**Scholar Conda Setup**

In order to have access to the conda environment created for the class, you will need to run a few commands.

Run the script (on Scholar):

. /depot/lslipche-class/apps/chm673/2021/global-install-students.sh

In case the script fails, you can manually do it by running:

module use /depot/lslipche-class/apps/chm673/2020/modulefiles

module load conda-env/chm673-py3.6.4

rcac-conda-env kernel -p /depot/lslipche-class/apps/chm673/2020/envs/chm673

The previous lines will generate a Jupyter kernel named "My chm637" that can be accessed from JupyterHub. In case you want to run the environment from the terminal, you would need to type the following *every time* you want to use the environment.

module use /depot/lslipche-class/apps/chm673/2020/modulefiles

module load conda-env/chm673-py3.6.4

**Alternative to Jupyter Hub**

Here is an alternative to access and run your Notebooks:

1. Login to <https://gateway.scholar.rcac.purdue.edu/>
2. In the top bar menu, under "Interactive Apps", select "Jupyter Notebook"
3. Next page will let you select queue (scholar) and duration of the job. Defaults are reasonable, so hit the blue "Launch" button.
4. Wait until the job starts (the page will refresh and eventually show a blue "Connect to Jupyter" button).
5. Hit that button and you'll be connected to your own Jupyter instance running on one of the compute nodes - so you just open your notebook and fire away.

**Local Conda Setup**

**If you're running a Linux (any flavor) or MacOS computer**:

1. Download Conda <https://docs.conda.io/en/latest/miniconda.html>
2. Run the script and follow the directions. You may have to restart your terminal.
3. Create conda environment with Psi4:

conda create -n chm673 psi4 -c psi4

1. Every time you want to use Psi4 and the modules installed in it, you should run:

conda activate chm673

1. Install conda modules (while chm673 environment is active):

conda install -y pandas

conda install -y nb\_conda

conda install -y matplotlib

conda install -y -c plotly plotly

conda install -y -c conda-forge py3dmol

conda install -y -c conda-forge nglview

1. Install "blobs":

git clone https://github.com/VHchavez/blobs.git

cd blobs

pip install .

**If you're running Windows**:

1. Make sure you have WSL installed:  
   <https://docs.microsoft.com/en-us/windows/wsl/install-win10>
2. Your terminal can be accessed with the program: 'wsl'. It is very likely that the default directory is system32. You can access your usual files by moving to:
3. cd /mnt/c/Users/your\_username

It would be wise to create an alias to take to you that directory:  
<https://ilikekillnerds.com/2017/08/create-alias-c-drive-ubuntu-bash-windows/>

1. Follow instructions for Linux/Mac.