

PHYMOL SAPT Workshop
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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 fortectubeview 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 python=3.11 -c conda-forge/label/libint_dev -c conda-forge`
5. Follow the steps to install fortectubeview:
`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 fortectubeview`

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