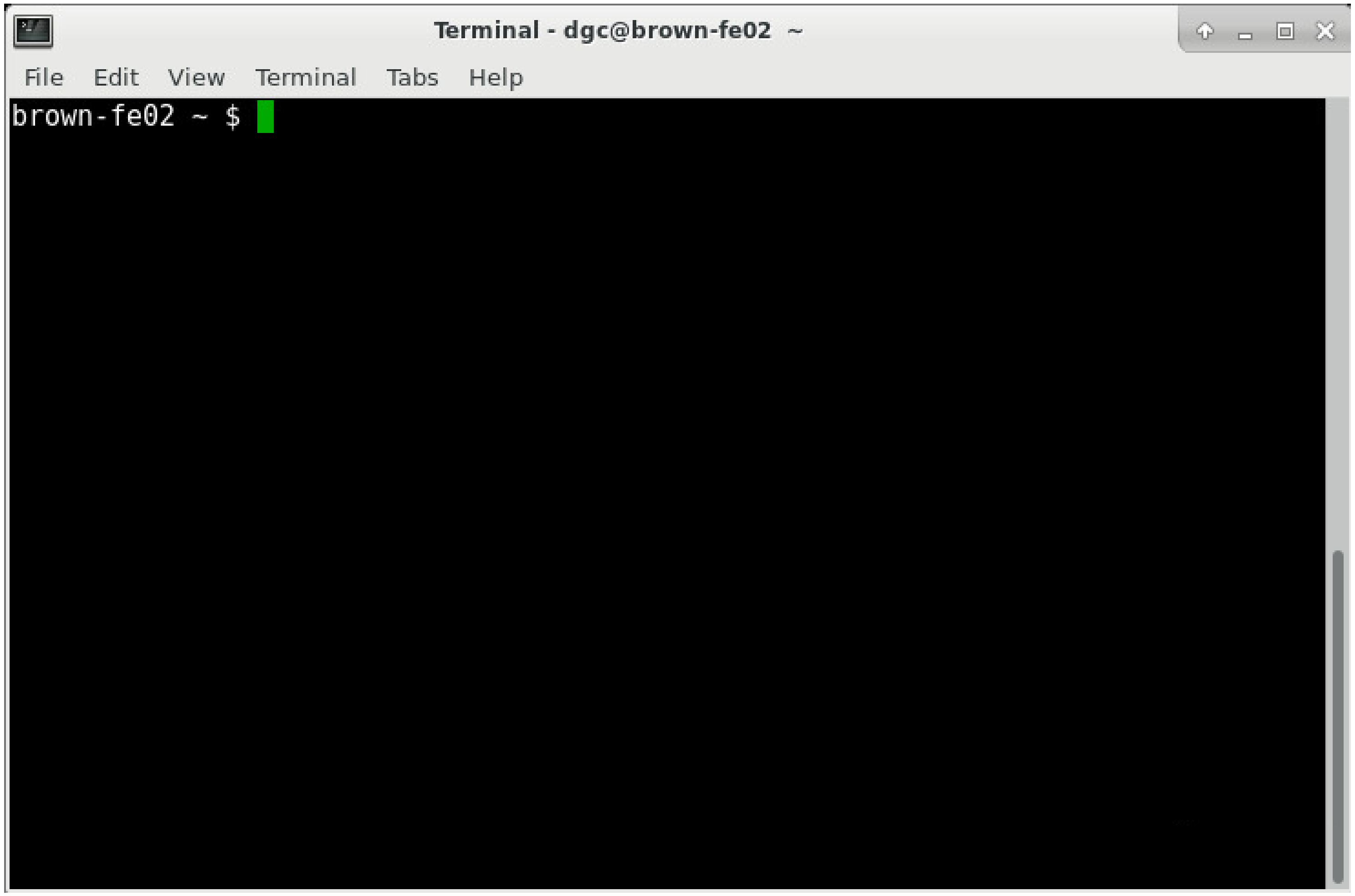
ThinLinc sessions can persist!

- Programs/windows that are open and running can persist after closing the ThinLinc Client
- Smile patiently while I demonstrate persistence
- If you explicitly click Applications->Log Out you will be logged completely out and application state will not persist

What is a “shell”?

- A text-based user interface used to launch programs. The shell we use is called “bash”
- Used to launch programs, pass arguments to programs, specify input/output files
- Terminal is one way of accessing a shell
- Launch via Applications->Terminal Emulator or Applications->System->Xfce Terminal (my preferred method)

A Terminal


Terminal - dgc@brown-fe02 ~
File Edit View Terminal Tabs Help

```
brown-fe02 ~ $
```

Multiple Terminal windows

- You can have many Terminal windows open at once
- To open an additional Terminal window on the same server as an existing Terminal, type:

```
    xfce4-terminal &
```

- If you omit the &, the first Terminal cannot be used again until the second is closed
- Type `exit` to log out of a shell

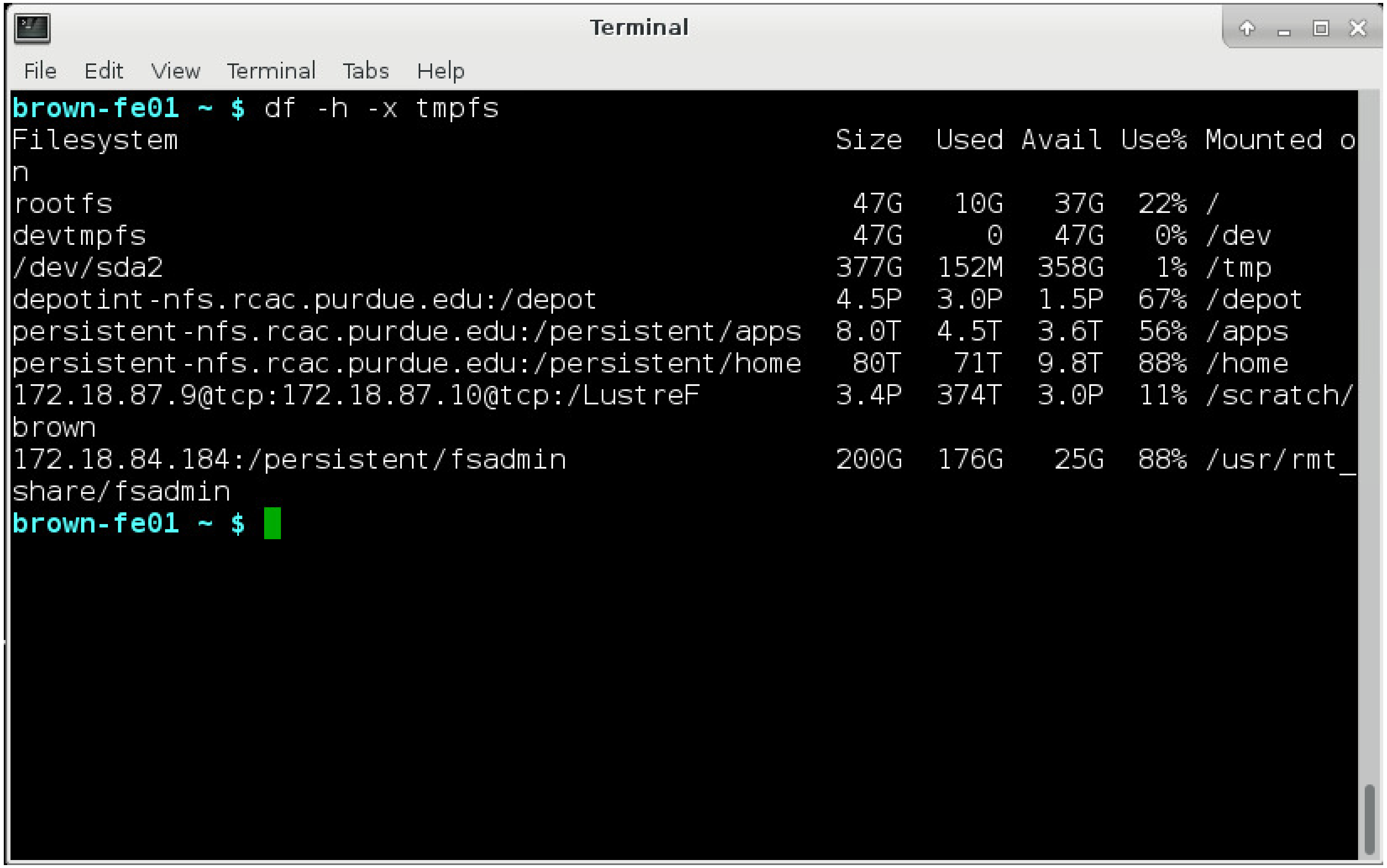
Using copy/paste

- Using the Windows shortcuts Control-C and Control-V will generally not work, because those keys mean other things under Linux
- Either select the text and select Edit/Copy and then Edit/Paste
- Or select the text which implicitly copies it, and press down on the mouse wheel to paste (don’t roll it, press down like it’s a button)

Filesystems

- Filesystems on Linux similar to network drives on Windows, but without drive letters
- Example directories on different filesystems: /home/dgc, /depot/nihomics, /scratch/brown/dgc
- Hierarchical. Directory names separated by “/”, not by “\” as with Windows. Avoid spaces in filenames and directory names.

Filesystems on Brown



```
brown-fe01 ~ $ df -h -x tmpfs
Filesystem                                        Size  Used Avail Use% Mounted o
n
rootfs                                             47G   10G   37G  22% /
devtmpfs                                           47G     0   47G   0% /dev
/dev/sda2                                         377G  152M  358G   1% /tmp
depotint-nfs.rcac.purdue.edu:/depot               4.5P  3.0P  1.5P  67% /depot
persistent-nfs.rcac.purdue.edu:/persistent/apps   8.0T  4.5T  3.6T  56% /apps
persistent-nfs.rcac.purdue.edu:/persistent/home    80T   71T  9.8T  88% /home
172.18.87.9@tcp:172.18.87.10@tcp:/LustreF         3.4P  374T  3.0P  11% /scratch/
brown
172.18.84.184:/persistent/fsadmin                 200G  176G   25G  88% /usr/rmt_
share/fsadmin
brown-fe01 ~ $
```

Shell features

- Shell environment variables used to control settings for how certain things work
- Thousands of potential commands can be executed
- Commands available varies from one Linux computer to the next, depending on what has been installed, and the value of your PATH environment variable

Shell features (cont.)

- Filename completion (using “Tab” key)
- Command completion (using “Tab” key)
- Command line editing using arrow keys (up-arrow key to go to the previous command)

Let’s get dirty!

Listing files in Terminal

- Type `ls` to list files in the current directory
- Type `ls -l` to list files with more detail
- Type `ll` to list files with even more detail

Navigating directories in Terminal

- Type pwd to see full path to current directory
- Type `cd` *`dirname`* to change directories
- Type `cd ..` to go to the parent directory, or `cd ../..` to go to the grandparent, etc.
- Type `cd ~` to go to your home directory
- `cd /depot/nihomics/data`
- Absolute paths start with `/`, relative paths are relative to the current directory

Special directories

- `/home/`*`USERNAME`* – Your home directory, where source code, programs, and final results go
- `/scratch/brown/`*`USERNAME`* – Enormous scratch directory. Can place original data sets and intermediate results there
- Type *`myquota`* to see used disk space and limits

Editing, copying, moving files

Editing, copying, moving files

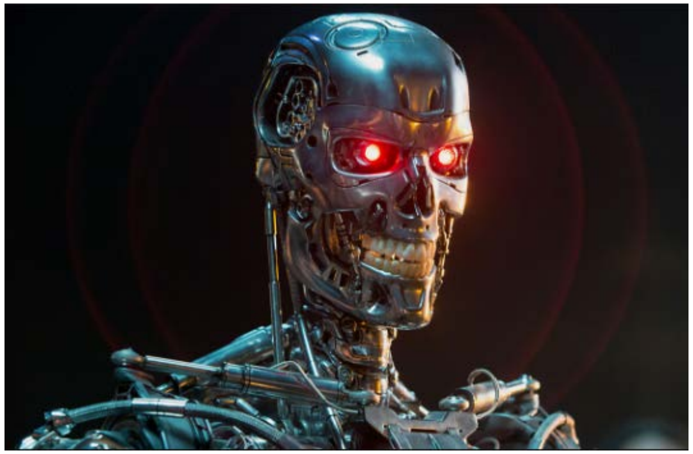
- `gedit` *`filename`* – Edits *`filename`*
- `mv` *`oldname newname`* – Moves a file or directory, possibly to a new directory, possibly renaming the file or directory in the process
- `cp` *`oldname newname`* – Copies files
- `cp -r` *`olddir newdir`* – Copies `olddir` and all files and subdirectories within to `newdir`

Create/Remove directories, files

- `rm` *`filename`* – removes *`filename`*
- *`mkdir dirname`* – creates *`dirname`*
- *`rmdir dirname`* – removes *`dirname`*, but only if *`dirname`* is empty
- Let’s practice, and use filename completion and command line editing while we are at it!

Terminating a program

- If you are running a program in a terminal window that you would like to terminate, press Control-C
- This won’t work if you started that program it with an &



See what programs are running

- `ps xuww` - Show what programs we are running now
- PID column shows the Process ID of each program
- Can use `top` to see most CPU intensive programs currently running by everyone on this server. Press q or just control-c to exit `top`

Terminate or `kill` or program

- Must first know the process id number (PID) using either `ps xuww` or `top`
- `kill NNNNN` Will kill most programs
- `kill –HUP NNNNN` Use if the previous doesn’t work
- `kill -9 NNNNN` Use if the previous doesn’t work

Let’s practice starting/killing progs

- On a Brown node, type `busy 1000 &`
- Type it again a few times (use the up-arrow!)
- Type `top` to see the PIDs of all the jobs running, press q to quit
- Kill all of the busy jobs by typing the PIDs *like*: `kill 24933 24937 24939 24944`
- Type `top` again to confirm they are gone

Redirecting input/ouput

- Some programs write output to the Terminal/shell screen
- We can save it using output redirection
- `qstat -a > out1` Saves results of the command `qstat -a` to the file `out1`
- `head < out1` See the first 10 lines of `out1`
- `head < out1 > out2` Save to `out2`

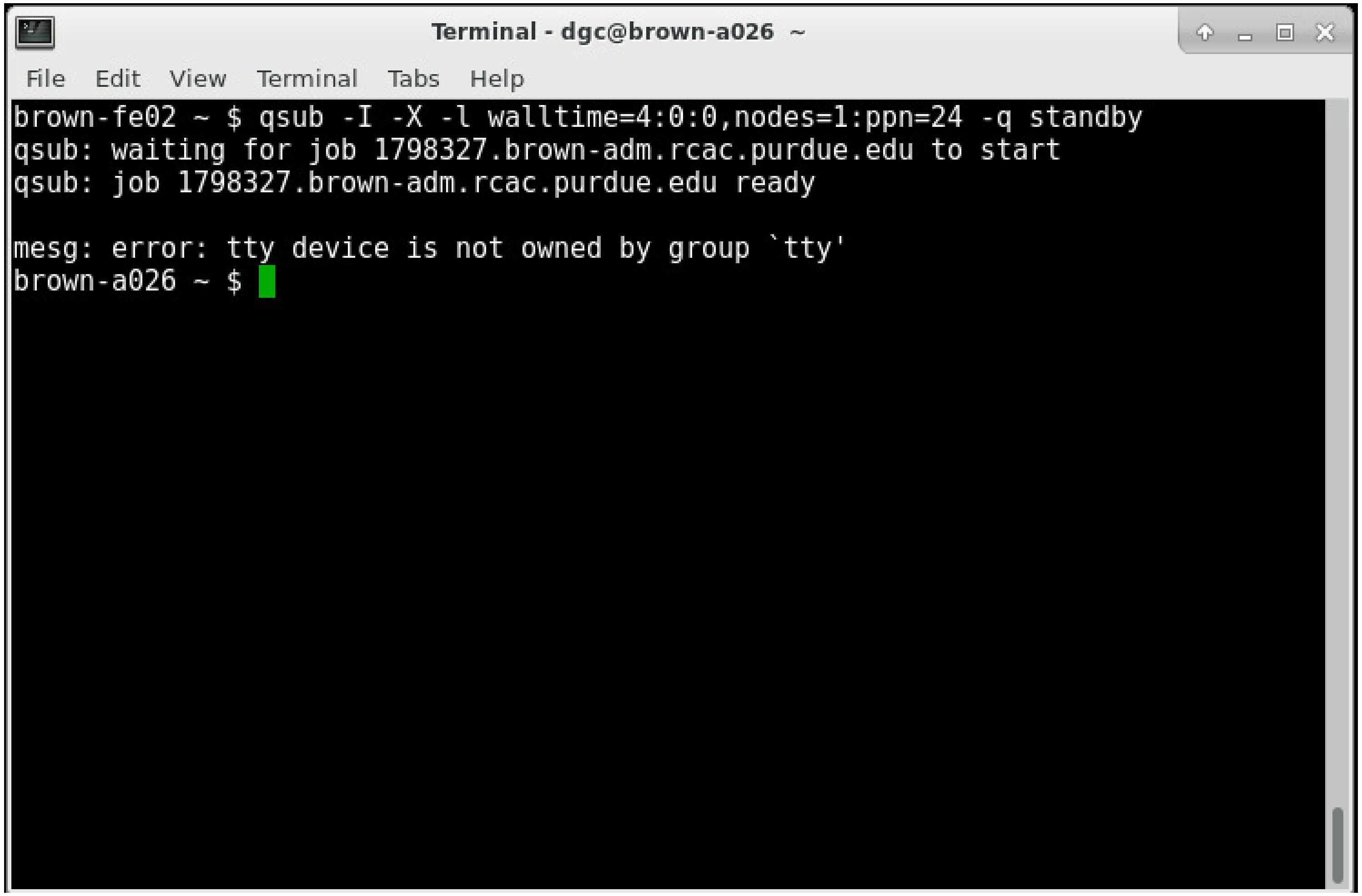
Redirecting input/ouput

- Can only save the text output that would have normally appeared on the screen. If a program wouldn’t normally generate any text output, nothing will be saved
- `Terminal > out3` (Nothing is saved!)

Interactive shell on back-end node

- So far we've been working only on a Brown front-end node. We really want a back-end.
- `qsub -I -X -l walltime=4:0:0,nodes=1:ppn=24 -q standby` (one long typed line)
- Now we have a whole single node to ourselves for interactive use – for 4 hours

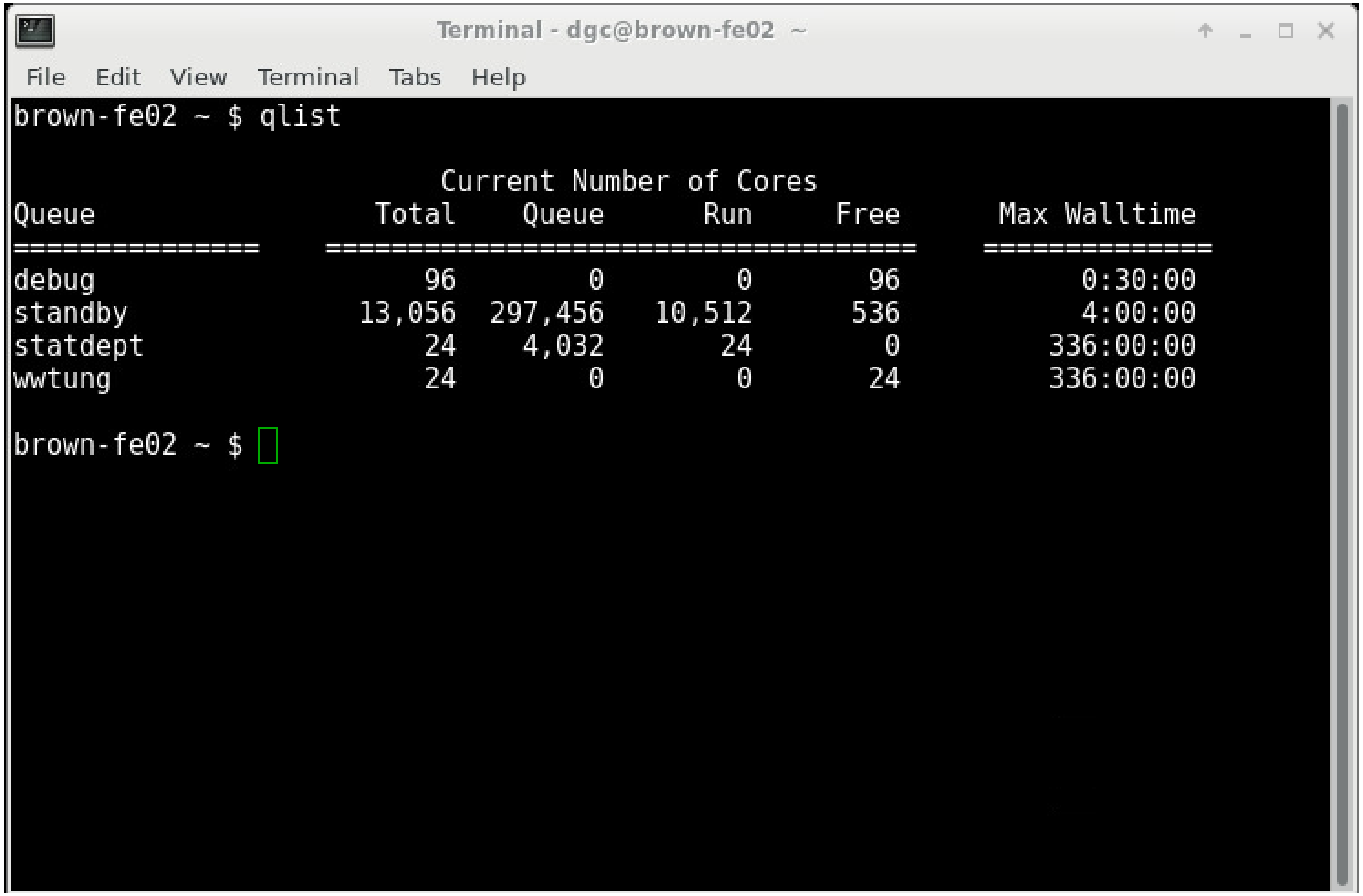
Interactive shell on back-end node


Terminal - dgc@brown-a026 ~
File Edit View Terminal Tabs Help

```
brown-fe02 ~ $ qsub -I -X -l walltime=4:0:0,nodes=1:ppn=24 -q standby
qsub: waiting for job 1798327.brown-adm.rcac.purdue.edu to start
qsub: job 1798327.brown-adm.rcac.purdue.edu ready

mesg: error: tty device is not owned by group `tty'
brown-a026 ~ $
```

Using qlist


Terminal - dgc@brown-fe02 ~
File Edit View Terminal Tabs Help

```
brown-fe02 ~ $ qlist

                          Current Number of Cores
Queue                 Total     Queue      Run      Free      Max Walltime
===============     ====================================    ==============
debug                    96         0        0        96           0:30:00
standby              13,056   297,456   10,512       536           4:00:00
statdept                 24     4,032       24         0         336:00:00
wwtung                   24         0        0        24         336:00:00

brown-fe02 ~ $
```

This talk continues at a later date