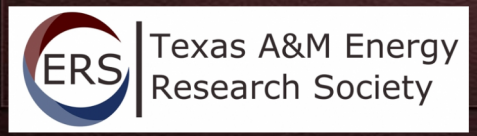
HPRC Data Workshop

Texas A&M Conference on Energy

Zhenhua He

12/03/2021



High Performance
Research Computing
DIVISION OF RESEARCH

Original slides created by Dr. Jian Tao

Data Labs

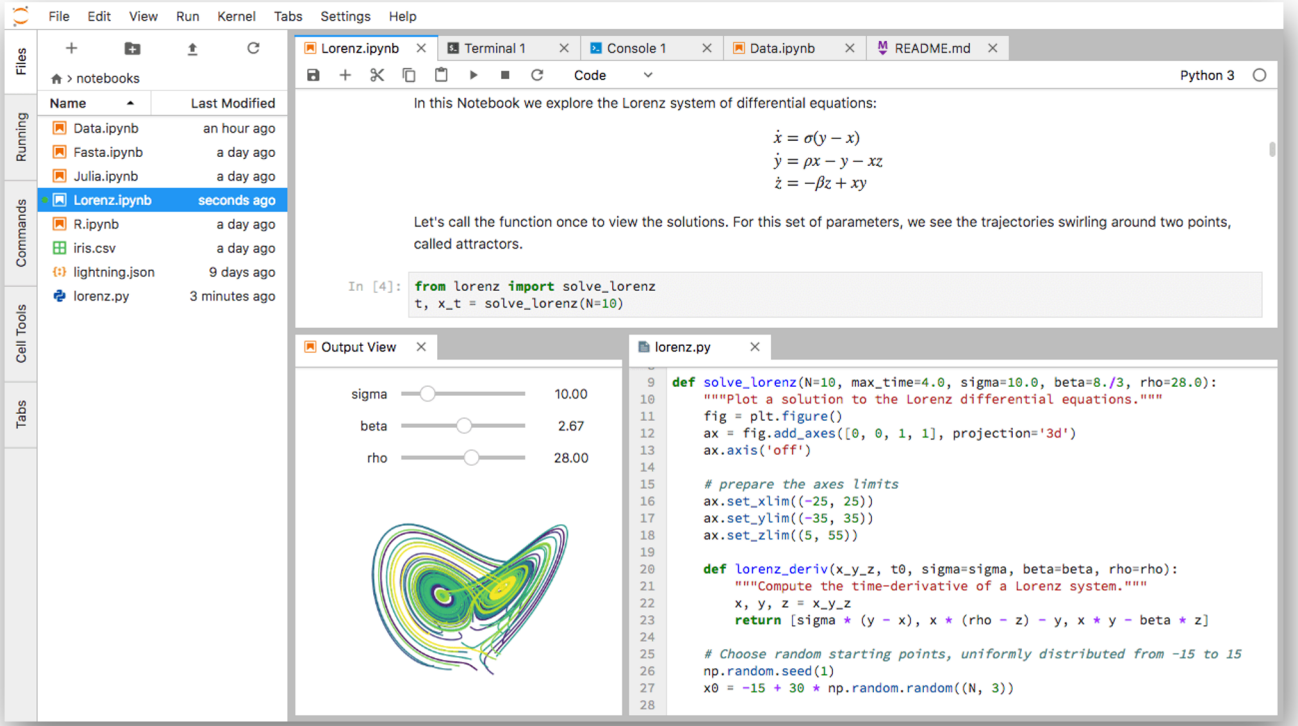
Lab I. JupyterLab

We will load a module with required libraries and run JupyterLab on the HPRC Terra Portal.

Lab II. Data Exploration

We will go through some examples with two popular Python libraries: Pandas and Matplotlib for data exploration.

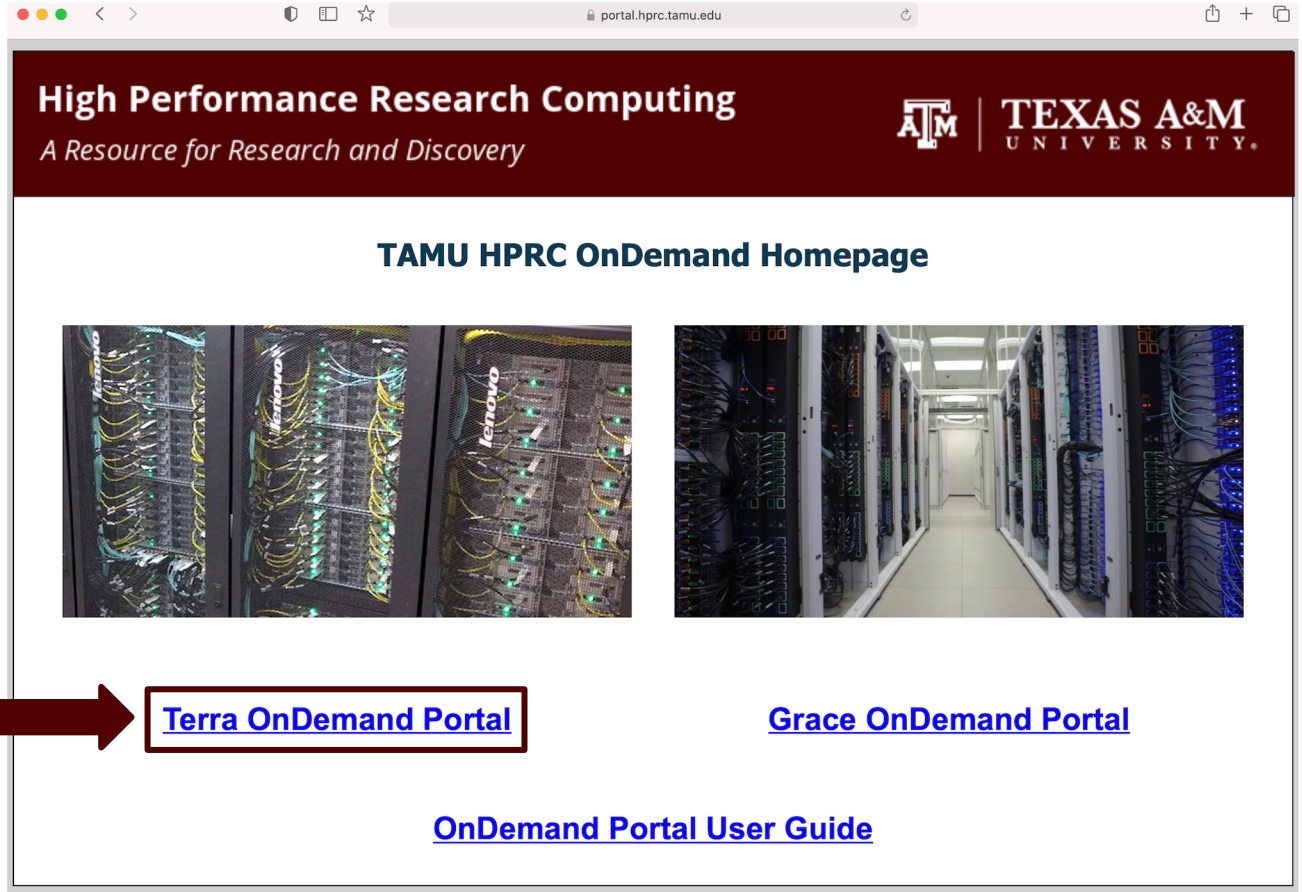
Lab I. JupyterLab



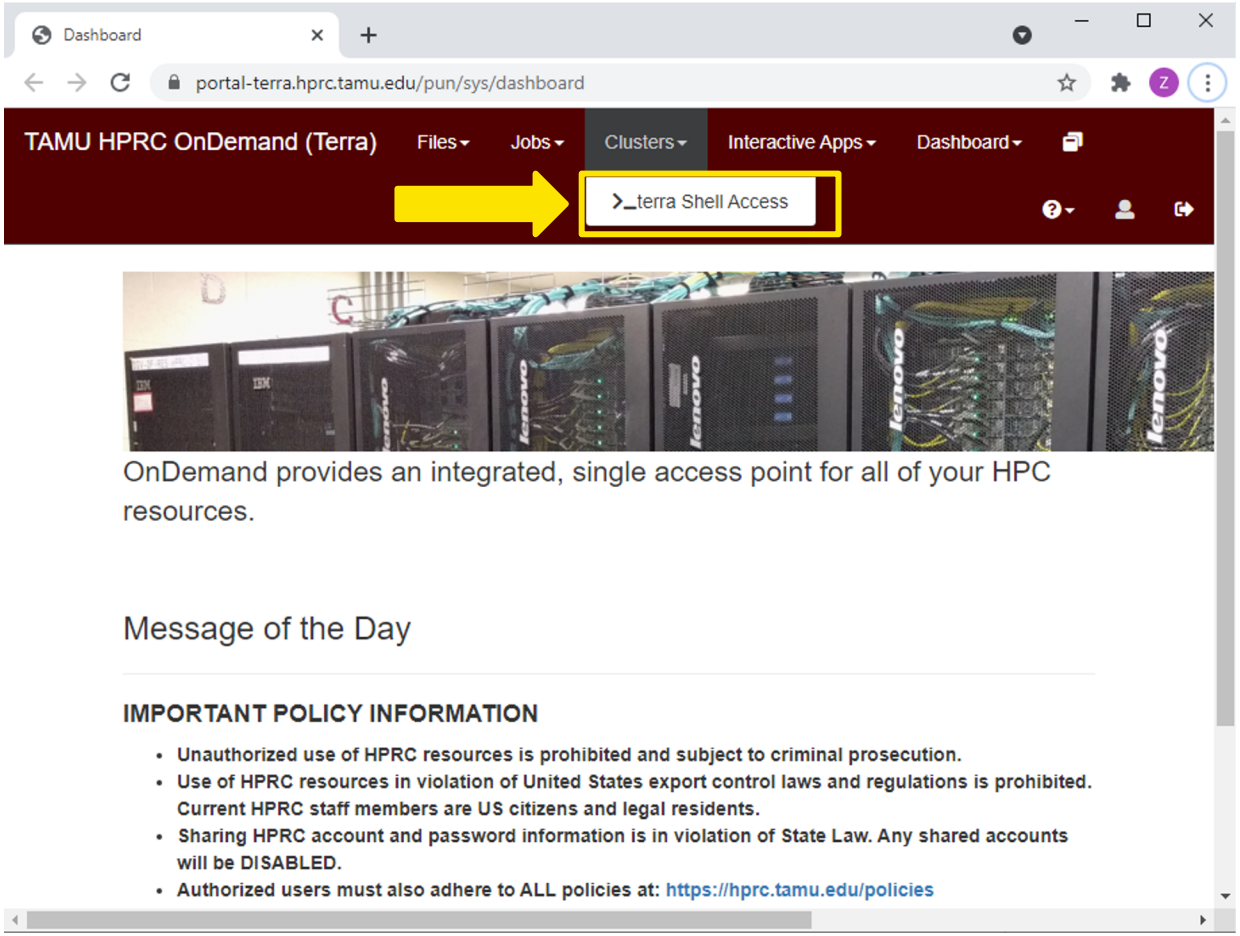
L1 - Resources

- Texas A&M High Performance Research Computing (HPRC)
- Terra Quick Start Guide
- HPRC Portal
- HPRC YouTube Channel
- Jupyter Project
- help@hprc.tamu.edu

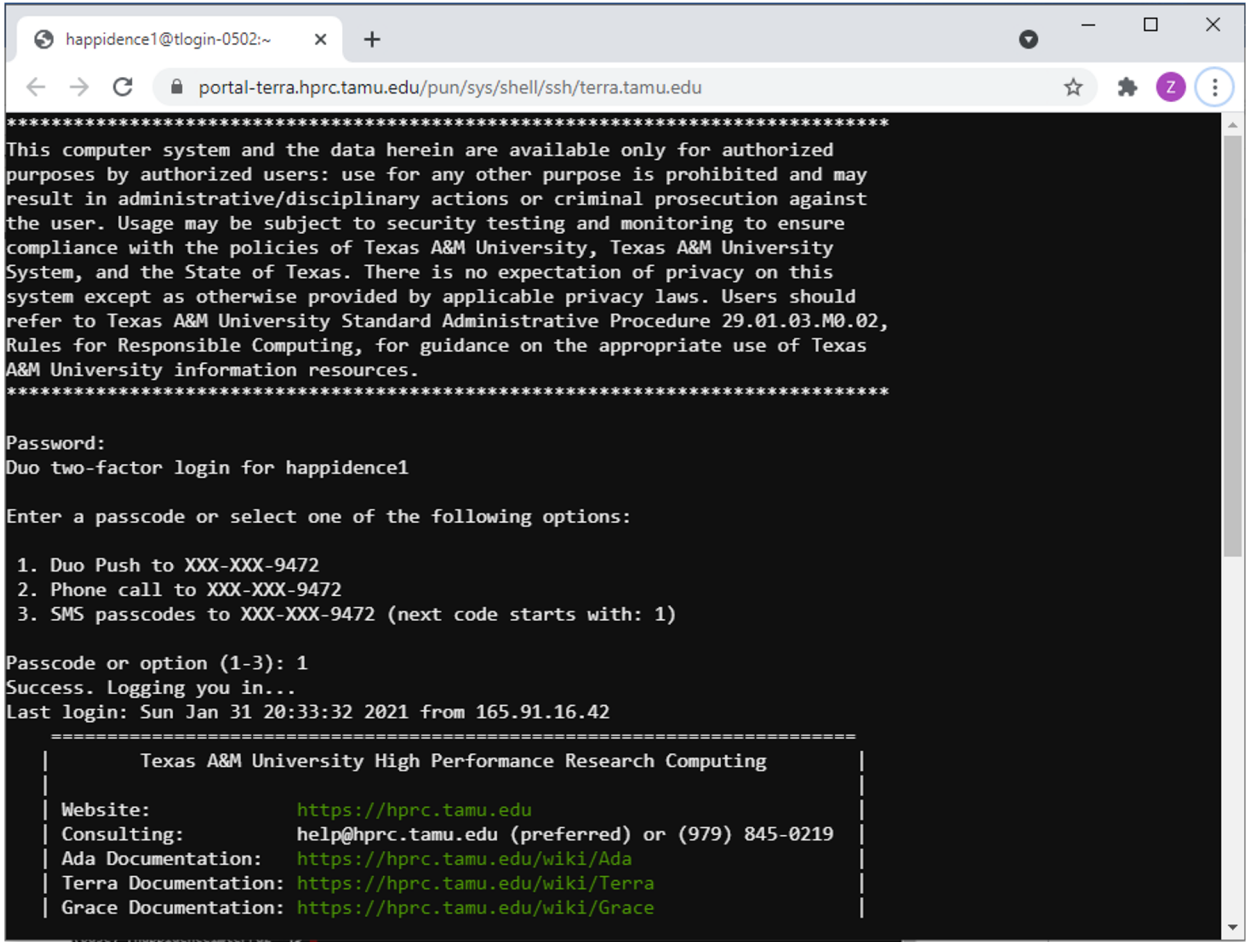
Login HPRC Portal



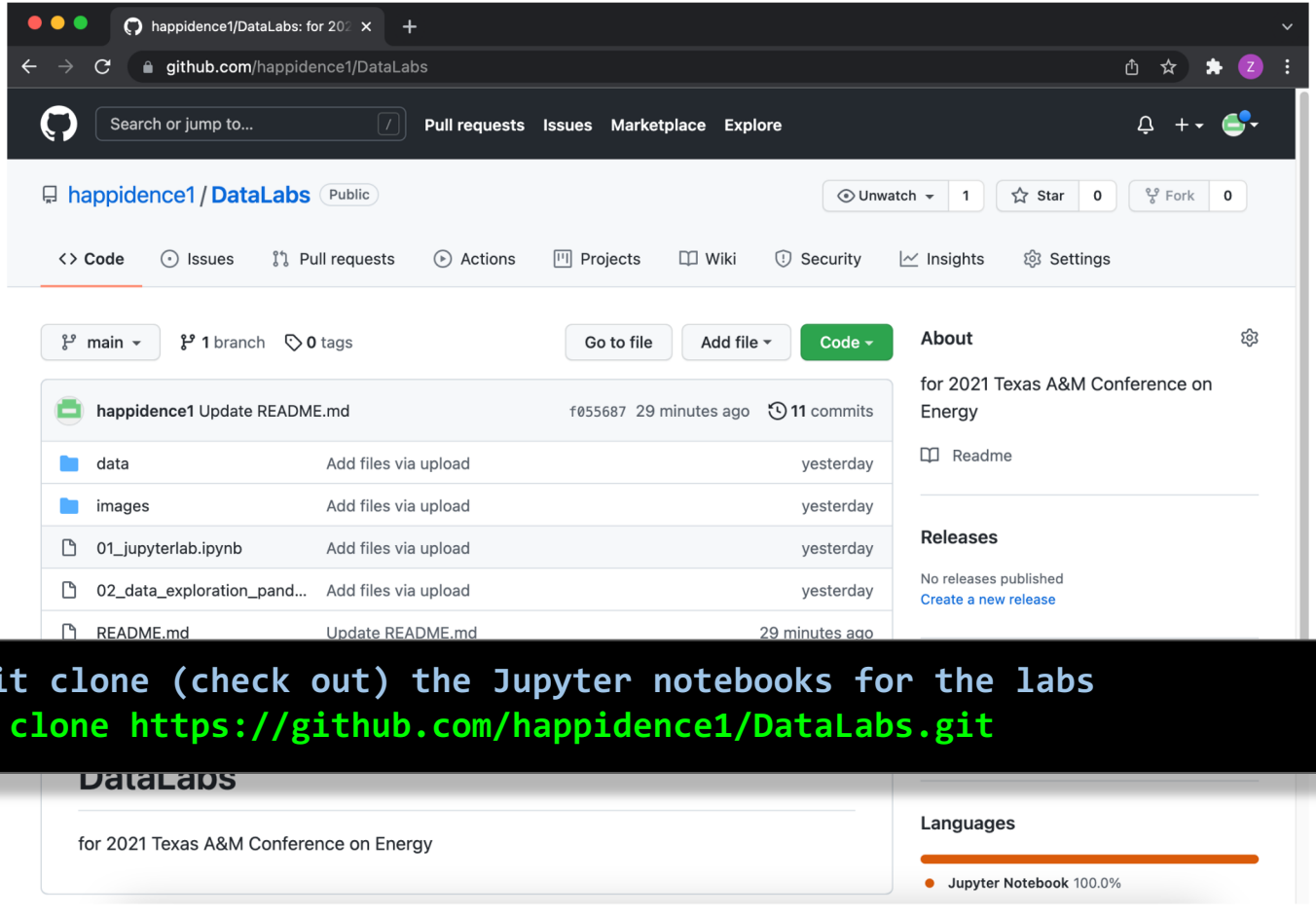
Shell Access - I



Shell Access - II

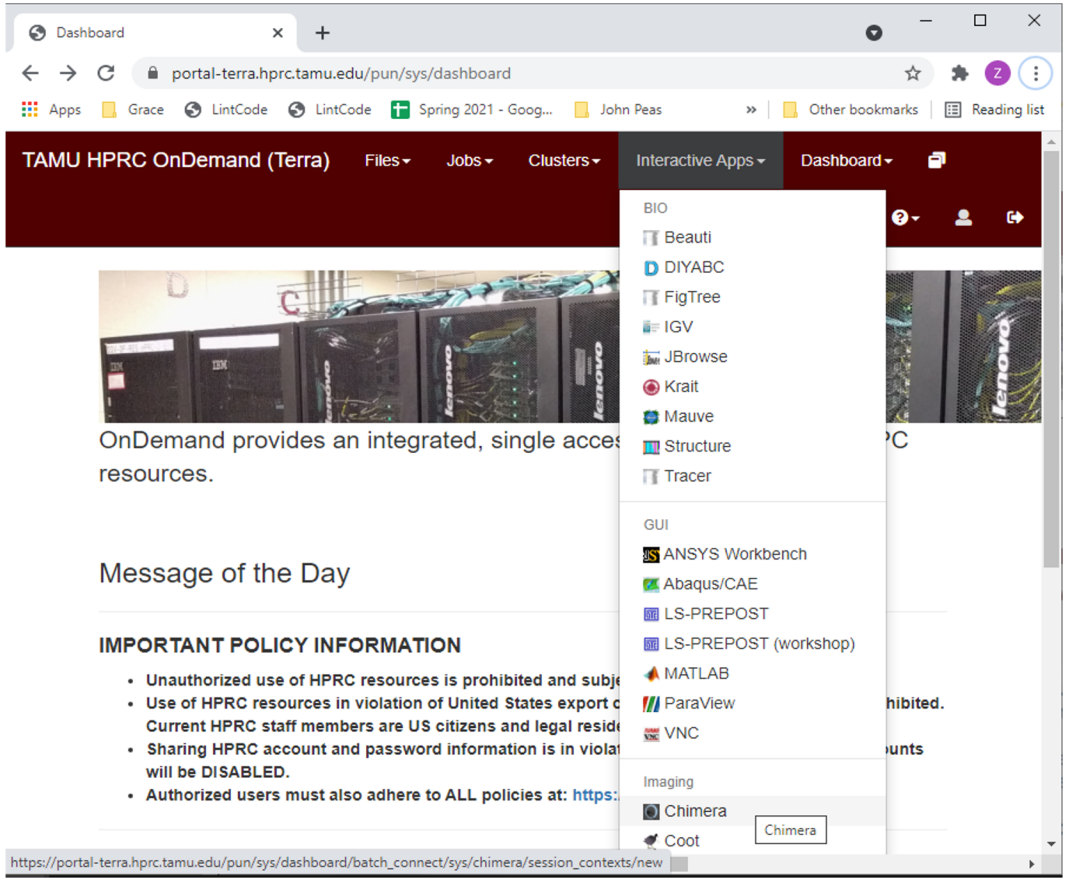


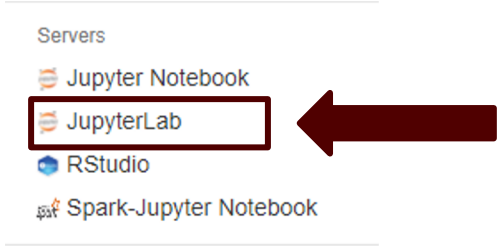
Check out Exercises



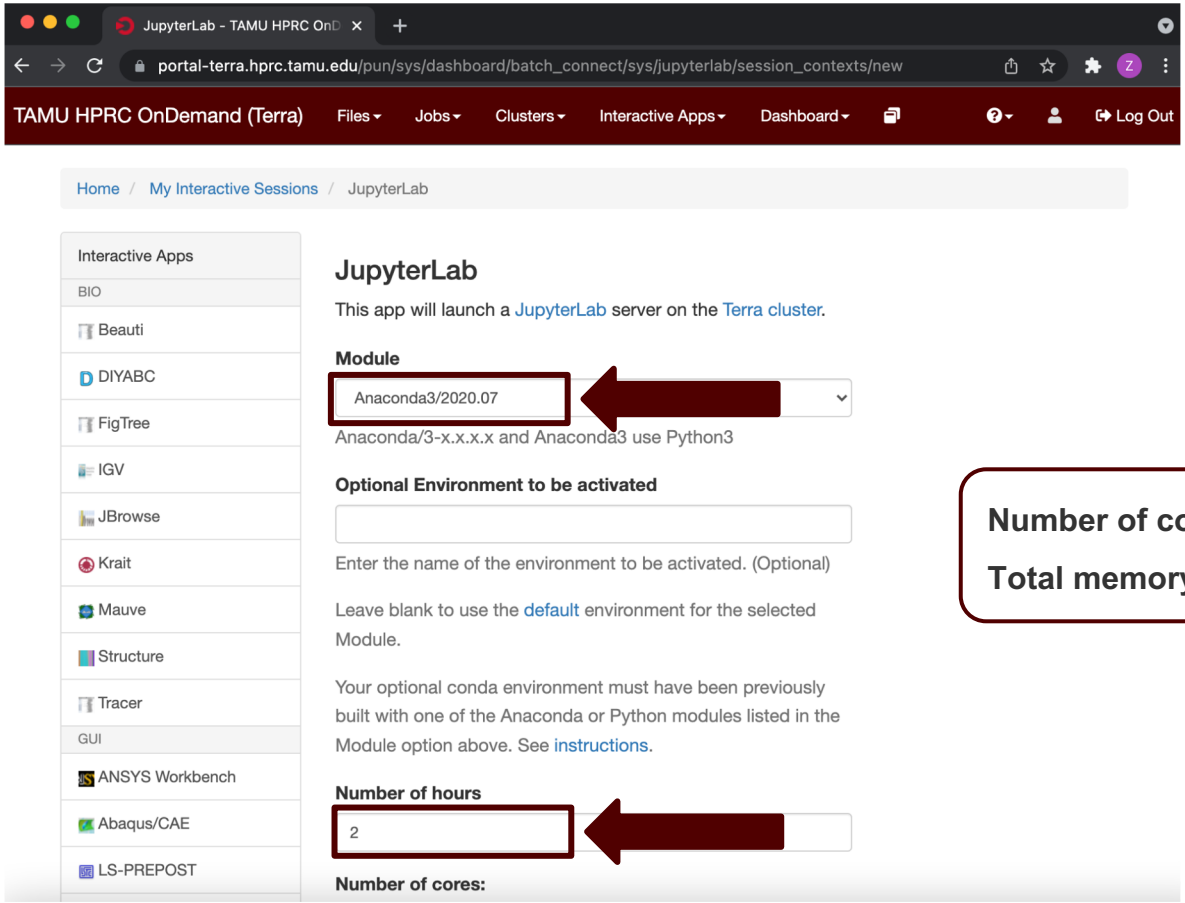

```
# git clone (check out) the Jupyter notebooks for the labs
git clone https://github.com/happidence1/DataLabs.git
```

Go to JupyterLab Page





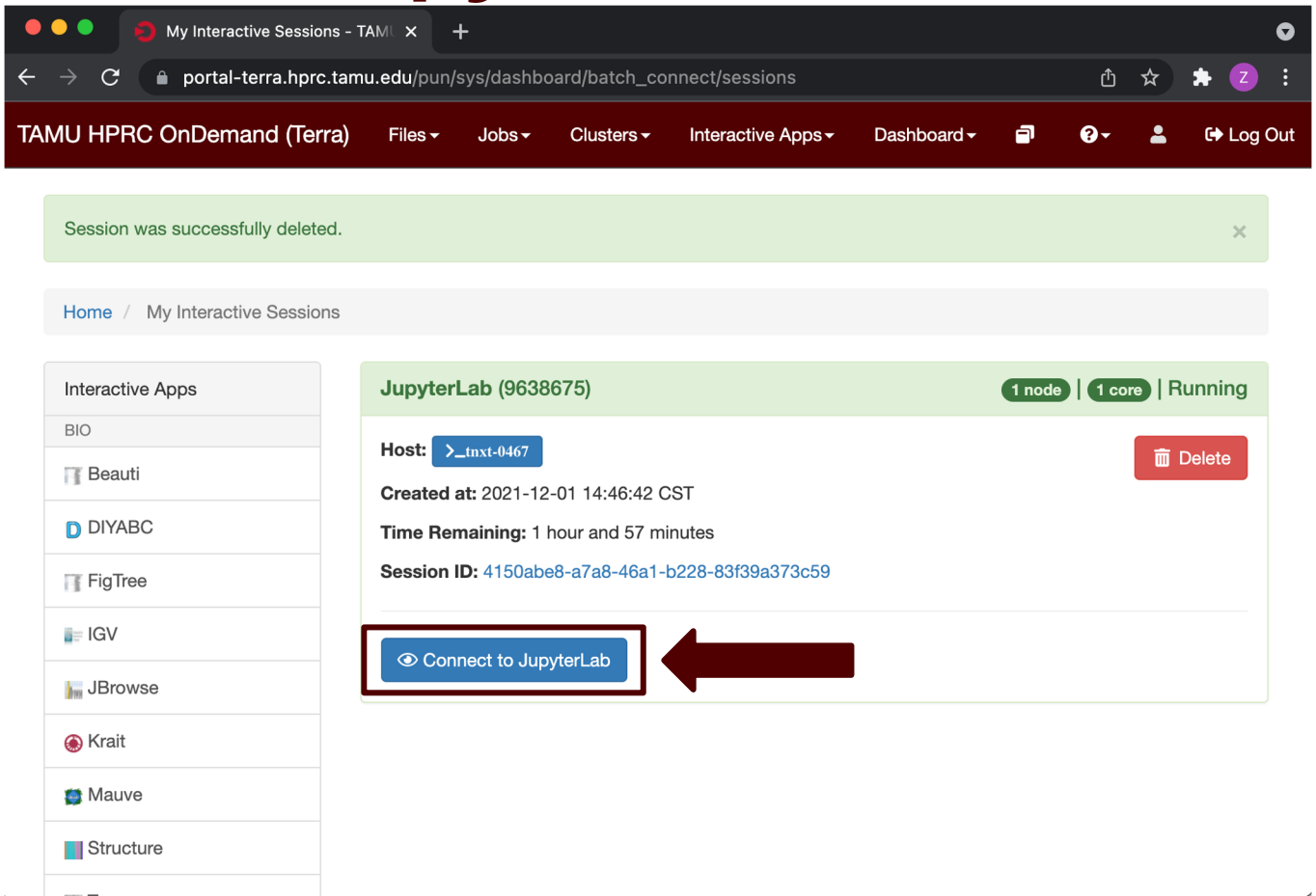
Load module



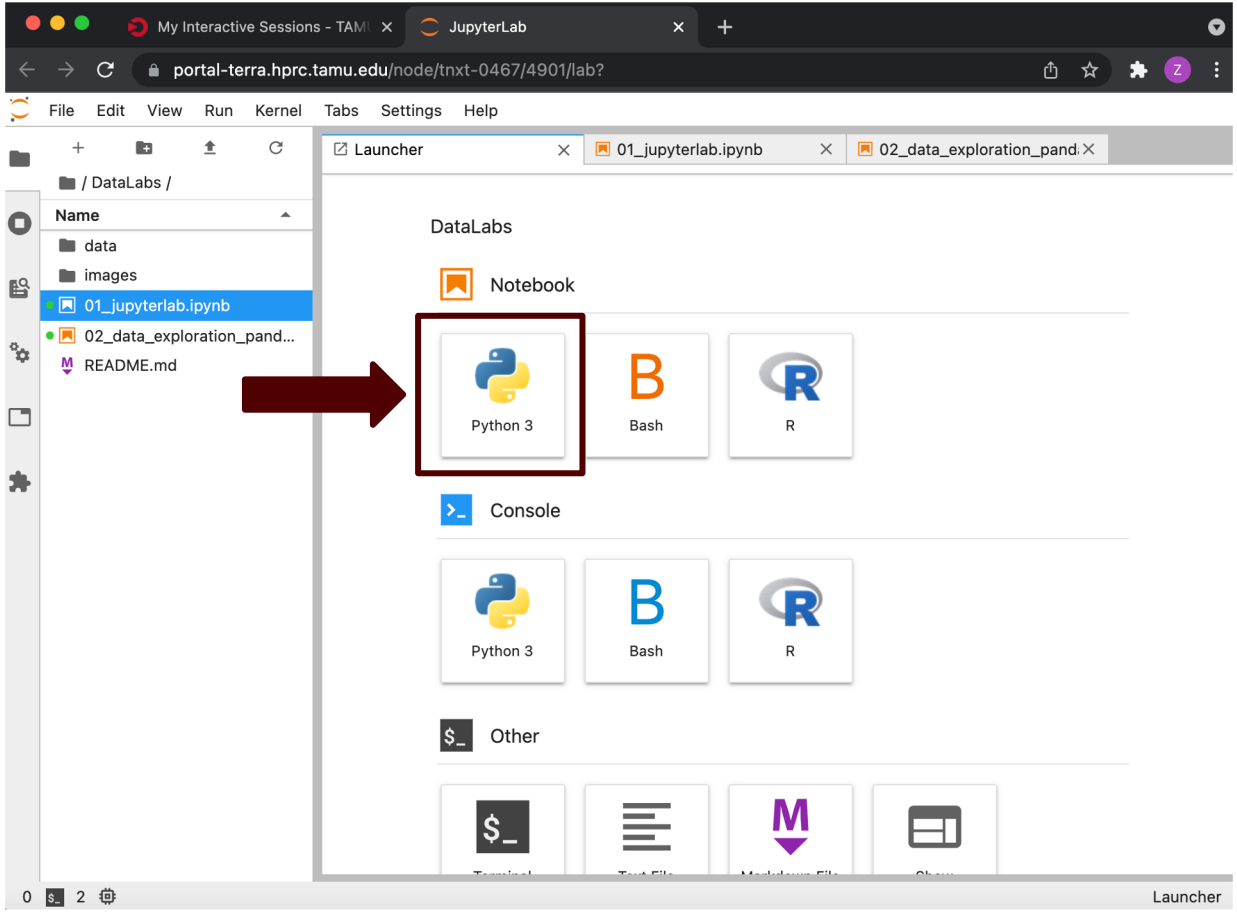
Number of cores: 2

Total memory (GB): 4

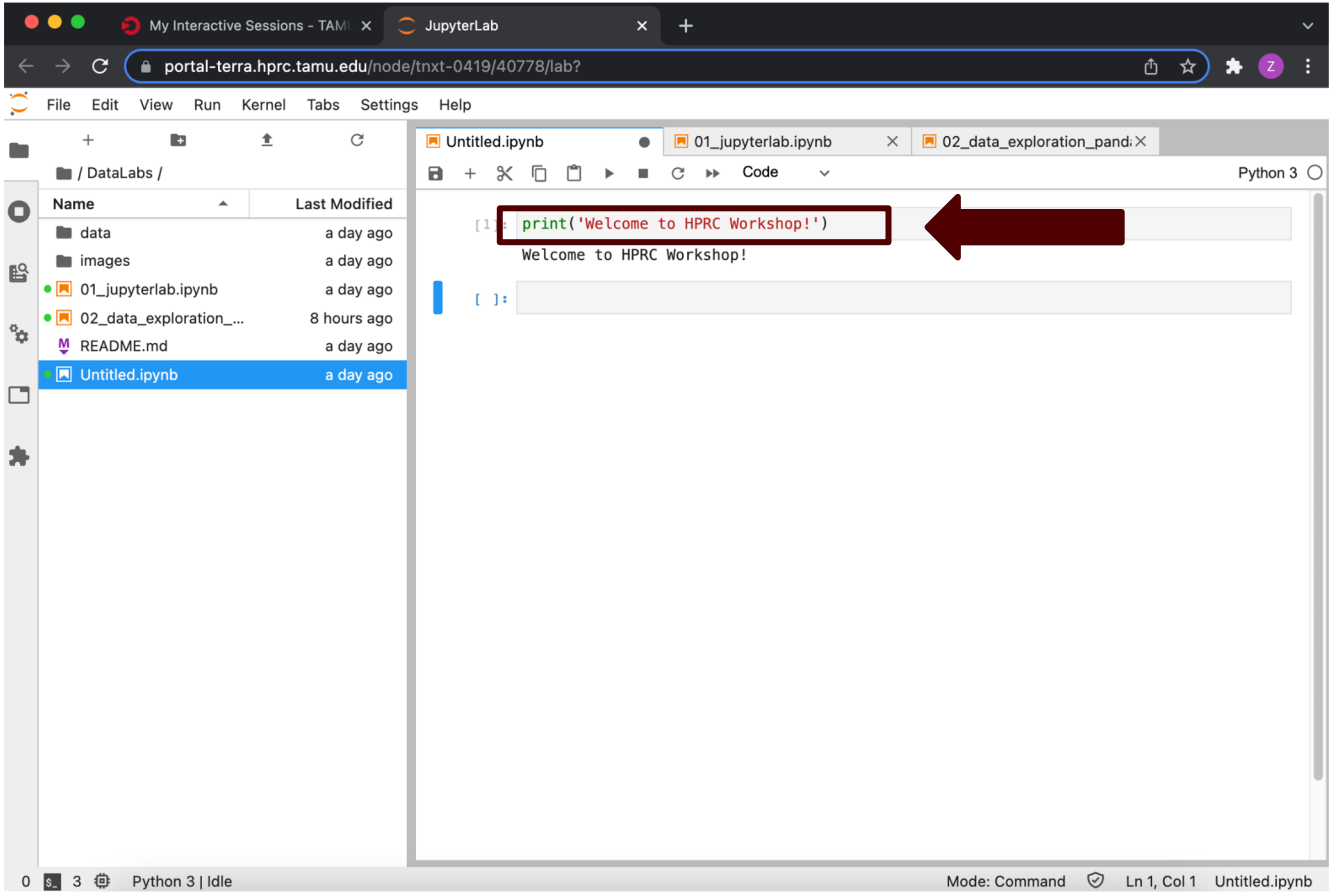
Connect to JupyterLab



Create a Jupyter Notebook



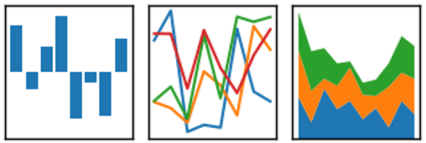
Test JupyterLab



Lab II. Data Exploration

pandas

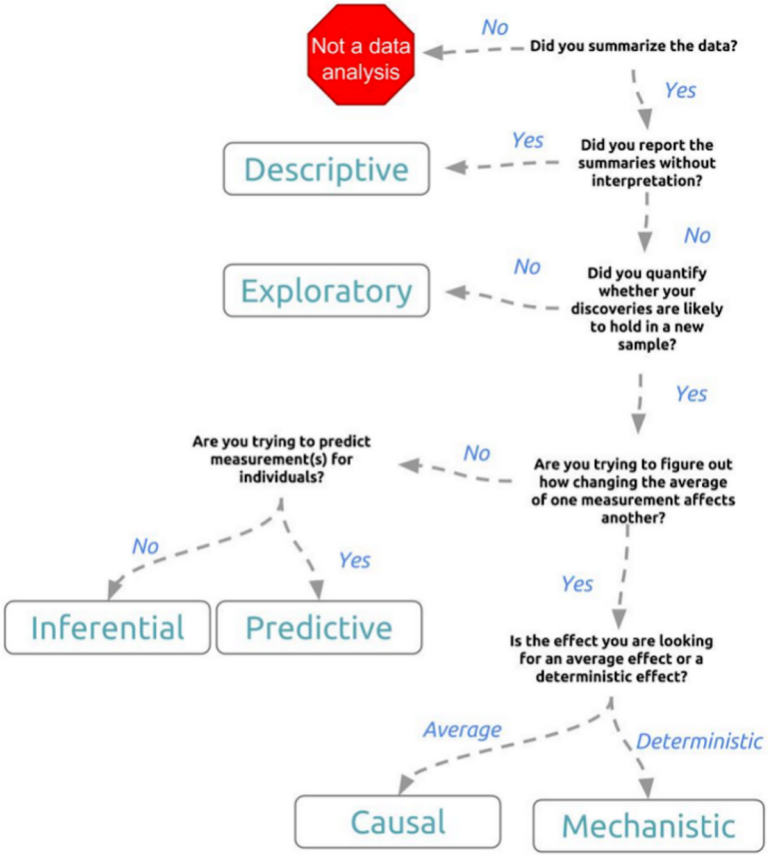
$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$



matplotlib

Types of Data Science Problems

- **Descriptive** (summaries, e.g., census)
- **Exploratory** (search for unknowns, e.g., four-planet solar system)
- **Inferential** (find correlations, e.g., many social studies)
- **Predictive** (make predictions, e.g., Face ID, Echo, Siri)
- **Causal** (explore causation, e.g., smoking versus lung cancer)
- **Mechanistic** (determine governing principles, e.g., experimental science)



Credit: Jeff Leek - The Elements of Data Analytic Style

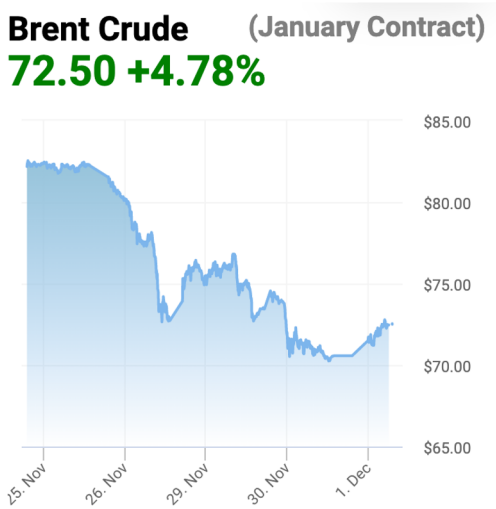
Data Structures

Pandas has two data structures that are descriptive and optimized for data with different dimensions.

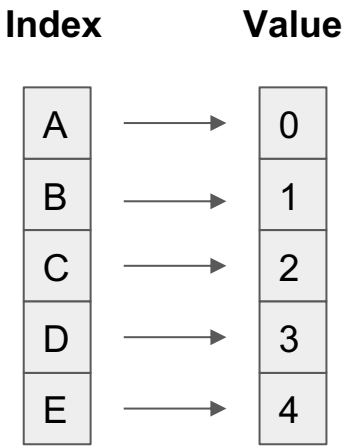
- **Series:** 1D labeled array
- **DataFrame:** General 2D labeled, size-mutable tabular structure with potentially heterogeneously-typed columns

Series in pandas

- One-dimensional labeled array
- Capable of holding any data type (integers, strings, floating point numbers, etc.)
- Example: time-series oil price data



(source: oilprice.com)



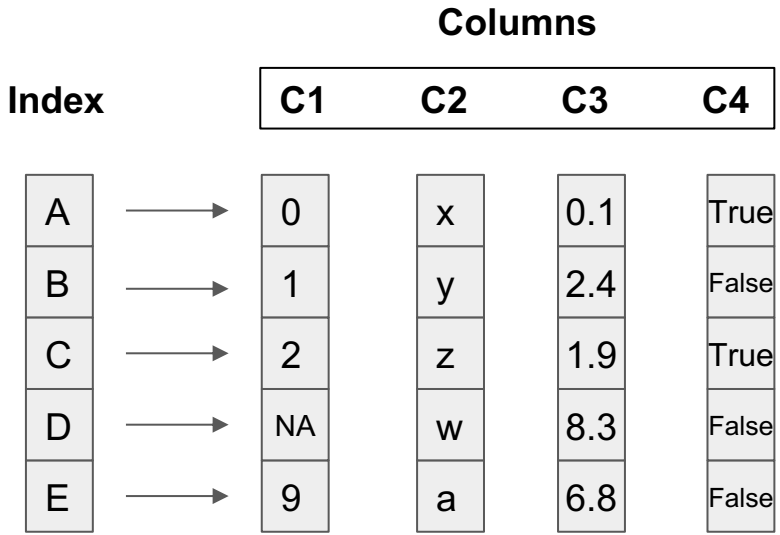
DataFrame in pandas

- Primary Pandas data structure
- A dict-like container for Series objects
- Two-dimensional size-mutable
- Heterogeneous tabular data structure

Top producing oil fields in the United States, 2019* being updated

Rank	Field	State	Discovery Year	Million Bbl/Day
1	Permian	Texas/New Mexico	1920	4.2
2	Eagle Ford Shale	Texas	2008	1.34
3	Bakken	North Dakota/Montana	1951	1.33
4	Prudhoe Bay Oil Field	Alaska	1967	.791
5	Wattenberg Gas Field	Colorado	1970	.473
6	Shenzi	Federal Gulf of Mexico	2002	.353
7	Kuparuk River oil field	Alaska	1969	.295
8	Midway-Sunset Oil Field	California	1901	.288
9	Atlantis Oil Field	Federal Gulf of Mexico	1998	.273
10	Sugarkane	Texas	2009	.258

(source: wikipedia)



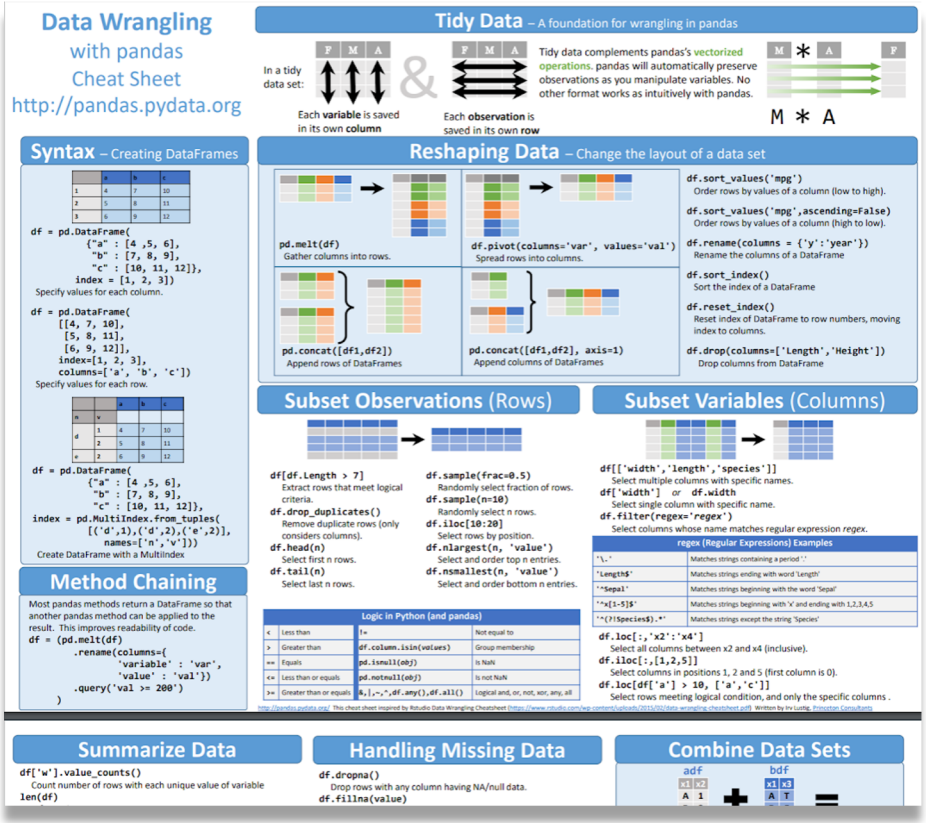
Pandas Learning Objectives

After this lesson, you will know how to:

- Create a DataFrame
- Drop Entries
- Index, Select, and Filter data
- Sort data
- Input and Output

JupyterLab Exercises

Pandas Cheat Sheet



https://pandas.pydata.org/Pandas_Cheat_Sheet.pdf

Key Plotting Concepts in Matplotlib

- **Matplotlib: Figure**

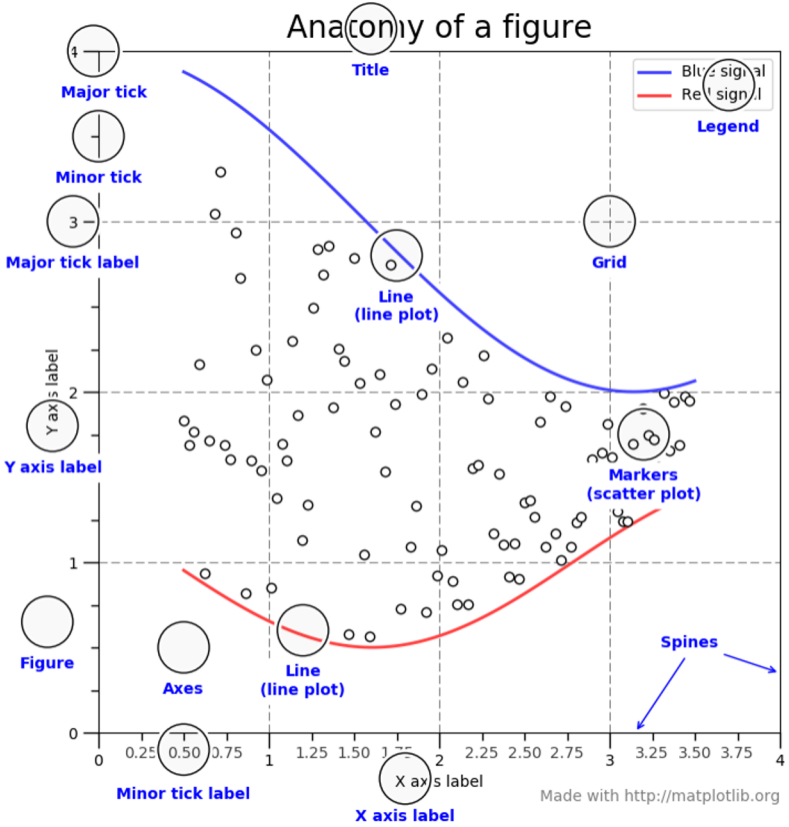
  Figure is the object that keeps the whole image output. Adjustable parameters include:

  1. Image size (set_size_inches())
  2. Whether to use tight_layout (set_tight_layout())

- **Matplotlib: Axes**

  Axes object represents the pair of axis that contain a single plot (x-axis and y-axis). The Axes object also has more adjustable parameters:

  1. The plot frame (set_frame_on() or set_frame_off())
  2. X-axis and Y-axis limits (set_xlim() and set_ylim())
  3. X-axis and Y-axis Labels (set_xlabel() and set_ylabel())
  4. The plot title (set_title())



(Credit: matplotlib.org)

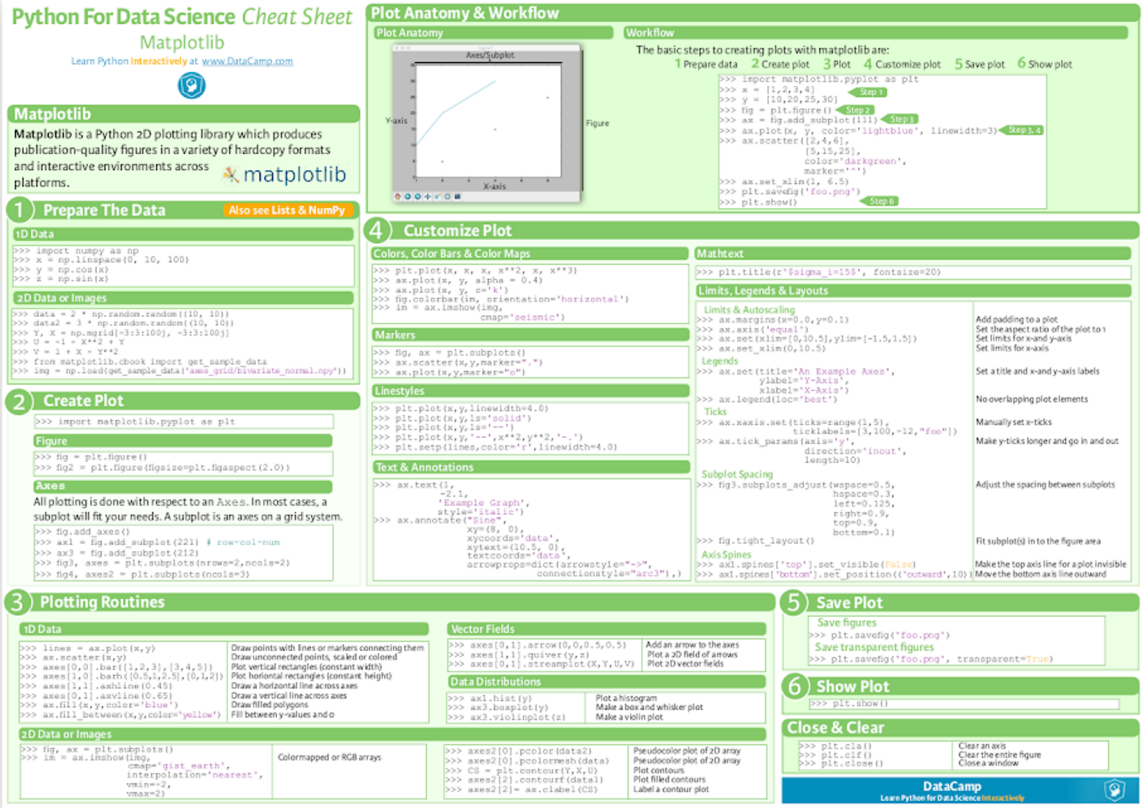
Matplotlib Learning Objectives

After this lesson, you will know how to:

- Scatter plot and Line plot
- Subplots
- Color map
- Contour figures
- 3D figures
  - Surface plots
  - Wire-frame plot
  - Contour plots with projections

JupyterLab Exercises

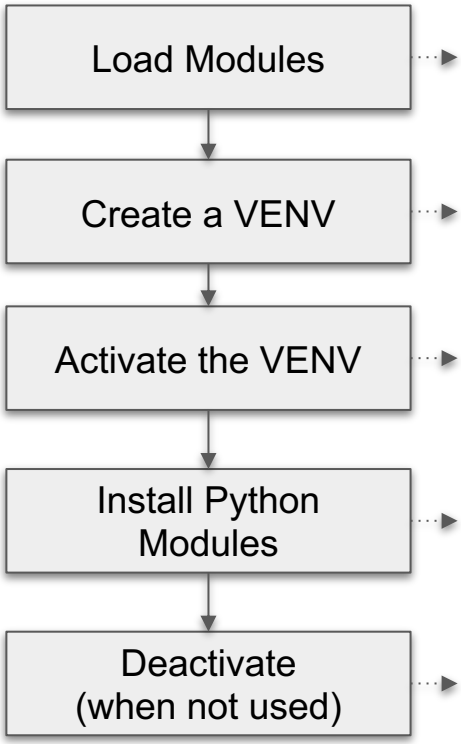
Matplotlib Cheat Sheet



https://s3.amazonaws.com/assets.datacamp.com/blog_assets/Python_Matplotlib_Cheat_Sheet.pdf

Additional Materials

Python Virtual Environment (VENV)




```
# Change to /scratch/user/netid directory
cd $SCRATCH

# clean up and load Anaconda
module purge
module load Anaconda/3-5.0.0.1

# create a Python virtual environment
conda create -n mylab

# activate the virtual environment
source activate mylab

# install required package to be used in the portal
conda install -c conda-forge jupyterlab=1.2.2
conda install pandas matplotlib
conda install scikit-learn
conda install tensorflow

# deactivate the virtual environment
# source deactivate
```

Common Anaconda Commands

```
# Conda virtual environment
conda info                          # show Conda installation
conda create -n VENV                # create a virtual environment
conda create -n VENV python=3.4 # create a venv with a py version
conda env list                      # list installed venv

# Conda package management
conda list                          # list all installed packages
conda search  PACKAGENAME           # search a Conda package
conda install PACKAGENAME           # install a Conda package
conda update  PACKAGENAME           # update a Conda package
conda remove  PACKAGENAME           # remove a Conda package
```