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National Laboratory

U.S. DEPARTMENT
of ENERGY

Week 2
👋Hello Python and Jupyter

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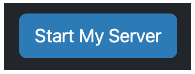
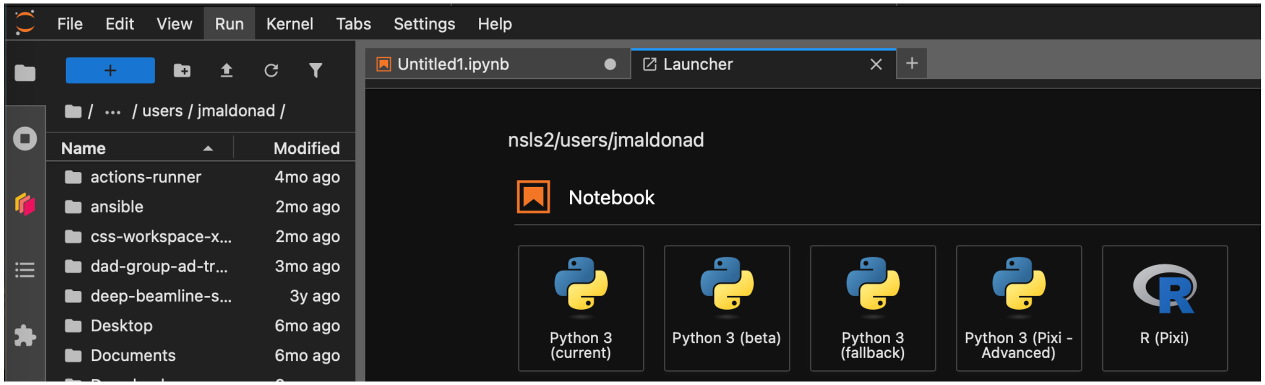
Let’s get setup…

1. Open up : jupyter.nsls2.bnl.gov
2. Log in with your BNL credentials and accept DUO push
3. Start My Server



4. Select Job Profile: Scientific Python, Start
5. Open a notebook



/ … / users / jmaldonad /

Name	Modified
actions-runner	4mo ago
ansible	2mo ago
css-workspace-x...	2mo ago
dad-group-ad-tr...	3mo ago
deep-beamline-s...	3y ago
Desktop	6mo ago
Documents	6mo ago

nsls2/users/jmaldonad

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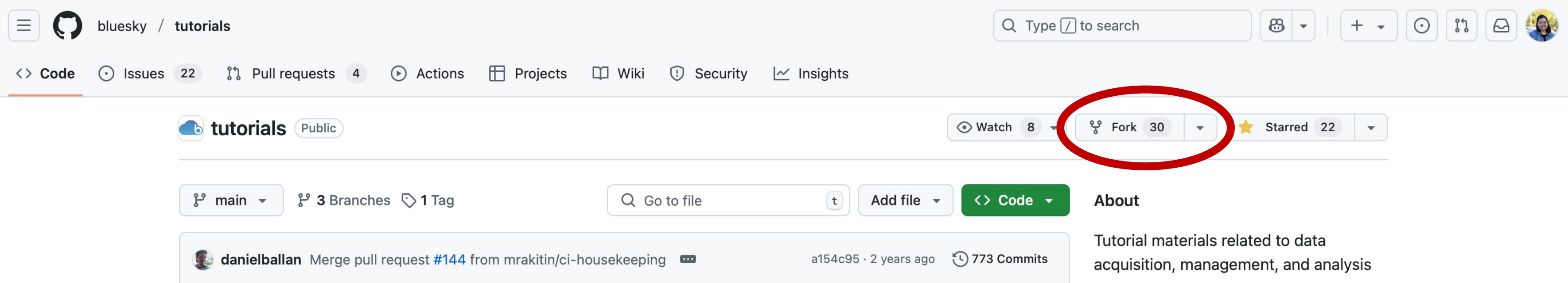
Using git…

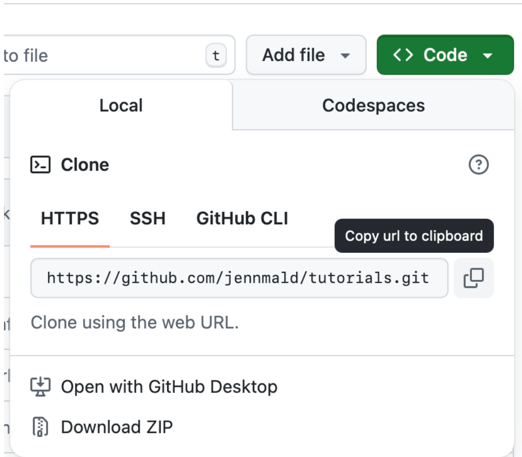
1. Open: https://github.com/NSLS2/bluesky-training-2025-2
2. Make a fork of this repository (if you have not done so already)



danielballan Merge pull request #144 from mrakitin/ci-housekeeping a154c95 · 2 years ago 773 Commits

Tutorial materials related to data acquisition, management, and analysis

Using git ...



```
https://github.com/jennmald/tutorials.git
```

Clone using the web URL.

1. Copy the HTTP clone link
2. In the first cell of your notebook try

```
!git clone https://github.com/<username>/bluesky-training-2025-2.git
```

3. You should see a new folder “bluesky-training-2025-2” appear in the file explorer
4. Open the folder and find **“hello-python-and-jupyter.ipynb”** in the week 2 folder

Types of Cells

Markdown

- Cells for text using Markdown which is like HTML (but easier)
- Headings, bold, italics, lists
- https://daringfireball.net/projects/markdown/

Code

- Allows you to enter and run code
- Run each code cell using Shift-Enter or pressing the play button in the tool bar
- https://jupyter-notebook.readthedocs.io/en/stable/examples/Notebook/Running%20Code.html

The Toolbar

Full list of shortcuts: https://gist.github.com/discdiver/9e00618756d120a8c9fa344ac1c375ac

💾	Save (ctrl + s)
+	Add new cell (shift + b, not in cell edit mode)
✂	Cut this cell (shift + x, not in cell edit mode)
⧉	Copy this cell (shift + x, not in cell edit mode)
📋	Paste cell from clipboard (shift + v, not in cell edit mode)
▶ ■ ↻	Run cell (shift + enter), Stop Kernel, Restart Kernel (00)
⏩	Restart kernel and run all cells
Markdown ⌄	Set cell type (shift + m for markdown, shift + y for code cell)

Run the notebook

Other Python Interfaces

- IPython – terminal based with magic
- Terminal – simple python shell
- IDEs
  - PyCharm
  - Visual Studio Code

Python Environments

Conda

- Cross-platform, package manager
- We use custom conda environments in DSSI to deploy necessary packages and python version on the experimental floor

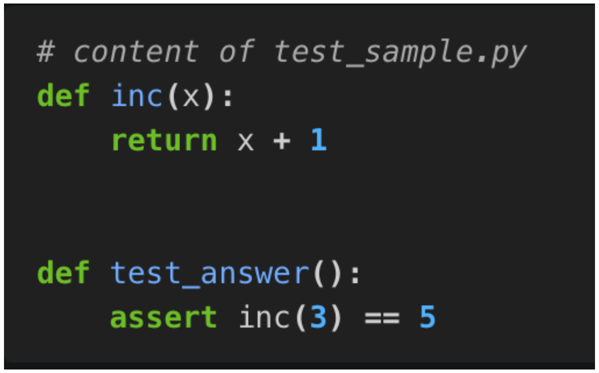
venv – virtual environments

- Module supports lightweight virtual environments each with their own independent set of python packages installed in their site directories
- Common install tool is pip

pixi – new package management workspace

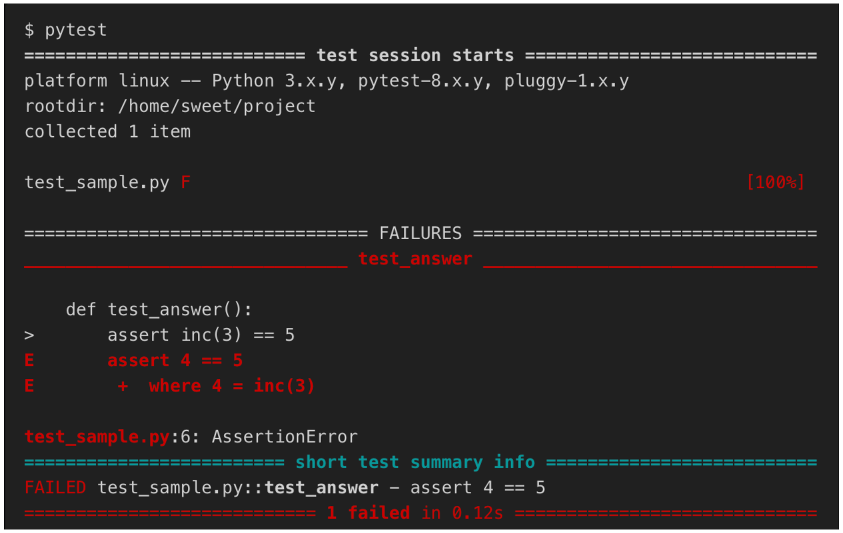
Testing in Python

- pytest: helps you write better programs
- Makes it easy to write small, readable tests, but also scales to complex functional testing for applications



```python
# content of test_sample.py
def inc(x):
    return x + 1


def test_answer():
    assert inc(3) == 5
```



```
$ pytest
=========================== test session starts ============================
platform linux -- Python 3.x.y, pytest-8.x.y, pluggy-1.x.y
rootdir: /home/sweet/project
collected 1 item

test_sample.py F                                                     [100%]

================================= FAILURES =================================
_______________________________ test_answer ________________________________

    def test_answer():
>       assert inc(3) == 5
E       assert 4 == 5
E        +  where 4 = inc(3)

test_sample.py:6: AssertionError
========================= short test summary info ==========================
FAILED test_sample.py::test_answer - assert 4 == 5
============================ 1 failed in 0.12s =============================
```

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Some notes about beamline profile collection repositories…

- Previously, all profile collections would be stored in NSLS-II-TLA, where TLA is the three-letter acronym of the beamline
- The DAD group is working on transitioning these repositories to the NSLS2 organization and renaming the repos to TLA-profile-collection
- This will help us maintain the profiles better and do more testing
- We will also be upgrading the conda environments to have the latest packages necessary

Questions?

Please feel free to reach out with any questions!

jmaldonad@bnl.gov or via Slack

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Challenge Problem

Crow’s Nest from Tiny Python Projects

- Write a program to announce something “off the larboard bow” to the captain of the ship
- Use test_crowsnest.py to check your work

Example:

Input: $ ./crowsnest.py narwhal

Output: Ahoy, Captain, a narwhal off the larboard bow!