

Assignment 1 Software Guide

CS 279, BIOE 279, BMDS 245, BIOPHYS 279, and CME 279

Policies

In this class, there will be exercises that involve some coding with existing software packages. We **strongly recommend** students work on the Learning and Technologies Spaces (LTS) machines so that you do not need to install any software on your personal machines. While you are free to install the programs on your own machine and develop locally, if you encounter issues with installation or development, we encourage you to work on the LTS machines. Feel free to post issues to [Ed](#) or come to office hours if you have any issues.

Installing PyMOL

If you are working on your personal machine for the first assignment, you will need to [download and install PyMOL 3.1](#) on your computer. Download the PyMOL 3.1 build for your platform:

PyMOL-3.1.8_0-MacOS-x86-64-py310.dmg for Mac, PyMOL-3.1.8-Windows-x86_64.exe for Windows, or PyMOL-3.1.8_0-Linux-x86-64-py310.tar.bz2 for Linux.

The first time you run PyMOL, connect to the 'Stanford' wifi network while on campus or use the Stanford VPN (Cisco AnyConnect) to download the [Stanford license key](#) for PyMOL. PyMOL 3.1 is also available on all the LTS Macs, which can be accessed remotely. Again, we recommend that students utilize LTS machines in person. See the [Working on LTS Machines](#) handout for additional details. If you cannot get PyMOL to run on your computer, please use any of the LTS machines or contact the CAs.

Basic Commands in the PyMOL Terminal

Within PyMOL, there is a terminal where you can navigate through your files and execute commands.

Here is a list of commands that may be helpful:

- `pwd` – prints the current working directory
- `cd <new directory>` – changes the working directory to the new directory. E.g. to navigate to a folder named CS279 on Desktop, use `cd Desktop/CS279`. To go back one directory, use `cd..` (include both periods).
- `ls` – lists the files in the current directory
- `mv <original> <new>` – moves the original file to the new file.
(This is also how you rename files).
- `man <command>` – Display additional information about any command or program (type “q” to exit the manual display).
- `*` – a wildcard that stands for “any characters”. `*.tif` means every .tif file in this folder.

- **Tab** – press the Tab key part-way through a file or folder name and the terminal will complete it for you.
- **Ctrl+C** – stops a program that is currently running.

If you want additional information about any command or program, you can use `man` which brings up the command's manual page.

To invoke a program within PyMOL, first navigate to the directory the program lives in, then call the program. For example, we will need to run `analysis.py` for assignment 1, which we can do by navigating into the correct directory via `cd Downloads/assign1_starter_code`, then `run analysis.py` (if your assignment is saved to Downloads).

Editing Files

To edit exercise files like `analysis.py`, you may use text editors that came with your computer e.g. TextEdit on Mac, Notepad on Windows. They will work, with two caveats:

- TextEdit: turn off Edit → Substitutions → Smart Quotes and Smart Dashes. Otherwise TextEdit silently replaces ' with a curly quote, which looks almost identical on screen but causes a syntax error. If the file opens in rich text, use Format → Make Plain Text first.
- Notepad: when you save, choose "All Files" in the "Save as type" dropdown, or Windows will rename your file to `analysis.py.txt` and PyMOL will not find it.

If you prefer a more user-friendly editor, [Sublime Text](#) and [VS Code](#) are popular choices.