

# Python for Data Scientists on **ACES**

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High Performance  
Research Computing  
DIVISION OF RESEARCH



# Outline

- Overview of Python for Data Science
- Getting Started
- Arrays and Series
- Plots

# Overview of Python for Data Science

# Arrays

Numpy Arrays support common operations, such as arithmetic, on an element-by-element (or “vectorized”) basis.

Example:

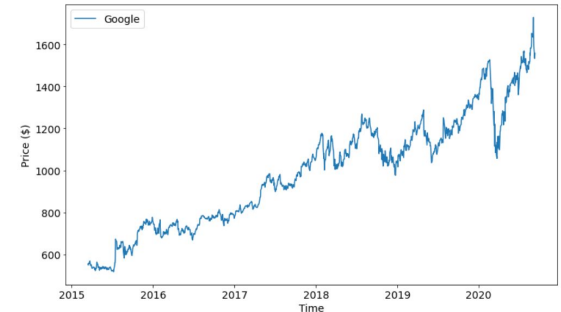
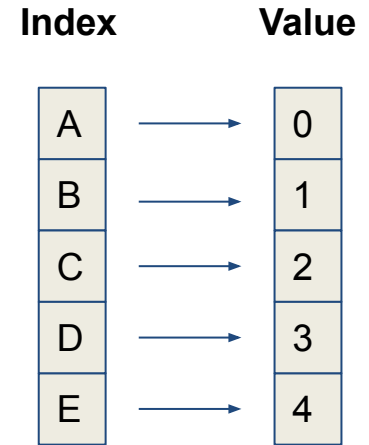
```
array C = array A + array B
```

This adds the elements of A and B pair-wise (Instead of concatenating the elements as would happen with lists).

Pandas Series and DataFrames further expand on this.

# Series

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



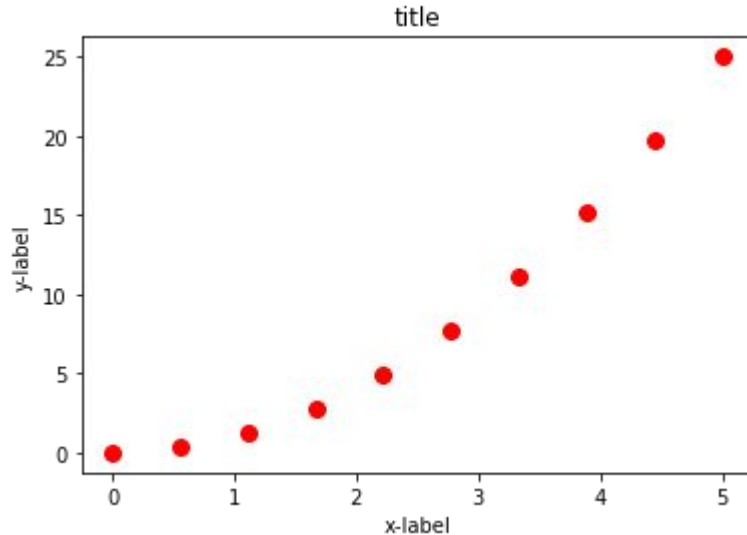
# Anatomy of a Plot

## Marker

- style
- size
- color

## Figure

- title
- xlabel
- ylabel



# Learning Resources

- Slides on the course web page  
[https://hprc.tamu.edu/training/aces\\_python4data.html](https://hprc.tamu.edu/training/aces_python4data.html)
- HPRC's Knowledge Base  
<https://hprc.tamu.edu/kb/Software/Python/>
- HPRC on YouTube  
<https://www.youtube.com/c/TexasAMHPRC>
- ACCESS Links  
<https://support.access-ci.org/ci-links>

# Getting Started

# ACES Portal

TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING

Home User Services Resources Research Policies Events Training About **Portal**

Quick Links

- New User Information
- Accounts
  - Apply for Accounts
  - Manage Accounts

Terra Portal

Grace Portal

FASTER Portal

FASTER Portal (ACCESS)

**ACES Portal (ACCESS)**

ACES Portal [portal-aces.hprc.tamu.edu](http://portal-aces.hprc.tamu.edu)  
is the web-based user interface for the ACES cluster

Open OnDemand (OOD) is an advanced web-based  
graphical interface framework for HPC users

ACES OnDemand Portal

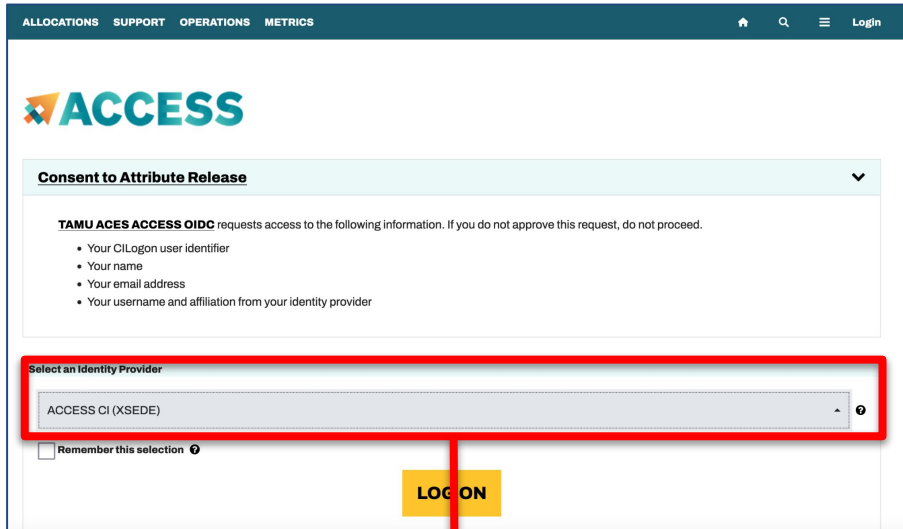
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OnDemand provides an integrated, single access point for all of your HPC resources.

powered by  
**OPEN OnDemand**

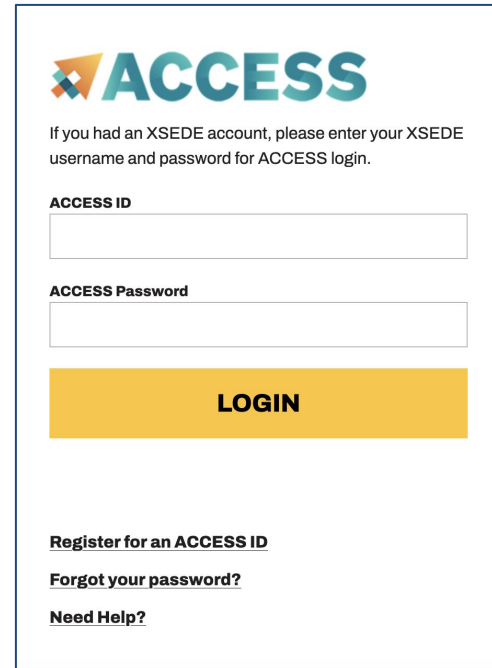
OnDemand version: 3.0.0

# Accessing ACES via the Portal (ACCESS)



The screenshot shows the ACCESS portal interface. At the top, there is a navigation bar with links for ALLOCATIONS, SUPPORT, OPERATIONS, METRICS, and a Login button. Below the navigation bar is the ACCESS logo. A section titled "Consent to Attribute Release" contains a message from TAMU ACES ACCESS OIDC requesting access to user information. Below this is a "Select an Identity Provider" dropdown menu with "ACCESS CI (XSEDE)" selected. A red box highlights the dropdown menu and the "LOG ON" button below it.

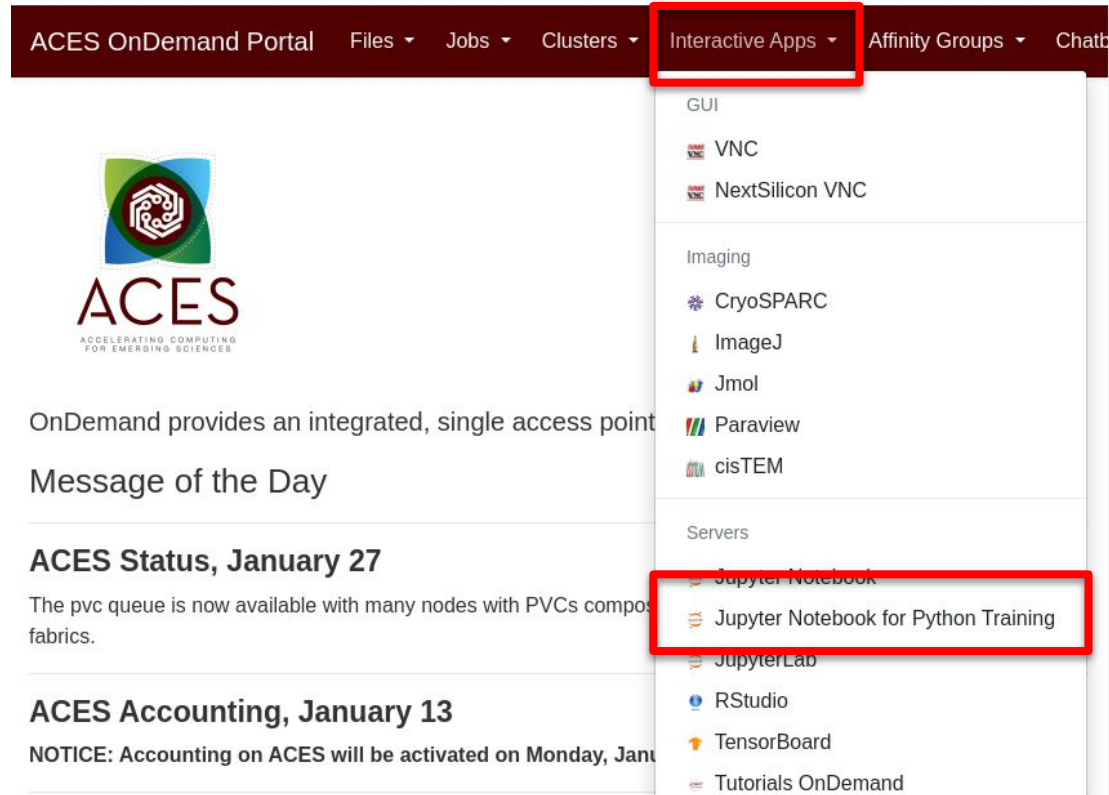
Select the Identity Provider appropriate for your account.



The screenshot shows the ACCESS portal login form. At the top, there is the ACCESS logo. Below the logo is a message: "If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login." The form contains two input fields: "ACCESS ID" and "ACCESS Password". Below the input fields is a yellow "LOGIN" button. At the bottom of the form, there are links for "Register for an ACCESS ID", "Forgot your password?", and "Need Help?".

Log-in using your ACCESS or institutional credentials.

# Jupyter Notebook for Python Training



The screenshot displays the ACES OnDemand Portal interface. At the top, a dark red navigation bar contains the following items: "ACES OnDemand Portal", "Files", "Jobs", "Clusters", "Interactive Apps", "Affinity Groups", and "Chatt". The "Interactive Apps" menu is open, showing a list of applications. The "Jupyter Notebook for Python Training" option is highlighted with a red box. Below the navigation bar, the main content area features the ACES logo (Accelerating Computing for Emerging Sciences) and several news items, including "OnDemand provides an integrated, single access point", "Message of the Day", "ACES Status, January 27", and "ACES Accounting, January 13".

ACES OnDemand Portal Files Jobs Clusters **Interactive Apps** Affinity Groups Chatt

GUI

- VNC
- NextSilicon VNC

Imaging

- CryoSPARC
- ImageJ
- Jmol
- Paraview
- cisTEM

Servers

- Jupyter Notebook
- Jupyter Notebook for Python Training**
- JupyterLab
- RStudio
- TensorBoard
- Tutorials OnDemand

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OnDemand provides an integrated, single access point

Message of the Day

**ACES Status, January 27**  
The pvc queue is now available with many nodes with PVCs composed of fabrics.

**ACES Accounting, January 13**  
NOTICE: Accounting on ACES will be activated on Monday, Jan

# Jupyter Notebook for Python Training

## Jupyter Notebook for Python Training

This app will launch a Jupyter Notebook server on the [ACES cluster](#).

Email

This field is optional.

Launch

\* The Jupyter Notebook for Python Training session data for this session can be accessed under the [data root directory](#).

Jupyter Notebook for Python Training (636884)

1 node | 1 core | Starting

Created

Time

Session

Your session

take a

Jupyter Notebook for Python Training (636884)

1 node | 1 core | Running

Host: >\_ac058

Delete

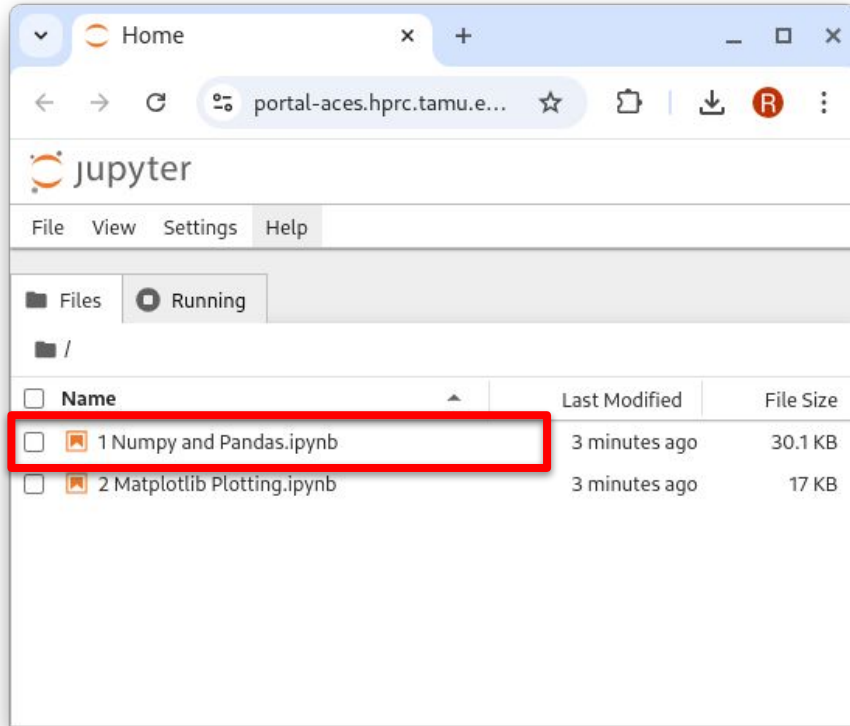
Created at: 2025-01-28 09:19:34 CST

Time Remaining: 7 hours and 9 minutes

Session ID: 428342db-6782-4d59-8bf8-2537d8ee857d

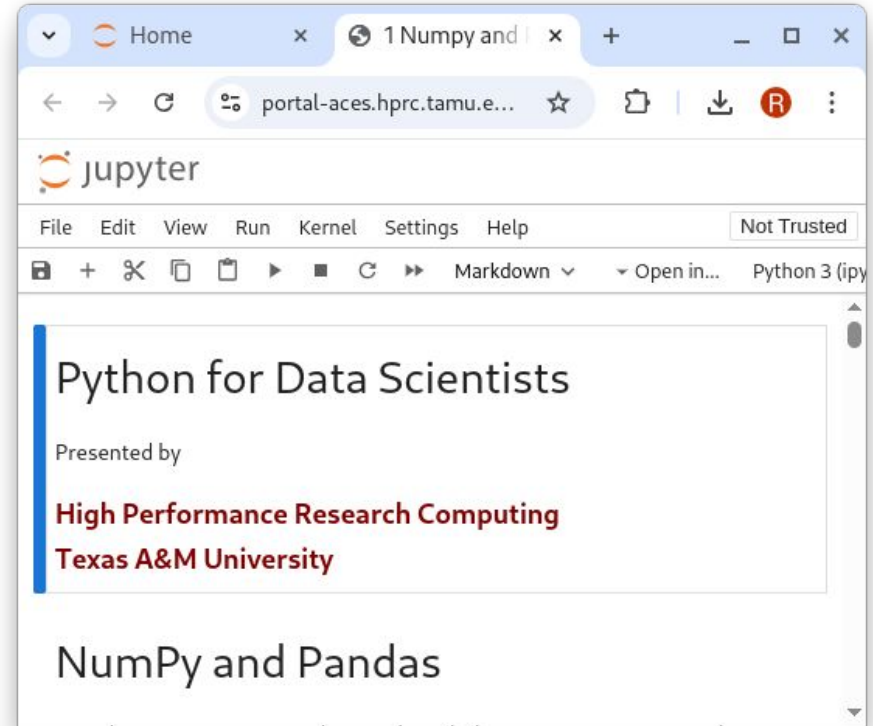
Connect to Jupyter

# Jupyter Notebook for Python Training



A screenshot of the JupyterLab interface showing the file browser. The browser displays a list of files in the current directory. The file "1 Numpy and Pandas.ipynb" is highlighted with a red box. The table below shows the details of the files:

Name	Last Modified	File Size
1 Numpy and Pandas.ipynb	3 minutes ago	30.1 KB
2 Matplotlib Plotting.ipynb	3 minutes ago	17 KB



A screenshot of a Jupyter Notebook titled "Python for Data Scientists". The notebook content includes the following text:

Python for Data Scientists

Presented by

**High Performance Research Computing**  
**Texas A&M University**

NumPy and Pandas



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<https://hprc.tamu.edu>

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

*Take our short course survey!*



[https://u.tamu.edu/hprc\\_shortcourse\\_survey](https://u.tamu.edu/hprc_shortcourse_survey)

HPRC Survey

[https://u.tamu.edu/hprc\\_shortcourse\\_survey](https://u.tamu.edu/hprc_shortcourse_survey)

Help us help you. Please include details in your request for support, such as, Cluster (ACES, FASTER, Grace, Launch), NetID (UserID), Job information (JobID(s), Location of your jobfile, input/output files, Application, Module(s) loaded, Error messages, etc), and Steps you have taken, so we can reproduce the problem.



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# Break

0:00 pm CST - 0:00 pm CST