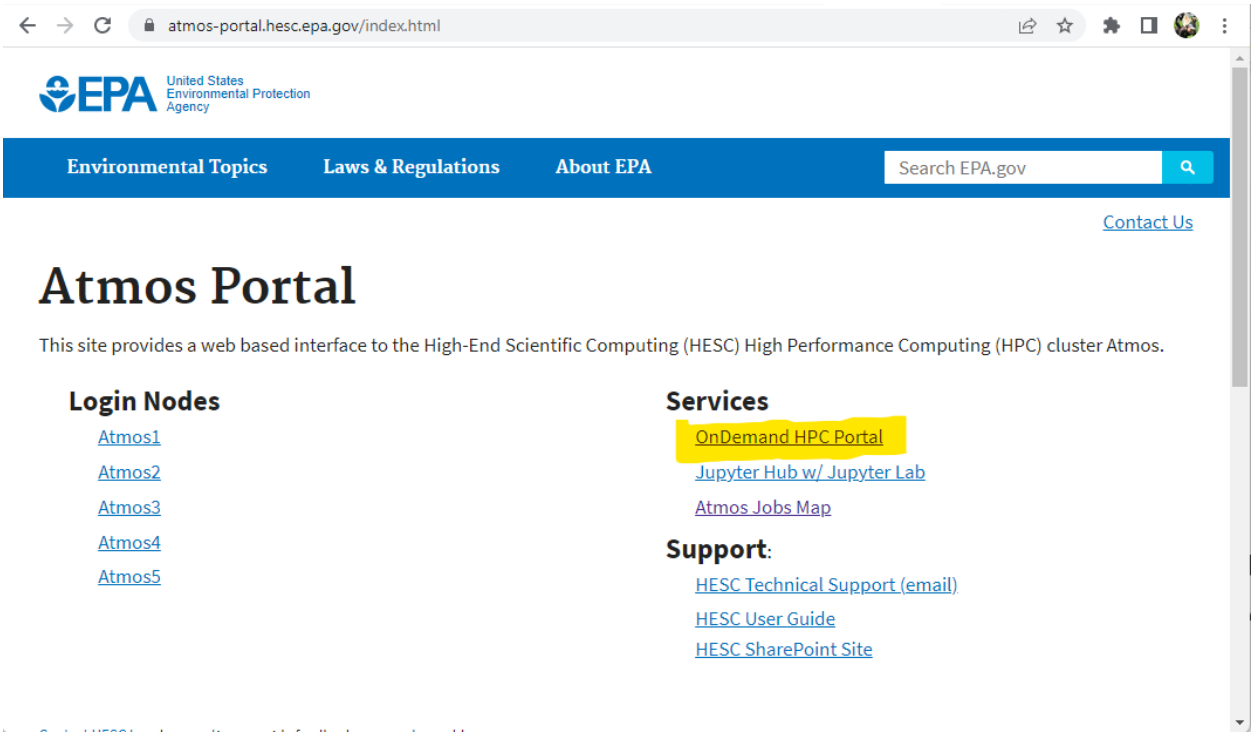
# Jupyter through OnDemand on Atmos

This is a tutorial on running JupyterHub on Atmos via the OnDemand interface. We will login to atmos and use a shell to copy some configurations, then login to a JupyterHub on Atmos, then open a Jupyter Notebook and use it to install libraries. Finally, we'll do some CMAQ analysis.

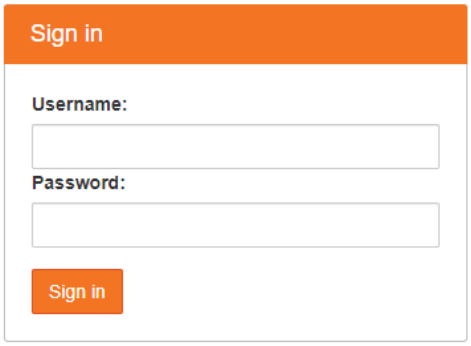
If the steps are not clear, please provide feedback to Barron H. Henderson.

## Tutorial Steps

1. Connect to the EPA Network or VPN
2. Navigate a web browser to https://atmos-portal.hesc.epa.gov/
3. Click on "OnDemand HPC Portal"



4. Log in with your Lan ID and password (not necessary every time)



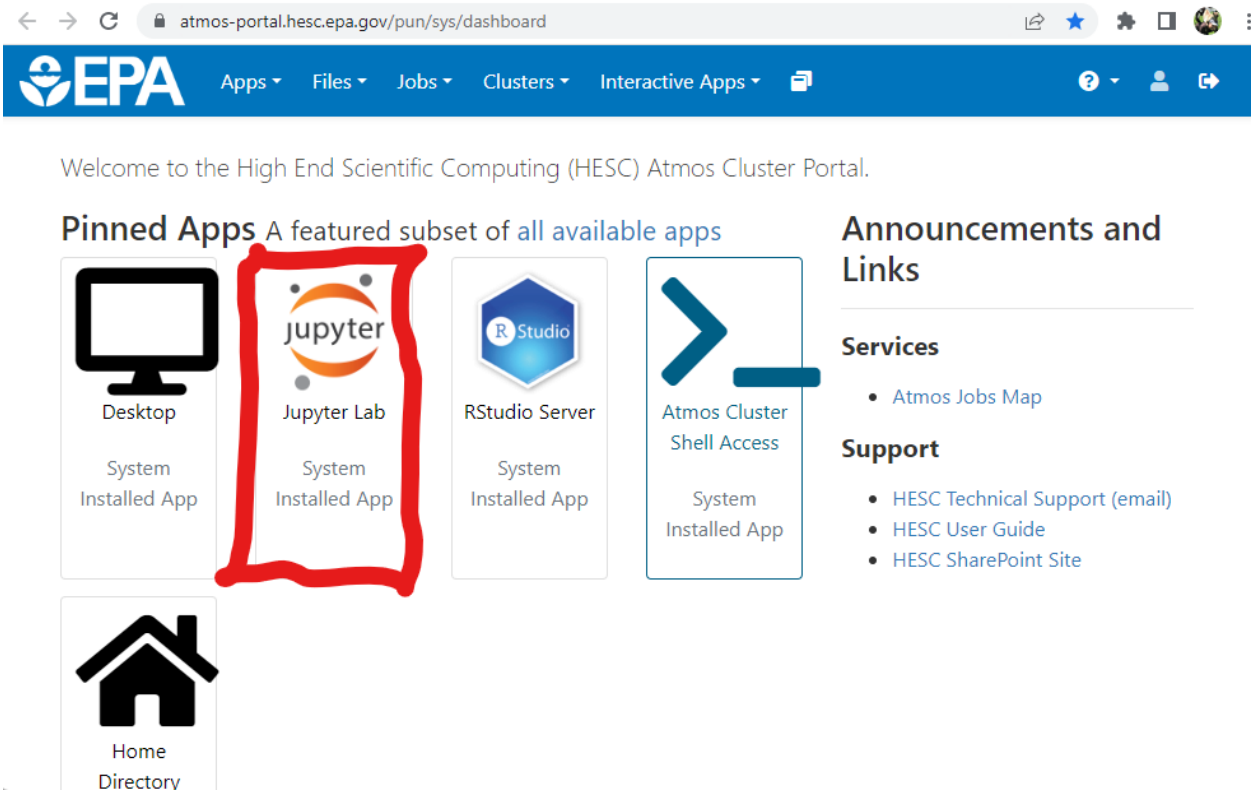
5. Choose “Atmos Cluster Shell Access” (first time only)
    a. Copy my RC file to your home directory as show below
    b. Then exit and close the tab

```
$ mkdir -p ~/.jupyter/rc
```

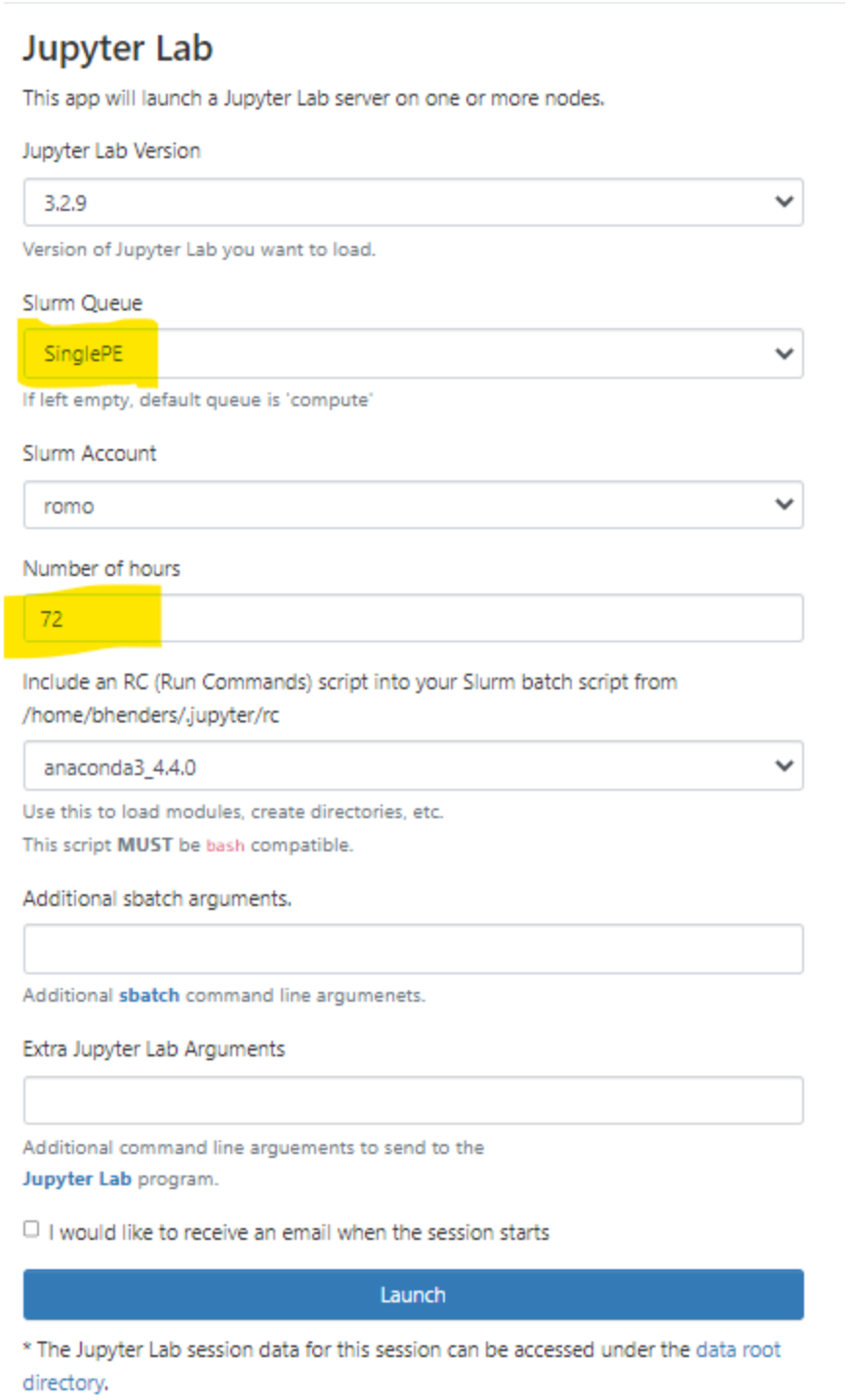
```
$ cp ~bhenders/.jupyter/rc/anaconda3_4.4.0 ~/.jupyter/rc/
```

```
$ exit
```

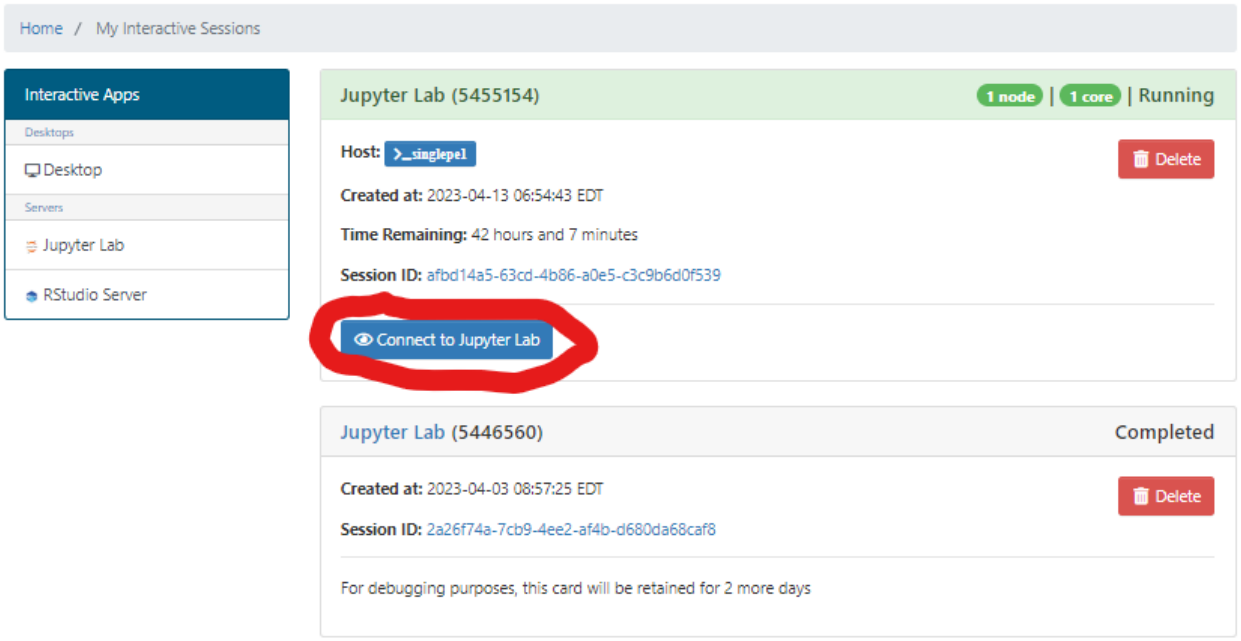
6. Now, choose Jupyter Lab to start a now session



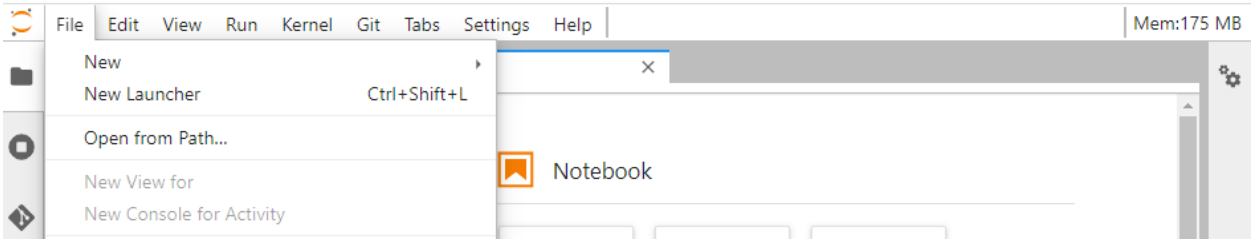

7. Make sure your configuration looks like this one. I have highlighted fields you might change a lot. “SinglePE” is good for small work. The duration might vary from 8 to 120 hours.

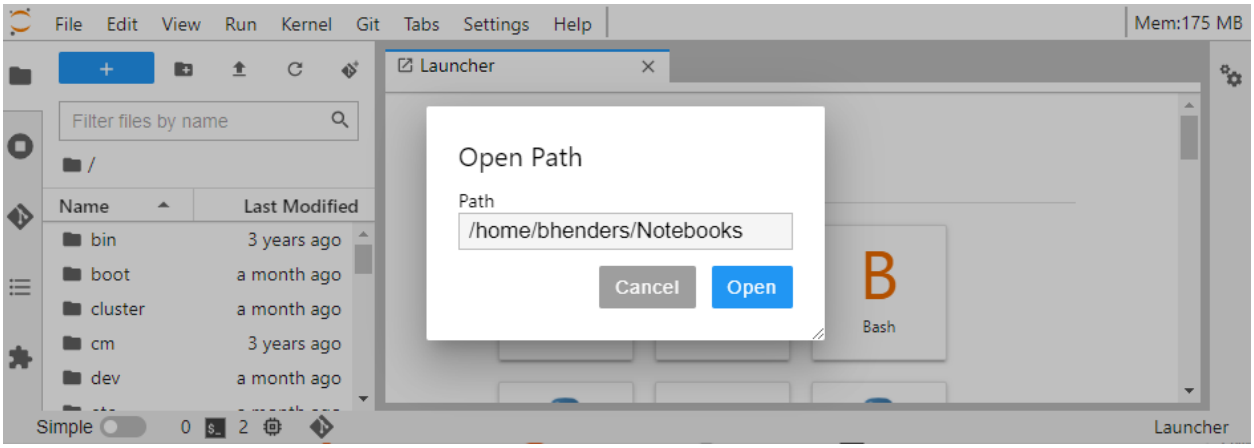



8. Wait until you see “Connect to Jupyter Lab” and click on it (as shown below).
    a. Incidentally, you can always come back to “My Interactive Sessions” to reconnect to a notebook if you get disconnected (e.g., VPN disconnect).

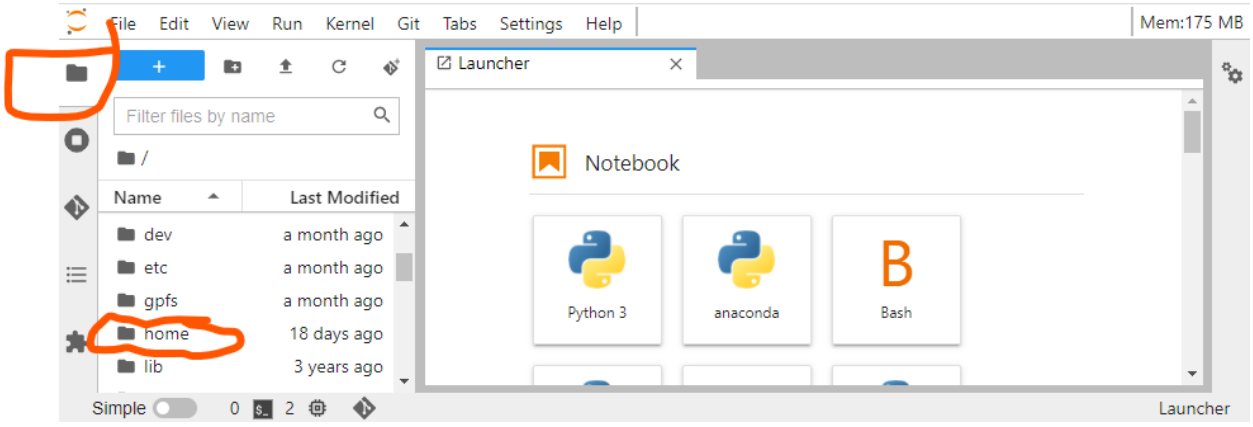



9. Navigate to a folder with a notebook
    a. Select “File” and “Open from Path…”

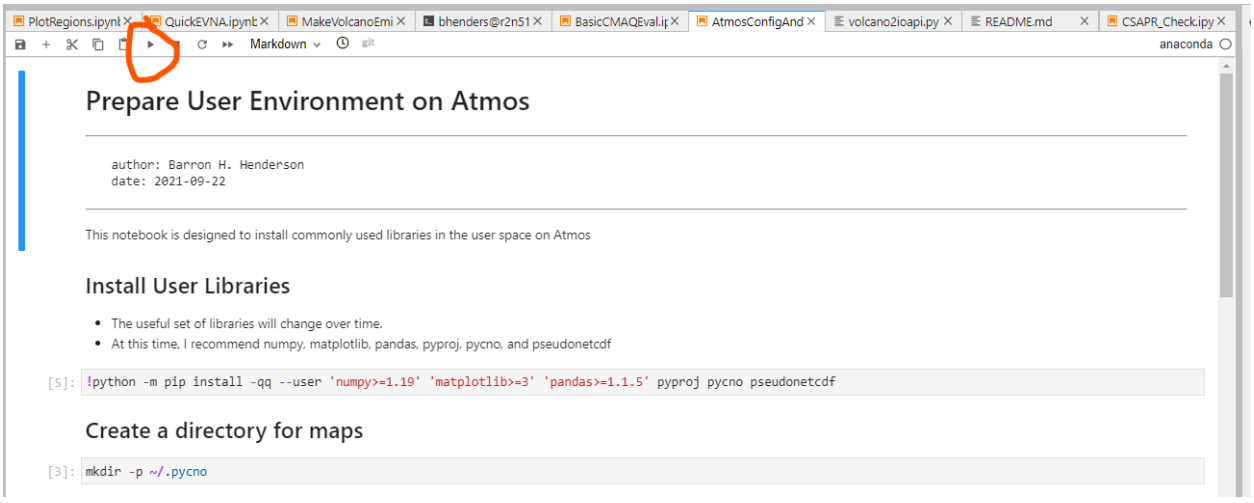


b. Or navigate by clicking in the file browser (folder on left)




10. For your first example, navigate to /home/bhenders/Notebooks, then double click on 0AtmosConfigAndTest.ipynb notebook. This will open the Notebook.
    a. This is your first time, and this notebook helps to update or install a few libraries
    b. Optionally, Use File “Save Notebook As” and save it in your own user space (/home/<username>). The notebook that is open is the newly saved notebook.
    c. Click the play button once for each cell (e.g., see [1] in next figure).




    d. The primary purpose of the notebook is to install libraries that are known to work

e. You can also avoid warnings in the future by running “mkdir -p ~/.pycno”

11. You can open any of the notebooks in /home/bhenders/Notebooks and follow a similar process to steps 6 and 7. The three notebooks below are intended to be updated as needed so that they can be used as tutorials.
    a. Pycno.ipynb
    b. AQS_Pregenerated_MonthMean.ipynb a
    c. BasicCMAQEval.ipynb performs a simplistic CMAQ evaluation against AQS observations.
    d. MachineLearningExample.ipynb
    e. CMAQ_Ozone_Evaluation.ipynb has a more detailed evaluation of a year.
    f. MASK_MAKER.ipynb is a simple tool to make arbitrary masks from shapefiles

12. Lastly, any time you make a new notebook:
    a. Choose the anaconda kernel. This will ensure you have access to important scientific libraries.
    b. Always add “%matplotlib inline” in the first cell. On Atmos, this ensures plots will be shown.

## Known Atmos Issues

- On atmos, the matplotlib figures may not show. If not, make sure you have `%matplotlib inline`
- Occasionally, you'll get logged out and keep seeing a popup error. Open a new tab and go back to OnDemand and re-login. The old tab should resume functionality.
- Occasionally, the cached credentials will go bad. Open a new web browser tab and clear your cache. Then re-login through OnDemand. You will have to refresh your notebook tab. If it asks for a login, close the web browser tab with your notebook. Then, go back to OnDemand and then "My Interactive Sessions" and reopen your session.