# Setting Up A Software Development Environment

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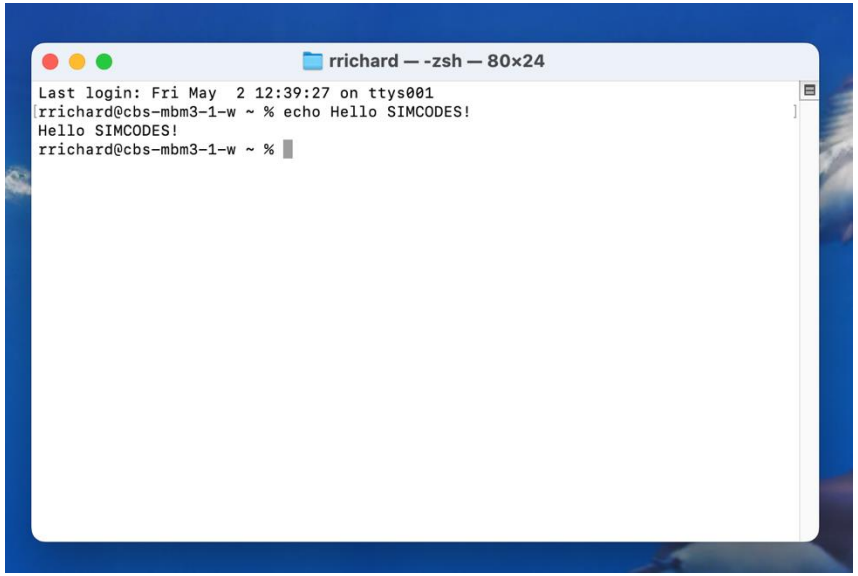
# Assumptions

- Have access to a computer.
- The computer is running MacOS (preferred) or Windows (I'll begrudgingly accept).
- Can install software on that computer.
- Current programming level is: "Terminal, that's where I board a plane, right?"
  - If you're more experienced than this, the assumption is you'll let me oversimplify many many things.

# Objectives

- Know what a Linux terminal is.
- Know how to access a Linux terminal.
- Know the most important Linux terminal commands.
- Install Python.
- Write a “Hello World” Python module.
- Run the “Hello World” Python module.

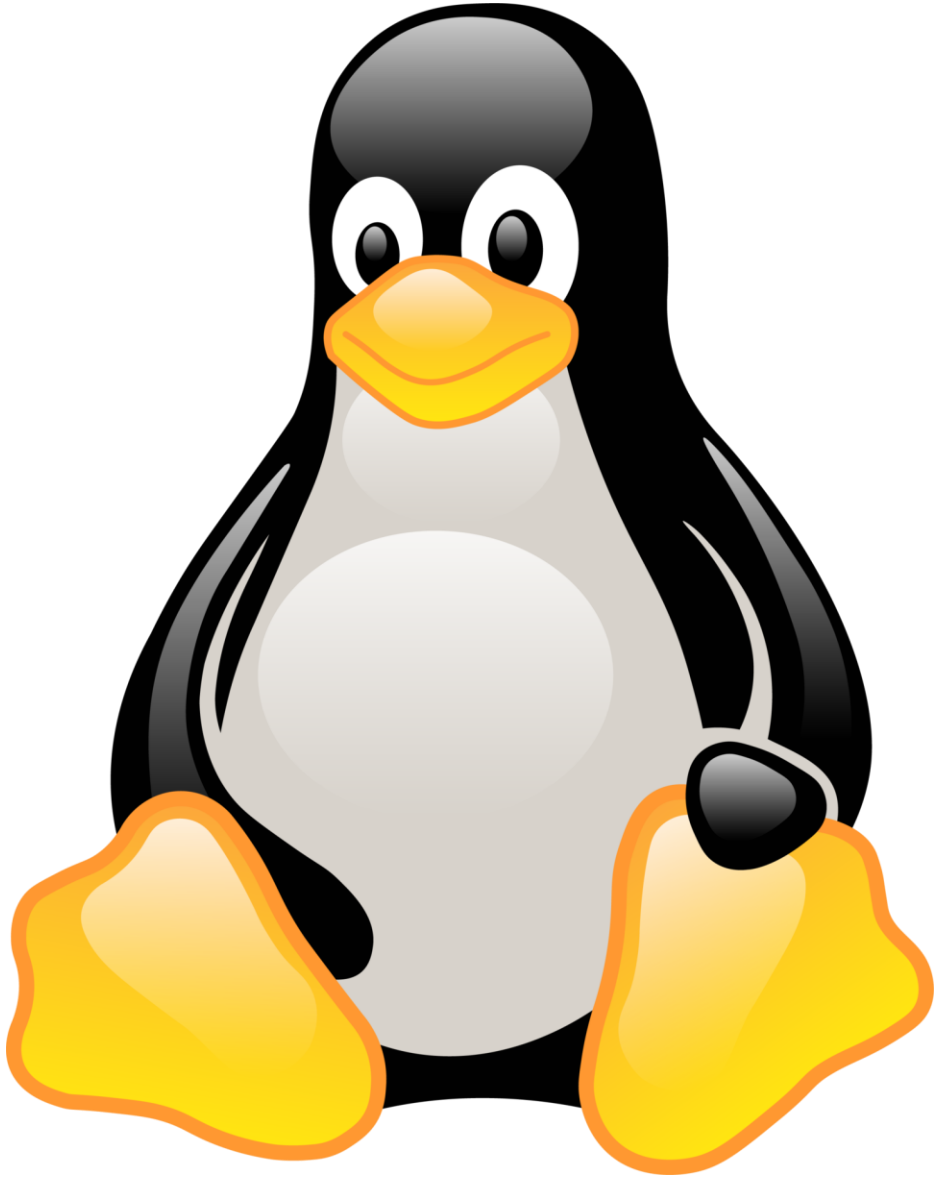




# What is a Terminal?

- Most people interact with their computer graphically.
  - Called a “Graphical User Interface” or GUI for short (pronounced gooey).
  - Graphics in the GUI represent pieces of the program.
  - Use mouse to select pieces of the graphics.
  - Typing is reserved for entering text/numerical data.
- Can also interact with a computer through text.
  - Use a program called a “terminal” to do this.

# What is Linux?

- Linux is an operating system (OS) alternative to MacOS and Windows.
  - (Pause for diehard Linux people to correct me…)
- Unlike MacOS/Windows, Linux is open source.
  - “Open source” means that the source code is publicly available.
  - Easier for people to add features.
- Programmer’s preference.
  - Virtually every programming language is supported.
  - Uses little resources.
  - Runs on most hardware.
  - Community supported.



# What is a Linux Terminal?

Strictly speaking, it's a terminal you can use to interact with the Linux OS.

More loosely, it's a terminal that supports Linux commands.

Contrast this with Window's PowerShell (if you know about it).

TL;DR.

| | | |
|---|---|---|
| "Linux" = best OS (according to programmers). | "Terminal" = way to interact with your computer via text. | "Linux Terminal" = is the best way to interact with your computer via text (according to programmers). |

Disclaimer: From here forward we assume Linux terminals, i.e., if you try the commands in PowerShell or another terminal they may not work.

# Why Do I Want To Use a Terminal?

Because I said so… (just kidding)

Automation!!!

Great for tutorials.

- Easy: `git clone https://github.com/SIMCODES-ISU/.github`
- Hard: “Open a web browser. Navigate to GitHub. Up by the cat-thing, type in the search bar…”.

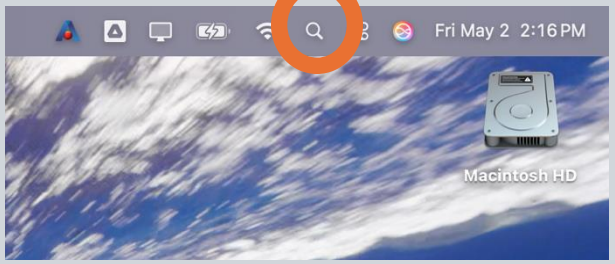
Usually how you interact with remote computers.

- Sending/receiving graphics requires sending a lot of extra data.

# Accessing a Linux Terminal (MacOS): Part 1

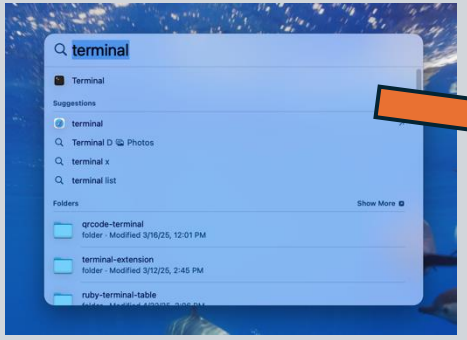
1

Open spotlight (magnifying glass)



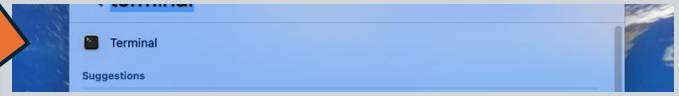

2

Type “terminal”



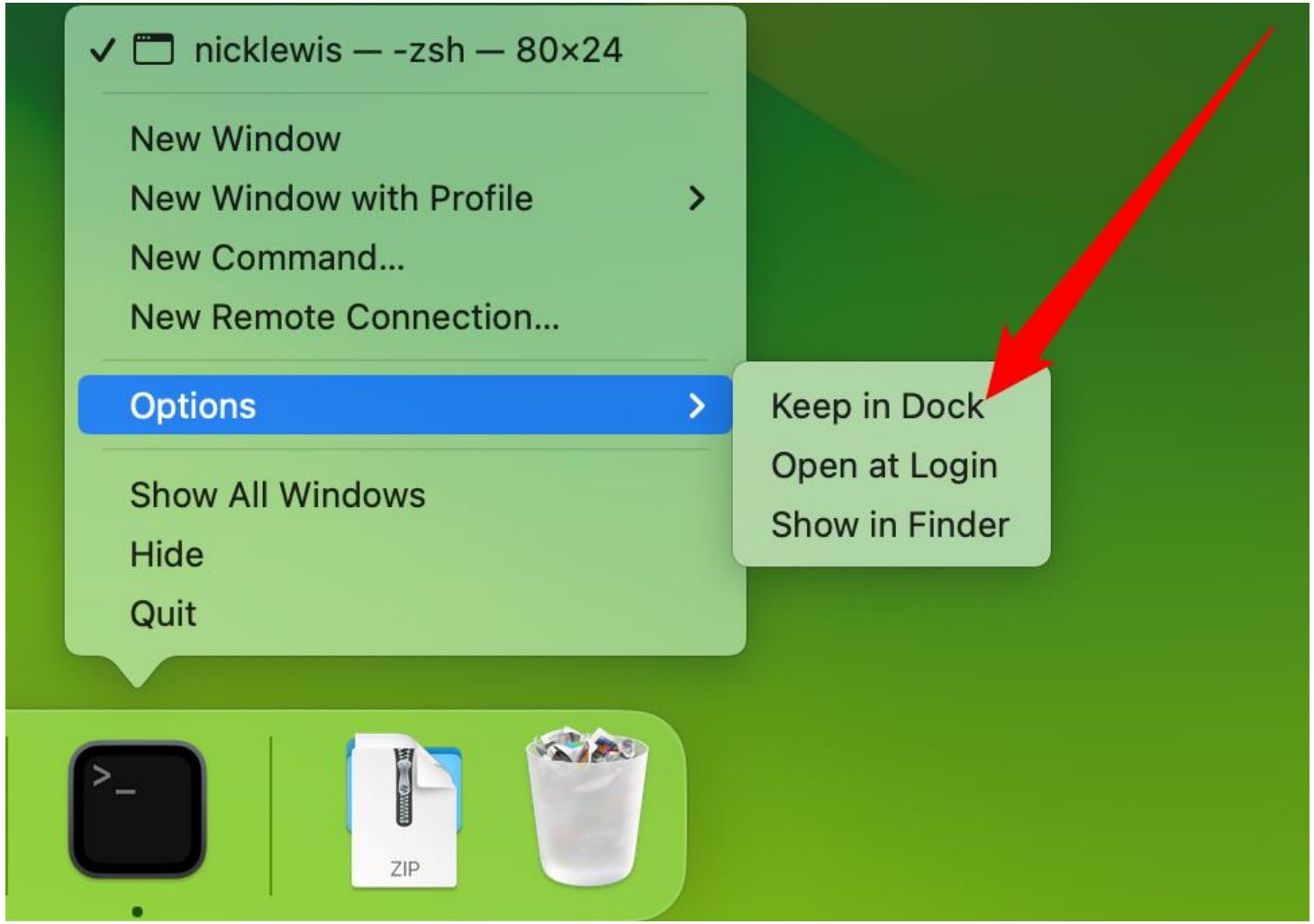

3

Click on terminal



# Accessing a Linux Terminal (MacOS): Part 2

- Please wait for your Windows colleagues (it's going to be a while).
- In the meantime, consider pinning terminal to your dock.

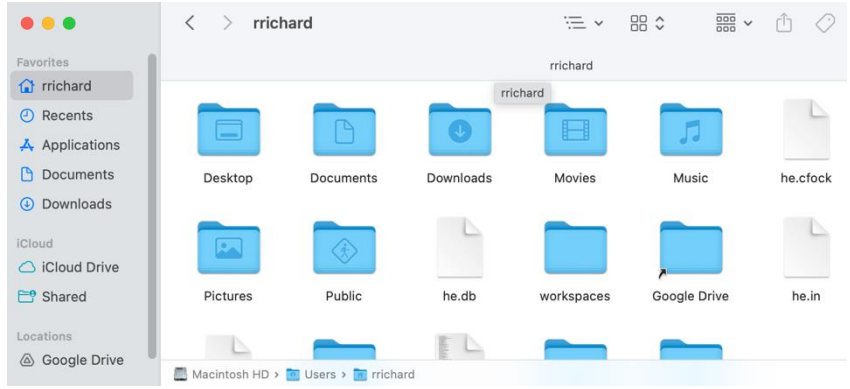


# Accessing a Linux Terminal (Windows 10)

1. Go to Microsoft Store

# Accessing a Linux Terminal (Windows 11)

# I Have a (Linux) Terminal. Now What?

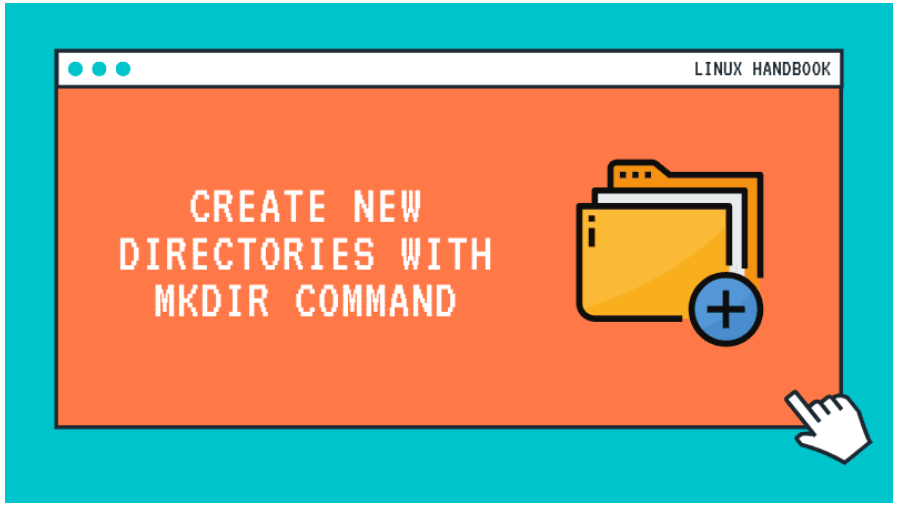



- Start by thinking of your terminal like a file system.
- When you start terminal, you are in a folder/directory, but which one?
  - Type `pwd` (and hit enter)
  - The result is your current directory.
  - `pwd` stands for:
    - Print (write to the terminal)
    - Working Directory (the directory you are currently working in).

# Other Filesystem Commands

```
rrichard@cbs-mbm3-1-w ~ % ls
Desktop      Downloads    Library      Music        Public       spack
Documents    Google Drive Movies       Pictures     simcodes.txt workspaces
```

- `ls` is used to see the files and directories in your current working directory.
  - `ls` is short for list (not sure why we needed to abbreviate it…)
  - You may not get color (if you do, the colors denote file types)
- `mkdir <dirname>` is used to create directories
  - `mkdir` is short for make directory.
  - `<dirname>` should be replaced with what you want to call the directory.



```
rrichard@cbs-mbm3-1-w ~ % mkdir my_simcodes_tutorial_directory
rrichard@cbs-mbm3-1-w ~ %
```

# Pop Quiz: Where's My Directory?

- When I run `mkdir` nothing happens. How can I check if `mkdir` did its job?

```
rrichard@cbs-mbm3-1-w ~ % mkdir my_simcodes_tutorial_directory
rrichard@cbs-mbm3-1-w ~ % ls
Desktop                         my_simcodes_tutorial_directory
Documents                       Pictures
Downloads                       Public
Google Drive                    simcodes.txt
Library                         spack
Movies                          workspaces
Music
```

# Pop Quiz: Answer

`ls`

# Even More Filesystem Commands

- To change directory use `cd`.
- Pro tip: “tab” key is auto-completes file/directory names. If you start typing the name of a long directory, like “`my_simcodes_tutorial_directory`”, try hitting tab after a few letters to let the terminal fill in the rest.
  - Auto-complete will only fill in as much as it can unambiguously. If it only gives you part of the name hit tab a second time to see the choices.

```
rrichard@cbs-mbm3-1-w ~ % cd my_simcodes_tutorial_directory
rrichard@cbs-mbm3-1-w my_simcodes_tutorial_directory % pwd
/Users/rrichard/my_simcodes_tutorial_directory
rrichard@cbs-mbm3-1-w my_simcodes_tutorial_directory %
```

# Notes on File Names

Whoever created the terminal made a terrible decision, spaces are used to separate arguments to commands.

E.g., `cd my_simcodes_tutorial_directory` the command (`cd`) is separated from the argument (`my_simcodes_tutorial_directory`) by a space.

If your file/directory names contain spaces, we now run into a problem

TL;DR get in the habit **NOW** of avoiding spaces or special characters (&*$#!) in file/directory names. For our purposes “-” and “_” are NOT special characters.

# Command Summary

- `pwd` prints the working directory.
- `ls` shows the files and directories in a directory.
- `mkdir` creates a directory.
- `cd` changes the directory.
- There are a ton more https://www.geeksforgeeks.org/linux-commands-cheat-sheet/

# Objectives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- Install Python.
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# What is Python?

- Named for Monty Python
- GeeksForGeeks: Most popular programming language.
- Design philosophy prioritizes code readability.
- “High-level” language.
  - Python programs are relatively performant without exposing “low-level” details like memory management.
  - “Natural language”-like syntax
- Becoming the *de facto* language of scientific computing.
  - Notable exception is high-performance computing where C++ still dominates, but Python is gaining.

# Installing Python (MacOS)

You're done.

Wait for your Windows colleagues (again).

# Installing Python (Windows)

- Open a WSL tab in Windows Terminal
- Run the command `sudo apt install python3`
  - `sudo` stands for superuser do. It's used to run the following command as a superuser (administrator).
  - `apt` is short for advanced package tool (sorta like an App/Play Store for Linux)
  - `install python3` tells apt to, well, install python3

# What is a Python Module?

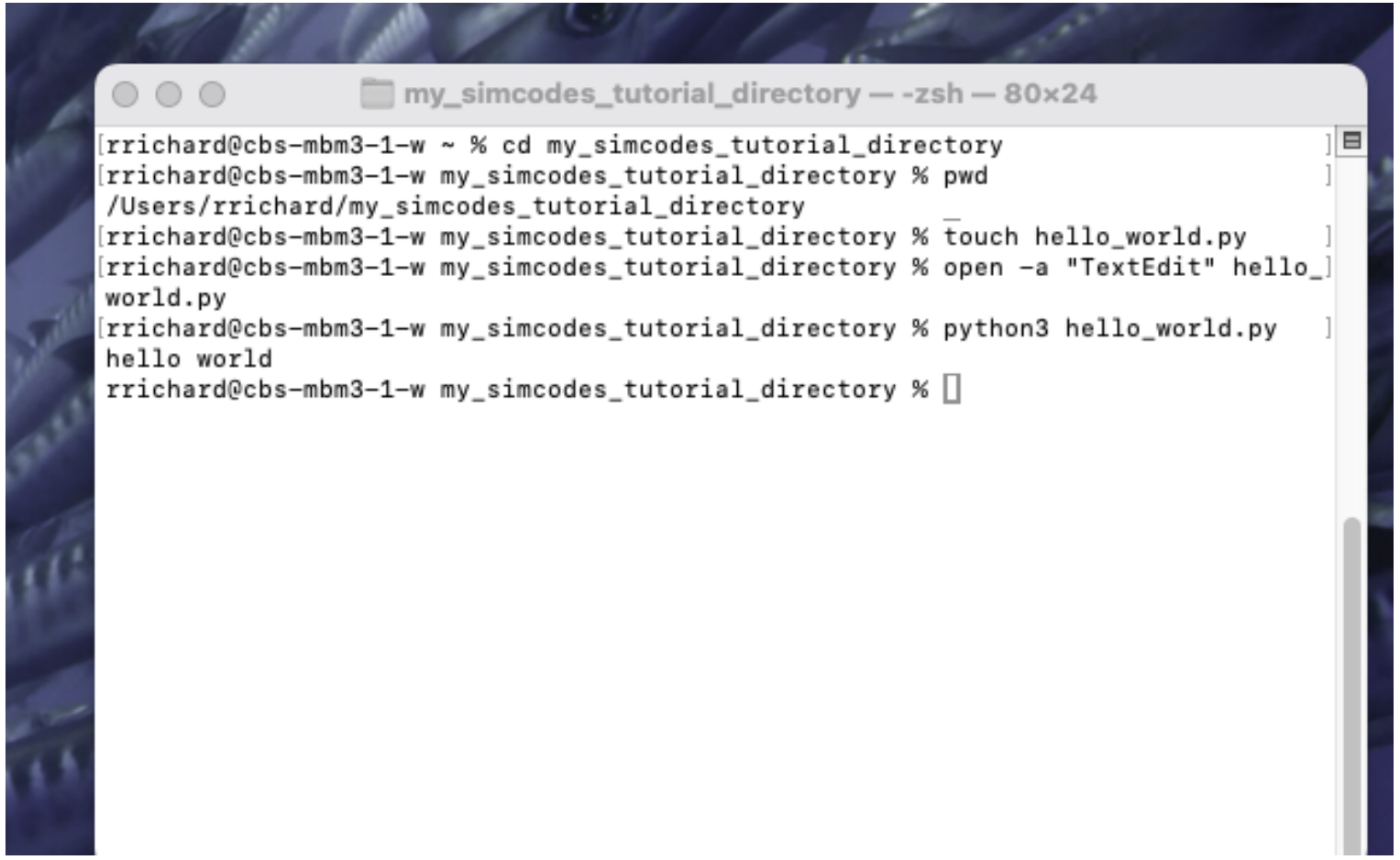
- It is a text file that contains Python source code.
  - Caveat: Need to be plain text files, e.g., **NOT** Word documents.
- Named like `name_of_file.py` (“.py” is standard extension).
- The Python “interpreter” is responsible for running the module.
  - MacOS and Linux: `python` (or sometimes `python3`) .
  - Windows: `python.exe` .
- To run a Python module you simply tell the interpreter the name of the module
  - E.g., `python name_of_file.py`

# Creating a Python Module (MacOS)

1. Open terminal.
2. `touch hello_world.py` (makes an empty file)
3. `open -a "TextEdit" hello_world.py`
4. Type `print("hello world")`, then ⌘ + s (saves)

# Creating a Python Module (Windows)

# Running Our Python Module



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# Software Development Environment (SDE)?

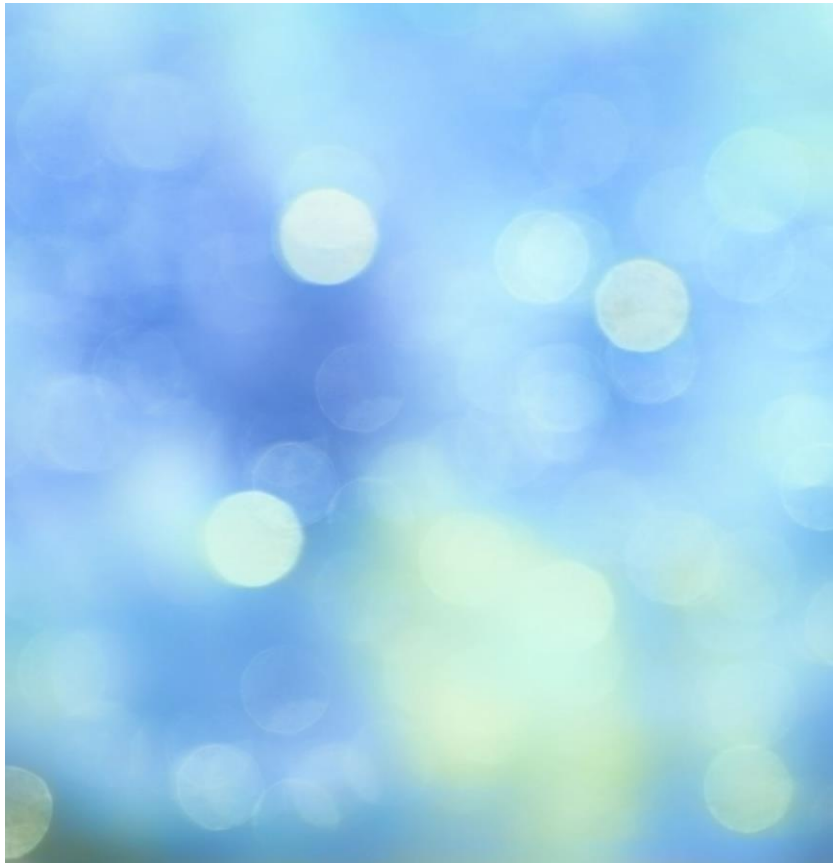
The title was “Setting Up A Software Development Environment” and we haven’t mentioned SDE yet…

An SDE is just a collection of tools to develop, test, and debug an application.

Terminal is arguably the most important tool for development.

Python comes with tools for testing and debugging. We’ll go over those tools in future lectures.

TL;DR you now have a bare-bones SDE!!!



# Acknowledgements


- MolSSI. I "borrowed" (i.e., stole) the content from them.
  - Installing terminal: https://education.molssi.org/python-package-best-practices/setup.html
  - Terminal: https://github.com/msse-chem-280-2024/msse-chem-280-2024.github.io/
- NSF for funding SIMCODES