Software Engineering for Spatial Data Analysis??

CEE 690

Software Engineering for Spatial Data Analysis??

CEE 690

Or “ESDA II: Now do it for real”

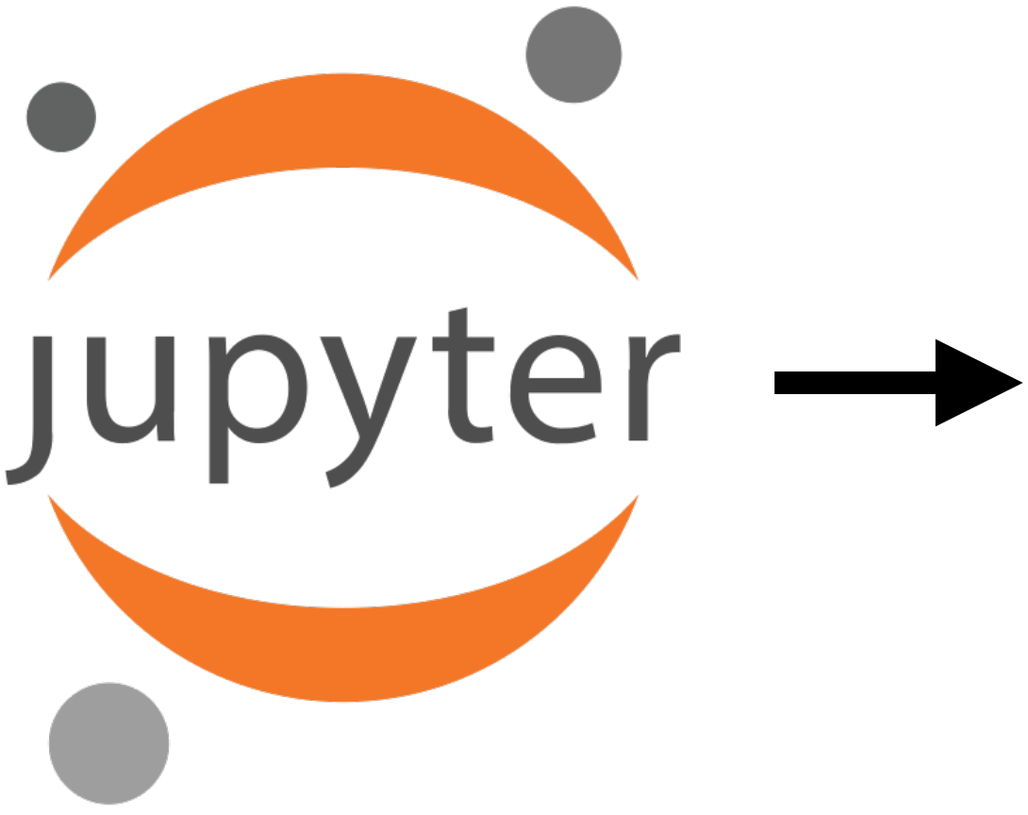
The ESDA experience

The ESDA experience

Issues using Jupyter Notebooks for software development (and really any IDE)

- **Non-linear workflow**
  - Out-of-order execution
  - Variables remain in memory
- **Poor software engineering**
  - Lack of testing
  - Difficult refactoring
- **Version control challenges**
  - Unreadable diffs
  - Merge conflicts
- **Performance and memory issues**
  - Memory overhead
  - Blocking execution

Farewell to Jupyter



Ultimately, it will be worth it

Ultimately, it will be worth it

But it is going to take a semester…

Tentative schedule

Part I: Python

Date	Topic
01/08	The headless environment
01/13	Text editors
01/15	Software architecture I
01/20	Software architecture II
01/22	Verification and profiling
01/27	Packaging, automation and documentation
01/29	Computing on spatial grids
02/03	GPU computing in Python
02/05	High-Speed kernels: Numba CPU & CUDA
02/10	Anatomy of an HPC cluster
02/12	Shared memory parallelism I
02/17	Distributed memory parallelism I
02/19	The scheduler
02/24	High-Performance I/O

Part II: Compiled languages

Date	Topic
02/26	Compiled languages I
03/03	Compiled languages II
03/05	The build process
03/17	Memory management and basic debugging
03/19	Tensors in memory and data layout
03/24	Computer architecture and cache
03/26	Code documentation and profiling
03/31	Code interoperability
04/02	Shared memory parallelism II
04/07	Distributed memory parallelism II
04/09	Containers
04/14	TBD

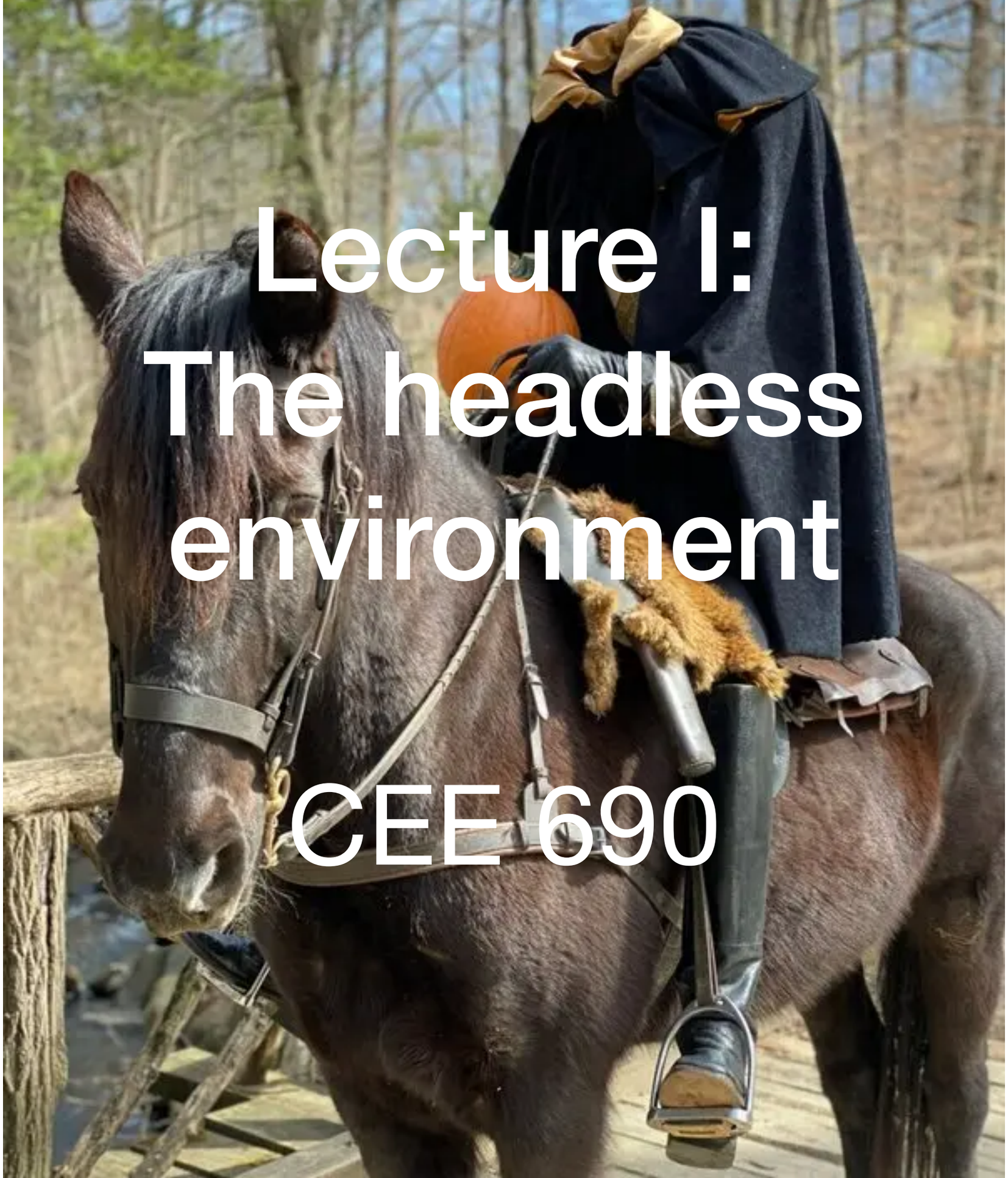
Grades and workload

The course grade will be based on:

- Homework: 30%
- Project I: 35%
- Project II: 35%

Homework

TBD



Lecture I: The headless environment

CEE 690

Headless computing

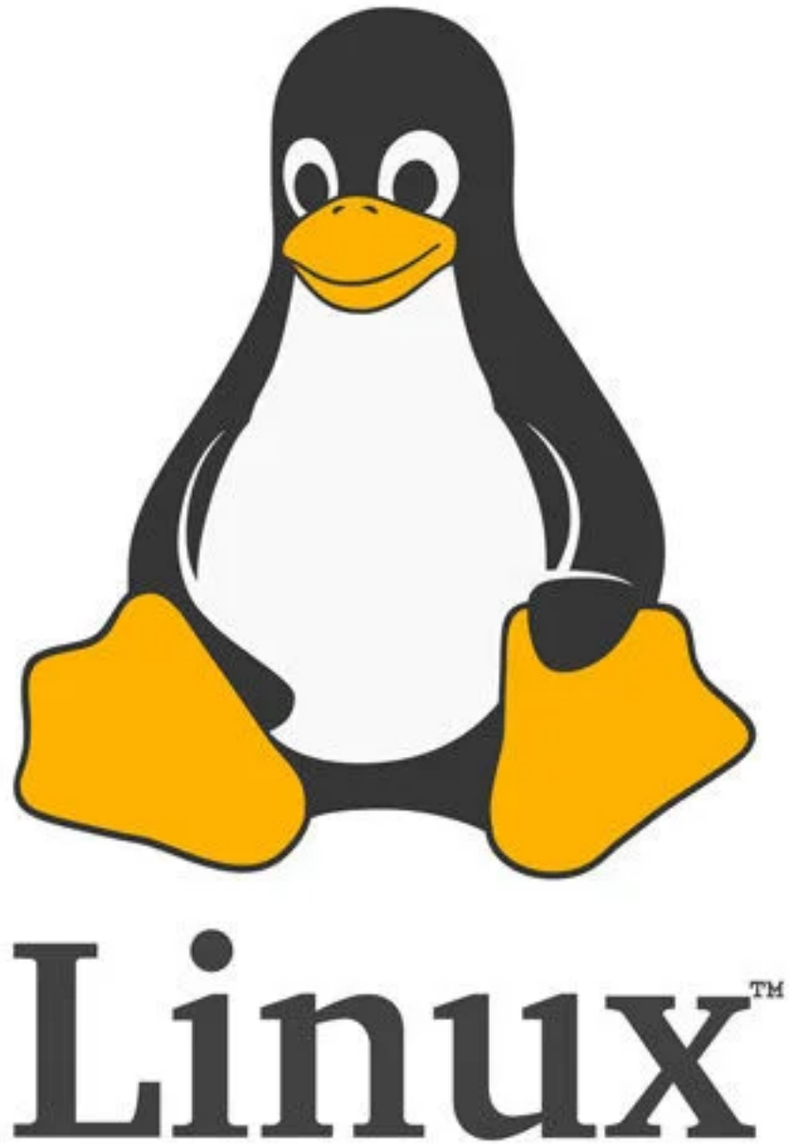
Headless computing

= No graphical user interface (GUI)

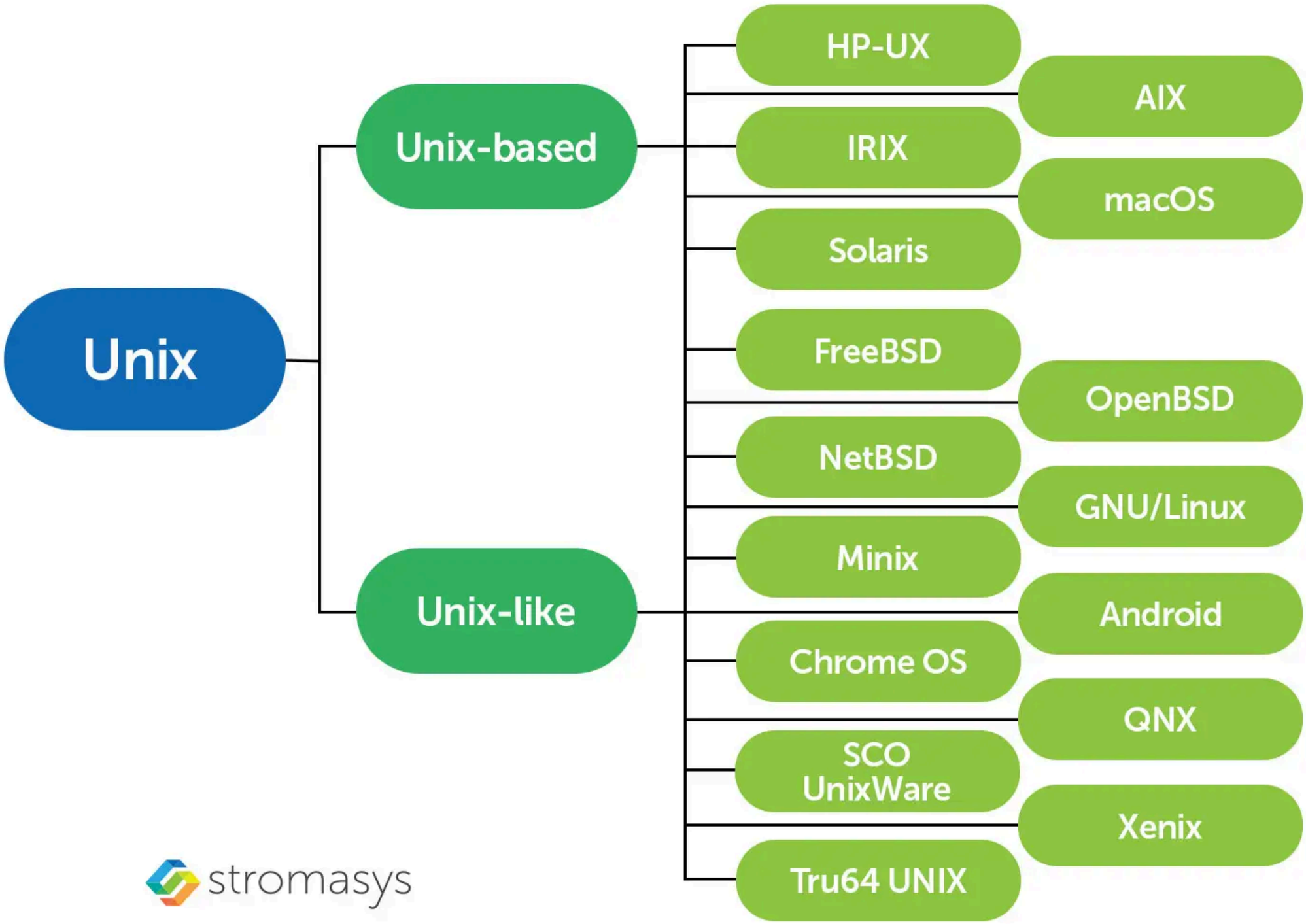
Why will this be critical?

You'll need to embrace linux

- Stripped-down efficiency
- Specialized tuning
- Access to source code
- Community driven tools
- High uptime
- Scale capability
- Cost effectiveness
- Interoperability



Origins of Linux



“All” Compute clusters/HPC use linux

Duke Compute Cluster

Overview

The Duke Compute Cluster is a general purpose high performance/high-throughput installation, and it is fitted with software used for a broad array of scientific projects. With a few notable exceptions, applications on the cluster are generally Free and Open Source Software.

Quick facts:

- 1360 nodes which combined have more than 45,000 vCPUs, 980 GPUs and 270TB of RAM
- Interconnects are 10 Gbps or 40 Gbps
- Utilizes a 7 Petabyte Isilon file system
- Runs Alma 9 and SLURM is the job scheduler

Need an account on the Duke Compute Cluster (or another machine)

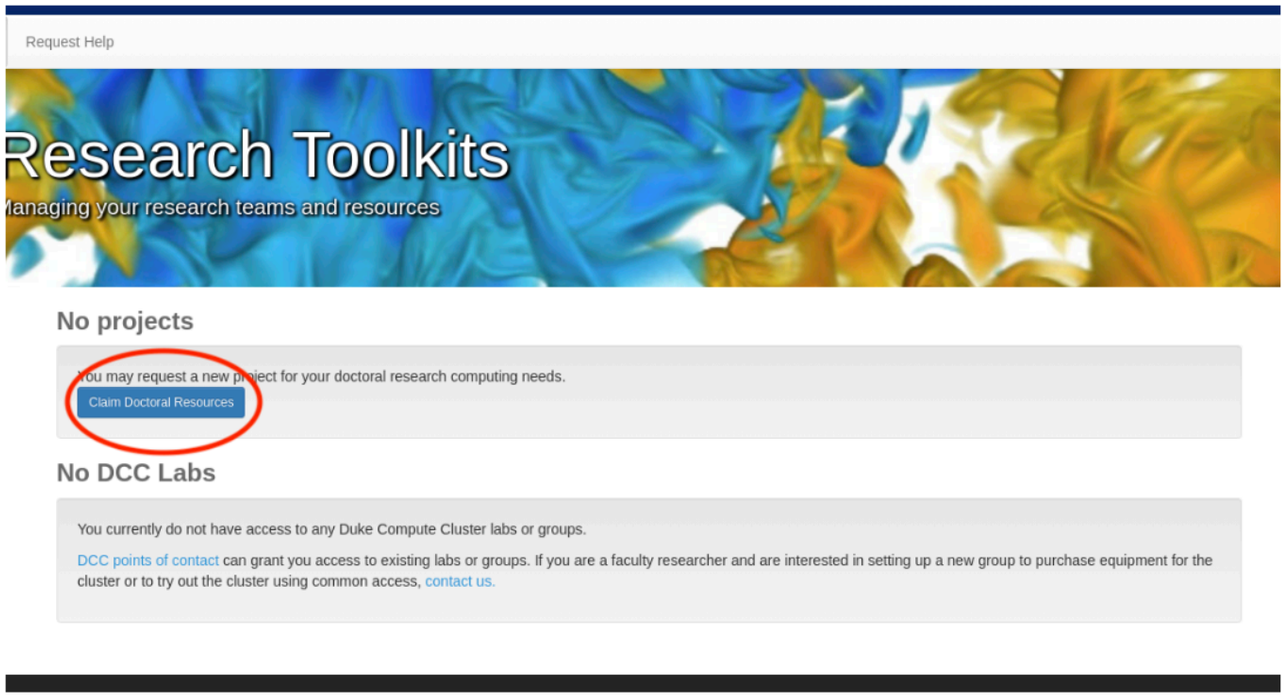
Claim PhD Student Allocation

Duke PhD students now direct allocations to the DCC for compute hours and 500GB of dedicated storage.

Dedicated storage can be found at: `\hpc\dctrl\<netid>`

To claim this allocation, PhD student should:

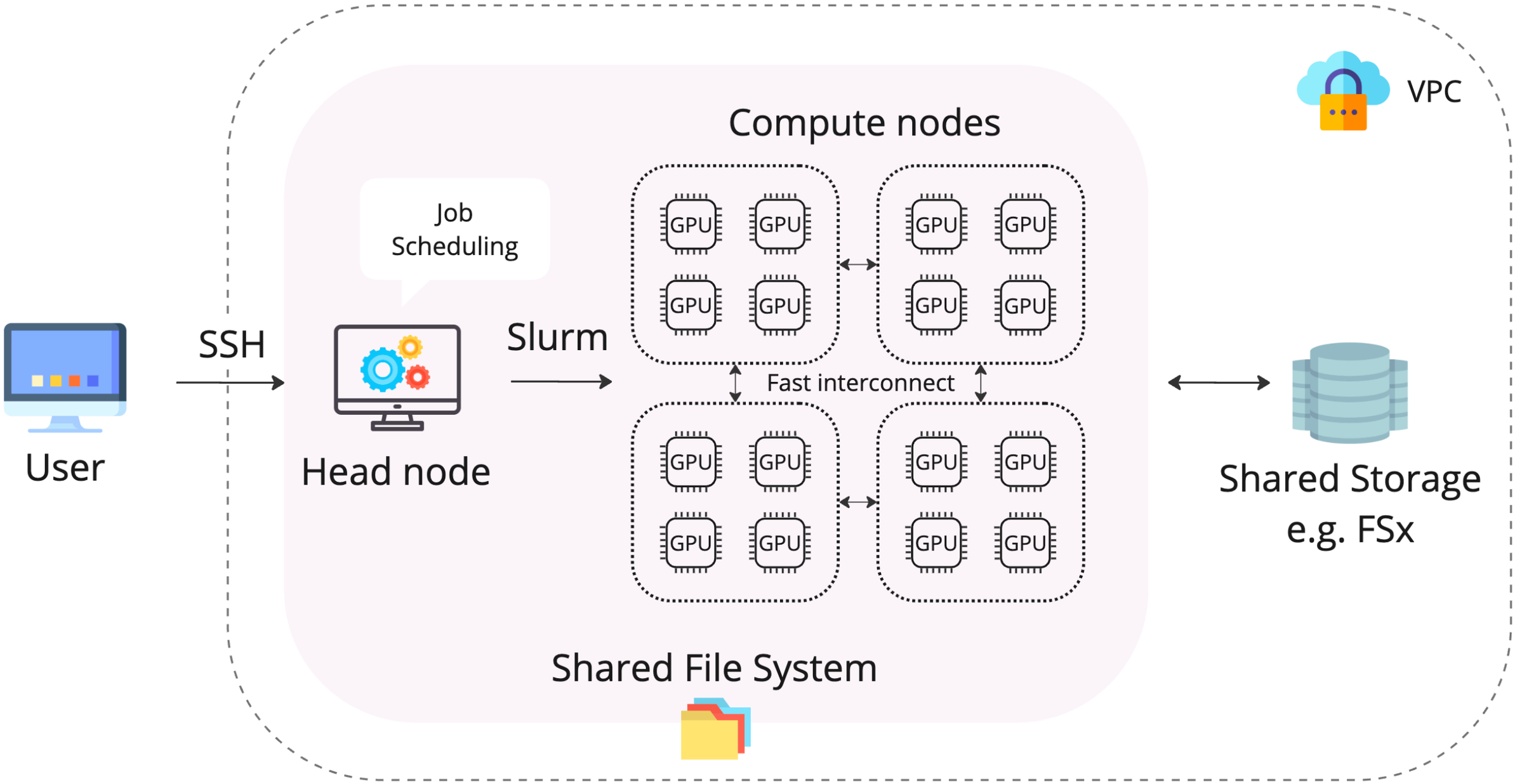
1. Login to Research Toolkits
2. Claim your Doctoral resources by selecting the `Claim Doctoral Resources` button



3. Once the project is created, open it and select the menu to `add a service`, and choose `DCC Grant`. Your project will now automatically update with status as your access is provisioned.

Once your access is provisioned check out our training and quick-start guides.

How to connect to these machines



Source: https://www.unitary.ai/

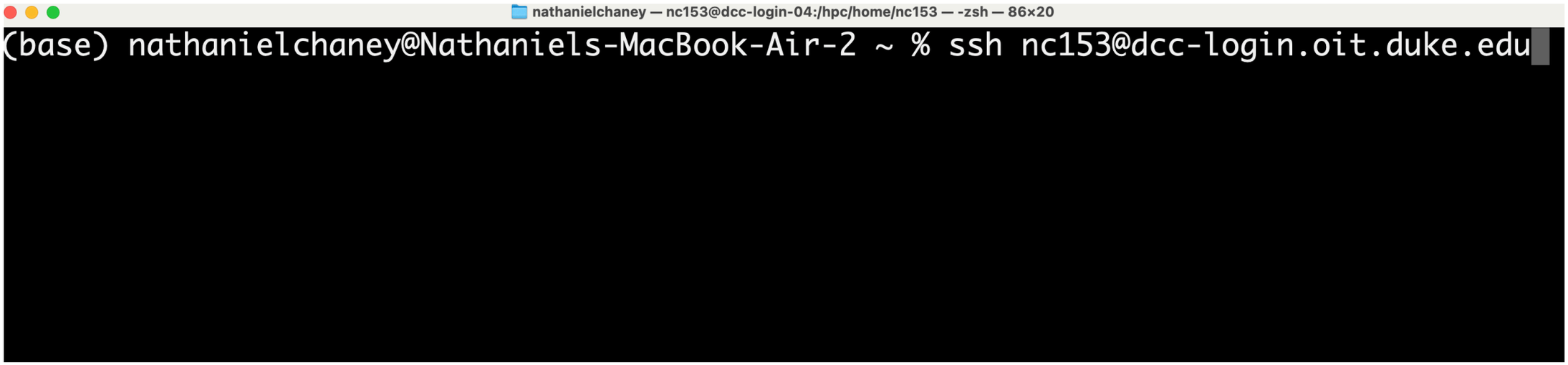
SSH (secure shell): Portal to the cluster

Tunnel to connect your laptop/desktop to a compute cluster or HPC system

- **Components**
  - Client (your local machine)
  - Server (login node of HPC system)
  - Handshake (two computers exchange keys to establish encrypted connection)

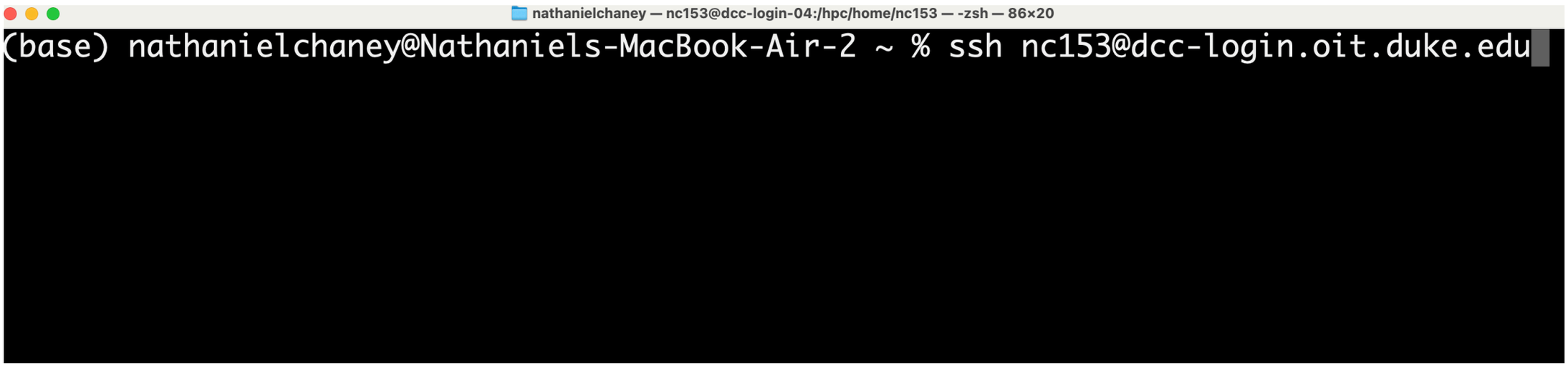
SSH

First open up a terminal/command line. This example is using MacOS.



SSH

First open up a terminal/command line. This example is using MacOS.



Want passwordless entry? Learn about public key authentication

Passwordless login on DCC?

Duke | RESEARCH COMPUTING **Duke Compute Cluster** Search

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User Guide

Login

Software

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H200

Scheduling Jobs

Usage Reports

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Logging into the DCC

As a shared computing resource, all work done on the DCC must be done by submitting jobs to the scheduler. Login nodes must not be used to execute computing tasks.

Acceptable use of login nodes include:

- lightweight file transfers,
- script and configuration file editing,
- job submission and monitoring,
- BaseSpace BaseMount - users can use basemount to mount BaseSpace into their home directories.

To minimize disruption and ensure a comfortable working environment for users, resource limits are enforced on login nodes, and processes started there will automatically be terminated if their resource usage (including CPU time, memory and run time) exceed those limits.

.config file

```
(base) nathanielchaney@Nathaniels-MacBook-Air-2 ~ % vi $HOME/.ssh/config
```

```
Host cluster
        HostName        chaney.egr.duke.edu
        User            nc153

Host dcc
        HostName        dcc-login.oit.duke.edu
        User            nc153
```

```
(base) nathanielchaney@Nathaniels-MacBook-Air-2 ~ % ssh dcc
```

More terminals!

```
...c153@dcc-login-05:/hpc/home/nc153 — ssh dcc ...  ...c153@dcc-login-05:/hpc/home/nc153 — ssh dcc  ...53@dcc-login-05:/hpc/home/nc153 — ssh dcc  ...53@dcc-login-05:/hpc/home/nc153 — ssh dcc
Last login: Thu Jan  8 09:05:51 on ttys003
ssh dcc%
(base) nathanielchaney@NathanielsAir2 ~ % ssh dcc
Last login: Thu Jan  8 09:05:53 2026 from nathanielsair2.wired.duke.local
##############################################################################
# Please report any issues or questions to: oitresearchsupport@duke.edu      #
#                                                                            #
# Duke Research Computing info and documentation: https://rc.duke.edu        #
#                                                                            #
# My next patch run is Thursday (01-22-2026) at  3 AM                        #
##############################################################################
 3.8GiB (15%) used of  25GiB in /hpc/home/nc153
 179GiB (17%) used of 1.0TiB in /hpc/group/chaneylab
     0B  (0%) used of  25TiB in /work/nc153
(base) nc153@dcc-login-05  ~ $
```

```
(base) nc153@dcc-login-05  ~ $ ps -aux | grep "sshd: nc153"
root     3810045  0.0  0.0  49600 14076 ?        Ss   09:05   0:00 sshd: nc153 [priv
]
nc153    3810071  0.0  0.0  49600  7864 ?        S    09:05   0:00 sshd: nc153@pts/3
1
root     3810192  0.0  0.0  49600 14068 ?        Ss   09:05   0:00 sshd: nc153 [priv
]
nc153    3810218  0.0  0.0  49600  7944 ?        S    09:05   0:00 sshd: nc153@pts/3
3
root     3810340  0.0  0.0  49600 14024 ?        Ss   09:05   0:00 sshd: nc153 [priv
]
nc153    3810366  0.0  0.0  49600  7828 ?        S    09:05   0:00 sshd: nc153@pts/3
4
root     3810499  0.0  0.0  49600 14024 ?        Ss   09:05   0:00 sshd: nc153 [priv
]
nc153    3810525  0.0  0.0  49600  7840 ?        S    09:05   0:00 sshd: nc153@pts/3
5
nc153    3810983  0.0  0.0   6420  2616 pts/35   S+   09:06   0:00 grep --color=auto
```

Terminal multiplexer

Once you are inside a tmux session, use these shortcuts with the **Prefix (`Ctrl + b`)**.

Working with Panes (Splits)

- `Prefix` **+** `%` : Split the screen **vertically** (left and right).
- `Prefix` **+** `"` : Split the screen **horizontally** (top and bottom).
- `Prefix` **+** `Arrow Key` : Move your cursor between panes.
- `Prefix` **+** `z` : **Zoom** (maximize) the current pane. Press again to shrink it back.
- `Prefix` **+** `x` : Close the current pane.

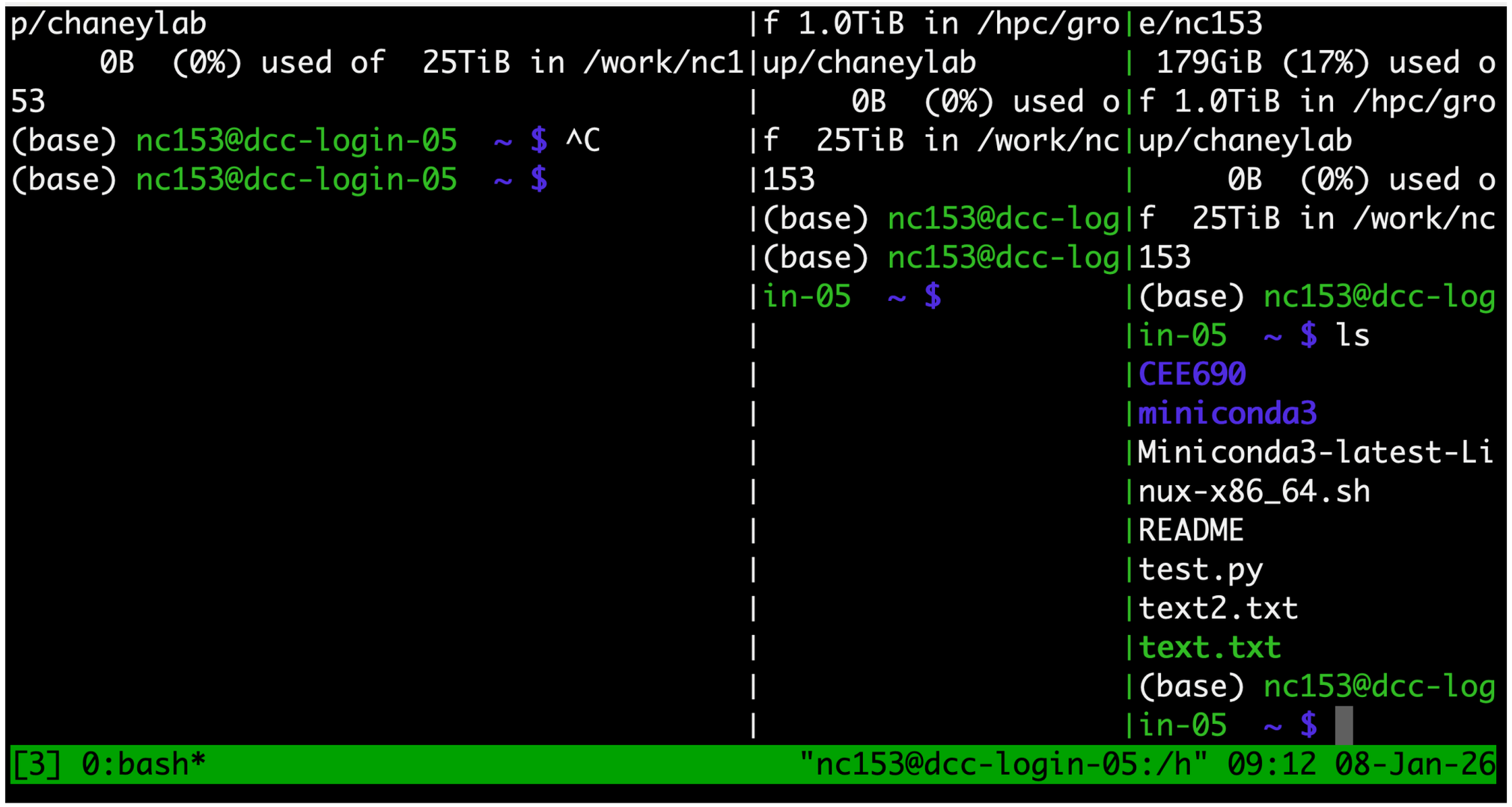
Working with Windows (Tabs)

- `Prefix` **+** `c` : Create a **new window**.
- `Prefix` **+** `n` / `p` : Switch to the **n**ext or **p**revious window.
- `Prefix` **+** `0-9` : Jump directly to a window by its number.
- `Prefix` **+** `,` : **Rename** the current window (makes it easier to find later).

Terminal multiplexer

```
p/chaneylab                                |f 1.0TiB in /hpc/gro|e/nc153
     0B  (0%) used of  25TiB in /work/nc1|up/chaneylab         | 179GiB (17%) used o
53                                         |     0B  (0%) used o|f 1.0TiB in /hpc/gro
(base) nc153@dcc-login-05  ~ $ ^C          |f  25TiB in /work/nc|up/chaneylab
(base) nc153@dcc-login-05  ~ $             |153                 |     0B  (0%) used o
                                           |(base) nc153@dcc-log|f  25TiB in /work/nc
                                           |(base) nc153@dcc-log|153
                                           |in-05  ~ $          |(base) nc153@dcc-log
                                           |                    |in-05  ~ $ ls
                                           |                    |CEE690
                                           |                    |miniconda3
                                           |                    |Miniconda3-latest-Li
                                           |                    |nux-x86_64.sh
                                           |                    |README
                                           |                    |test.py
                                           |                    |text2.txt
                                           |                    |text.txt
                                           |                    |(base) nc153@dcc-log
                                           |                    |in-05  ~ $
[3] 0:bash*                                    "nc153@dcc-login-05:/h" 09:12 08-Jan-26
```

Terminal multiplexer



I personally never use this. But I know many people that do and are huge fans

Navigating the linux filesystem

Navigation

- CD

```
(base) nc153@dcc-login-03  ~ $ cd CEE690/
```

- ls

```
(base) nc153@dcc-login-03  ~ $ ls
CEE690  miniconda3  Miniconda3-latest-Linux-x86_64.sh  README  test.py
```

- pwd

```
(base) nc153@dcc-login-03  ~ $ pwd
/hpc/home/nc153
```

Finding data

- find

```
(base) nc153@dcc-login-03  ~ $ find . -name "*.py"
```

- grep

```
(base) nc153@dcc-login-03  ~ $ grep 'Remember' README
# Remember, you only have 10 GB in your new home directory.
```

Regular expressions (Regex)

- . (Dot) - Matches any single character

```
(base) nc153@dcc-login-03  ~ $ grep '.y' README
# DON'T PANIC! Your old home directory still exists.
# The contents are located at /hpc/group/<groupname>/<your netid>
# Remember, you only have 10 GB in your new home directory.
```

- * (Asterisk) - Matches zero or more of the preceding element

```
(base) nc153@dcc-login-03  ~ $ grep 'a*' README
# DON'T PANIC! Your old home directory still exists.
# The contents are located at /hpc/group/<groupname>/<your netid>
# https://rc.duke.edu/working-with-new-dcc-storage-options/
# Remember, you only have 10 GB in your new home directory.
```

- [ ] (Brackets) - Matches any one character inside the brackets

```
(base) nc153@dcc-login-03  ~ $ grep '[yuh]' README
# DON'T PANIC! Your old home directory still exists.
# The contents are located at /hpc/group/<groupname>/<your netid>
# https://rc.duke.edu/working-with-new-dcc-storage-options/
# Remember, you only have 10 GB in your new home directory.
```

Regular expressions (Regex)

- . (Dot) - Matches any single character

```
(base) nc153@dcc-login-03  ~ $ grep '.y' README
# DON'T PANIC! Your old home directory still exists.
# The contents are located at /hpc/group/<groupname>/<your netid>
# https://rc.duke.edu/working-with-new-dcc-storage-options/
# Remember, you only have 10 GB in your new home directory.
```

There are many…

- [ ] (Brackets) - Matches any one character inside the brackets

```
(base) nc153@dcc-login-03  ~ $ grep '[yuh]' README
# DON'T PANIC! Your old home directory still exists.
# The contents are located at /hpc/group/<groupname>/<your netid>
# https://rc.duke.edu/working-with-new-dcc-storage-options/
# Remember, you only have 10 GB in your new home directory.
```

Piping and redirection

- The pipe (|)

```
(base) nc153@dcc-login-03  ~ $ ls | wc -l
5
```

- Redirection - Overwrite a file (>)

```
(base) nc153@dcc-login-03  ~ $ ls > text.txt
```

- Redirection - Append to a file (>>)

```
(base) nc153@dcc-login-03  ~ $ ls >> text.txt
```

Moving data

- cp - copy files within the host

```
(base) nc153@dcc-login-03  ~ $ cp text.txt text2.txt
```

- scp - copy files to/from client/server

```
(base) nathanielchaney@Nathaniels-MacBook-Air-2 ~ % scp test.py nc153@dcc-login.oit
duke.edu:.
```

- Rsync - Checks which parts have changed and only sends those

Permissions

- Chmod - Modify permissions on a file

```
(base) nc153@dcc-login-03  ~ $ chmod 755 text.txt
```

Common Octal Values:

Number	Permissions	Description
777	`rwxrwxrwx`	Anyone can read, write, and execute (generally not recommended for security).
755	`rwxr-xr-x`	Owner has full access; group and others can read and execute (common for public directories/programs).
644	`rw-r--r--`	Owner can read and write; group and others can only read (common for data files).
700	`rwx------`	Only the owner has full access; others have no rights (for private files/directories).

Understanding commands

```
(base) nc153@dcc-login-05  ~/miniconda3 $ grep --help
Usage: grep [OPTION]... PATTERNS [FILE]...
Search for PATTERNS in each FILE.
Example: grep -i 'hello world' menu.h main.c
PATTERNS can contain multiple patterns separated by newlines.

Pattern selection and interpretation:
  -E, --extended-regexp     PATTERNS are extended regular expressions
  -F, --fixed-strings       PATTERNS are strings
  -G, --basic-regexp        PATTERNS are basic regular expressions
  -P, --perl-regexp         PATTERNS are Perl regular expressions
  -e, --regexp=PATTERNS     use PATTERNS for matching
  -f, --file=FILE           take PATTERNS from FILE
  -i, --ignore-case         ignore case distinctions in patterns and data
      --no-ignore-case      do not ignore case distinctions (default)
  -w, --word-regexp         match only whole words
  -x, --line-regexp         match only whole lines
  -z, --null-data           a data line ends in 0 byte, not newline
```

Linux commands you should know… maybe?

Lego brick nature of terminal commands

Lots of unique commands

Combine many to create a “custom command”

Example I: User info

```
(base) nc153@dcc-login-05  ~/miniconda3 $ ps -aux | grep nc153
nc153    3808656  0.0  0.0  25368 15248 ?        Ss   09:03   0:00 /usr/lib/systemd
/systemd --user
nc153    3808659  0.0  0.0 198040  8528 ?        S    09:03   0:00 (sd-pam)
nc153    3809911  0.0  0.0   6016  3368 ?        Ss   09:05   0:00 tmux
nc153    3809912  0.0  0.0  17664  5528 pts/32   Ss+  09:05   0:00 -bash
root     3810045  0.0  0.0  49600 14076 ?        Ss   09:05   0:00 sshd: nc153 [pri
v]
nc153    3810071  0.0  0.0  49600  7864 ?        S    09:05   0:00 sshd: nc153@pts/
31
nc153    3810072  0.0  0.0  17784  5652 pts/31   Ss   09:05   0:00 -bash
nc153    3861915  0.0  0.0  19088  4504 pts/31   R+   09:26   0:00 ps -aux
nc153    3861916  0.0  0.0   6420  2604 pts/31   S+   09:26   0:00 grep --color=aut
o nc153
```

Example II: Count and save

```
(base) nc153@dcc-login-05  ~/miniconda3 $ ls -la | wc -l >& log.txt
```

```
(base) nc153@dcc-login-05  ~/miniconda3 $ cat log.txt
19
```

Example III: Read and process

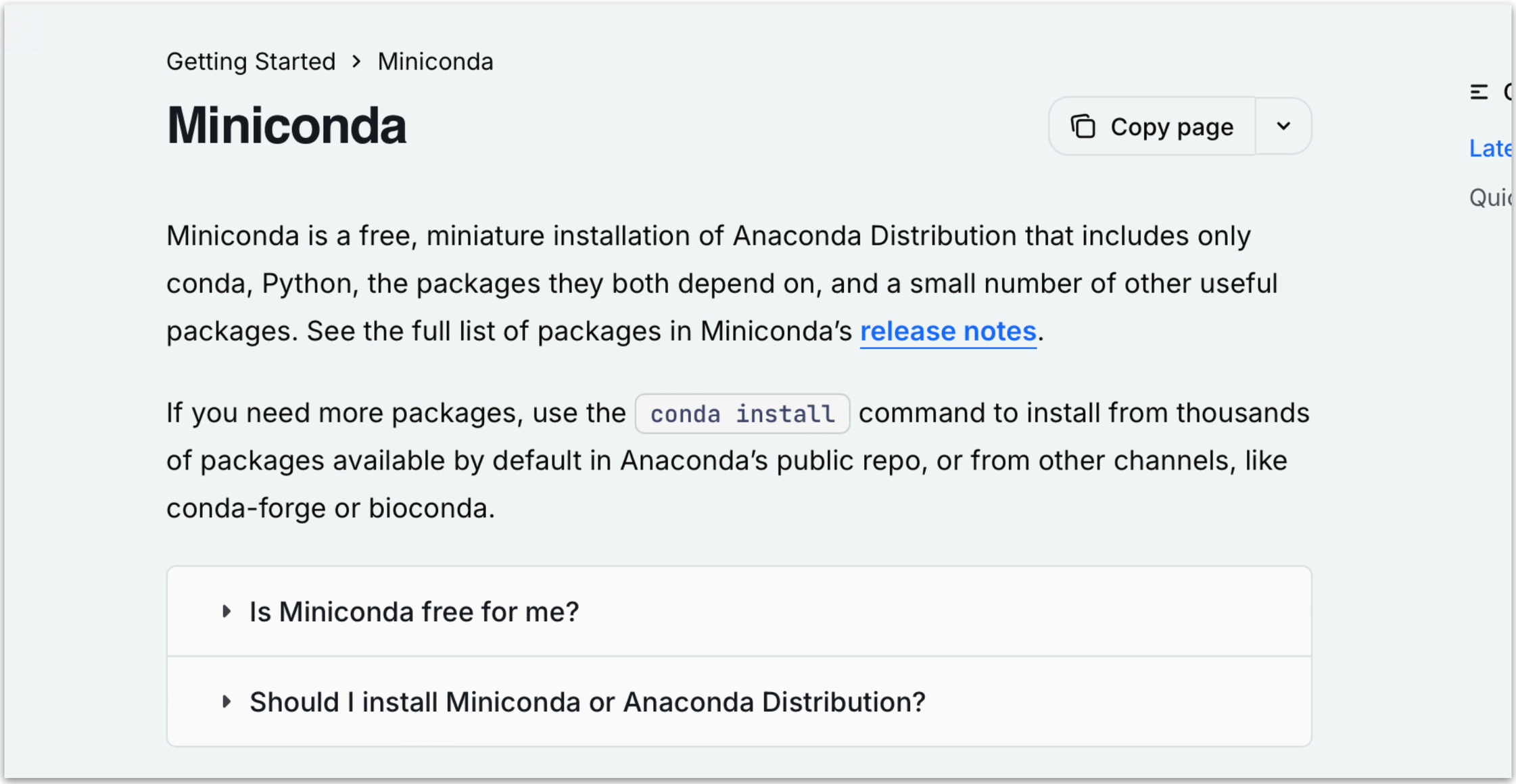
```
(base) nc153@dcc-login-05  ~/miniconda3 $ tail -10 LICENSE.txt | grep [acp]
    A stand-alone version of pycryptodome.
    A software library for encryption, decryption, signatures, password hashing and
 more.
pynacl
    A Python binding to the Networking and Cryptography library, a crypto library w
ith the stated goal of improving usability, security and speed.
Last updated September 28, 2020
```

Example III: Read and process

```
(base) nc153@dcc-login-05  ~/miniconda3 $ tail -10 LICENSE.txt | grep [acp]
    A stand-alone version of pycryptodome.
```

In practice, I just do most of these things directly in Python nowadays. However, you can save yourself a lot of time if you learn to use these well

Python on the system: Miniconda



Miniconda environment

```
(base) nc153@dcc-login-05  ~/miniconda3 $ conda create -n cee690
Collecting package metadata (current_repodata.json): done
Solving environment: done
```

```
(base) nc153@dcc-login-05  ~/miniconda3 $ conda activate cee690
(cee690) nc153@dcc-login-05  ~/miniconda3 $
```

Miniconda environment

```
(base) nc153@dcc-login-05  ~/miniconda3 $ conda create -n cee690
Collecting package metadata (current_repodata.json): done
Solving environment: done
```

```
(base) nc153@dcc-login-05  ~/miniconda3 $ conda activate cee690
(cee690) nc153@dcc-login-05  ~/miniconda3 $
```

Conda works really well until it doesn’t

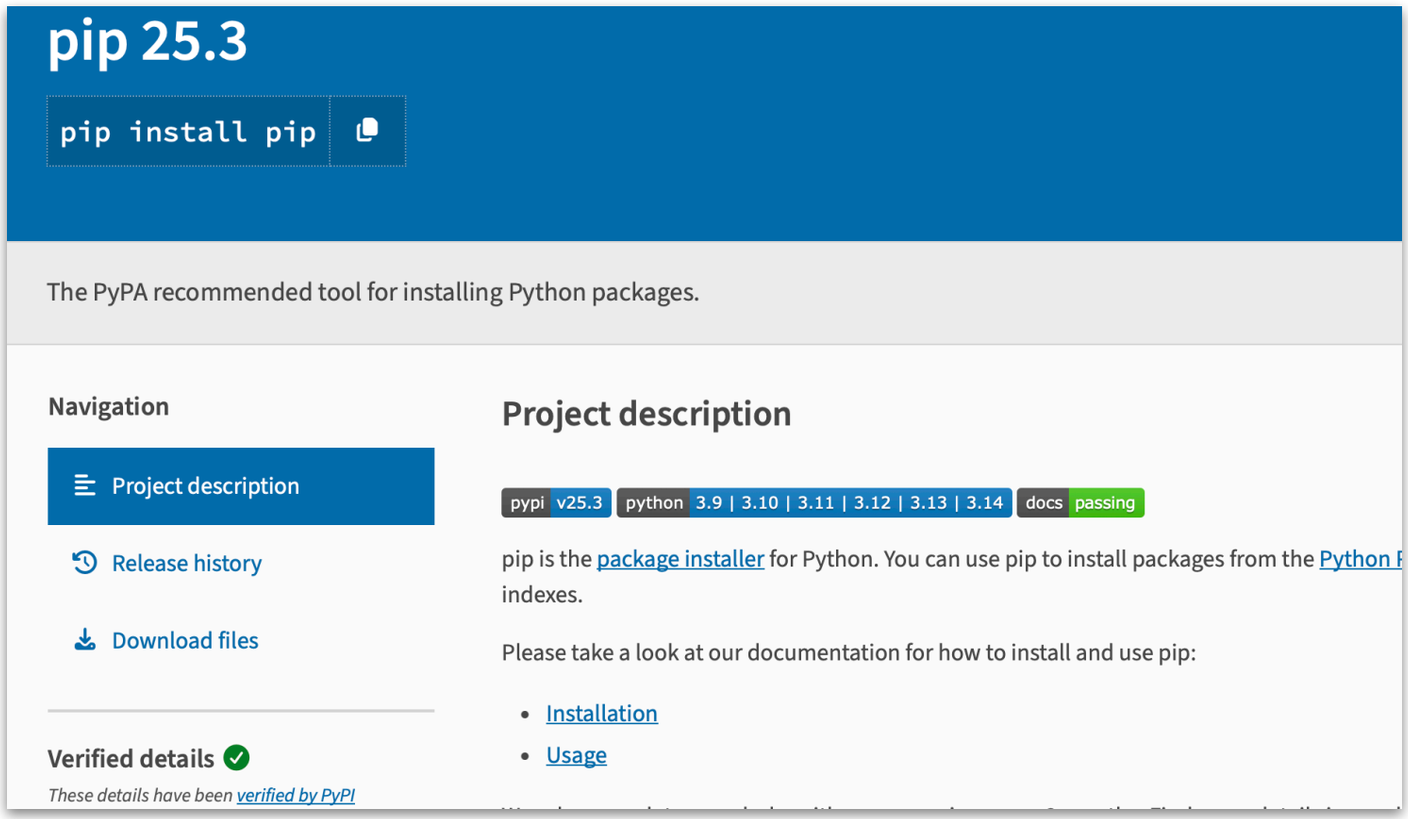
Install packages

```
(cee690) nc153@dcc-login-05  ~/miniconda3 $ conda install -c conda-forge rasterio
Collecting package metadata (current_repodata.json): done
Solving environment: done
```

```
Proceed ([y]/n)? y


Downloading and Extracting Packages
libxml2-2.15.1       | 44 KB     | ########################################## | 100%
libcblas-3.11.0      | 18 KB     | ########################################## | 100%
minizip-4.0.10       | 91 KB     | ########################################## | 100%
ncurses-6.5          | 871 KB    | ########################################## | 100%
libev-4.33           | 110 KB    | ########################################## | 100%
libjxl-0.11.1        | 1.7 MB    | ########################################## | 100%
certifi-2026.1.4     | 147 KB    | ########################################## | 100%
libxml2-16-2.15.1    | 543 KB    | ########################################## | 100%
liblapack-3.11.0     | 18 KB     | ########################################## | 100%
libstdcxx-ng-15.2.0  | 27 KB     | ########################################## | 100%
openssl-3.6.0        | 3.0 MB    | ########################################## | 100%
liblzma-5.8.1        | 110 KB    | ########################################## | 100%
libnghttp2-1.67.0    | 651 KB    | ########################################## | 100%
```

More control? pip



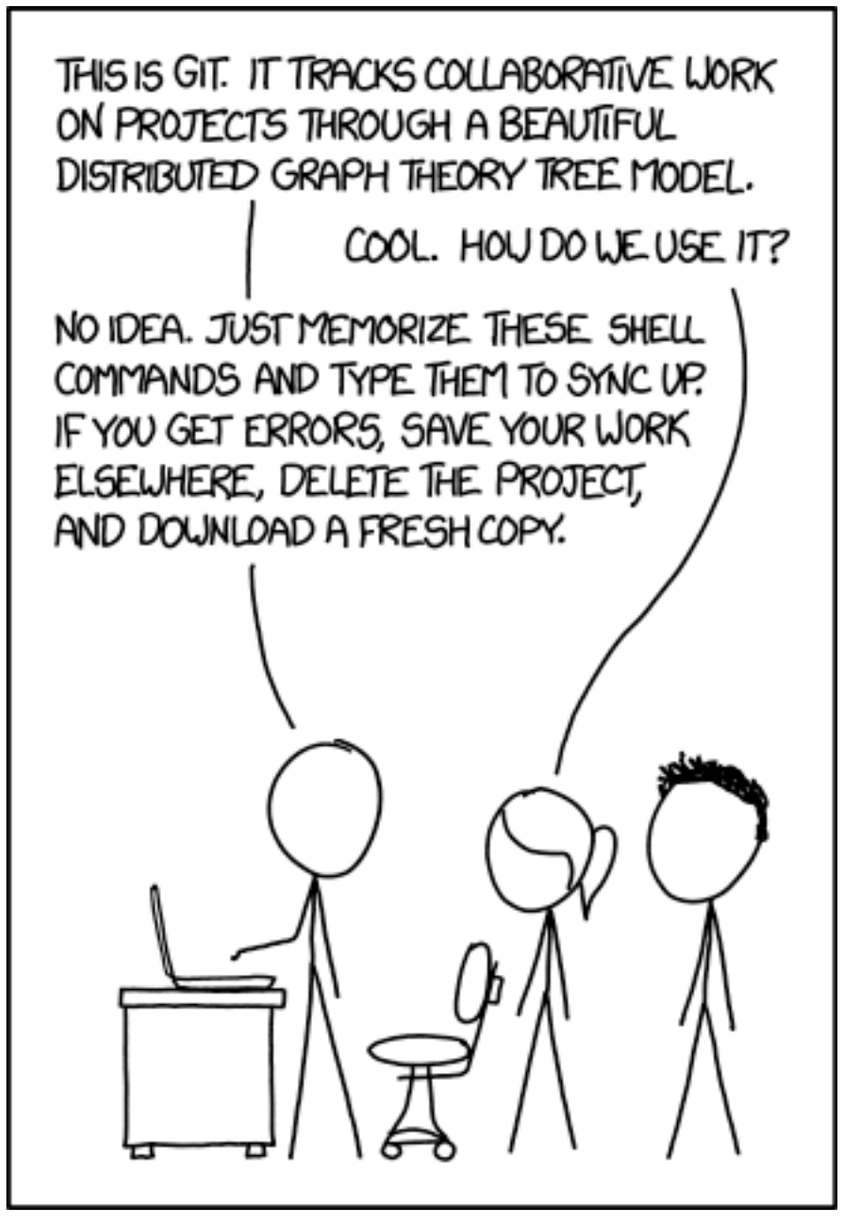

```
(cee690) nc153@dcc-login-05  ~/miniconda3 $ pip install matplotlib
Collecting matplotlib
  Downloading matplotlib-3.10.8-cp314-cp314-manylinux_2_27_x86_64.manylinu
6_64.whl.metadata (52 kB)
Collecting contourpy>=1.0.1 (from matplotlib)
  Downloading contourpy-1.3.3-cp314-cp314-manylinux_2_27_x86_64.manylinux_
64.whl.metadata (5.5 kB)
```

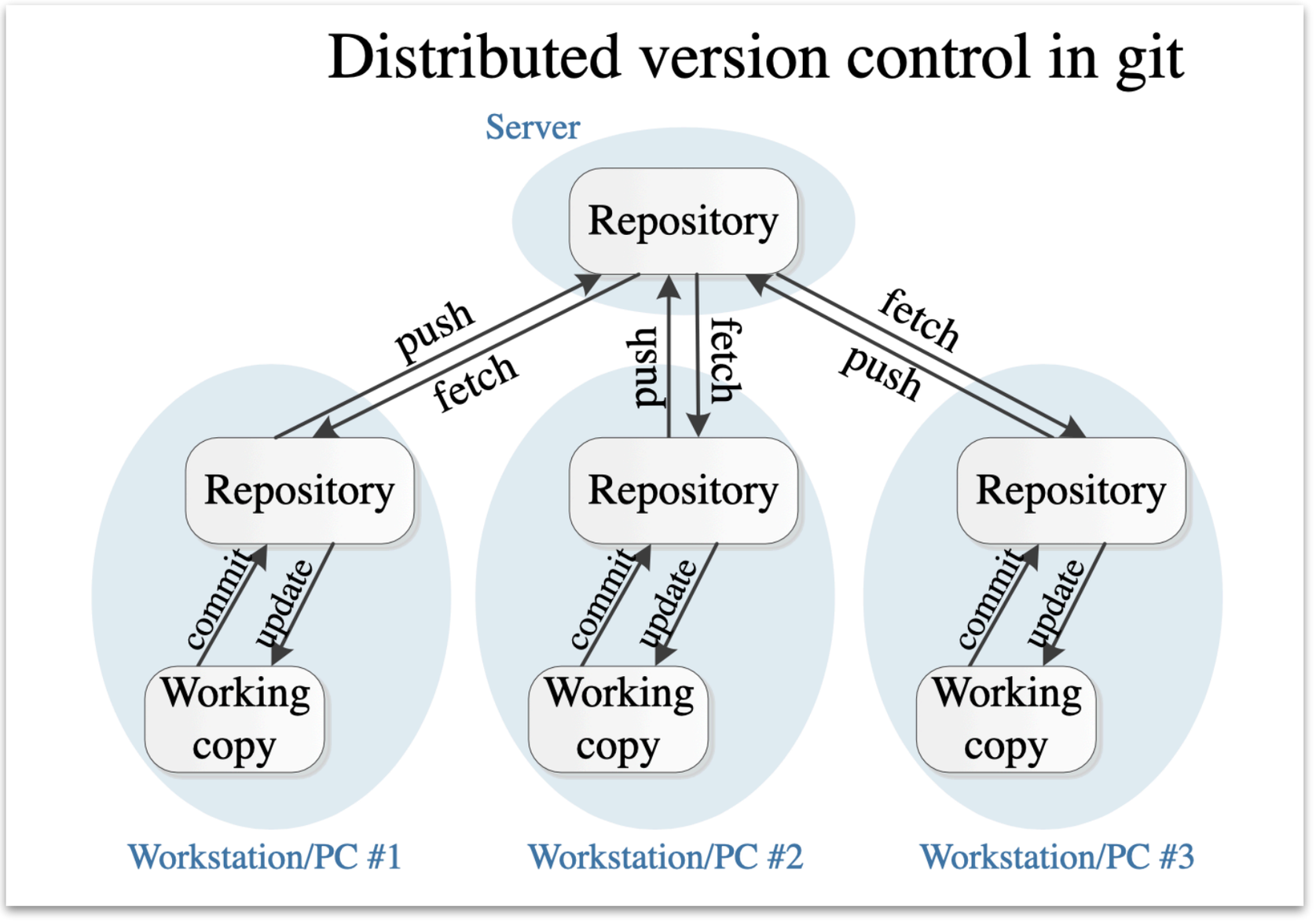
Python scripts

```
print("hello world")
~
~
~
~
~
~
~
```

```
(cee690) nc153@dcc-login-05  ~/miniconda3 $ python test.py
hello world
```

Version control





Source: https://homes.cs.washington.edu/~mernst/advice/version-control.html

Homework

Figure out what remote system you will be using and get things working

LLMs are your friend and are encouraged