# **HIGH PERFORMANCE RESEARCH COMPUTING** Primer: Running Jupyter Notebook on the HPRC Portal

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High Performance Research Computing DIVISION OF RESEARCH



### Accessing the HPRC Portal

- HPRC webpage: <u>hprc.tamu.edu</u>
- Shortcuts:
  - for TAMU NetID: portal-faster.hprc.tamu.edu
  - for ACCESS ID: portal-fa





# Jupyter Notebook Interactive App

• In the portal, go to Interactive Apps-> Server->Jupyter Notebooks



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### Jupyter Notebook Interactive App

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TAMU HPRC OnDemand (FASTER) Files - Jobs - Clusters - Interactive Apps -

#### Home / My Interactive Sessions / Jupyter Notebook

Interactive Apps	Jupyter Notebook
BIO	This app will launch a Jupyter Notebook server on the
👔 Beauti	FASTER cluster.
IGV	Module load + Python virtualenv
Mauve	Select the type of environment in which Jupyter is installed.
Structure	Module selected
	Dether (0.0.0
SYS Workbench	Select a module to load. All modules listed will also load the
MATLAB	appropriate Python and Jupyter by default.
VNC	Additional Core modules to be loaded: GCCcore/9.3.0
ging	Default Jupyter virtualenv available.
ChimeraX	Optional Environment to be activated



### Python Environments on FASTER

#### **Supported Environment Types**

- Pre-created Modules
- Module + Virtualenv
- Anaconda + Conda Env
- Singularity Container

Choose this one: 🖌

Leave this blank:

#### Jupyter Notebook

This app will launch a Jupyter Notebook server on the FASTER cluster.

#### Type of environment

Module load + Python virtualenv

Select the type of environment in which Jupyter is installed. Help me choose

Module selected

Python/3.8.2

Select a module to load. All modules listed will also load the appropriate Python and Jupyter by default.

Additional Core modules to be loaded: GCCcore/9.3.0 Default Jupyter virtualenv available.

Optional Environment to be activated

# Slurm Options on FASTER

- Provide number of hours for running notebooks on clusters
- Specify number of cores [1-64] allocated on node on clusters
- Requested total memory (2-240GB)
- Provide **node type** (CPU only, T4, A100, A40 or A30)
- Specify account details and email to receive a pop-up when session is ready to launch

Number of hours	(max 168)
-----------------	-----------

Number of	cores (max 64)	
1		
Total GB n	nemory (max 240)	
2		
Node type		
CPU on	ly	•
• T4, A	100, A10, A40, or A30, select a GPU node fo	or 2D/3D
visua	lization for software that supports GPU usage	. FASTE
has t	he following GPUs available:	
0	200 x T4 16GB GPUs (max 8 per job)	
0	40 x A100 40GB GPUs (max 12 per job)	
0	10 x A10 24GB GPUs (max 4 per job)	
0	8 x A40 48GB GPUs (max 4 per job)	
0	4 x A30 24GB GPUs (max 2 per job)	
• CPU	<ul> <li>select CPU node to reduce wait time for job</li> </ul>	to launch
Account		
This field is	s optional.	
Email		
This field is Email	s optional.	



### **Interactive Sessions on HPRC Portal**

After clicking Launch, use menu item My Interactive Sessions to find this page.

- Jupyter notebook session with JobID (94914 in this case) and session is running.
- Session ID is link to a directory where you can find the jobs logs
- click **Connect to Jupyter** when it appears (about 60 seconds)





### Welcome to Jupyter Notebook

#### File Navigator in Jupyter

- Default directory: user's \$SCRATCH directory or optionally provided virtual environment directory
- Create new Notebook files using New-> Python3
- If you are uploading existing .ipynb file, ensure python version is compatible

💭 Jupyter	Quit Logout
Files Running Clusters Softwares	
Select items to perform actions on them.	Upload New - 2
	Name      Last Modified File size
ondemand-faster	3 days ago
	6 minutes ago
Project1	9 minutes ago
Project2	a minute ago

# Notebook Files In Jupyter

#### Jupyter Notebook- Familiarize the setup

- Jupyter server is up and running.
  - To create a notebook:

#### New -> Python 3 (ipykernel)

- Upload notebook (Python version must be the same/compatible):
   Upload -> Select notebook
- File naming convention

All lowercase module names. Long module names can have words separated by underscores (really\_long\_module\_name.py). CamelCase for class names.

# Cells in Jupyter Notebook

Notebooks are organized into Cells. Click on the Cell to highlight it. Use the Jupyter Notebook Menu: **Insert -> Insert Cell Below** 

💭 jupyter Unti	tled	Logout
File Edit View	Insert Cell Kernel Help Trusted	Python 3 (ipykernel) O
8 + % 4 6	Insert Cell Above A Code	•
In [ ]:		
In [ ]:		



# Python in Jupyter Notebook

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

File Edit	/iew Insert Cell Kernel Help				
🖺 🕇 🗶 🖄	Market Area and A				
In [2]:	<pre>print("Hello! Welcome to the course!!")</pre>				
	Hello! Welcome to the course!!				
In [3]:	print(1+1)				
	2				
In [4]:	<pre>mylist = [1,2,3] print(mylist[0])</pre>				
	1				
In [10]:	<pre>myint=1 myvar="Hello" print(type(myint)) print(type(myvar))</pre>				
	<class 'int'=""> <class 'str'=""></class></class>				

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### **Exercise** 1

1. In Jupyter, create a new directory.

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

3. Execute some Python Code. Print a message: Welcome to HPRC



# Jupyter Notebook Sessions

#### Jupyter Notebook- Familiarize the setup

Kernel Attributes Interrupt

Restart

Restart & Clear Output

Restart & Run All

Reconnect

Shutdown

ile	Ed	it Vie	ew Insert	Cell	Kernel Help	Not Trusted	Python 3 (ipykernel)
	+ 9	< 2	₿ ↑ ↓	► Run	Interrupt I, I + E Restart 0, 0		
In [2]: In [1]:	print('Welcome t Welcome to HPRC		Restart & Clear Output Restart & Run All Reconnect Shutdown				
	n [1]:	! pwd		Change kernel			
		/scratch/	/user/pi				
	Т	. [].					

Change kernel (switch between various python versions available)



# Markdown in Jupyter Notebook

Use the Jupyter Notebook Menu: Cell -> Cell Type -> Markdown

Ctrl+enter or Run to format Text.	File     Edit     View     Insert     Cell     Kernel     Help       P     Image: Cells     Image: Cells     Image: Cells     Image: Cells     Image: Cells     Image: Cells       Bun Cells     Cells     Cells     Image: Cells     Image: Cells     Image: Cells     Image: Cells
Hello World	Run Cells and Insert Below    In []: print('Wel
Hello World	In []: <b>!pwd</b> Run All Below
	In []: %mkdir tes Cell Type > Code Y
	In []: !echo test Current Outputs All Output

Font changes from monospace to something more beautiful.



# Markdown in Jupyter Notebook

Use the Jupyter Notebook Menu: Cell -> Cell Type -> Markdown

### • Headers

# (Header 1, title) stands for html code <h1>Header 1,title<h1>

### • Line Break

The line breaks after using <br> br tags and it is awesome

### • Inline Formatting

Bold: \*\*HPRC Italics: \*HPRC Horizontal Line: \*\*\*

#### • Embed external link

<a href=>"https://www.google.com" >Link to Google</a> [section title](#section-title) [HPRC Link](<u>https://hprc.tamu.edu/</u>)



### Exercise 2: Markdown

- 1. Create a Markdown Cell and add some text.
- 2. Change the formatting as indicated below:

Bold

Italics

Headerl format

Include a link (<u>https://hprc.tamu.edu/</u>) next to the text



### More Text Formats in Jupyter Notebook

#### 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)
````
```

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



# Navigating Files in HPRC Portal

#### File Explorer

- Can view a file explorer for the users home or scratch directory
- View, delete, edit and create new files or directories on clusters
- Upload or download files

| TAMU HPRC OnDemand                      | I (FASTER)   | Files - Jobs - | Clusters - Inte  | eractive Apps <del>-</del> | ∎ «Þ • 0           |      |
|---|--|----------------|------------------|----------------------------|--------------------|------|
| >_ Open in Te                           | rminal 🕨 🕇 New   | File           | ctory 👤 Upload 🛃 | Download                   | Copy/Move          | ete  |
| Home Directory<br>/scratch/user/rarensu | ectory ser/rarensu / scratch / user / rarensu / ondemand-faster / data / sys / dashboar batch_connect / sys / jupyter / output / b321805a-fcd3-4dc9-b6b6-1d9141b C Change directory  Show Owner/Mode Show Dotfiles Filter: |                |                  |                            |                    |      |
|   | Type≜ <sub>v</sub>   | Name           | •                | Size *,                    | Modified at        | A.v. |
|   | O li   | after.sh       | •                | 493 Bytes                  | 11/17/2022 1:39:52 | 2 PM |
|   |  | before.sh      | I -              | 2 KB                       | 1/30/2023 4:05:47  | PM   |
|   | 0  | config.py      | •                | 383 Bytes                  | 1/30/2023 4:05:49  | PM   |

### **Exercise 3: Log Files**

### Log files can be found on disk at

\$SCRATCH/ondemand-faster/data/sys/dashboard/batch\_connect/sys/jupyter/output/

Find the Log Files for your Recent Session.
 (Hint: the Session ID link from the My Interactive Sessions is a shortcut)

What log files are available?



# Wrapping Up on HPRC Portal

#### **Final Steps**

#### • End Interactive Session:

In your Jupyter File Navigator, click 'Quit' in the top navigation bar. This will stop the running job and prevent wasting your SU's. (Logout does not do this)

#### • Saving the Notebook files:

Notebooks will be saved in the default directory (\$SCRATCH or virtual environment) This space persists between sessions.

#### • Logging Out of the Portal:

To properly log out the portal, follow the below mentioned steps:

- log out the portal by clicking 'Log out' from the top navigation bar
- close the browser to completely terminate the session



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# Thank you. Any questions?



### Need Help?

First check the FAQ hprc.tamu.edu/wiki/HPRC:CommonProblems

- FASTER User Guide hprc.tamu.edu/wiki/FASTER
- Email your questions to help@hprc.tamu.edu

Help us, help you -- we need more info

- Which Cluster
- 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 Video Tutorial Series

### HPRC's Wiki Page

