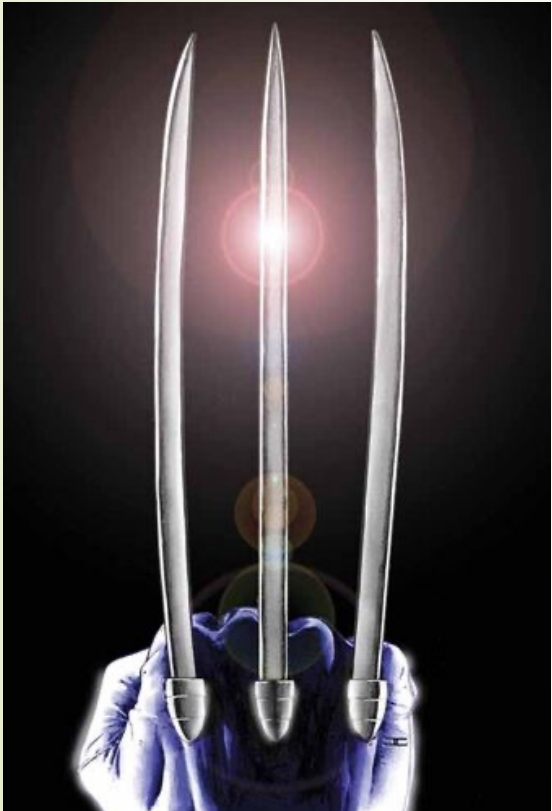


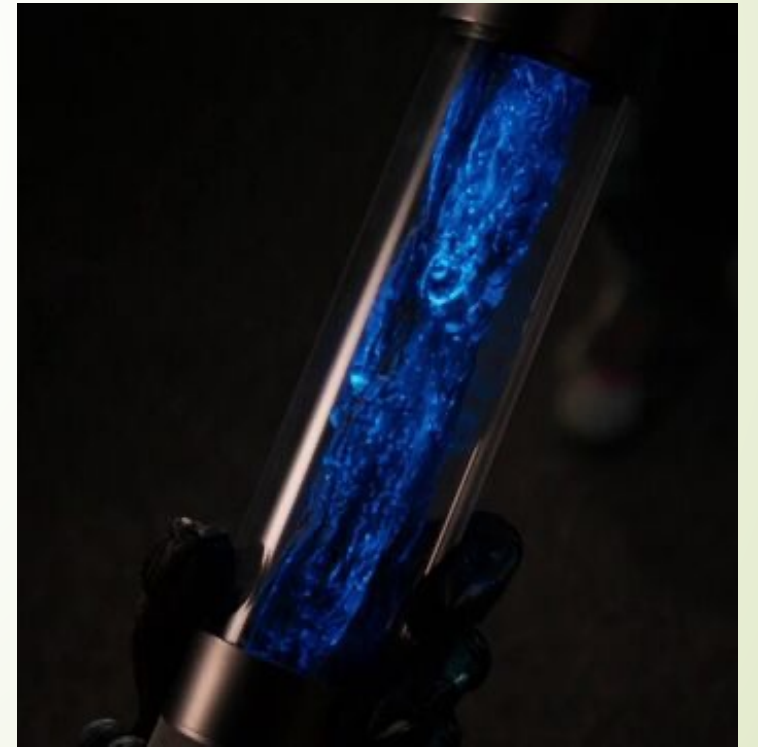
WHAT KIND OF MATERIAL WOULD YOU LIKE TO DESIGN?



Wolverine - Adamantium



Wonder Woman - Amazon suit



Black Panther - Vibranium

Day 1:
YALE PATHWAYS TO
SCIENCE SUMMER
WORKSHOP 2021

Aakash Kumar
aakash.kumar@yale.edu

Introduction to Linux

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

LEARNING GOALS

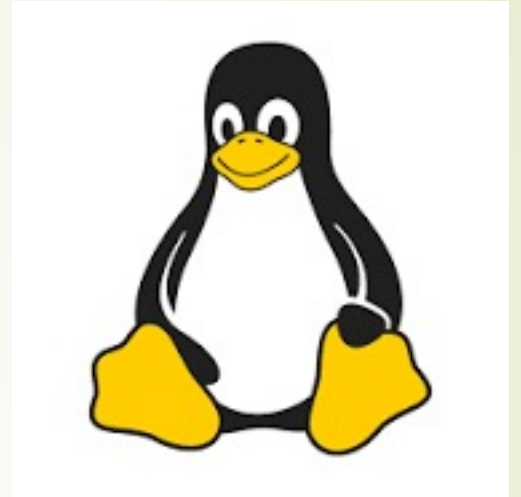
- Different type of Operating Systems (OS)
- Introduction to Linux
- Commands to change directories, view and edit files

QUIZ: WHICH OS DO YOU CURRENTLY USE?

- A) Windows 10
 - B) MacOS
 - C) Ubuntu
 - D) Chrome OS
-
- Personal laptop/desktop generally have Windows or MacOS
 - Both Ubuntu and Chrome OS are based on Linux

LINUX

- Linux is the most common OS on large computing resources
- Developed by Linus Torvalds in the early 90s
- Advantages:
 1. Security
 2. Free (open-source)
 3. Performance
 4. Low specs (memory, storage) required



Tux the penguin



Android is Linux based

LOGGING ON TO GRACE

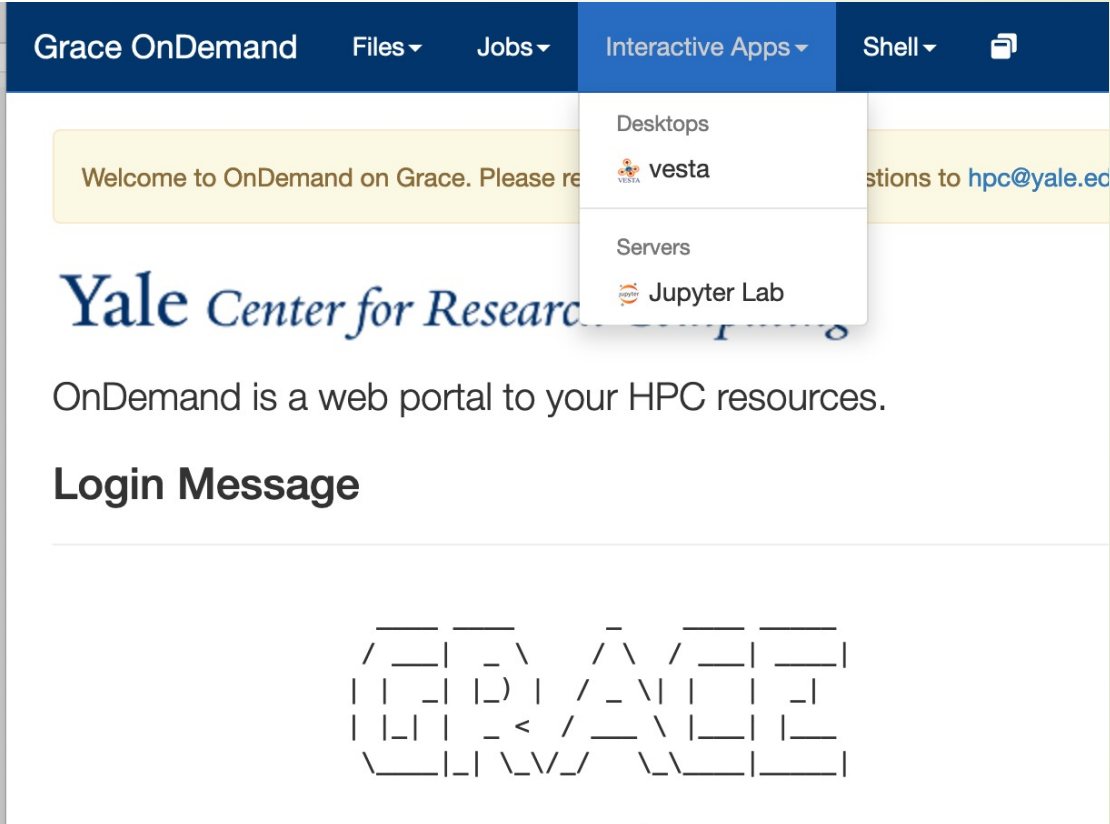
- Grace Supercomputer on Yale (<https://research.computing.yale.edu/>)
- Named after Grace Hopper, a pioneer of computer programming
- Grace has ~ 27000 cores (compare it to a 2-core or a quad-core laptop)

Go to:

- <https://pathways.ycrc.yale.edu> and type in your netID and password

- To use the supercomputer, we will use an interface called **JupyterLab**!

- Specify number of cores as 6, time as 2 hours



The screenshot shows the Grace OnDemand web portal. The top navigation bar includes 'Grace OnDemand', 'Files', 'Jobs', 'Interactive Apps', and 'Shell'. A dropdown menu is open under 'Interactive Apps', showing options for 'Desktops', 'vesta', 'Servers', and 'Jupyter Lab'. Below the navigation bar, a yellow banner reads 'Welcome to OnDemand on Grace. Please refer to the documentation for more information. For questions to hpc@yale.edu'. The main content area features the Yale Center for Research Computing logo and the text 'OnDemand is a web portal to your HPC resources.' Below this is a 'Login Message' section, which is currently blank. At the bottom of the page, there is a large, stylized graphic consisting of a grid of squares and lines, resembling a circuit board or a data visualization.

LOGGING ON TO GRACE


Welcome to OnDemand on Grace. Please report any issues or suggestions to hpc@yale.edu

Session was successfully deleted. ✕

[Home](#) / [My Interactive Sessions](#)

Interactive Apps

Desktops

 vesta

Servers

 Jupyter Lab

Jupyter Lab (31033723)

1 node | 6 cores | Starting

Created at: 2021-07-11 21:43:20 EDT

 Delete

Time Remaining: 1 hour and 59 minutes

Session ID: [d77af227-45d5-42b5-b02e-347a9fe08904](#)

Your session is currently starting... Please be patient as this process can take a few minutes.

LOGGING ON TO GRACE

Welcome to OnDemand on Grace. Please report any issues or suggestions to hpc@yale.edu

Session was successfully deleted. ✕

[Home](#) / My Interactive Sessions

Interactive Apps

Desktops

 vesta

Servers

 Jupyter Lab

Jupyter Lab (31041121)

1 node | 6 cores | Running

Host: [>_c18n03.grace.hpc.yale.internal](#)

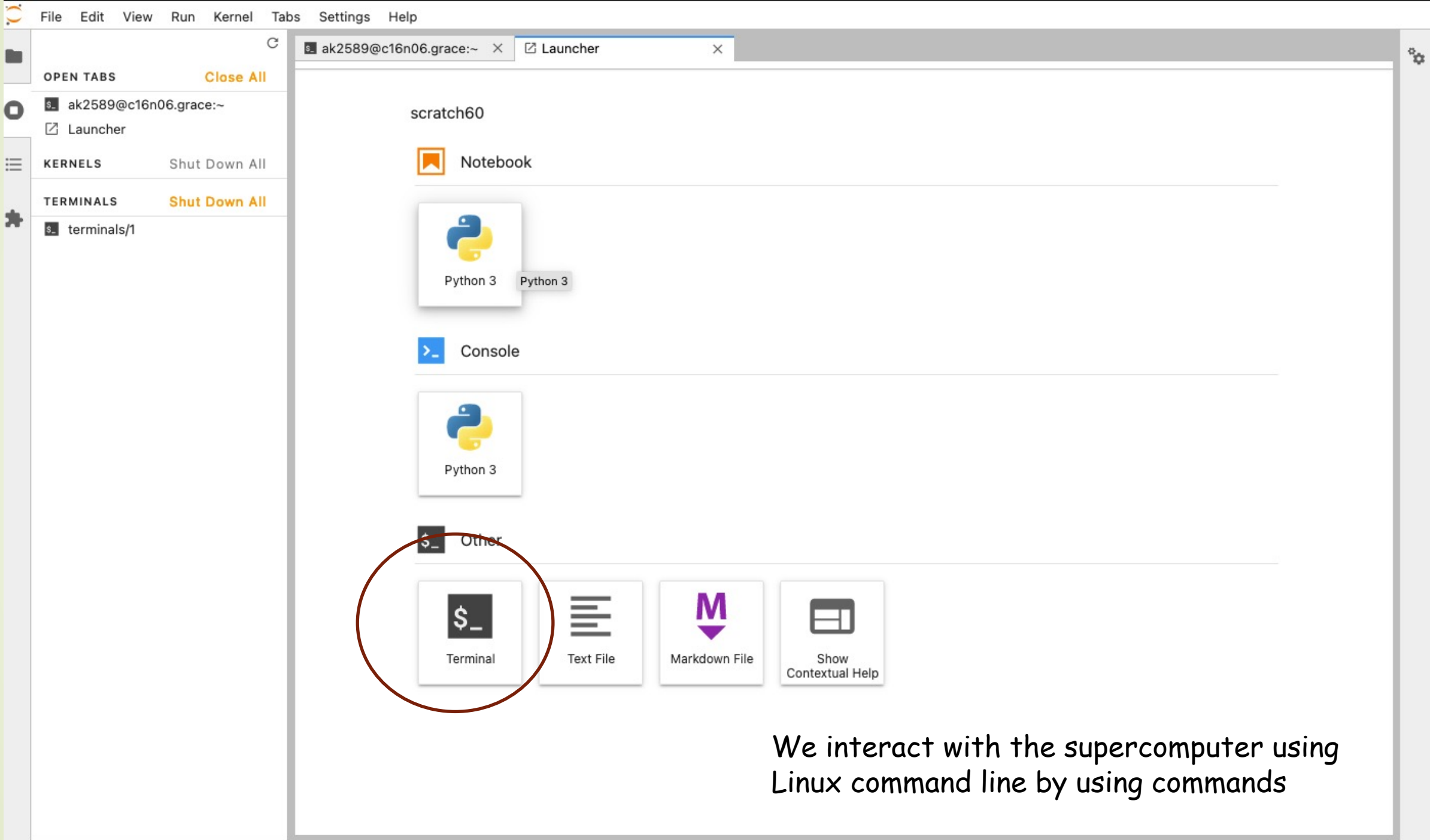
 Delete

Created at: 2021-07-11 23:49:49 EDT

Time Remaining: 1 hour and 59 minutes

Session ID: [7de716c2-af26-4197-847f-f7c3fdadf640](#)

 Connect to Jupyter



We interact with the supercomputer using Linux command line by using commands

LINUX COMMAND LINE



Your netid@computer node

```
[ak2589@c05n11 ~]$ ls
bin          intel
Desktop      material-for-ljubljana-ge-summer-school-master.tar.gz
greetings.py miniconda3
[ak2589@c05n11 ~]$
```

Miniconda3-latest-Linux-x86_64.sh parallel_python.ipynb
ondemand Pathways_workshop
parallel.ipynb project

- ls (lists the contents of the current directory)
- cd <directory> (takes you into <directory>)
- cd **Commands**
- cd .. (takes you one folder up)

```
[ak2589@c05n11 Pathways_workshop]$ ls
Commands Day1 Day2 Day3 Day4 Introduction_to_linux
[ak2589@c05n11 Pathways_workshop]$
```

- Activity: type the following command
cd -
- What does this do?

File Edit View Run Kernel Tabs Settings Help

Filter files by name

Name	Last Modified
/	
bin	11 days ago
intel	a year ago
miniconda3	12 days ago
ondemand	2 months ago
Pathways_workshop	a day ago
project	a year ago
Results	a year ago
scratch60	a year ago
Software	a month ago
Study_Group	a year ago
Wolfram Mathematica	6 months ago
Desktop	2 months ago
greetings.py	2 months ago
material-for-ljubljana-...	3 months ago
Miniconda3-latest-Lin...	a year ago
parallel_python.ipynb	2 months ago
parallel.ipynb	2 months ago

```
ak2589@c05n11.grace:~/P: X
[ak2589@c05n11 ~]$ cd Pathways_workshop/
[ak2589@c05n11 Pathways_workshop]$ ls
Commands Day1 Day2 Day3 Day4 Introduction_to_linux
[ak2589@c05n11 Pathways_workshop]$ cd ..
[ak2589@c05n11 ~]$ pwd
/home/ak2589
[ak2589@c05n11 ~]$ ls
bin intel
Desktop material-for-ljubljana-qe-summer-school-master
greetings.py miniconda3
[ak2589@c05n11 ~]$ python
Python 3.7.6 (default, Jan 8 2020, 19:59:22)
[GCC 7.3.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more ir
>>> import mpi4py
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'mpi4py'
>>>
[ak2589@c05n11 ~]$ ls
bin intel
Desktop material-for-ljubljana-qe-summer-school-master
greetings.py miniconda3
[ak2589@c05n11 ~]$ ls
bin intel
Desktop material-for-ljubljana-qe-summer-school-master
greetings.py miniconda3
[ak2589@c05n11 ~]$ cd Pathways_workshop/
[ak2589@c05n11 Pathways_workshop]$ s
bash: s: command not found...
[ak2589@c05n11 Pathways_workshop]$ cd ..
[ak2589@c05n11 ~]$ cd Pathways_workshop/
[ak2589@c05n11 Pathways_workshop]$ ls
Commands Day1 Day2 Day3 Day4 Introduction_to_linux
[ak2589@c05n11 Pathways_workshop]$
```

➤ File Navigator on the left side

➤ Go to Pathways_workshop

COPYING AND DELETING FILES

➤ `cp <filename1> <copy_of_filename1>` (make a copy)

➤ `cp Introduction_to_linux intro`

➤ `cp <filename1> <directory>` (copy to a directory)

➤ `cp intro Day1`

➤ `cd <directory>` (takes you into <directory>)

➤ `cd Day1`

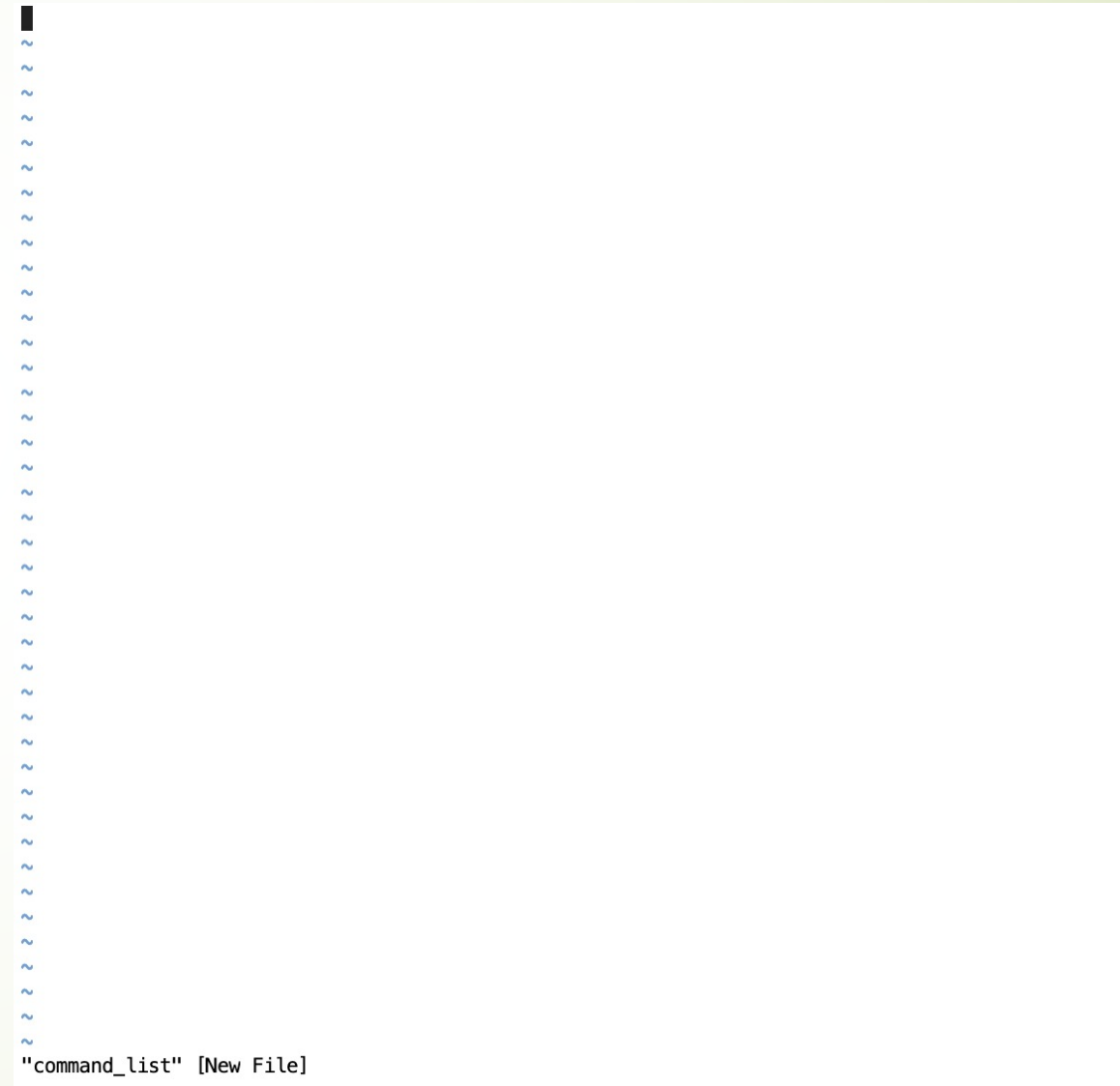
➤ `ls` (should show the file `intro` you just copied)

➤ `rm intro` (deletes/removes the file)

```
[ak2589@c05n11 Pathways_workshop]$ ls
Commands Day1 Day2 Day3 Day4 Introduction_to_linux
[ak2589@c05n11 Pathways_workshop]$ █
```

VIEWING AND EDITING FILES

- We will use `vim` as the editor
 - very powerful and simple text editor
 - we use commands to view, edit and save files!
-
- `vi <filename>`
 - `vi command_list`
-
- To start typing, press `'i'` key
 - `bsudgwudghekce`
 - press `'Esc'` key to exit writing (insert) mode
 - save by `:x` and hit enter

A screenshot of a Vim editor window. The window title is '"command_list" [New File]'. The editor area is mostly blank, with a vertical line of blue tilde characters (~) on the left side, indicating the start of a new file. The status bar at the bottom shows the filename and file type.

```
"command_list" [New File]
```

VIEWING AND EDITING FILES

- To ensure, file is not changed accidentally after some typing type `:q!` and hit 'enter'
- vi `command_list`
- Activity: Make some changes to the file (Hint: press 'i' to begin writing)
- `dd` deletes the current line
- What does `5dd` do? Try it!
- Exit the file saving the new changes (some lines deleted)!
- Also, try opening the file from the Navigation pane on the left

KEY POINTS

- ▶ Linux is very powerful, free OS and secure OS.
- ▶ We can use its command line interface to work with directories and files.
- ▶ vim editor is a highly configurable text editor to create, edit and save files.

RESOURCES

- Google search because linux & vim have a huge number of users
- <https://www.linux.org/forums/#linux-tutorials.122>
- https://vimhelp.org/vim_faq.txt.html
- <https://vim-adventures.com/> (play games and learn vim)