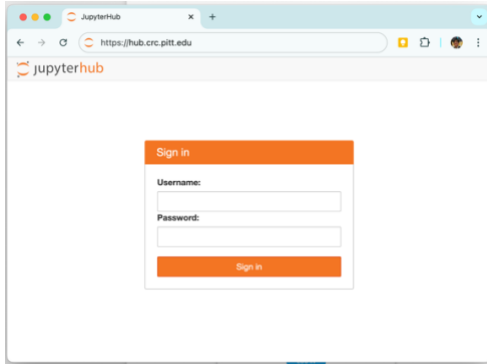
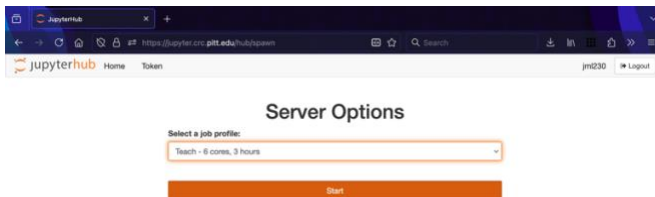


Generating a virtual environment for Jupyter Hub on H2P (The Pitt Shared Computing Cluster)

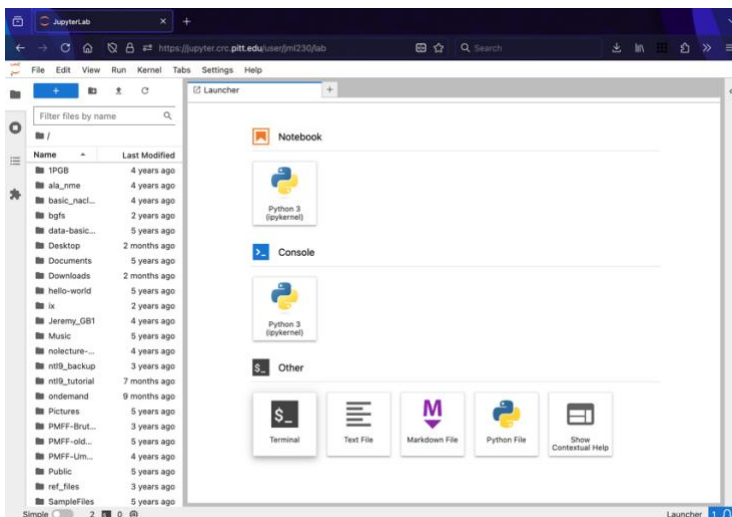
1. Go to <https://hub.crc.pitt.edu>. Login with your Pitt username (all lower case) and password.



2. Select Teach – 6 cores, 3 hours.



3. Once loaded, select “terminal”.



4. Run the following commands.

```
cd ~
```

```
python -m pip install nglview
```

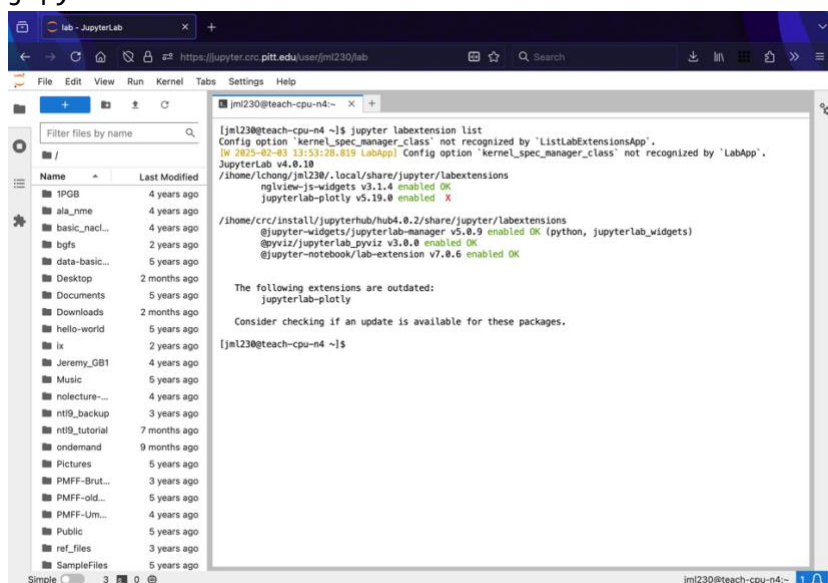
```
git clone https://github.com/jeremyleung521/drug-design2025
```

```
cd drug-design2025
```

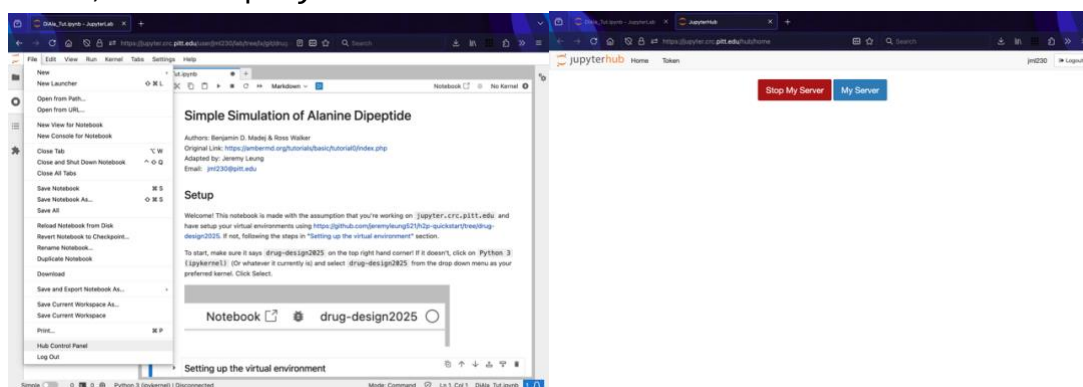
```
bash run_bash.sh
```

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

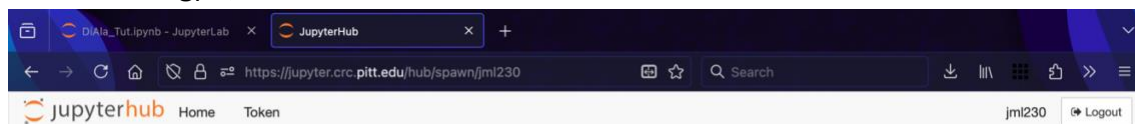
`jupyter labextension list`



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'.



Server Options

Select a job profile:

Teach - 1 gpu, 3 hours

Start

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 ~/drug-design2025/activate_env.sh` in the terminal.