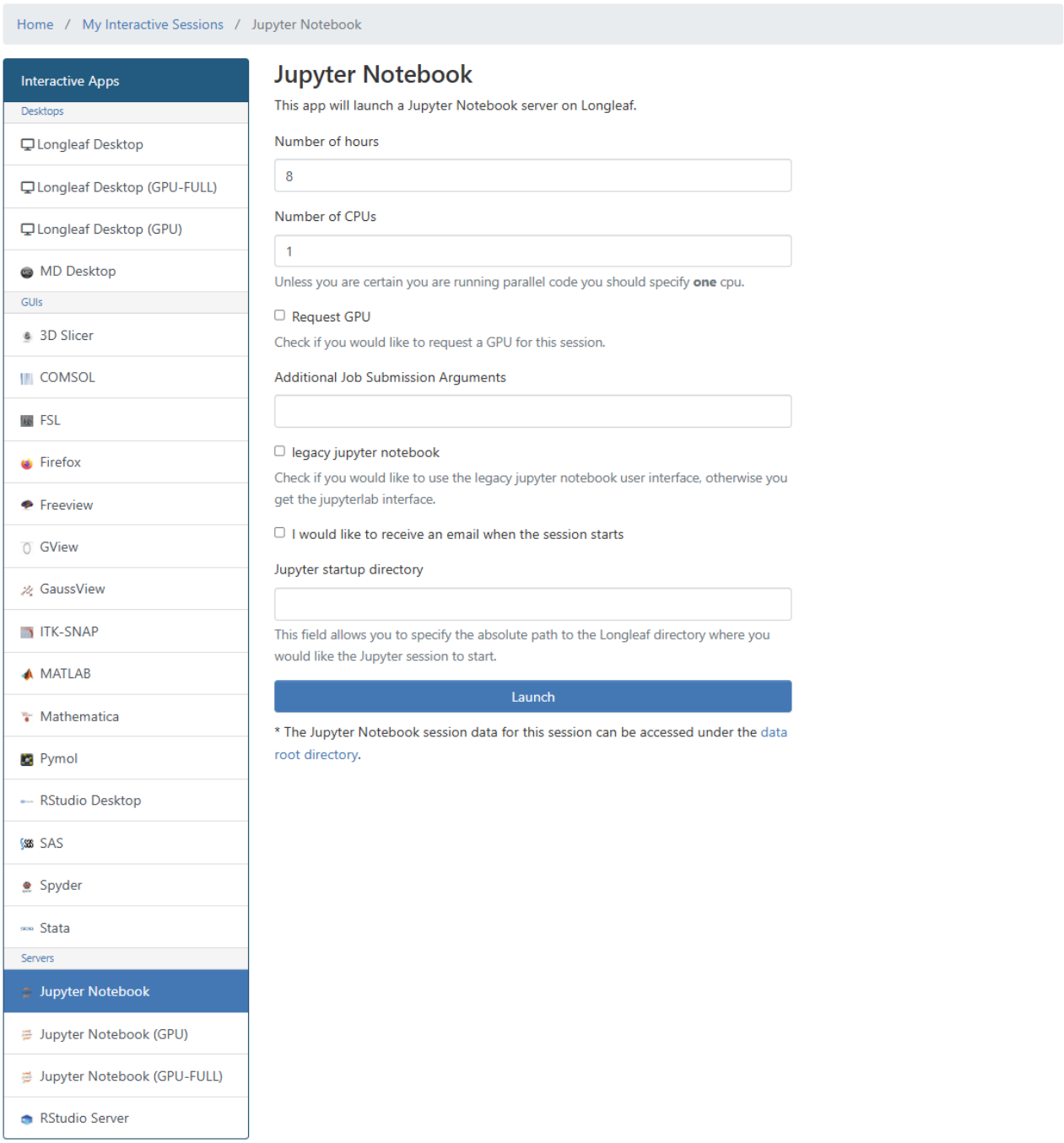
Setup Jupyter via Longleaf On Demand

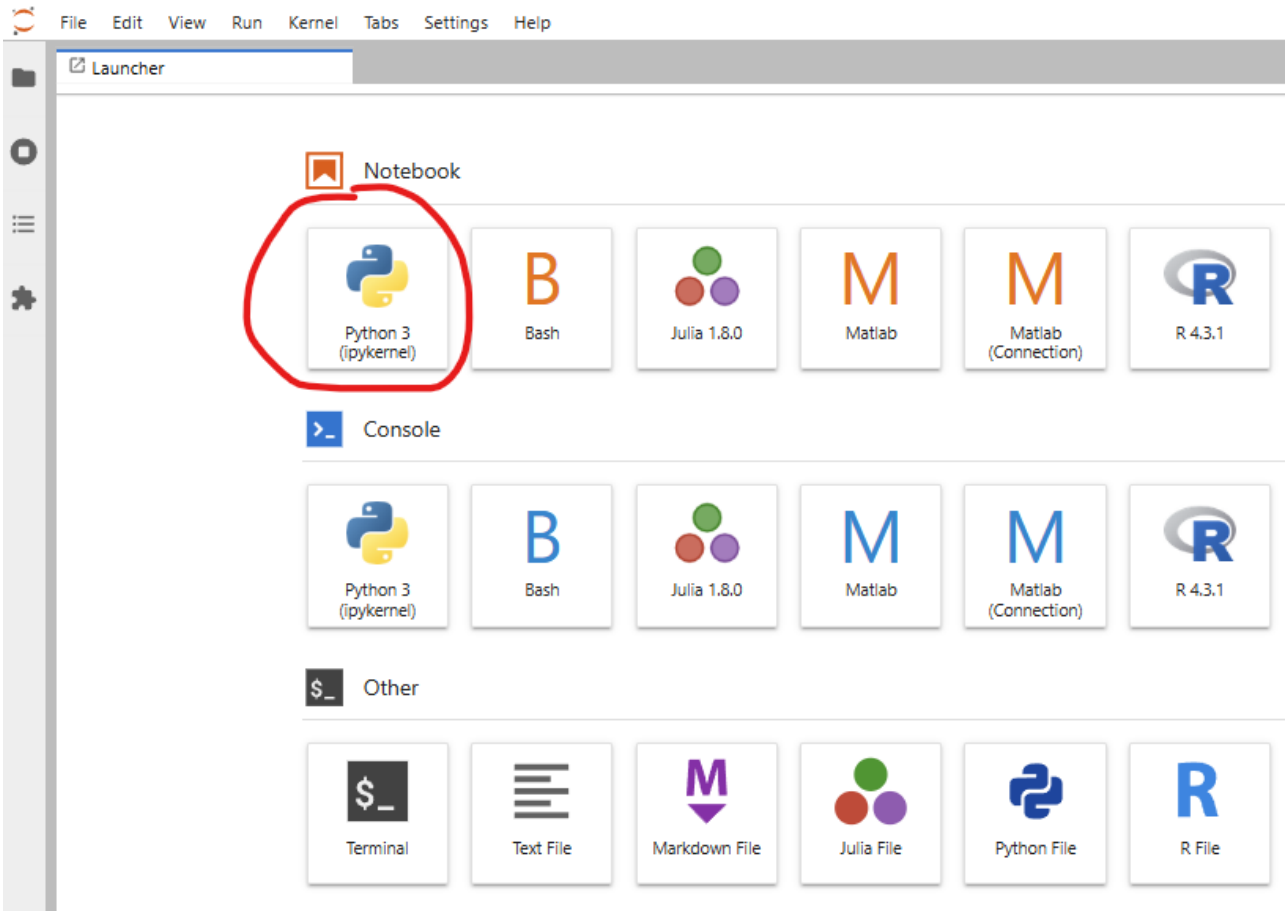
Super Important: Make sure you complete the First-time setup section at the end of this document or you will not be able able to start the coursework for CHEM 467.

Once your account is approved you will be able to access Longleaf. There are many ways to access Longleaf but for this course we will be using Longleaf On-Demand.

1. Go to https://ondemand.rc.unc.edu/pun/sys/dashboard.
2. Sign in using your onyen.
3. Click on `Jupyter Notebook`.
4. Request resources and click `Launch`.



5. Wait for computing resources to be allocated (~1 minute).
6. Click "Connect to Jupyter".
7. In the **Launcher** and under the section labeled **Notebook**, click "Python3 (ipkernel)" to open a notebook running Python.



Setting up your Jupyter notebook

Jupyter notebooks are made up of two main types of cells: **Markdown cells** and **Code cells**. You run a Jupyter notebook one cell at a time by click inside the cell and press `shift+enter`.

Markdown cells

Jupyter notebooks allow us to use a language called Markdown to type notes and descriptions in markdown cells. It's a good practice to have your first cell be markdown to explain the purpose of the notebook.

Basic markdown syntax

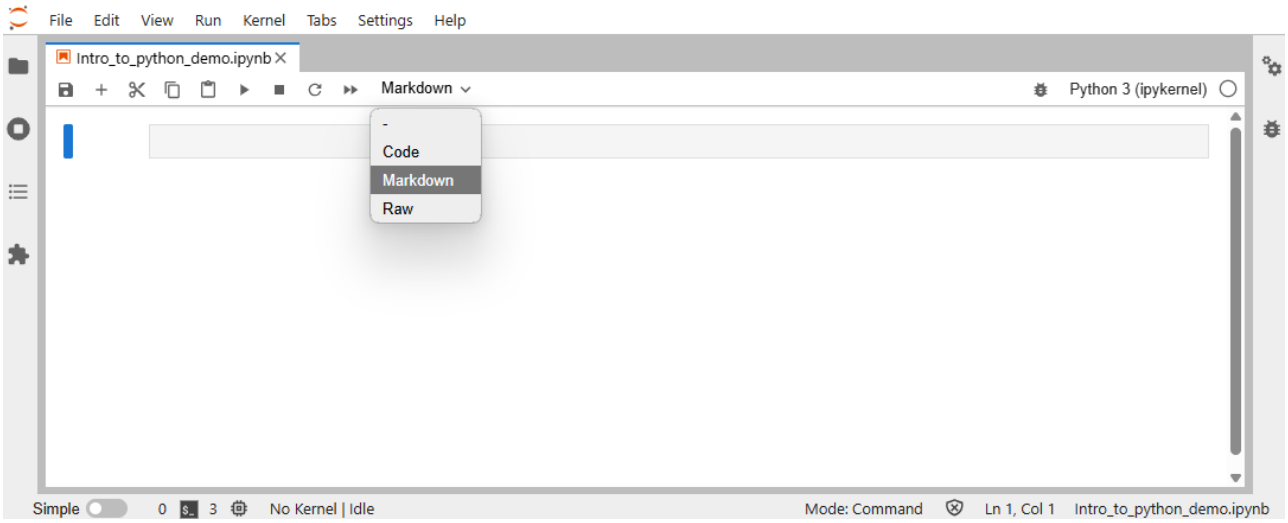
In the Markdown language, we create headers and lists using the following syntax.

Element	Basic Markdown Syntax
Heading	# H1 ## H2 ### H3

Element	Basic Markdown Syntax
Ordered List	1. First item 2. Second item 3. Third item
Unordered List	- First item - Second item - Third item

Let's practice!

1. Open a new Jupyter notebook using the instructions above.
2. Click the first cell.
3. Select `Markdown` from the cell type dropdown menu in the notebook ribbon (shown below).

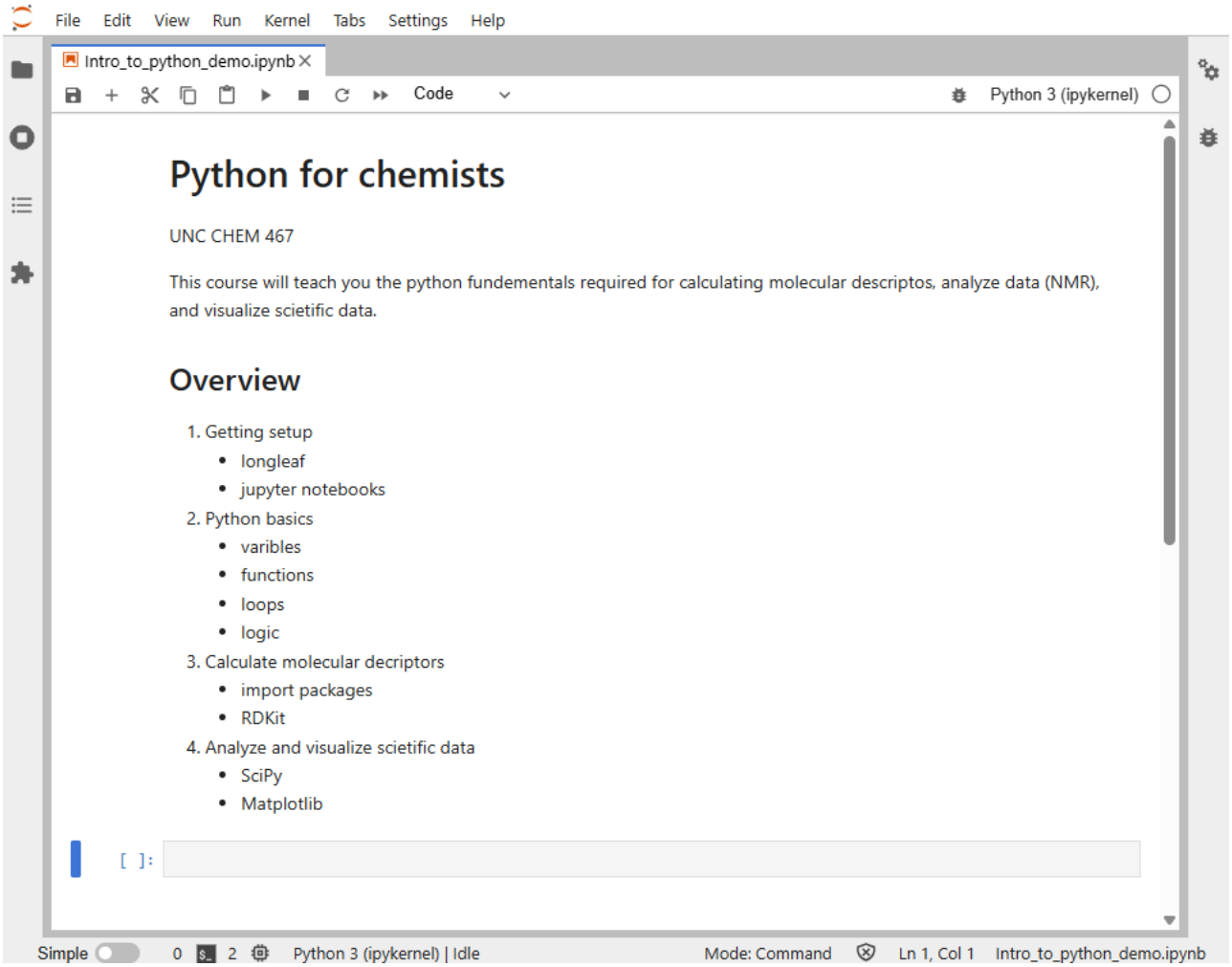


4. Paste the following into the markdown cell.

```
# Python for chemists

UNC CHEM 467

This course will teach you the python fundementals required for
calculating molecular descriptos, analyze data (NMR), and visualize
scietific data.

## Overview

1. Getting setup
    - longleaf
    - jupyter notebooks

2. Python basics
    - varibles
    - functions
    - loops
```

```
    - logic

4. Calculate molecular decriptors
    - import packages
    - RDKit

5. Analyze and visualize scietific data
    - SciPy
    - Matplotlib
```

5. Press `shift+enter` to evaluate the markdown cell. Now your notebook should look like the following:



Code cells

Jupyter notebooks allow us to run python code interactively and display the outputs all in one file. These features make Jupyter notebooks good for prototyping new code and for keeping a record of how you analyzed your data.

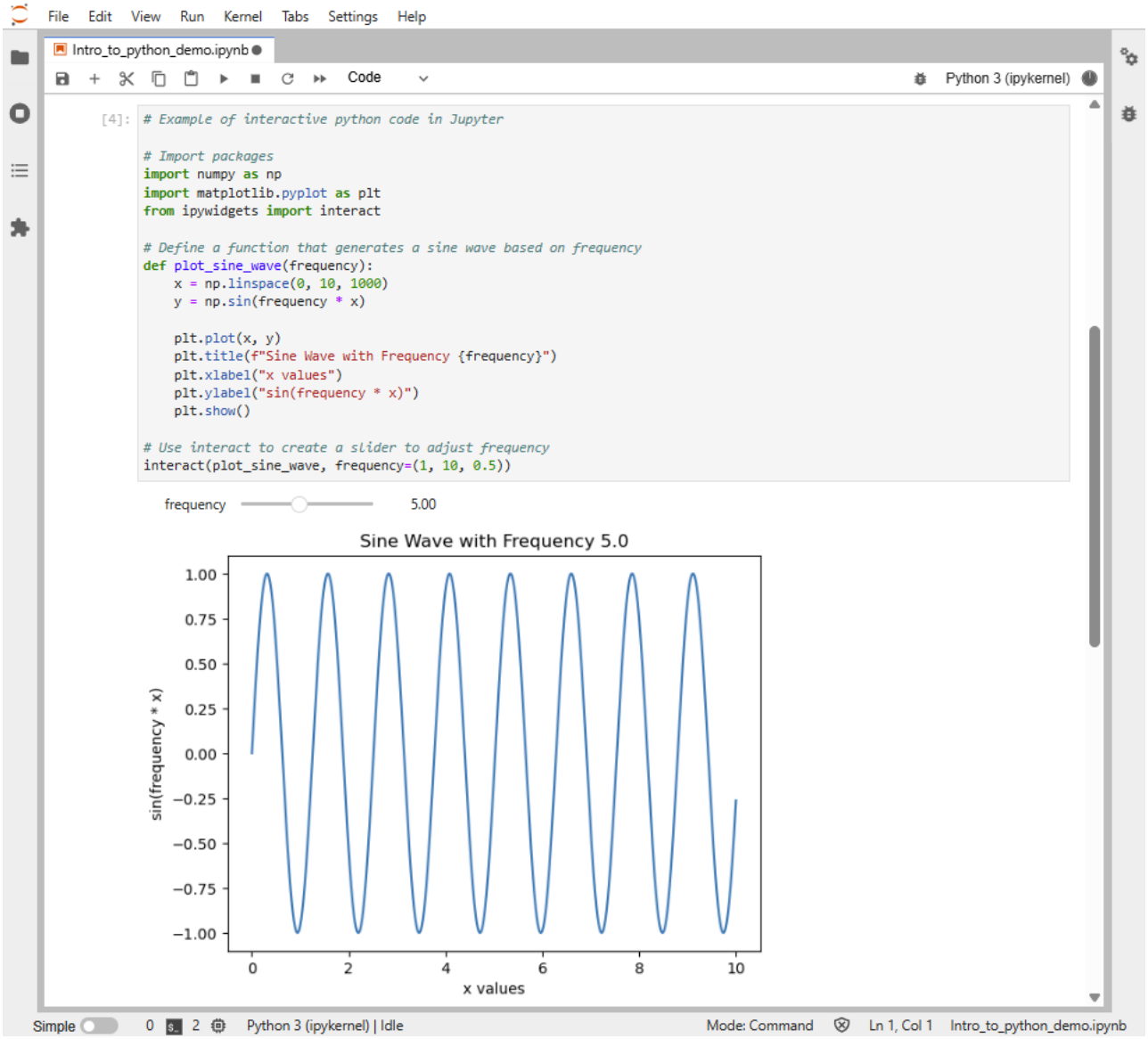
Let's practice!

1. Paste the following interactive python code into the empty code cell below our Markdown cell.

```
# Example of interactive python code in Jupyter

# Import packages
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact

# Define a function that generates a sine wave based on frequency
def plot_sine_wave(frequency):
    x = np.linspace(0, 10, 1000)
    y = np.sin(frequency * x)

    plt.plot(x, y)
    plt.title(f"Sine Wave with Frequency {frequency}")
    plt.xlabel("x values")
    plt.ylabel("sin(frequency * x)")
    plt.show()

# Use interact to create a slider to adjust frequency
interact(plot_sine_wave, frequency=(1, 10, 0.5))
```

Note: in Python (and therefore in Jupyter code cells) the # symbol is used to denote comments that will not be interpreted as code.

2. Press `shift+enter` to evaluate the code cell. Now your notebook should look like the following:

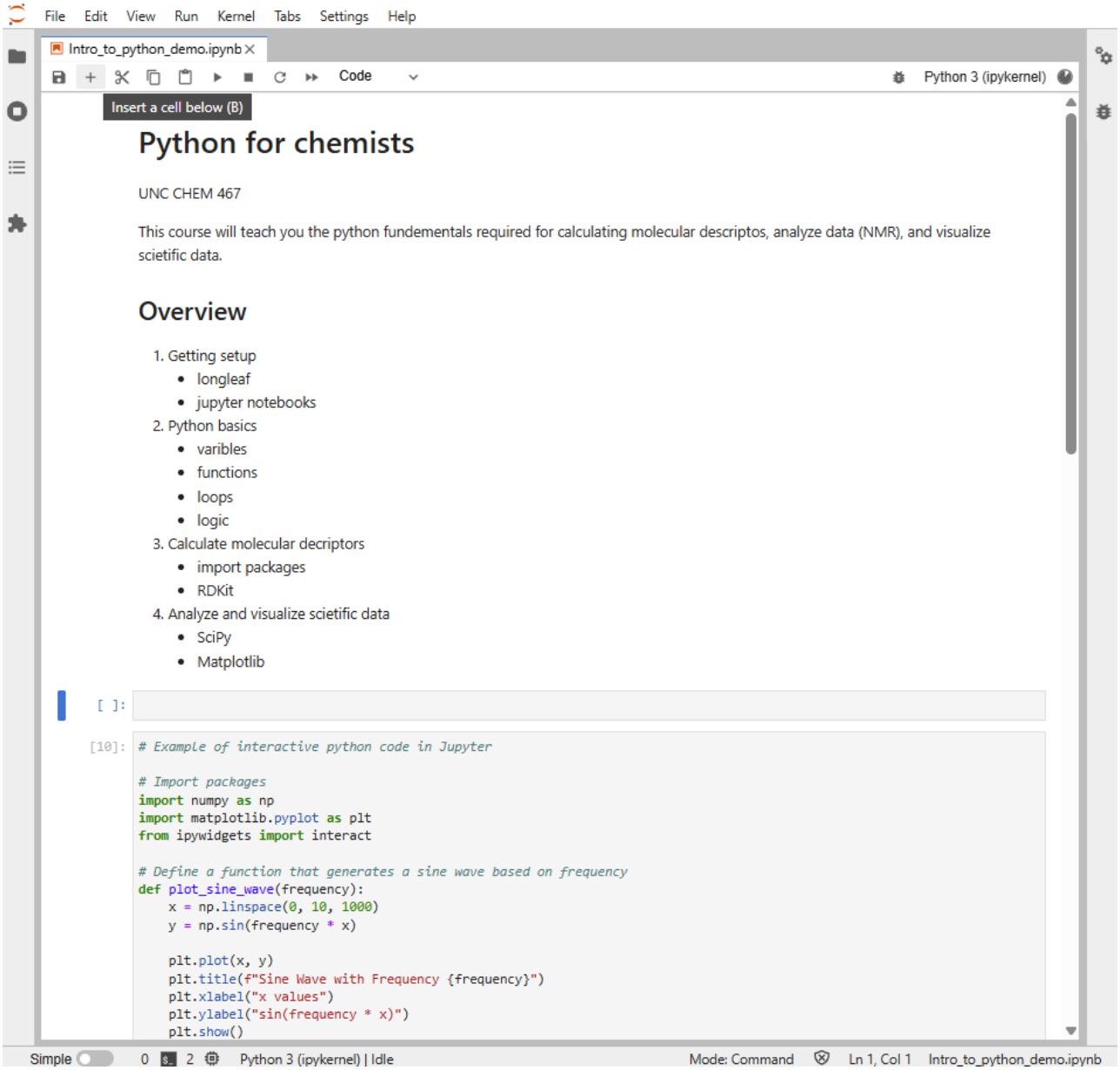


Note: move to the frequency slider to interact with the output.

How to insert and delete cells

1. Insert a new cell below our markdown cell.
    - click the markdown cell
    - click the + button in the ribbon to insert a cell below

Now your notebook should look like the following:



2. Delete the empty cell.
    - right-click the cell
    - click `Delete Cells`

First-Time Setup (Super important)

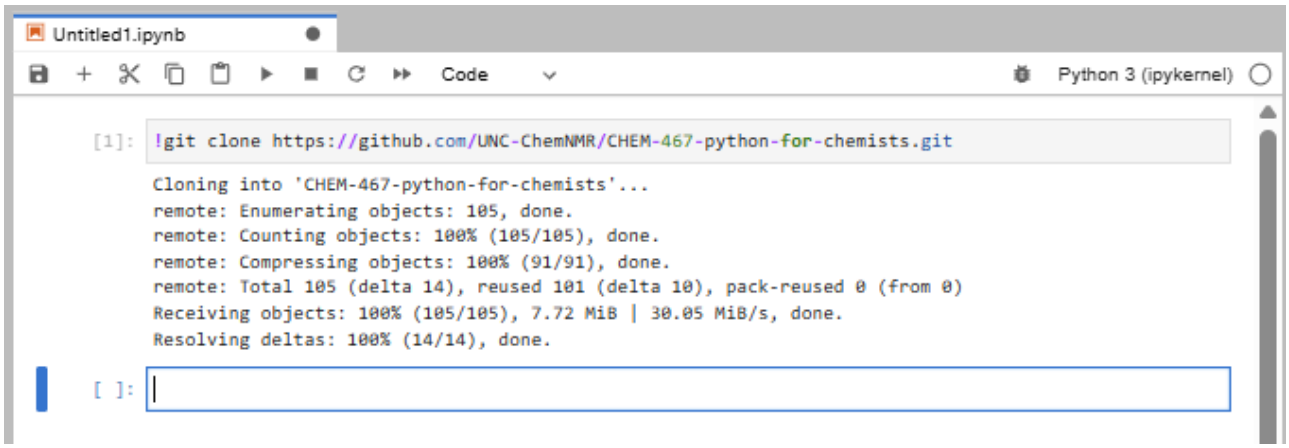
Clone the class repository

This will copy all the course material into your Longleaf storage.

1. Create a new code cell.
2. Paste this code into the code cell:

```
!git clone https://github.com/UNC-ChemNMR/CHEM-467-python-for-chemists.git
```

3. Run the code cell by pressing `shift+enter`
4. You should see an output that looks similar to this:

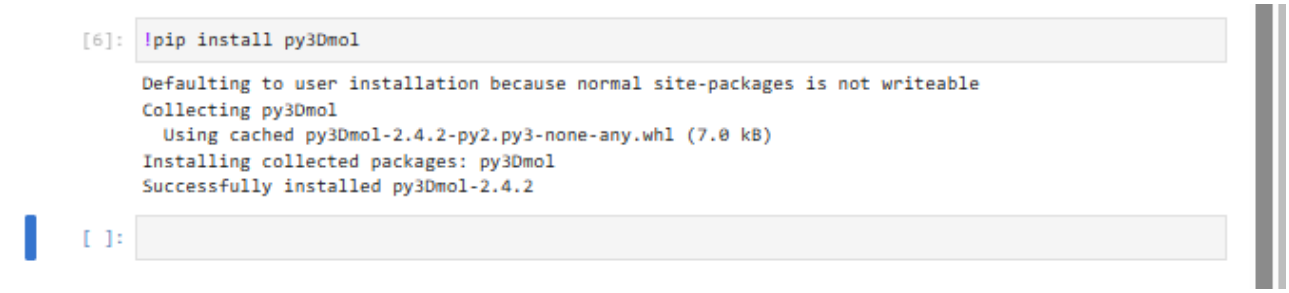


Install py3Dmol

1. Create a new code cell.
2. Paste this code into the code cell:

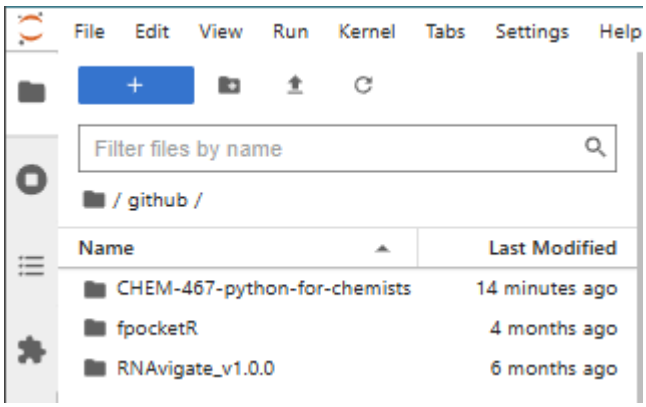
```
!pip install py3Dmol
```

3. Run the code cell by pressing `shift+enter`
4. You should see an output that looks similar to this:



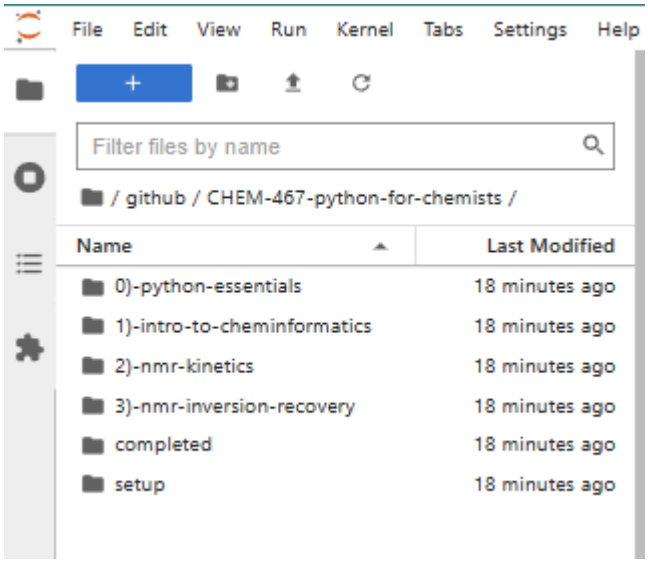
Navigating the course material in Jupyter

1. You should now see a folder (or directory) containing all the course material:

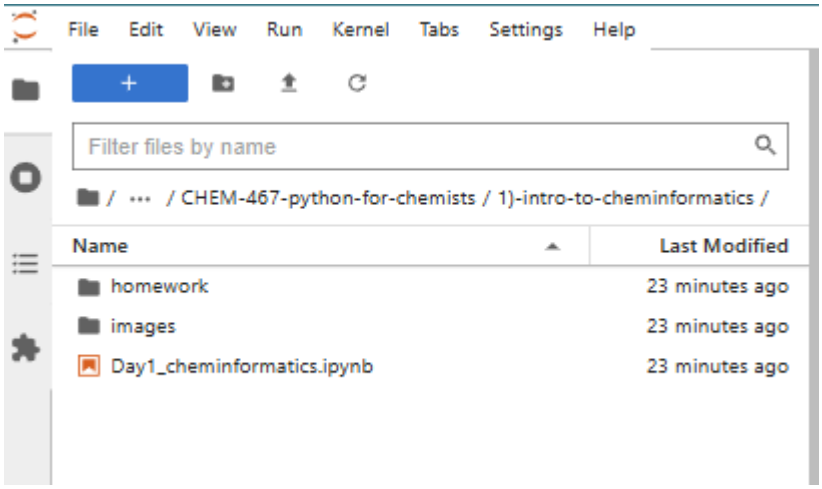


You're are done setting up your jupyter environment for CHEM 467.

2. You can double-click on the course folder to open it.



3. In-class notebooks and homework templates are located inside the numerated sub-directories.



You are not done setting up for CHEM 467!

Additional resources

Hopefully you have a good idea of how to run a Jupyter notebook in Longleaf now! If you have more questions take a look at the following resources.

- Longleaf OnDemand
- Jupyter notebook user interface