Jupyter: Notebooks, Lab, and Hub

Barron H. Henderson and Ben Murphy

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Outline

- Meet a Jupyter Notebook
  - Explorer tab, png, csv, json, terminal, console
  - Run a notebook (COVID or AQS)
- Jupyter Lab Introduction
  - Basic overview
  - Components and understanding
  - Ready cloud Environments
- Atmos access instructions
  - How to get to access JupyterHub
  - Prepare frequently used libraries
- Walk through Air Quality System (AQS) observation notebook

Hands on!

EPA Scientists need Jupyter Lab

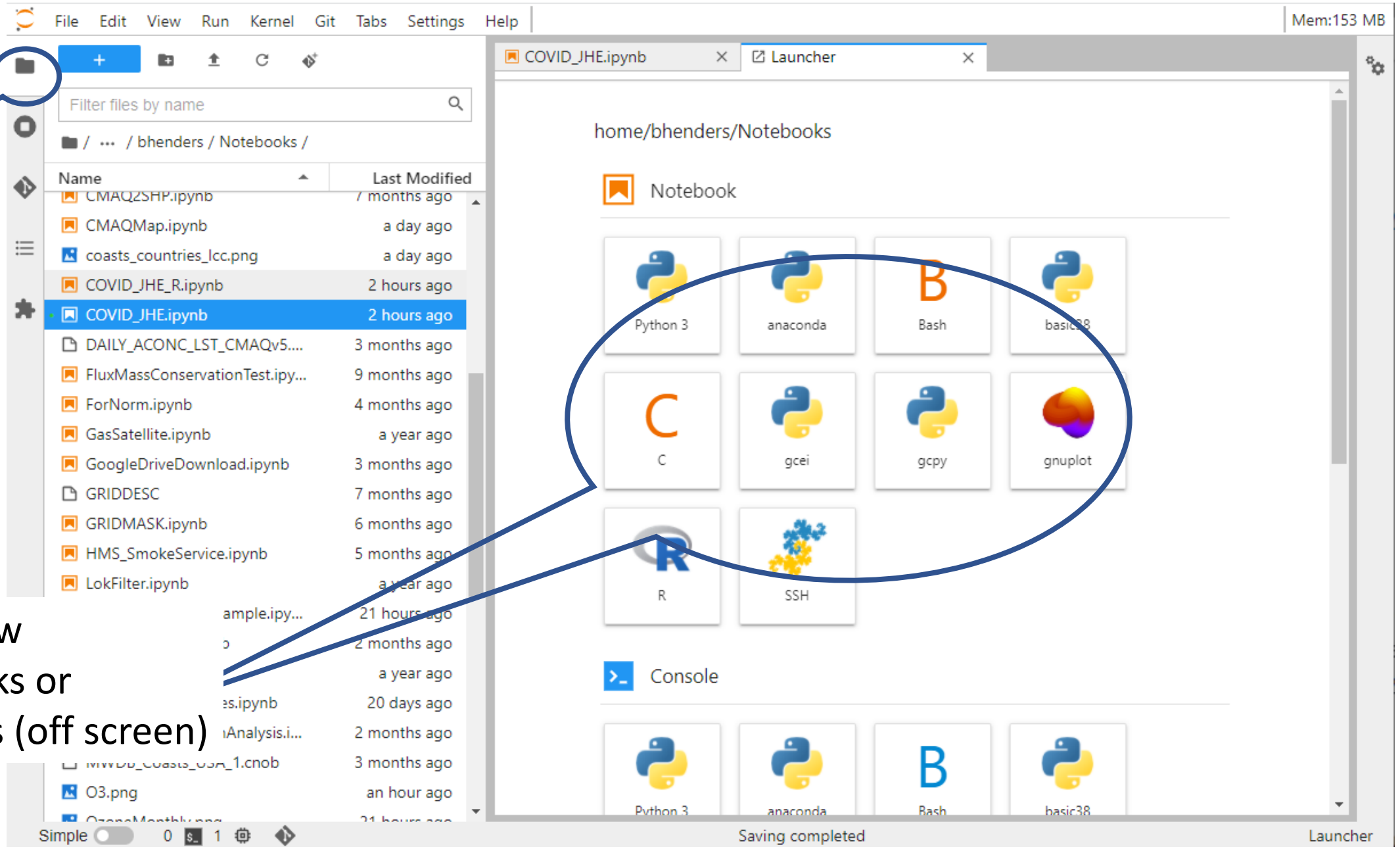
- Jupyter Lab is a notebook with web-based file browser and terminals
  - Docs, code, results, and images
  - Reusable with a minimum effort
  - R, Python, Bash, even C
- Easy install windows, linux, mac
- Jupyter Notebooks are a great way to share analysis systems.
  - Easily exported to PDF or HTML for sharing
  - Easily reproducible when dependencies are clear*

Meet a lab notebook

- To get folks excited, we're going to walk through a notebook.
- When we're done you should be able to answer the following questions:
  - Does jupyter lab have a file explorer?
  - Can I access the Terminal in a jupyter lab?
  - Can I write documentation and math in notebooks?
  - How do I run code in a notebook?
  - Can I interactively make figures?
  - What languages work in Jupyter?
- Because not everyone here uses CMAQ, we're going to look at COVID data. (atmos://home/bhenders/Notebooks/COVID_JHE.ipynb)

File Browser

Make New Notebooks or Terminals (off screen)



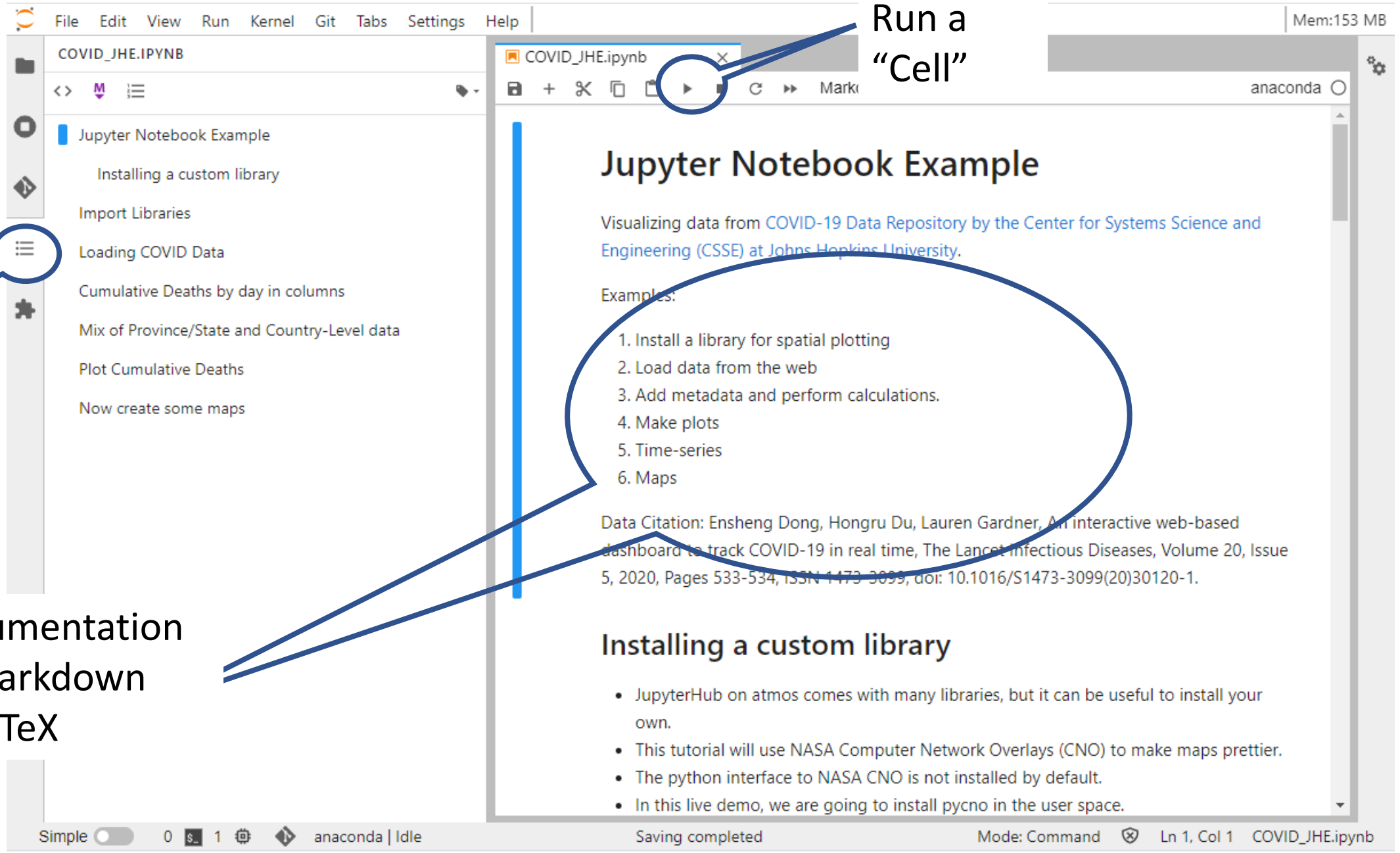
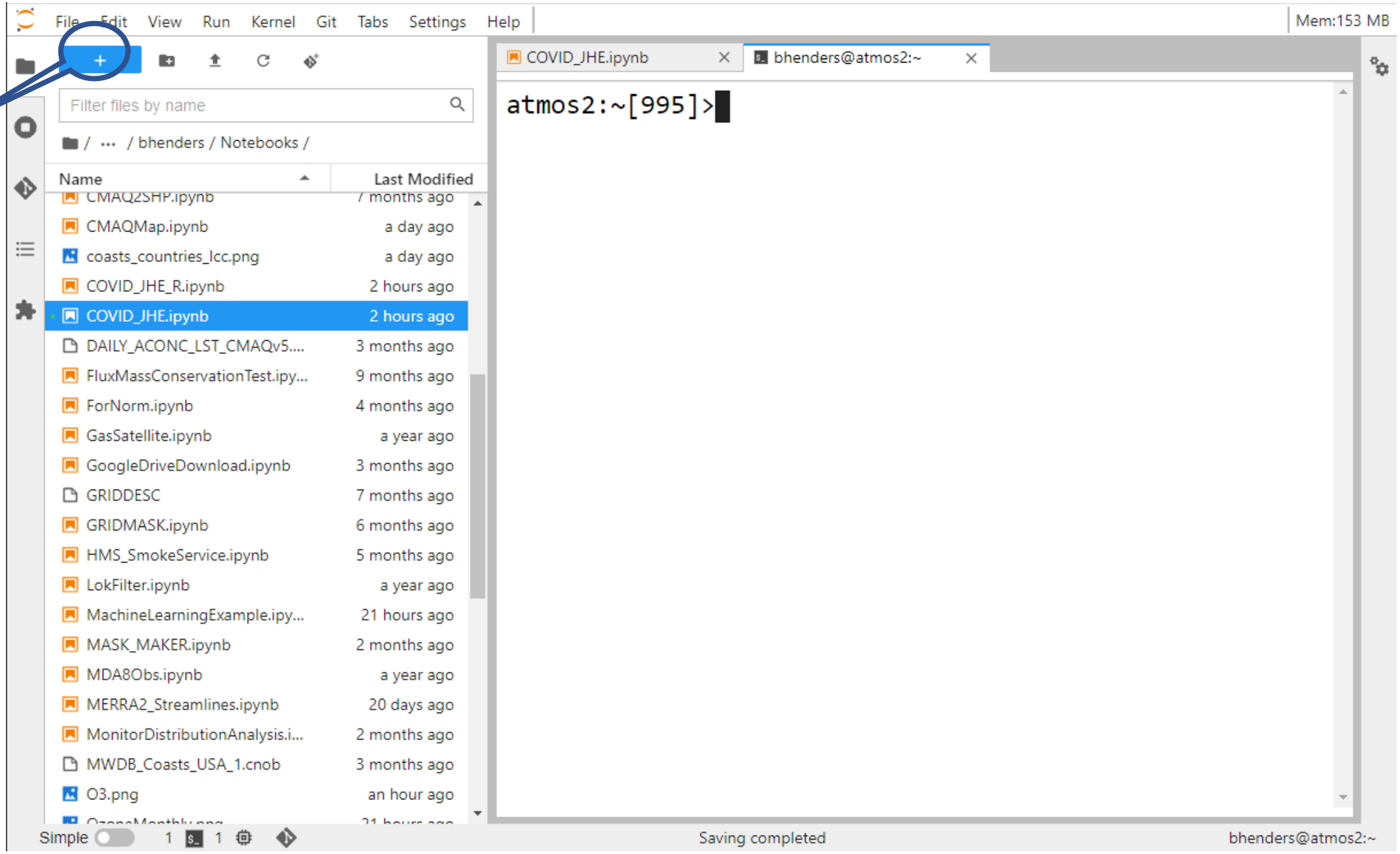


Table of Contents

Add Documentation

- Use Markdown
- Use LaTeX

Make new Notebooks or Terminals



How do Notebooks Work?

- Users access notebooks by a “web browser” (e.g., Chrome).
- The browser accesses a Notebook “server.”
  - A server can be on your machine.
  - A server can be on atmos
  - A server can be on the cloud
- The Notebook server
  - Stores data in a Notebook file
  - Passes commands to the Kernel
- The Kernel processes commands
  - Kernels can operate in many languages
  - Python, R, CSH etc

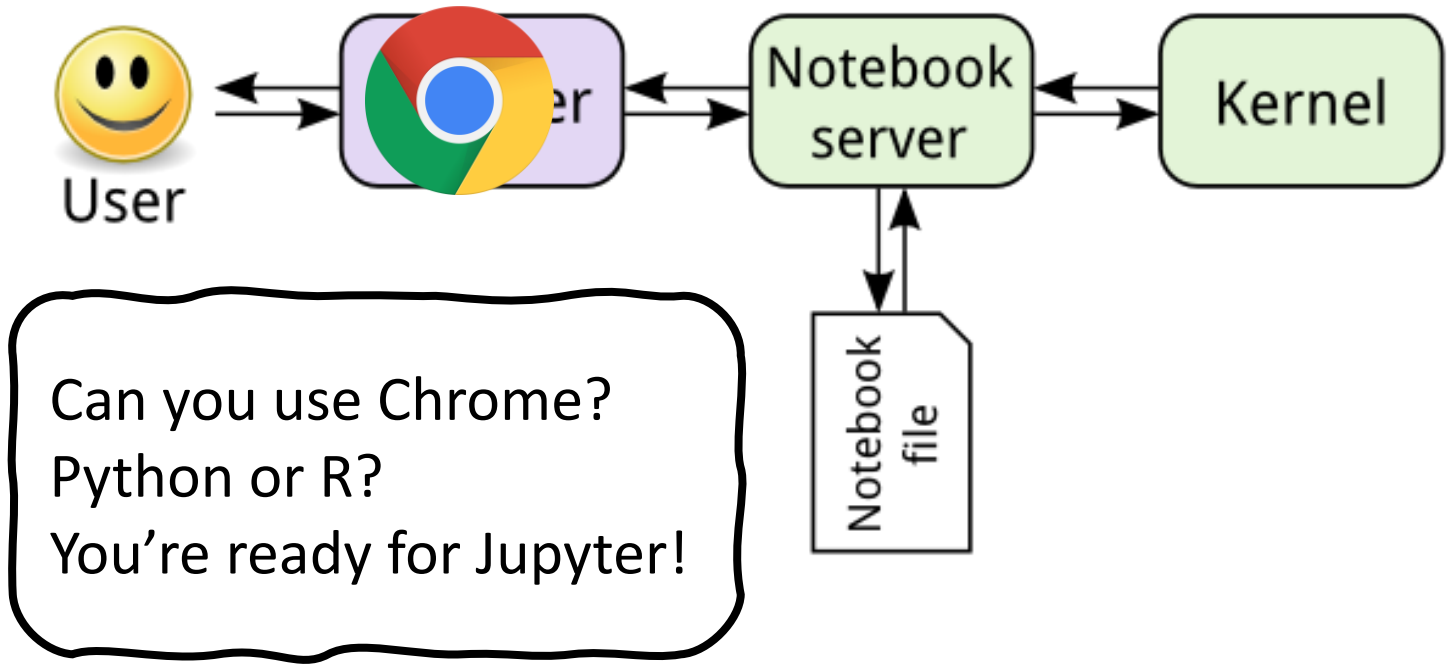


Figure source: https://coderefinery.github.io/jupyter/interface/

On Windows

Install Once

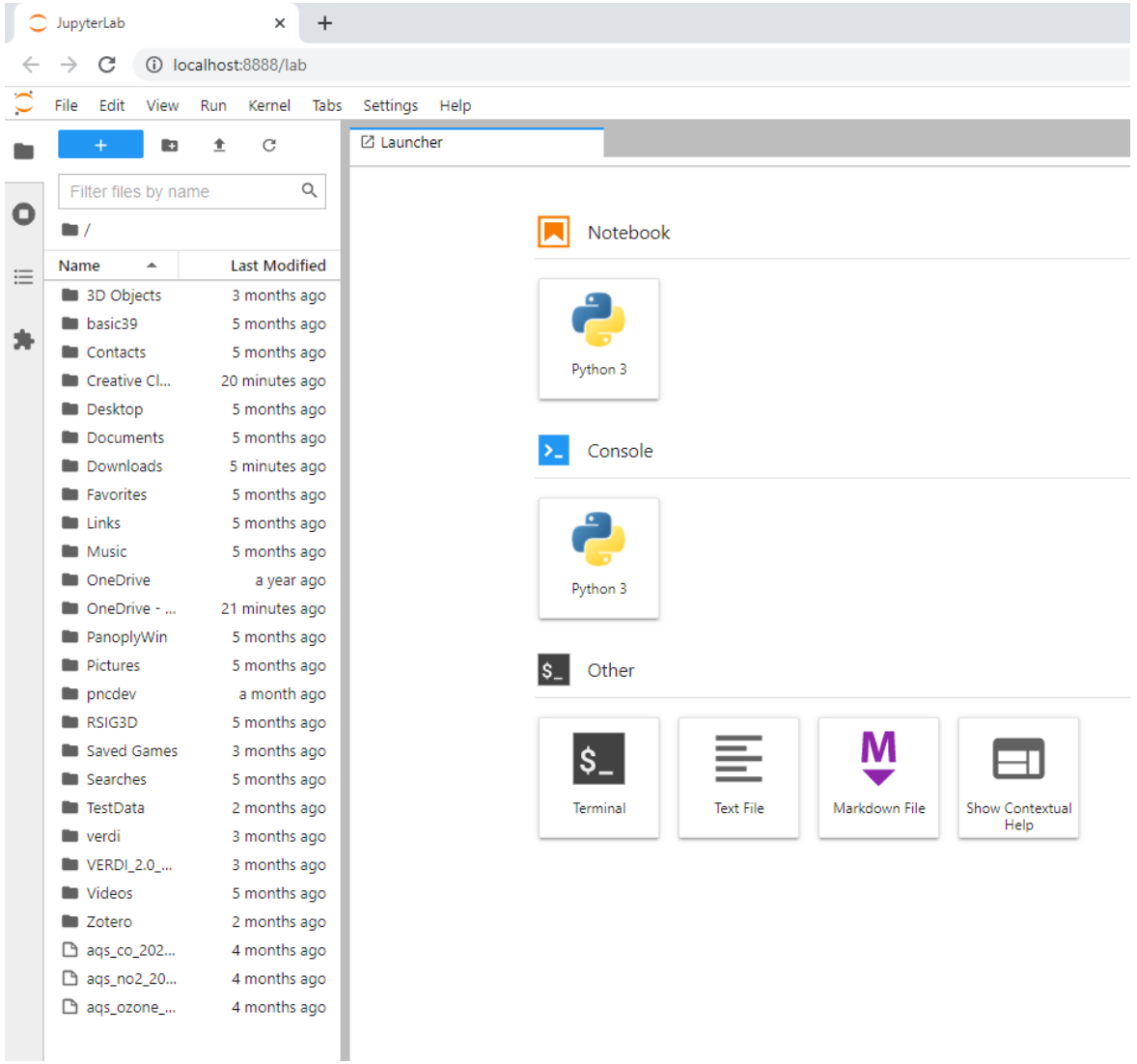
- Installer from python.org installed for user in basic39.
- `.\basic39\Scripts\pip.exe install --user jupyterlab`

Start a server any time…

```
C:\Users\BHenders>.\basic39\Scripts\jupyter.exe lab
```

```
[I 2021-11-16 20:39:33.950 ServerApp] jupyterlab | extension was successfully linked.
[W 2021-11-16 20:39:33.982 ServerApp] The 'min_open_files_limit' trait of a ServerApp insta
NoneType None.
[I 2021-11-16 20:39:34.715 ServerApp] nbclassic | extension was successfully loaded.
[I 2021-11-16 20:39:34.732 LabApp] JupyterLab extension loaded from c:\users\bhenders\basic
ab
[I 2021-11-16 20:39:34.732 LabApp] JupyterLab application directory is C:\Users\BHenders\ba
[I 2021-11-16 20:39:34.737 ServerApp] jupyterlab | extension was successfully loaded.
[I 2021-11-16 20:39:34.737 ServerApp] Serving notebooks from local directory: C:\Users\BHer
[I 2021-11-16 20:39:34.737 ServerApp] Jupyter Server 1.8.0 is running at:
[I 2021-11-16 20:39:34.737 ServerApp] http://localhost:8888/lab?token=3ab2554914c937288f55b
[I 2021-11-16 20:39:34.737 ServerApp]     http://127.0.0.1:8888/lab?token=3ab2554914c937288
ac
[I 2021-11-16 20:39:34.737 ServerApp] Use Control-C to stop this server and shut down all k
ation).
[C 2021-11-16 20:39:34.815 ServerApp]

    To access the server, open this file in a browser:
        file:///C:/Users/BHenders/AppData/Roaming/jupyter/runtime/jpserver-12384-open.html
    Or copy and paste one of these URLs:
        http://localhost:8888/lab?token=3ab2554914c937288f55be1967ad88ea09117cb30d982aac
        http://127.0.0.1:8888/lab?token=3ab2554914c937288f55be1967ad88ea09117cb30d982aac
```



This also works on atmos… we would all need our own “server”, our own “port”, and SSH tunnels… not easy…

On Mac or Linux

Install Once

- Installer from python.org installed for user in basic39.
- `python -m pip install --user jupyterlab`

Start a server any time…

```
$ jupyter lab
```

```
[I 2021-11-16 20:39:33.950 ServerApp] jupyterlab | extension was successfully linked.
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        http://127.0.0.1:8888/lab?token=3ab2554914c937288f55be1967ad88ea09117cb30d982aac
```

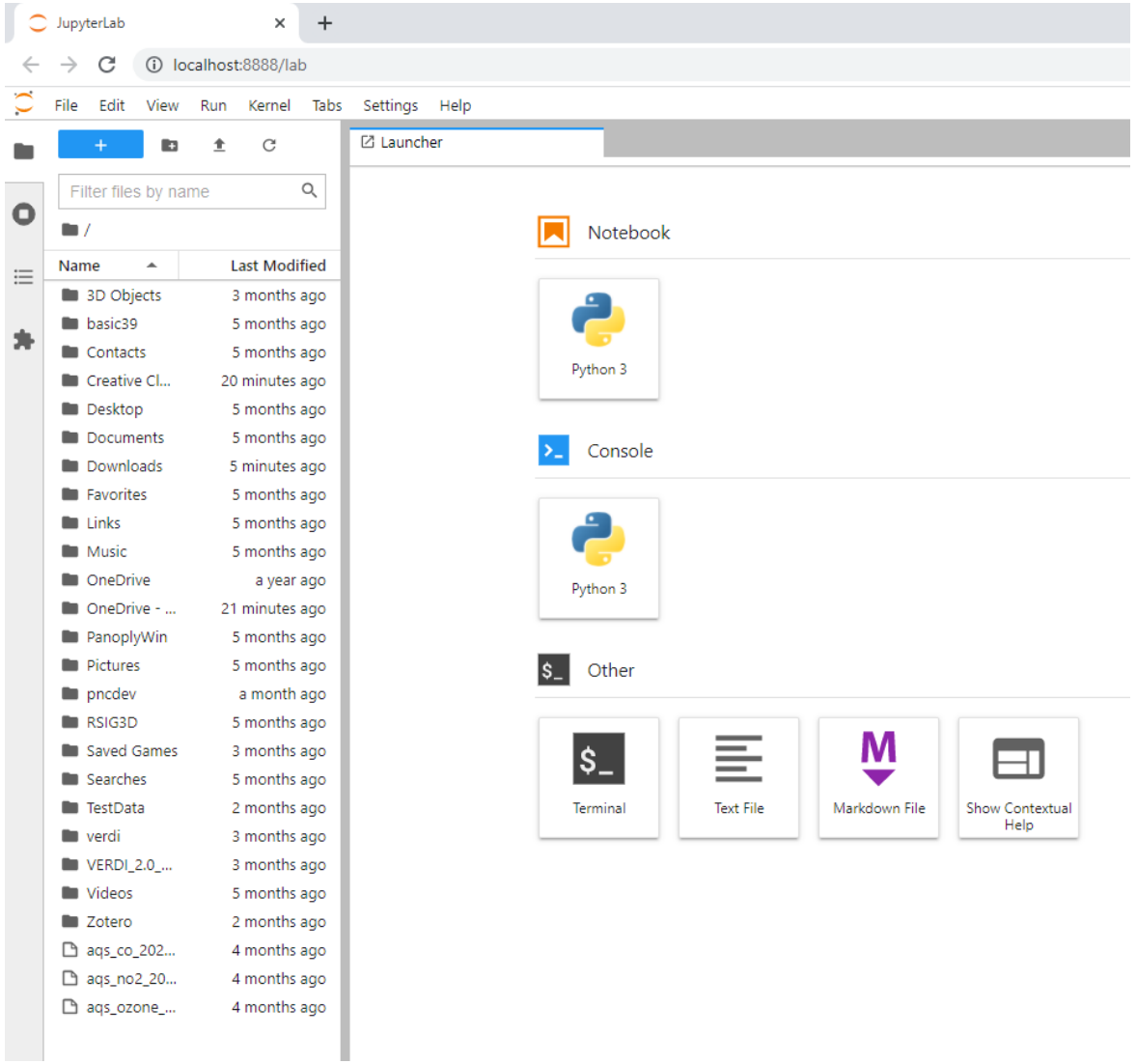

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What if I can’t install?

What if I don’t *want* to install?

Use  jupyterhub

GIPHY

JupyterHubs give anyone access to cloud computing services.

- The interface is the same in the cloud as on your machine.
- Available all kinds of places
  - Google Colab (integrated GitHub)
  - Amazon Sage Maker
  - Microsoft Azure (discontinued?)
  - mybinder.org (integrated GitHub)
  - Atmos and EPA DMAP…
- When your data is on the same machine… WOW!

Figure source: https://coderefinery.github.io/jupyter/interface/

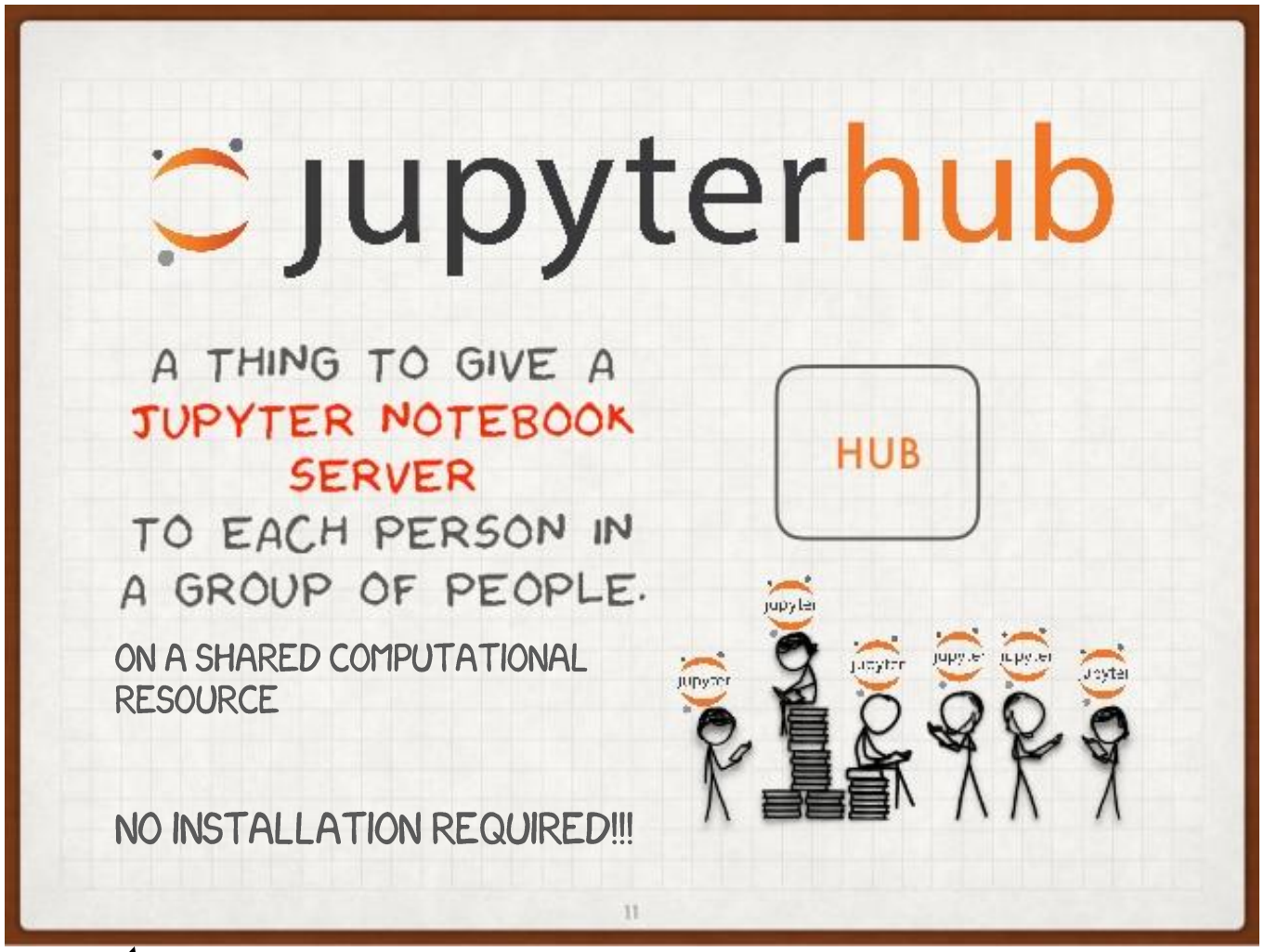
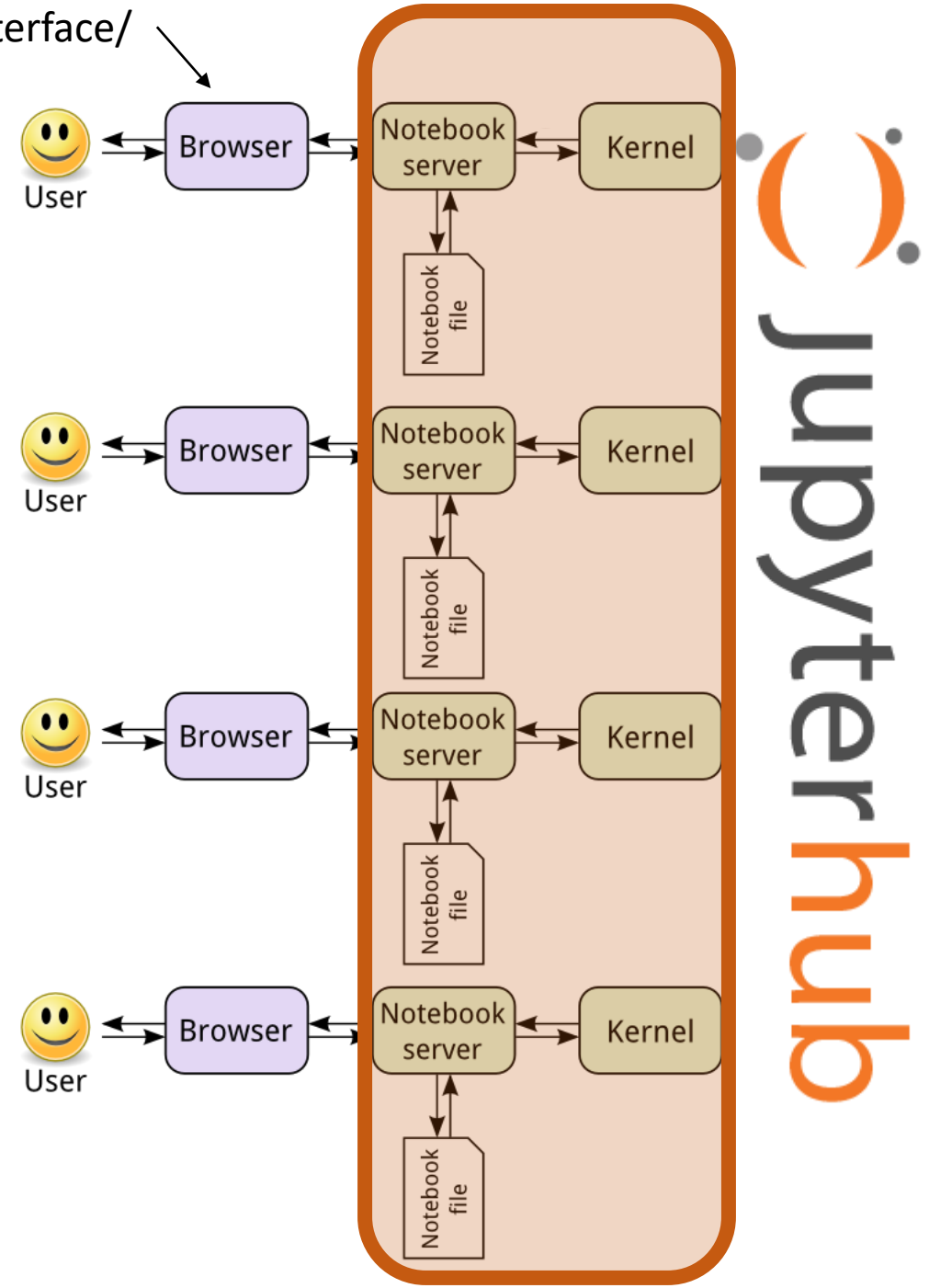


Figure source: https://geohackweek.github.io/Introductory/05-Jupyter-tutorial/



Cloud Options at EPA

Amazon-based Data Management and Analytics Platform (DMAP)

- Spinup your own Jupyter Server
- Access computational resources and data on AWS
- Up to $100/month approved
- Requires an account request to OMS
- Currently notebooks not labs, but basically the same.
- May expand to Amazon Sagemaker

*Google Colab requires a Google account

High Performance Computing (HPC) on atmos

- JupyterHub is already running on atmos.
- Access login nodes and computational nodes.
- Access data on atmos
- Already paid for.
- Requires an account that many of you already have… ask your branch chief or emvl_help@epa.gov.

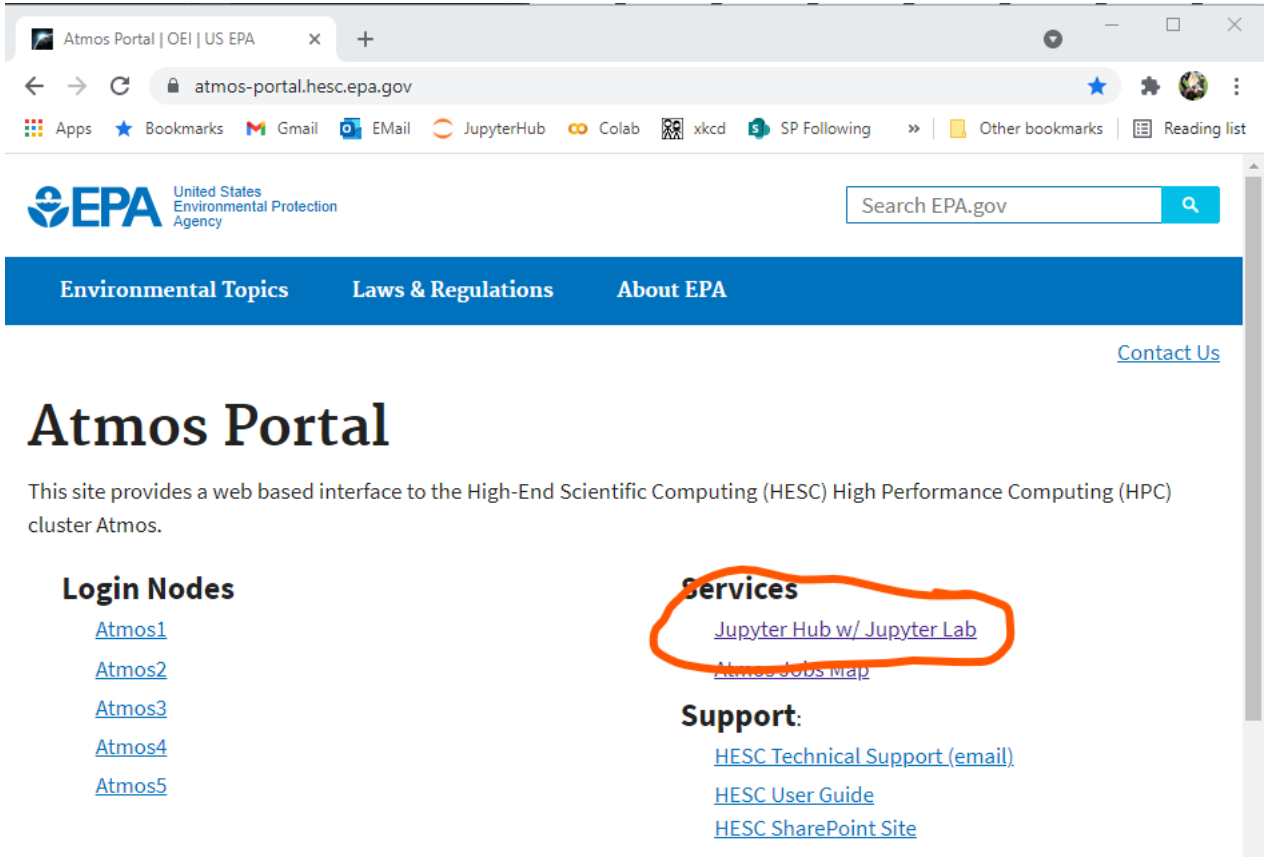
*Mybinder.org requires an account

Atmos Instructions

- The next few examples assume you have access to atmos.
- If you do not, you can use mybinder.org or Google Colab to explore publicly available notebooks.
  - https://colab.research.google.com/
  - For the CMAQ crew http://github.com/barronh/pseudonetcdf_examples
- If you have an atmos account, and your already know how to access JupyterHub, consider exploring
  - /home/bhenders/Notebooks/
  a. AQS_Pregenerated_MonthMean.ipynb
  b. BasicCMAQEval.ipynb
  c. CMAQ_Ozone_Evaluation.ipynb
  d. MachineLearningExample.ipynb
  e. MASK_MAKER.ipynb
- The rest of us are going to access atmos Jupyter Hub for the first time.

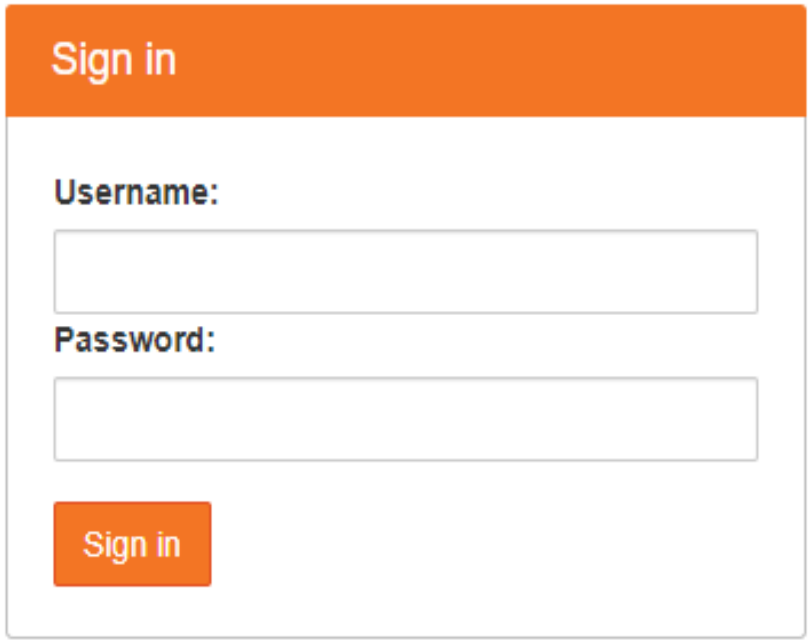
Access Jupyter Hub from the atmos-portal

1. Connect to the EPA Network or VPN
2. Navigate a web browser to https://atmos-portal.hesc.epa.gov/
3. Click on “Jupyter Hub w/ Jupyter Lab”



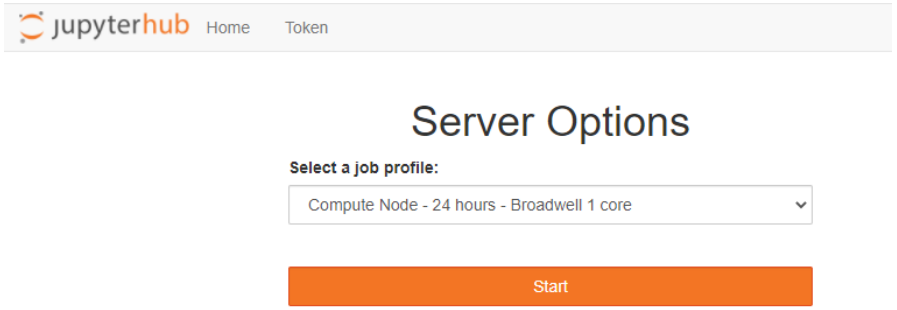
Logging in and starting a “user server”

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



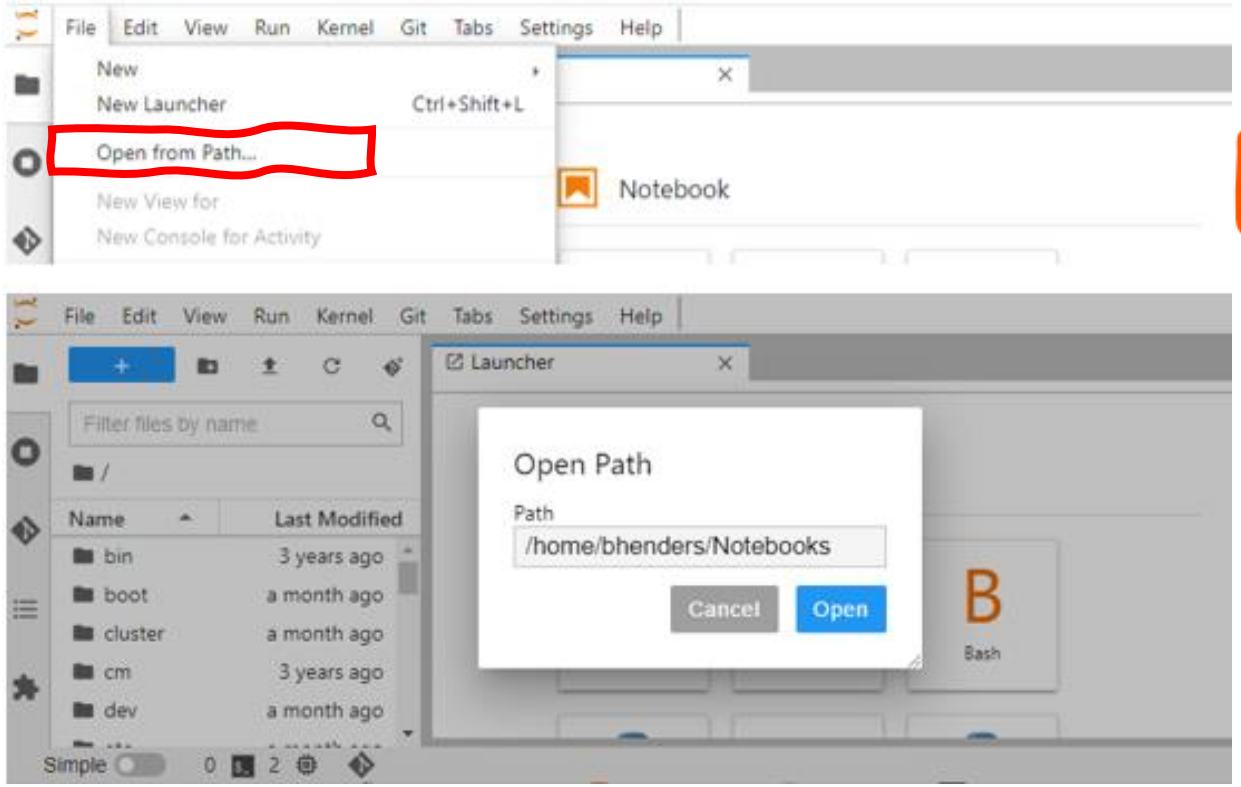
5. Normally, select a “Compute Node – 24 hours - Broadwell 1 core” and click start.

- **Select a singlepe node**
- **Select a debug node for 4 hours**
- **Select a compute node for 1 days.**

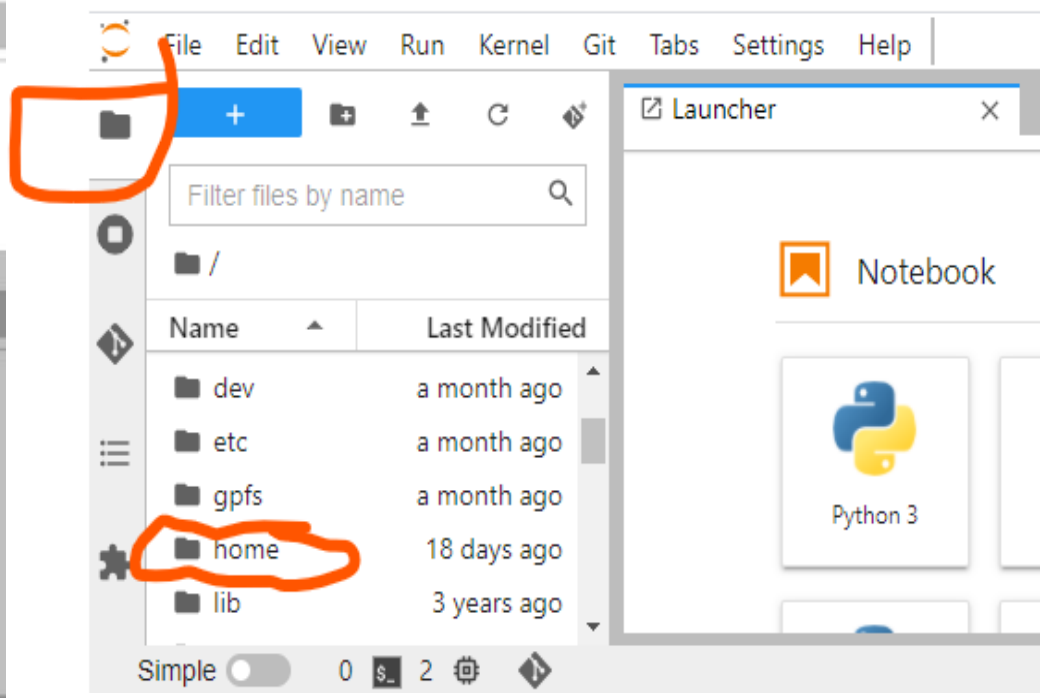


6. Navigate to a folder with a Notebook

a) Select “File” and “Open from Path…”

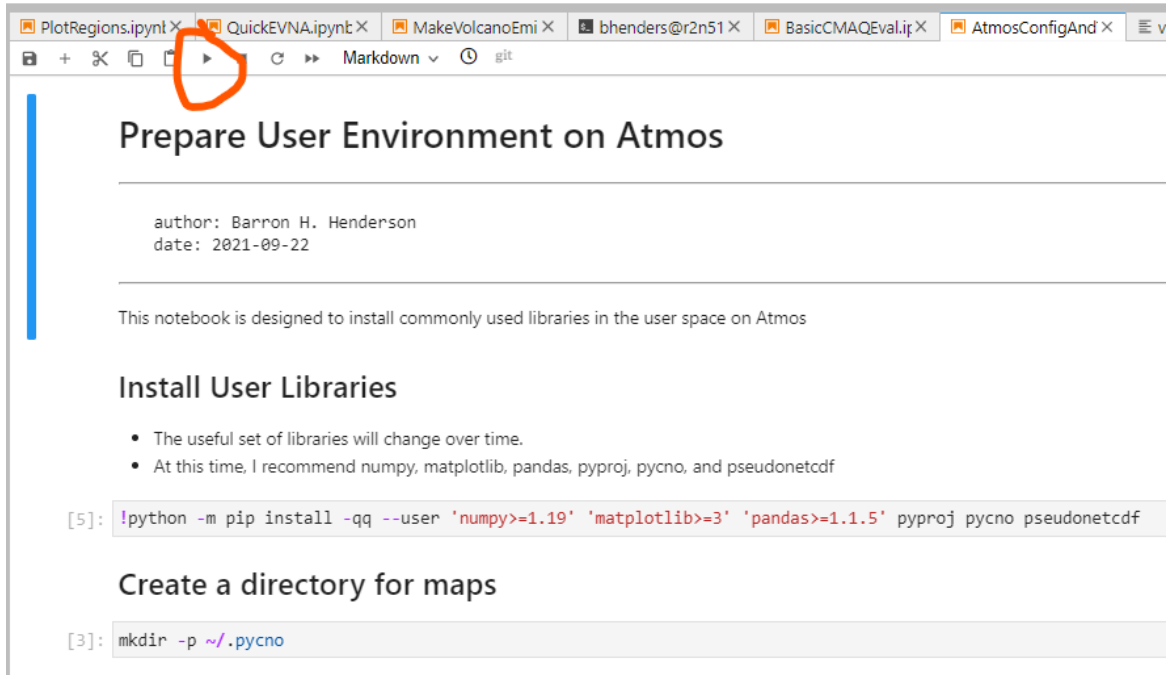


b) Or navigate by clicking in the file browser (folder on left)



7. Example notebook and system configuration

7. 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



Explore and make other notebooks

8. 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. ***AQS_Pregenerated_MonthMean.ipynb a simple observation analysis system***
    b. BasicCMAQEval.ipynb performs a simplistic CMAQ evaluation against AQS observations.
    c. MachineLearningExample.ipynb
    d. CMAQ_Ozone_Evaluation.ipynb has a more detailed evaluation of a year.
    e. MASK_MAKER.ipynb is a simple tool to make arbitrary masks from shapefiles

9. 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

We're going to do this one together.

Live Examples

- A repository of fully functional runnable code.
- Oriented toward solving CMAQ types of problems.
- Right now, the CMAS Forum Python Channel allows us to link to these sorts of things
  - cmascenter.org -> Help -> CMAS Forum -> Category Python
  - https://forum.cmascenter.org/c/python/