PHYMOL SAPT Workshop
Dr. Konrad Patkowski, Auburn University
Software Installation Instructions

Goal: You want to have on your laptop an Anaconda environment with all typical numerical-python stuff (numpy, scipy, matplotlib, jupyter), the newest version of Psi4, and the fortecubeview package for visualizing cube files.

Step-by-step instructions from a terminal (Mac) or Anaconda PowerShell (Windows):

0. Make sure that you have the latest version of Anaconda Navigator installed:
   https://www.anaconda.com/download

1. Create a new environment workshop:
   ```
   conda create –n workshop python=3.11
   ```

2. Activate the new environment:
   ```
   conda activate workshop
   ```

3. Add most of the basic stuff:
   ```
   conda install jupyter matplotlib
   ```

4. Install psi4 itself:
   ```
   conda install psi4=1.8.1 python=3.11 –c conda–forge/label/libint_dev –c conda–forge
   ```
   (these two lines are a single command)

5. Follow the steps to install fortecubeview:
   ```
   conda install scikit–image
   conda install –c conda–forge pythreejs
   conda install nodejs –c conda–forge ––repodata–fn=repodata.json
   jupyter nbextension install ––py ––symlink ––sys–prefix pythreejs
   jupyter nbextension enable ––py ––sys–prefix pythreejs
   pip install fortecubeview
   ```

If you run into any issues, email me (patkowsk@auburn.edu) or ask me on Tuesday!