Primer: Running JupyterLab on the ACES Portal

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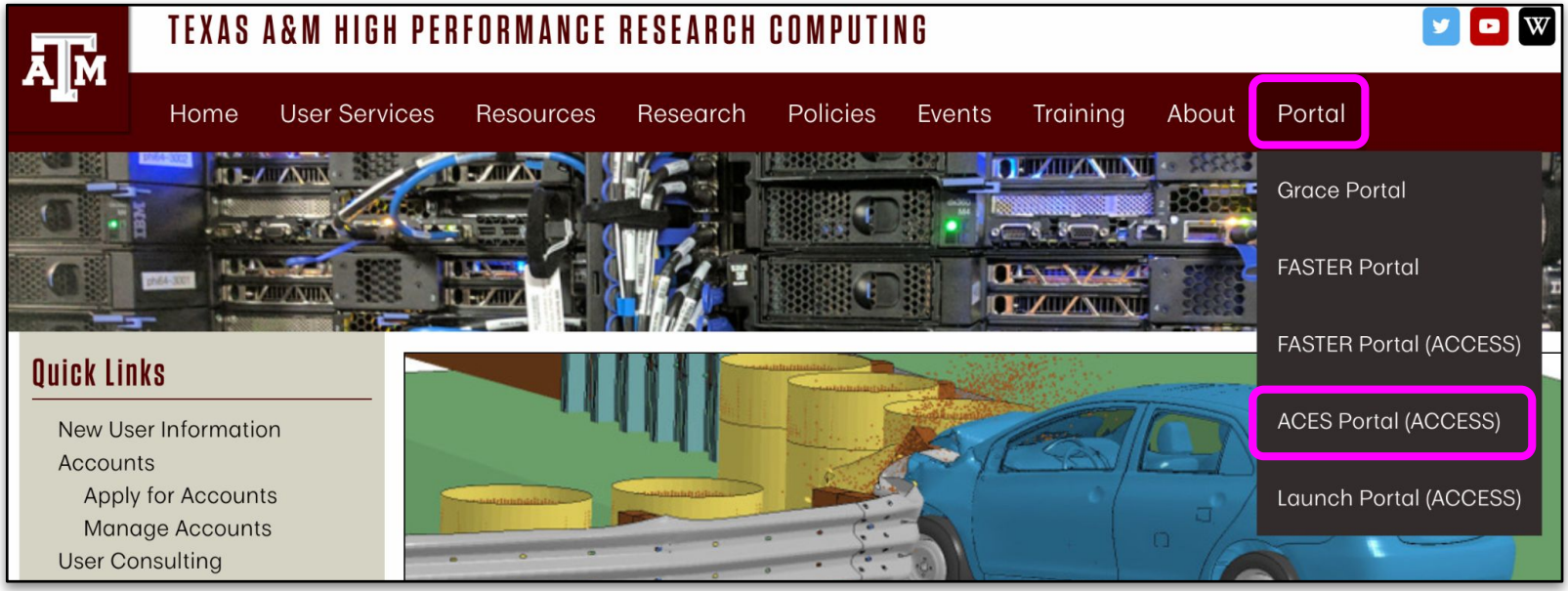
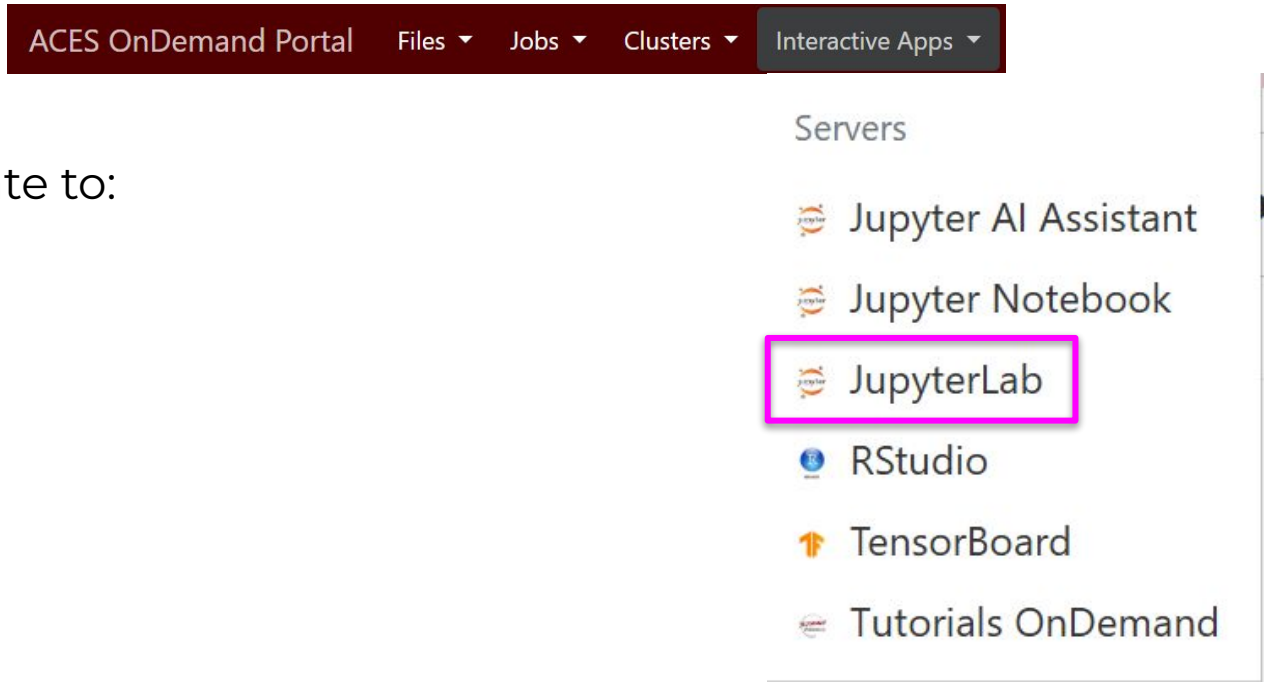
High Performance
Research Computing
DIVISION OF RESEARCH

The ACES Portal

- Get your ACCESS ID ready!
- Head to HPRC webpage: hprc.tamu.edu and navigate to Portal menu
- ACES portal shortcut - portal-aces.hprc.tamu.edu



JupyterLab Interactive App



In the portal, navigate to:

> Interactive Apps

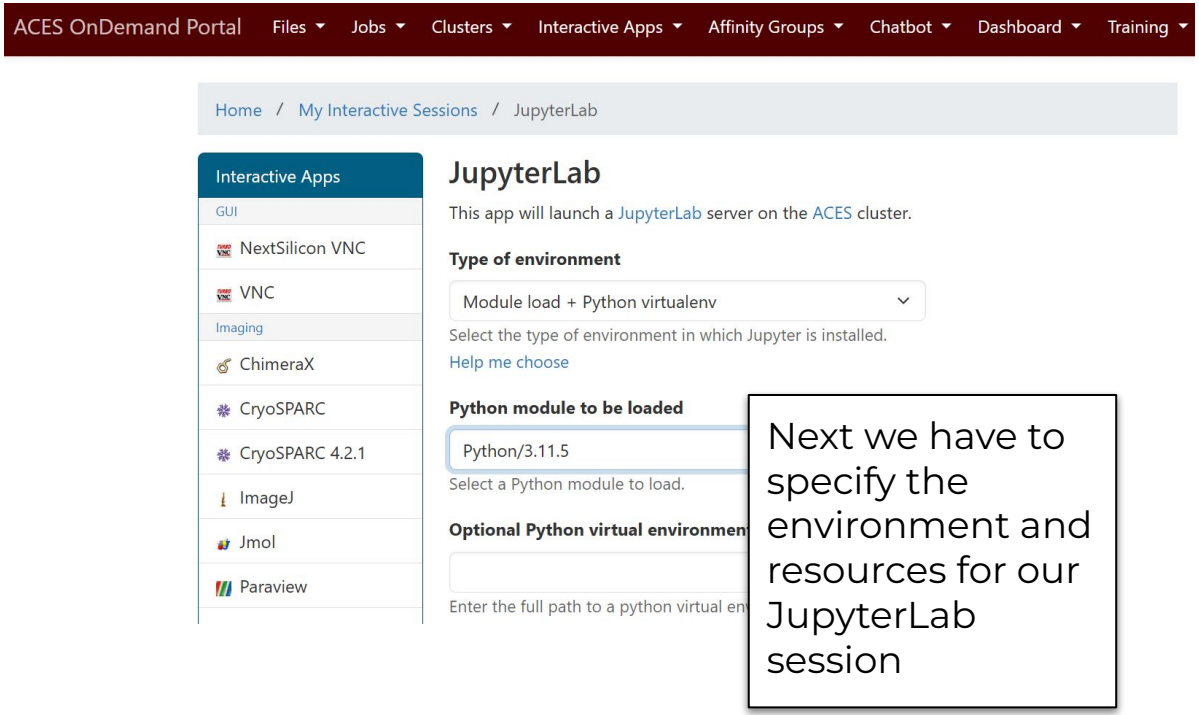
>> Servers section:

>>> JupyterLab

JupyterLab Interactive App

Supported Environment Types

- TAMU Modulair
- Container (Singularity)
- Anaconda environment
- Module load + Python Virtualenv

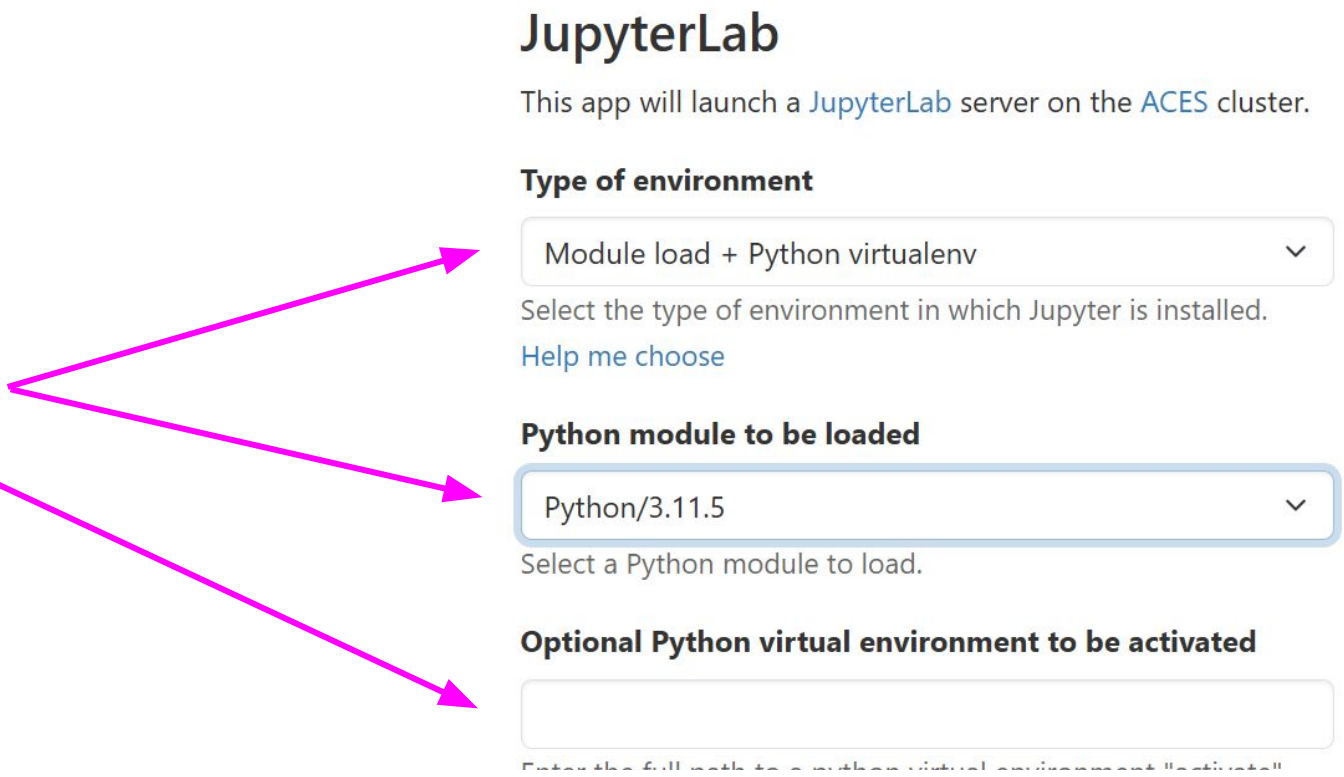


Python Environments on ACES

For now:

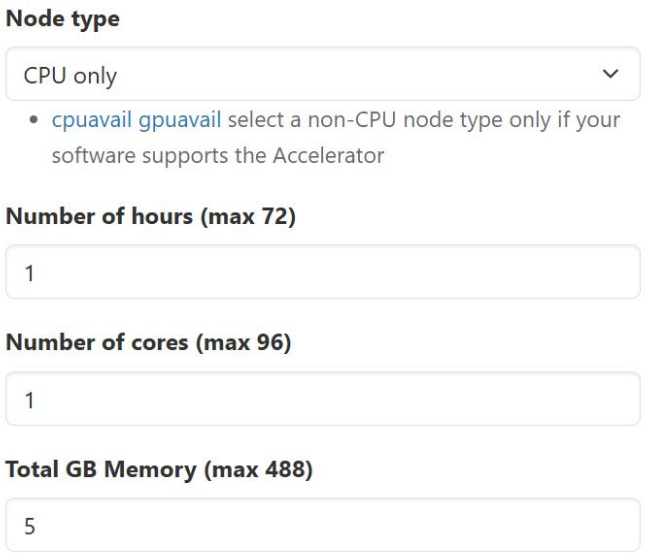
Choose these two:

Leave this blank:



Session Parameters on ACES

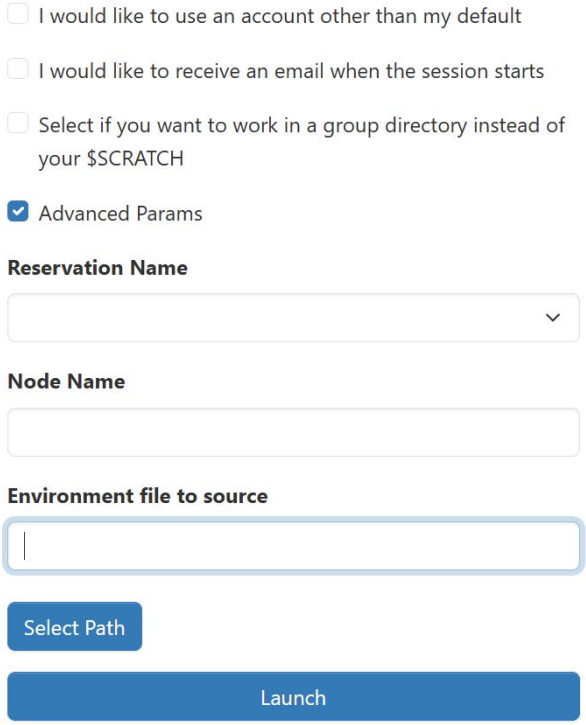
- Provide **node type** (CPU only, H100 GPU or A30 GPU)
  - **CPU**
- Provide **number of hours** [1-72] for running jupyter lab on the cluster
  - **1 core**
- Specify **number of cores** [1-96] allocated on node on the cluster
  - **1 core**
- Requested **total memory** [5-485 GB]
  - **5 GB**



Optional Session Parameters on ACES

You can ignore these today, but you can also:

- Specify an account number to charge SUs
- Provide an email to be notified when session is ready to launch
- Choose to work in a group directory instead of user's `$SCRATCH`
- Advanced Parameters:
    - Reservation name
    - Node name
    - Environment file to source (e.g. additional path for `$PATH` or `$LD_LIBRARY_PATH`)

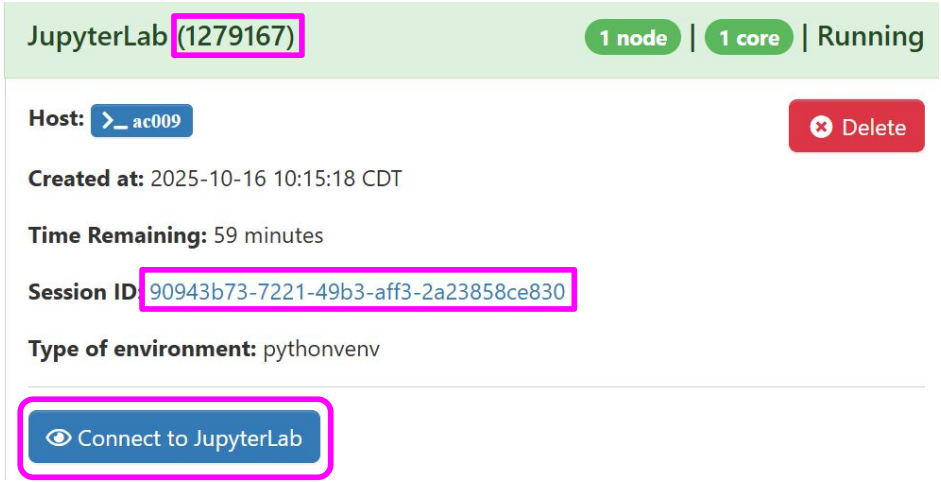


Interactive Sessions on ACES Portal

After clicking **Launch**, you are sent to the **My Interactive Sessions** page.

- Your job will first show as a blue box with “JupyterLab (<job ID>)” at the top
- ‘Session ID’ is link to a directory where you can find the jobs logs
- Click **Connect to JupyterLab** when it appears

  (box will turn green; speed depends on cluster usage)



Jupyter Notebook vs JupyterLab

Jupyter Notebook

- Web-based interactive environment
- Simpler more lightweight interface
- Can only open Jupyter Notebooks
- Used for data analysis and visualization
- Supports languages like Python, Julia, R, etc.

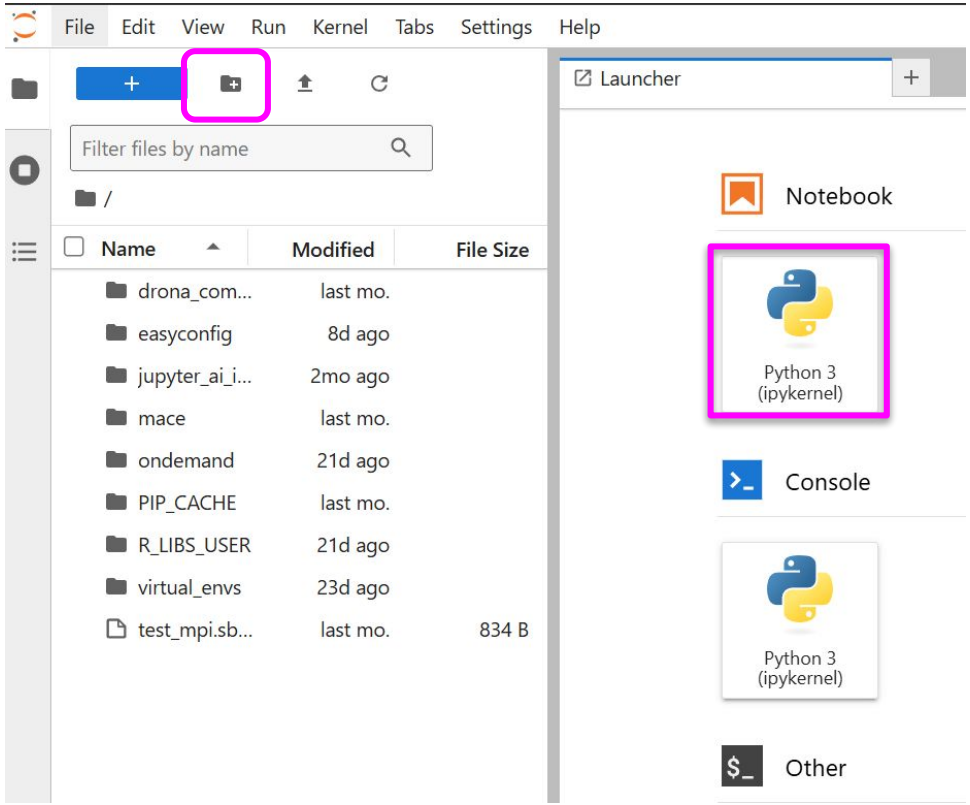
JupyterLab

- IDE like experience
- Versatile and feature-rich interface
- Modular structure where you can open different file types:-
  - Jupyter Notebook
  - Terminal sessions
  - PDF, HTML, txt files
  - and more!
- Supports languages like Python, Julia, R, etc.

Welcome to JupyterLab

File Navigator in JupyterLab

- Default directory: user's `$SCRATCH` directory or optionally-provided group directory
- Create new directories using the New Folder icon
- Create a new Jupyter Notebook using the first icon in the Notebook section on the right panel
- If you are uploading an existing .ipynb file, ensure the Python version is compatible

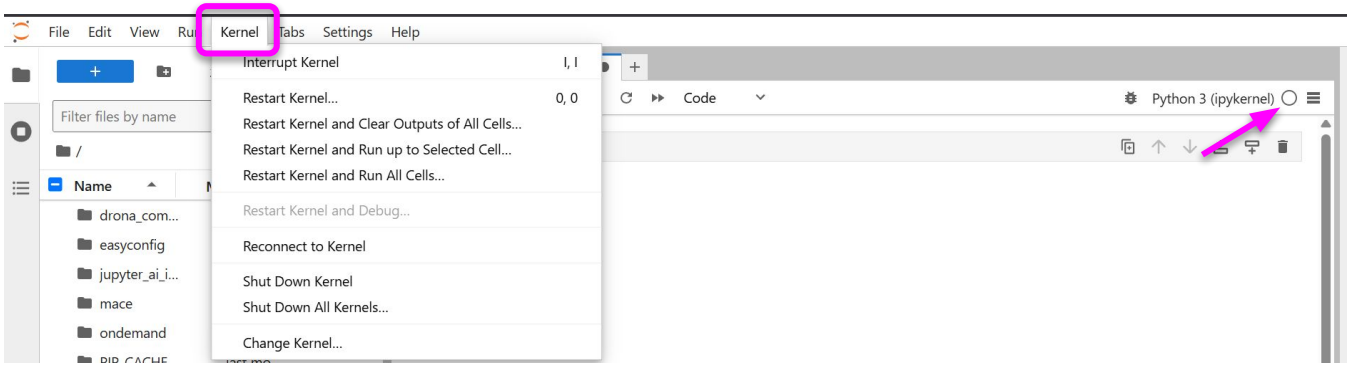


Exercise 1

1. In JupyterLab, create a new directory and go into it.

2. Create a new Jupyter Notebook file inside the directory. Save the file regularly to avoid losing changes.

Jupyter Notebook Kernels



Thinking...

Idle

Broken!

The “kernel” is like the brain of your notebook. It determines what language you are thinking in–and if it is not working, you cannot process anything.

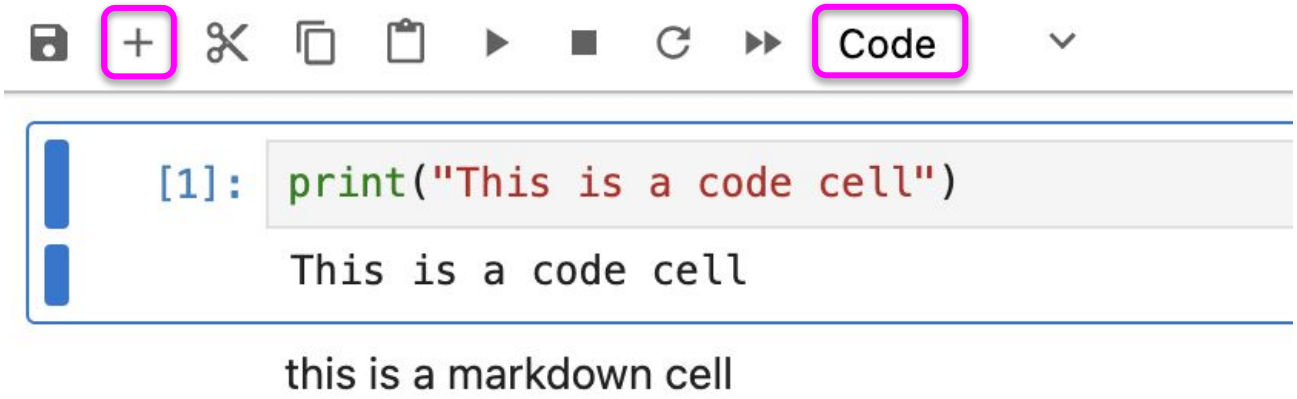
In the top-right of your window is the kernel status, showing what language you are using and what the kernel is doing.

When you first start a notebook, it will take a moment for the kernel to start up. If something goes wrong, you may have to restart it.

Cells in Jupyter Notebook

Notebooks are organized into Cells.

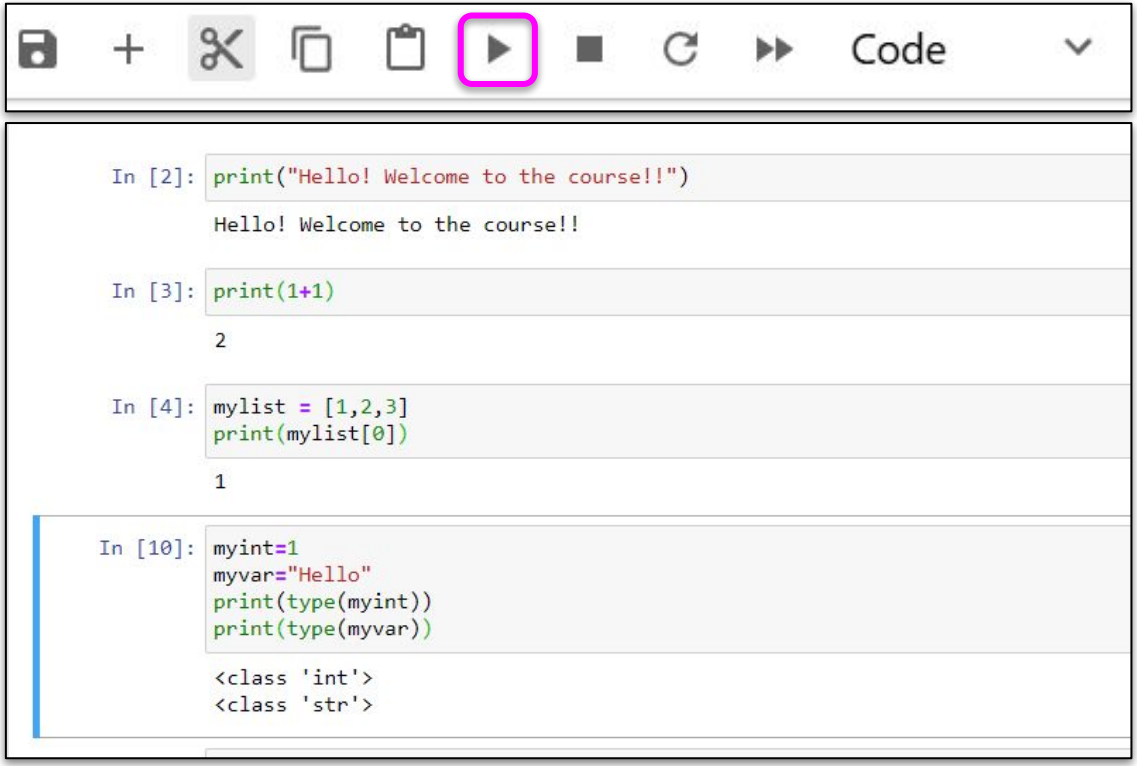
- These can be either *code* cells or *markdown* cells (we'll start with code).
- Click to the left of a cell to highlight it (blue, for "command mode")
- Click inside the body of the cell to edit it
- Add new cells using the "+" icon



Executing Code in Jupyter Notebooks

ctrl+enter or click the **Run** button to run a cell.

The brackets to the left will show [*] if the cell is running and change to a number (showing what order the cells were executed) once it's done.



Python in Jupyter Notebooks

Cells are just blocks of code you choose to execute all at once. You can execute them in any order, and any defined objects persist across them.

All that matters is what order you send code to the kernel.

Plotting in Jupyter Notebooks

Making plots in Jupyter depends somewhat on your environment.

You may need a “notebook magic” to make images show up.
(magics are a big, kernel-dependent topic we won’t cover here!)

```
[6]: # A simple plot with matplotlib
from matplotlib import pyplot as plt

x = [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
y = [2, 4, 7, 11, 6, 2, 0, -4, -1, 2]

plt.plot(x, y)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

No magic, no plot!

```
[15]: %matplotlib inline

[16]: # A simple plot with matplotlib
from matplotlib import pyplot as plt

x = [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
y = [2, 4, 7, 11, 6, 2, 0, -4, -1, 2]

plt.plot(x, y)
plt.xlabel("x")
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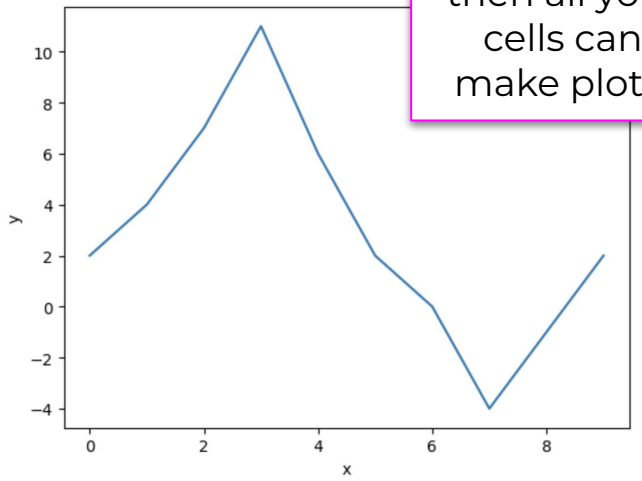

Magic first, then all your cells can make plots!

Exercise 2

1. Enter some Python code in a cell. Print a message: “Welcome to HPRC”.

2. Try to make a simple plot, like on the previous slide.

Markdown in Jupyter Notebooks

Markdown cells are used for annotation, documentation, organization, etc.

- Convert a cell from drop down menu in the toolbar (can also be found in the Cell menu)
- As with code cells, **Ctrl+enter** or **Run** to execute and format Text.

Font changes from `monospace` to something more *beautiful*.

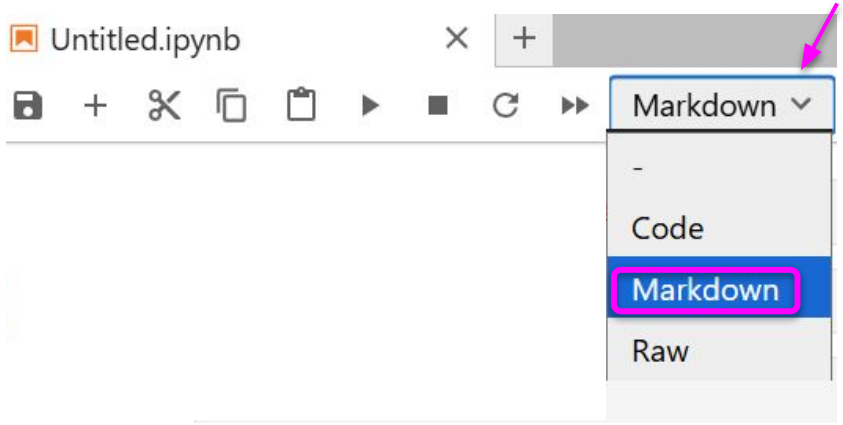

Markdown in Jupyter Notebooks

- *Headers*
  # (Header 1, title) stands for html code
  <h1>Header 1,title<h1>
  Add more '#' for smaller headers

- Line Break
  Insert line breaks using *
*

- Inline Formatting
  Bold: ***HPRC***
  Italics: **HPRC**
  Horizontal Line: *****

- Embed external link
  Works like html:
  link text

```
# Look! Markdown!

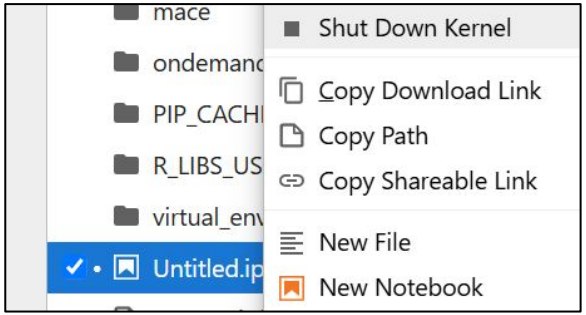
Normal text<br>
Normal text on a new line

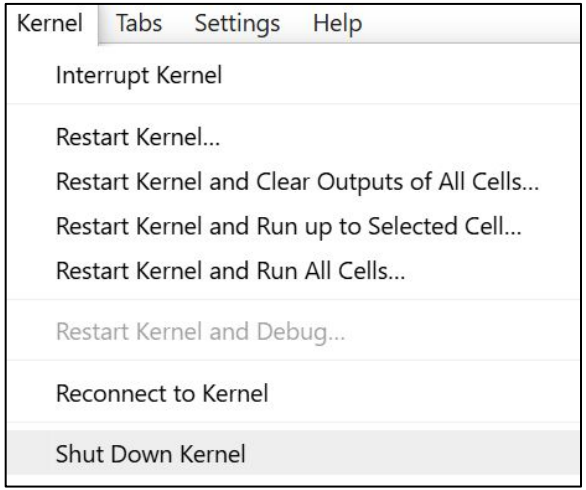
**Bold text!**
*Italic text*
***
<a href="https://hprc.tamu.edu/">Link to HPRC</a>
```

Look! Markdown!

Normal text
Normal text on a new line

Bold text! *Italic text*

Link to HPRC

Exercise 3: Markdown

1. Create a Markdown Cell and add some text.
2. Change the formatting as indicated below:
    - Bold
    - Italics
    - Header 1 format
    - Include a link (https://hprc.tamu.edu/) next to the text

More Text Formats in Jupyter Notebooks

LaTeX: for mathematical operations

- In a Markdown cell:
- `$ math expression $`

```
$\sqrt{k}$
```

$\sqrt{k}$

Embed Code in Text:

- In a Markdown cell:
- use the triple backticks ``` followed by a language name.

````
```Python
str = "This is block level code"
print(str)
```
````

```Python
str = "This is block level code"
print(str)
```

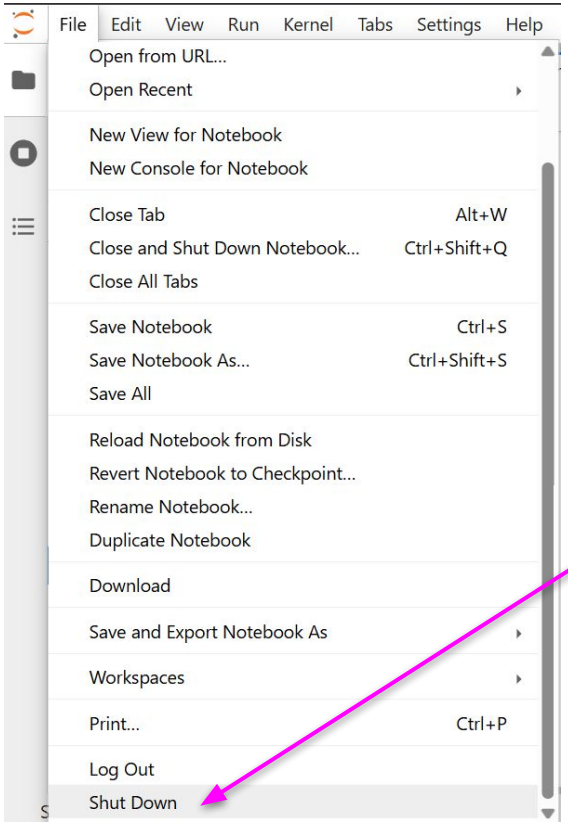
Shutting Down

- Notebooks (i.e. their kernels) keep running even if you exit their browser tab
- To shut one down, find it in the Jupyter file browser
- Right click and choose “Shutdown Kernel”
- Can also shutdown kernel in the “Kernel” menu at the top and shut them down there.





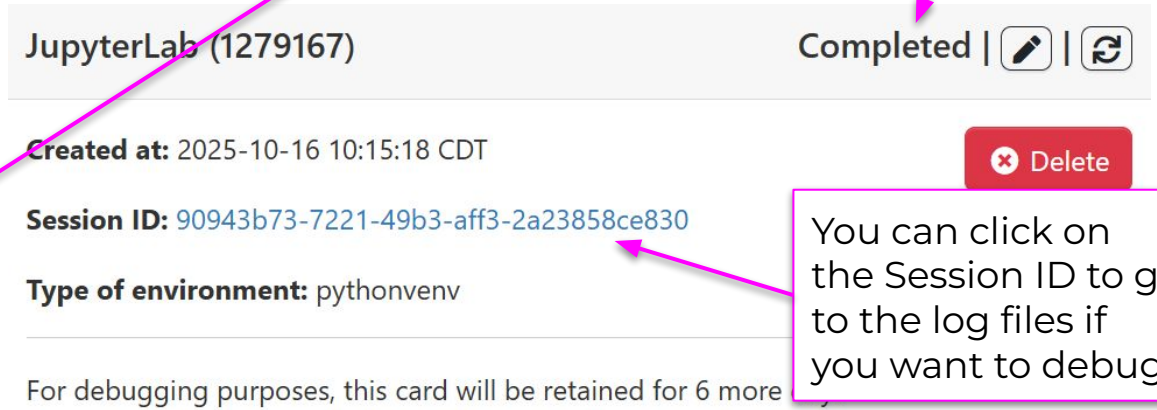
Ending the Jupyter Session



As long as your Jupyter session is running (not just notebooks!) you're taking up compute resources!

To quit before the time you specified at the beginning, go to File → Shut Down

Back in "My Interactive Session" in the HPRC Portal, the box for your session will turn grey to indicate it is done.



You can click on the Session ID to go to the log files if you want to debug!

Exercise 4: Shutting Down

1. Shut down your Jupyter session

2. Find the log files for your recent session.
   (Hint: the Session ID **link** from the My Interactive Sessions is a shortcut; you should end up in:
   `$SCRATCH/ondemand/data/sys/dashboard/batch_connect/sys/jupyter/output/`
   (You may need these some day to diagnose errors.)

Need Help?

First check the FAQ https://hprc.tamu.edu/kb/FAQ/Accounts/

- ACES User Guide https://hprc.tamu.edu/kb/User-Guides/ACES/
- Email your questions to help@hprc.tamu.edu

Help us help you -- when you contact us, tell us:

- Which Cluster you're using
- Your Username
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used if any
- Module(s) loaded if any
- Error messages
- Steps you have taken, so we can reproduce the problem

Continued Learning

Intro to HPRC YouTube Channel

HPRC's Knowledge Base

High Performance
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Give us feedback on the class with this survey:
https://u.tamu.edu/hprc_shortcourse_survey

Thank you

Questions?

HPRC Survey