PHYS 4332 – Computational Physics Python Tutorial



1.1 – Introduction and Installation Instructions

Python is a high-level, interpreted programming language that has now become the language of choice in many fields of science. This is largely due to its ease of programming and readability, the large number of libraries and community support, and the variety of programming environments (e.g. command line interpreters, scripts, web-based interpreters, notebooks). This tutorial is a crash course in Python designed to give you an overview of the programming essentials, as well as some useful tools for scientific computing, data processing, and visualization.

Although a variety of web browser-based Python development environments exist, there are significant advantages to installing Python locally on your computer. This tutorial provides step-by-step instructions on how to install and configure Python from source, as well as how to install third-party libraries that are essential for data science.

The majority of the modules in this tutorial are written in Jupyter Notebooks (formally IPython Notebooks). This is a web-based interactive development environment (IDE) for writing code (e.g., Python, Markdown, LATEX, etc.) and displaying graphics. It uses a notebook format similar to Wolfram Mathematica or Windows OneNote, where interactive cells of code can be executed one at a time by a kernel (a centralized "computational engine"). While the kernel is running, all the data generated by your code is stored temporarily in your computer's random access memory—allowing you to access data generated in previous cells.

Jupyter Notebooks can be run in a web browser if you have Python and Jupyter installed locally. However, it is highly recommended to install and use Visual Studio Code (VS Code) to work through this tutorial. This IDE integrates the three most common Python environments (command line, scripts, and notebooks), allowing you to choose the most convenient option. It also has built-in features for debugging and streamlines the installation of third-party extensions for additional features like code linting.

The latest stable (and trustworthy) version of Python is 3.10.9. We recommend selecting this option when installing it on your system using the instructions below.

Installing Python (3.10.9) for Windows

- 1. Go to https://www.python.org/downloads/windows/
- 2. Click on "Python 3.10.9" under "Stable Releases"
- 3. Scroll down to "Files" and select the "Windows Installer" corresponding to your operating system type (32-bit) or (64-bit). (To check your operating system type, click the Start menu, select Settings → System → About. It should be listed under "System type".)
- 4. Once the Installer has downloaded, run the .exe file (usually located in your Downloads folder).
- 5. In the Python Installer Setup window, click on the checkbox "Add Python 3.10 to PATH" at the bottom. This will add the location of the Python.exe to your system's PATH environment variable so you can run python from the command prompt.

- 6. Next, click "Install Now" to install Python. Choose the default setting for any remaining setup options.
- 7. Once Python has finished installing, click on the Start Menu, type cmd, and open a command prompt by selecting cmd.exe.
- 8. To verify Python installed correctly, type python --version and hit Enter. "Python 3.10.9" should appear.

Installing Python (3.10.9) for MAC

MACs usually come pre-installed with Python version 2. To check which version you have, open a terminal and type python --version + Enter.

- 1. Go to https://www.python.org/downloads/macos/
- 2. Click on "Python 3.10.9" under "Stable Releases"
- 3. Scroll down to "Files" and select the "macOS 64-bit universal2 installer" (for macOS 10.9 and later).
- 4. Once the Installer has downloaded, run the .pkg file. Choose the default setup options.
- 5. Upon completion, the installer will create a "Python 3.10" directory in your applications folder.
- 6. To verify Python installed correctly, open a new terminal and type python3 --version + Enter. "Python 3.10.9" should appear. (Note that you must use the "python3" command to access Python 3.10 from the command prompt. The command "python" will default to Python 2 unless you create an alias.)

Running Python from a Terminal

• From a command prompt or terminal, type python and hit Enter (python3 on a MAC). You should get something like the following:

```
Python 3.10.9 [MSC v.1929 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

- This is an interactive prompt that allows us to write one line of Python at a time.
- To create a "Hello World" application, we can simply write print (hello world!")" + Enter:

```
>>> print("hello world!")
hello world!
```

 \bullet We can also do simple calculations with integers and floats:

```
>>> 1+2 - 2*3
-3
>>> 4/3
1.333333333333333333333
```

• define variables:

```
>>> x=10
>>> y=2
>>> print(x**y)
100
```

• or import modules:

```
>>> import numpy as np
>>> t = np.pi
>>> print(np.cos(t))
-1.0
```

• To exit out of Python and return to the command prompt, simply type exit().

Installed VS Code

- Go to https://code.visualstudio.com/
- Click on the down arrow next to the "Download for Windows" button. This will display options for all available operating systems. Download the installer appropriate for your system.
- Follow the default installation instructions.
- Next, open VS Code and install the Python extension:
 - Click on the "Extensions" icon on the left sidebar (or type Ctrl + Shift + X).
 - Type python into the search bar and select the first result "Python". This extension includes Intellisense (PyLance), Linting, Debugging, Jupyter Notebooks, and more.
- Next, install the Code Runner extension:
 - Click on the "Extensions" icon on the left sidebar (or type Ctrl + Shift + X).
 - Type Code Runner into the search bar and select the first result. This extension includes additional options, controls, and shortcuts for running code.
- You are now ready to open Python files (.py) or Jupyter Notebook files (.ipynb) and start writing code.
- To run a Python file, open it and click on the "Run Code" button in the top right corner (or type Ctrl + Alt + N if you have Code Runner installed).
- When running for the first time, you may be asked to select a Python interpreter:
 - Open the command palette by typing Ctrl + Shift + P and type Python: Select Interpreter.
 You can also select the "Python Environment Option" on the bottom right corner of the status bar.
 - A list of available interpreters should appear (VS Code finds these automatically on your system). Select the version of Python that you just installed.

Additional resources

- To get your barrings with VS Code, check out their Getting Started videos: https://code.visualstudio.com/docs/getstarted/introvideos
- To get started with Python in VS Code: https://code.visualstudio.com/docs/python/python-tutorial
- Additional documentation on the VS Code interface can be found here: https://code.visualstudio.com/docs/getstarted/userinterface
- To further customize your VS code environment, check out Corey Schafer's video: https://www.youtube.com/watch?v=-nh9rCzPJ20