

# Jupyter through OnDemand on Atmos

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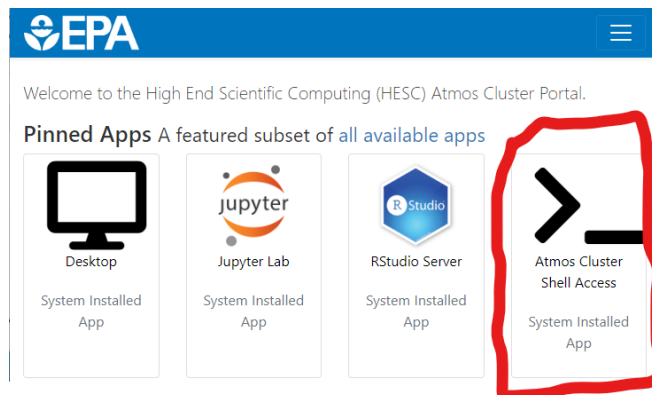
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This is a tutorial on running JupyterHub on EPA's Atmos cluster via the OnDemand interface on Red Hat Enterprise Linux 8 (RHEL8). We will login to atmos (steps 1-2), use a shell to enable some configurations (steps 3-4), start a Jupyter Lab instance (step 5-7), 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://atmos5.hesc.epa.gov/>
3. Choose "Atmos Cluster Shell Access" (first time only)

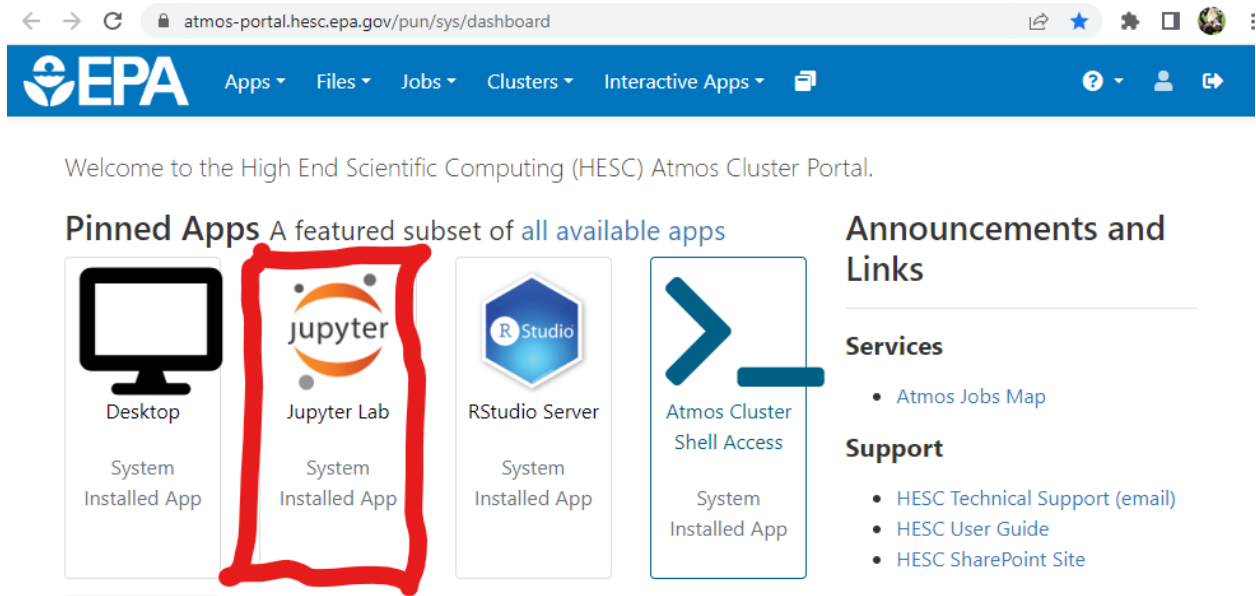


#### 4. Run commands to enable intelpython/3.9 in JupyterLab

```
Host: localhost Themes: Default
atmos5:~[1001]>mkdir -p ~/.jupyter/rc/
atmos5:~[1002]>cp ~bhenders/.jupyter/rc/intel39 ~/.jupyter/rc/

atmos5:~[1003]>source ~/.jupyter/rc/intel39
atmos5:~[1004]>python -m pip install -qq --user ipykernel
atmos5:~[1005]>python -m ipykernel install --user --name=intel39
Installed kernelspec intel39 in /home/bhenders/.local/share/jupyter/kernels/intel39
atmos5:~[1006]>exit
```

#### 5. Now, choose Jupyter Lab to start a now session



6. Make sure your configuration looks like this one.
- a. “Slurm Queue”: Login for tiny jobs; SinglePE for small jobs
  - b. Curation might vary from 8 to 120 hours.
  - c. “Include an RC”: choose intel39.
  - d. Click “Launch”

## Jupyter Lab

This app will launch a Jupyter Lab server on one or more nodes.

Jupyter Lab Version

3.2.9

Version of Jupyter Lab you want to load.

☐ Use my custom installed Jupyter binaries

If checked, will run `~/local/jupyter` instead of system Jupyter

Slurm Queue

SinglePE

If left empty, default queue is “compute”

Slurm Account

romo

Number of hours

72

Include an RC (Run Commands) script into your Slurm batch script from  
`/home/bhenderson/jupyter/rc`

intel39

Use this to load modules, create directories, etc.

This script **MUST** be **bash** compatible.

Additional sbatch arguments.

Additional **sbatch** command line arguments.

Extra Jupyter Lab Arguments

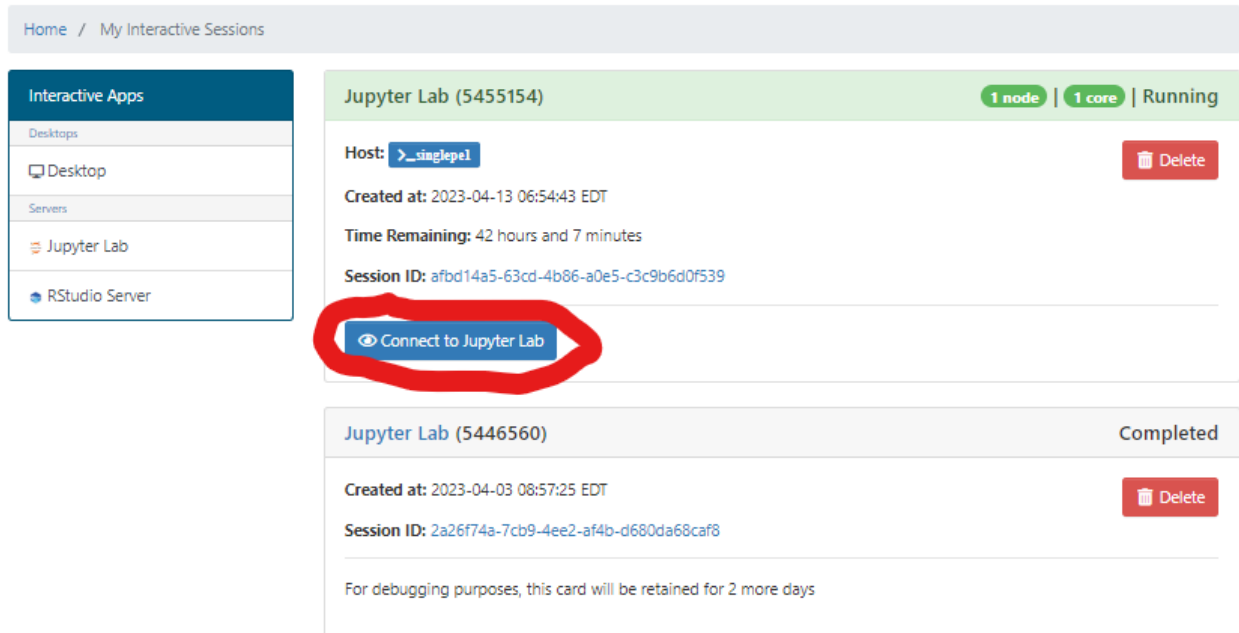
Additional command line arguments to send to the

**Jupyter Lab** program.

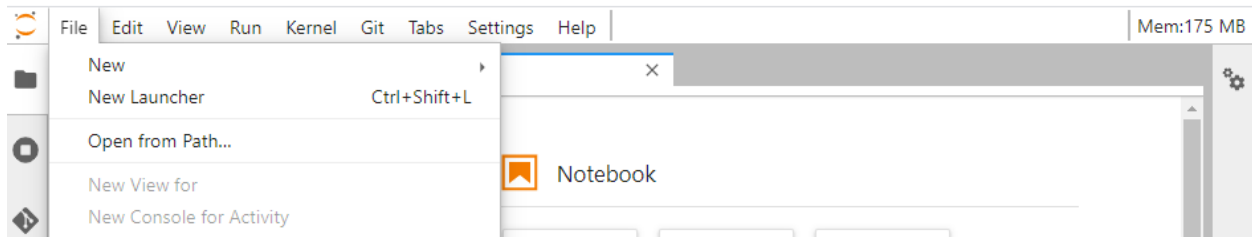
☐ I would like to receive an email when the session starts

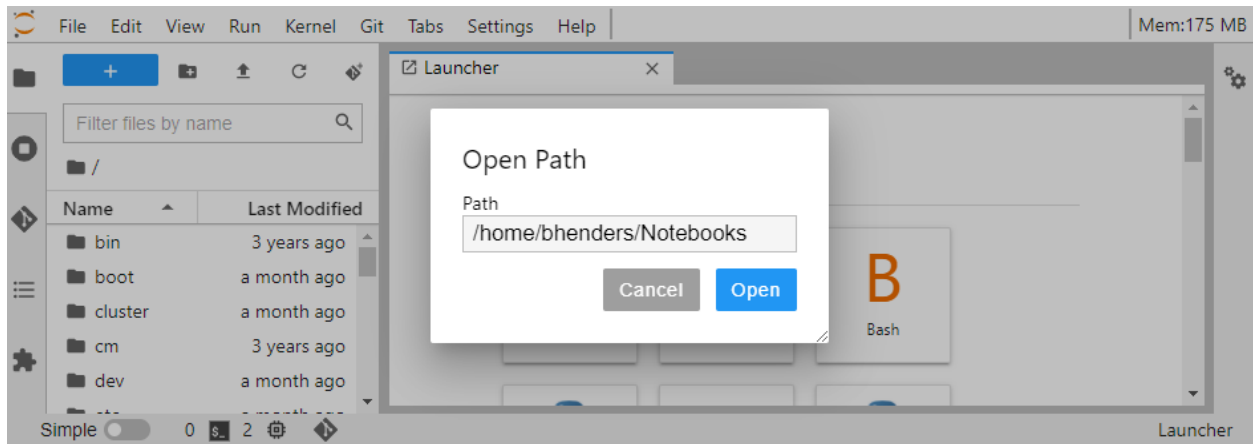
Launch

7. 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).

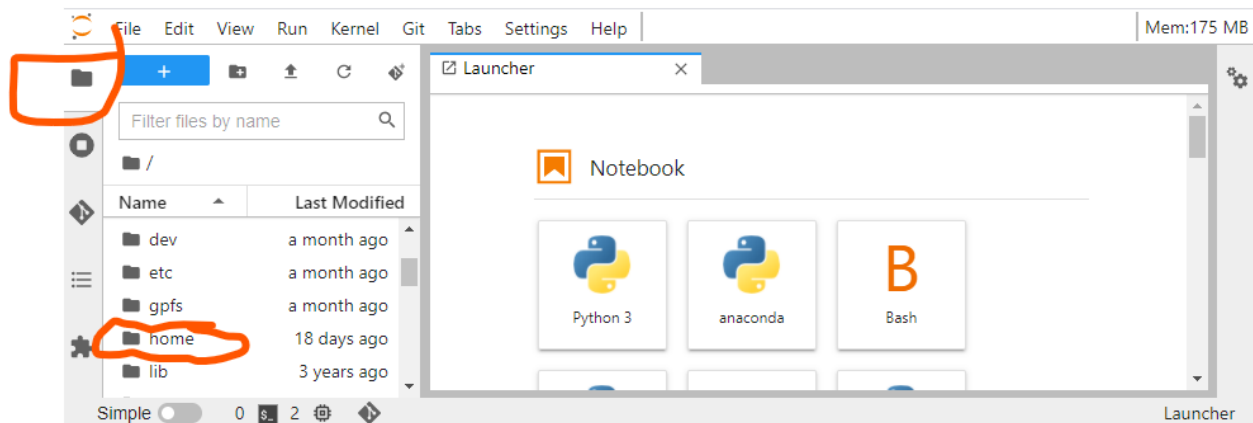


8. Navigate to a folder with a notebook
  - a. Select “File” and “Open from Path...”

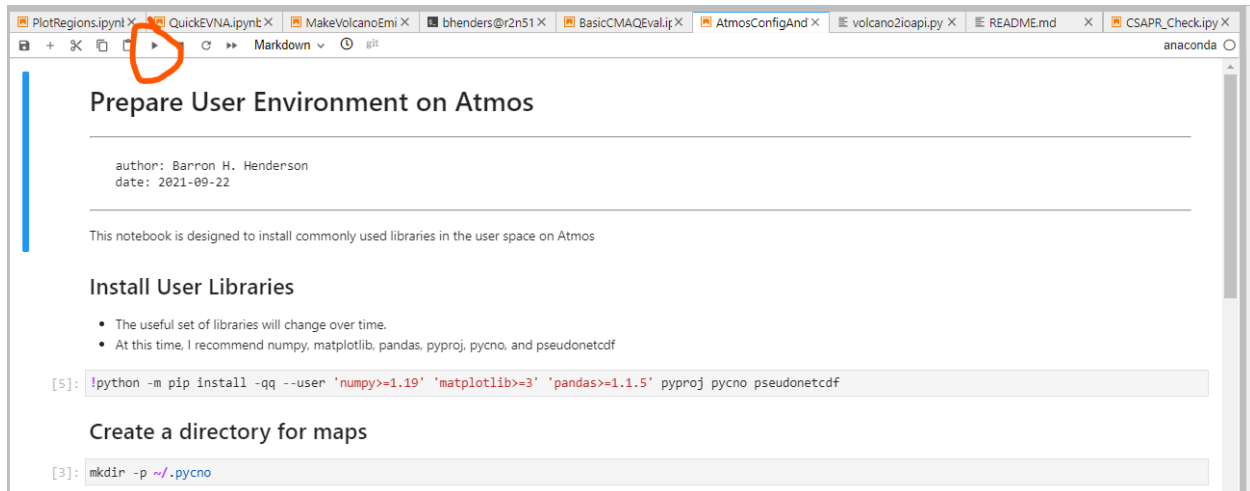




b. Or navigate by clicking in the file browser (folder on left)



9. For your first example, navigate to `/home/bhendersons/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”
10. 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
  - 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
11. 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``