Generating a virtual environment for Jupyter Hub on H2P (The Pitt Shared Computing Cluster)
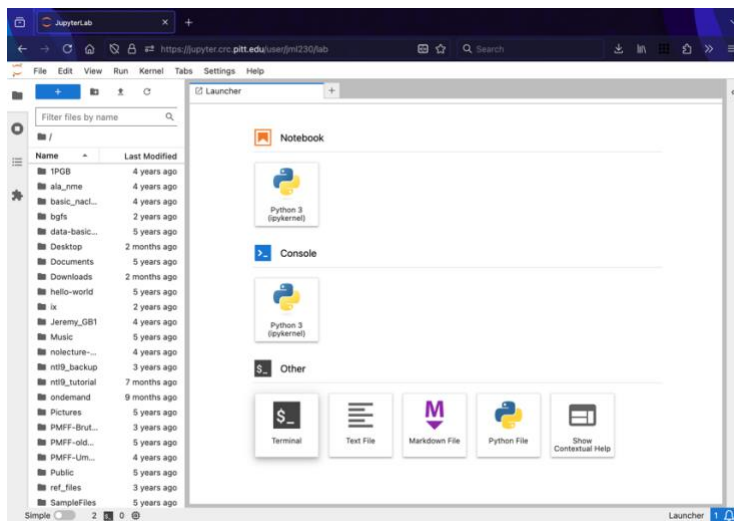
1. Go to https://hub.crc.pitt.edu. Login with your Pitt username and password.
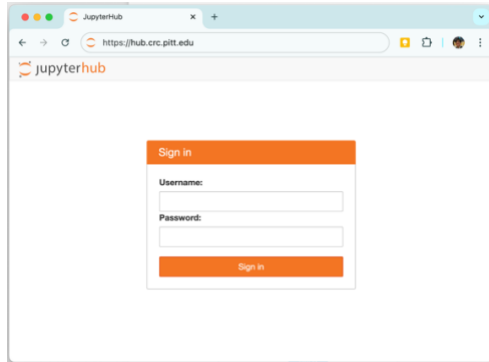
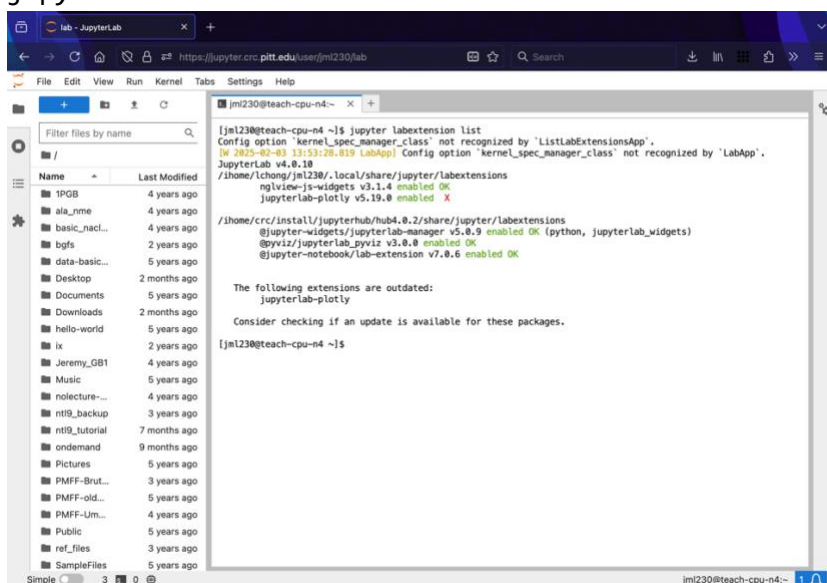2. Select Teach – 6 cores, 3 hours.
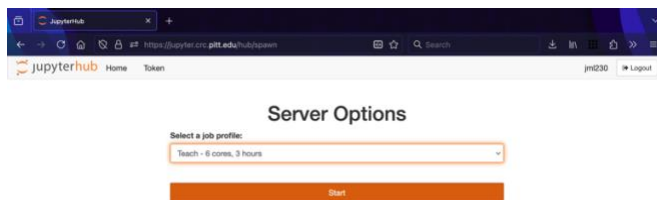

3. Once loaded, select "terminal".

4. Run the following commands.
```
cd ~
python -m pip install nglview
git clone https://github.com/jeremyleung521/drug-design2025
cd drug-design2025
bash run_bash.sh
```

5. Try running the following command. If you can see `nglview-js-widgets v3.1.4 enabled OK` in the output, you're good!

```
jupyter labextension list
```


6. Next, we need to shut down the server and create a new one (so our new installations apply). From the drop-down menu, select `File > Hub Control Panel`. In the next screen, select `Stop My Server`.
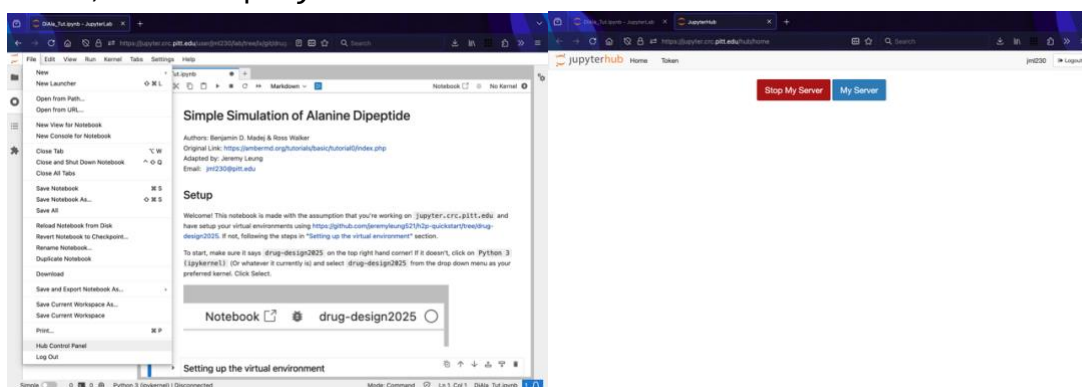
7. Once the page has reloaded, select `Start My Server`. This time, select `Teach – 1 gpu, 3 hours`.
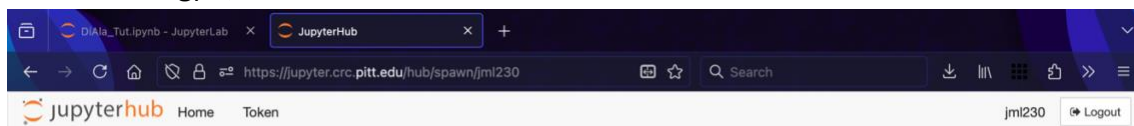
8. Once the server's started, navigate to the `drug-design2025` folder on the left-hand side. Then, navigate to `alanine-dipeptide` folder and launch the `DiAla_Tut.ipynb` Jupyter notebook. Select `drug-design2025` on the top right (more instructions in the notebook). Then go through the notebook.

Optional: If you need to access the virtual environment from the terminal, run `source ~/activate_env.sh` in the terminal.