

# Tutorial: Python for New Programmers on ACES

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High Performance  
Research Computing  
DIVISION OF RESEARCH



# Outline: HPRC Python Classes

- Python for New Programmers
- Python for Programmers New to Python
- Python for Data Scientists
- Python for HPC



You are here

Today: programming basics recognizable in almost every language

# Outline: Today's Class

- Overview of Python
- Getting Started
- Jupyter Notebooks:
  - Jupyter and Hello
  - Elements of Code
  - Control

# Overview of Python

# What Computers Don't

- Comp
- Comp  
you sa

what



Disney's *Fantasia* (1940)

# Where to get Python

- Windows, Mac, and Linux all have it in their app stores (for free)
- Python is also **online** for free in various places
  - <https://colab.research.google.com/>
  - <https://replit.com/>

*Note:* stay away from Python 2 because Python 3 is much better.

Today we will be using Python 3.11

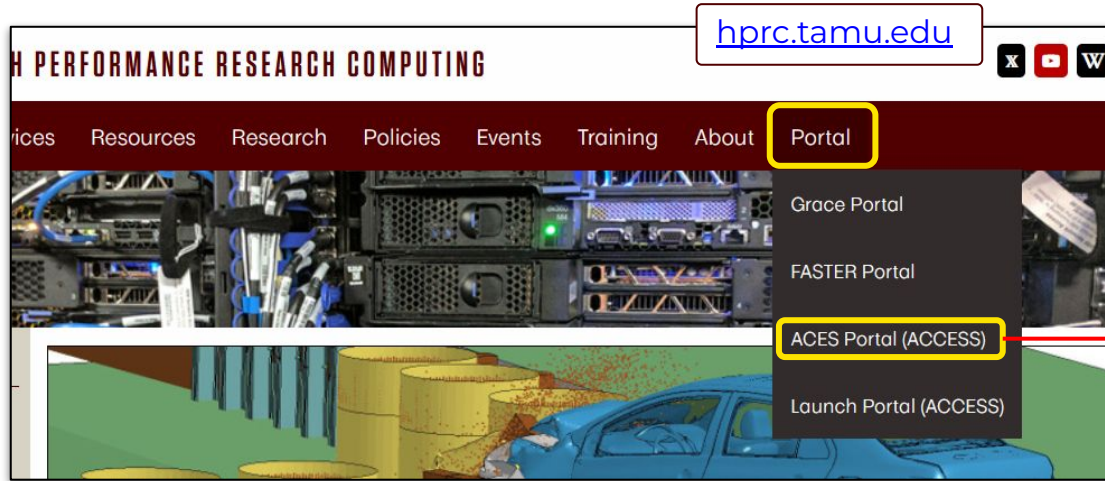
# Learning Resources

- Slides on the course web page  
[https://hprc.tamu.edu/training/aces\\_intro\\_python.html](https://hprc.tamu.edu/training/aces_intro_python.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



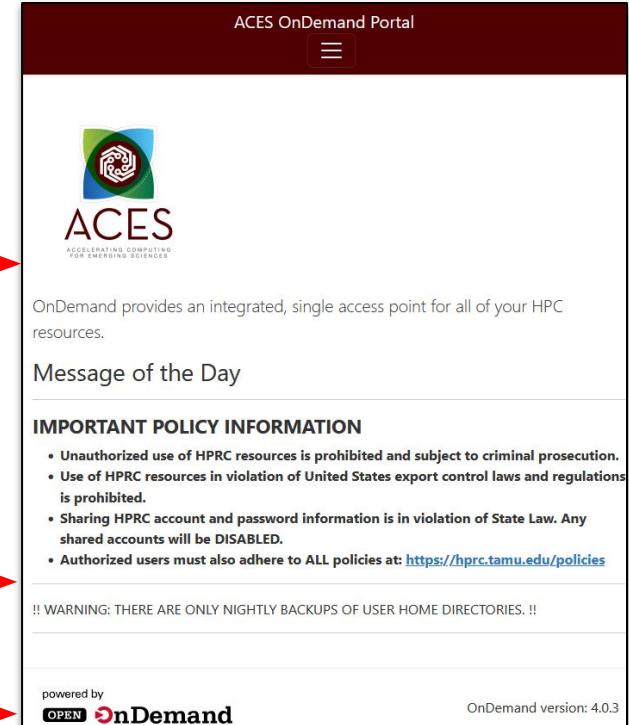
# Login to ACES Portal



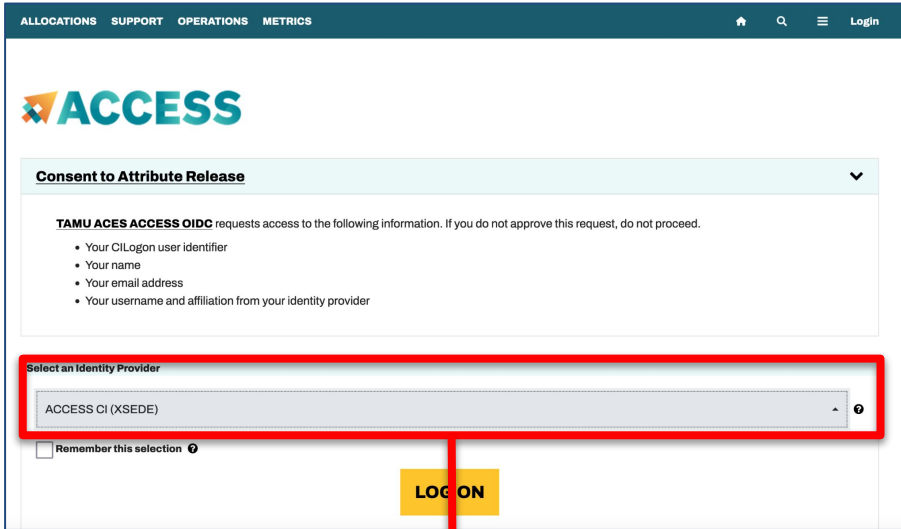
(You will have to log in with ACCESS if you haven't already)

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

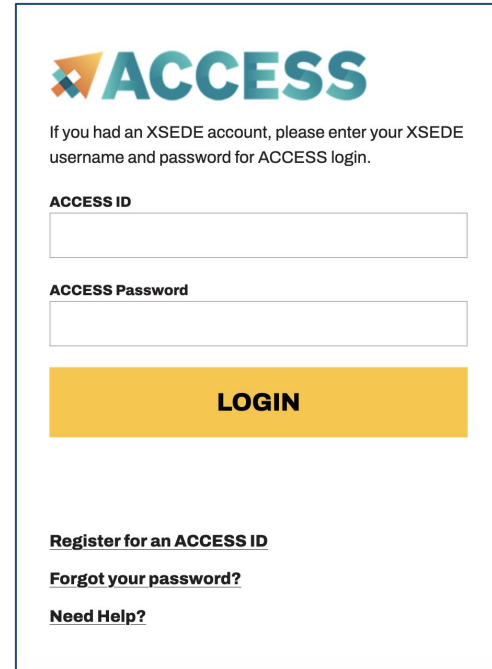


# Accessing ACES via the Portal (ACCESS)



The screenshot shows the ACCESS portal interface. At the top is a navigation bar with links: ALLOCATIONS, SUPPORT, OPERATIONS, METRICS, and a Login link. Below the navigation bar is the ACCESS logo. A section titled "Consent to Attribute Release" is expanded, showing a list of attributes that TAMU ACES ACCESS OIDC requests access to: Your CILogon user identifier, Your name, Your email address, and Your username and affiliation from your identity provider. Below this is a "Select an Identity Provider" dropdown menu with "ACCESS CI (XSEDE)" selected. A red box highlights this dropdown menu. Below the dropdown is a checkbox labeled "Remember this selection". A yellow "LOG ON" button is positioned below the dropdown menu.

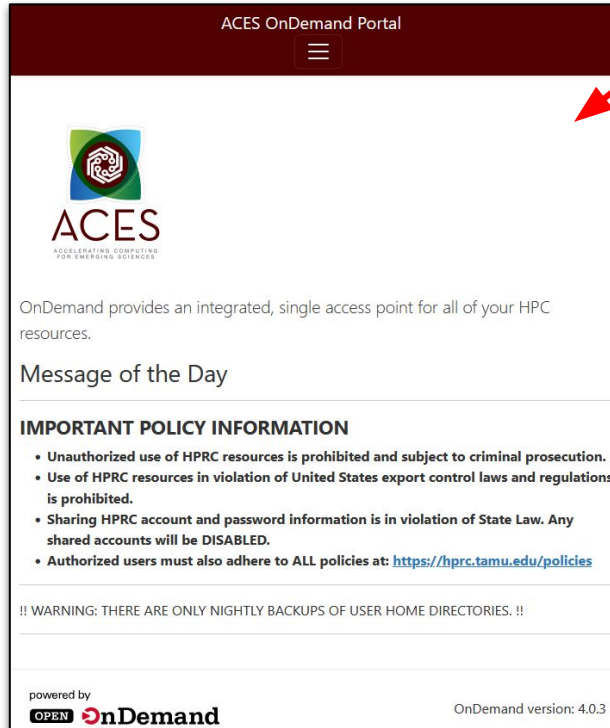
Select the Identity Provider appropriate for your account.



The screenshot shows the ACCESS portal login page. At the top 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." Below this message are two input fields: "ACCESS ID" and "ACCESS Password". Below the input fields is a yellow "LOGIN" button. At the bottom of the page are three links: "Register for an ACCESS ID", "Forgot your password?", and "Need Help?".

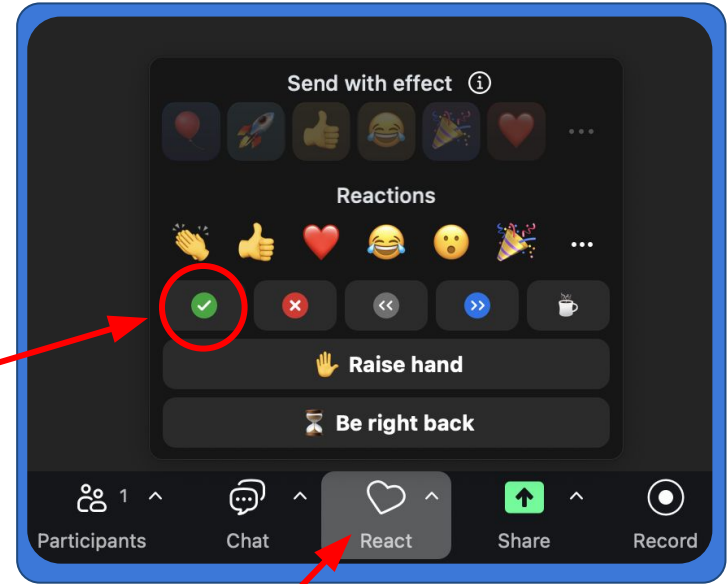
Log-in using your ACCESS or institutional credentials.

# Login to ACES Portal



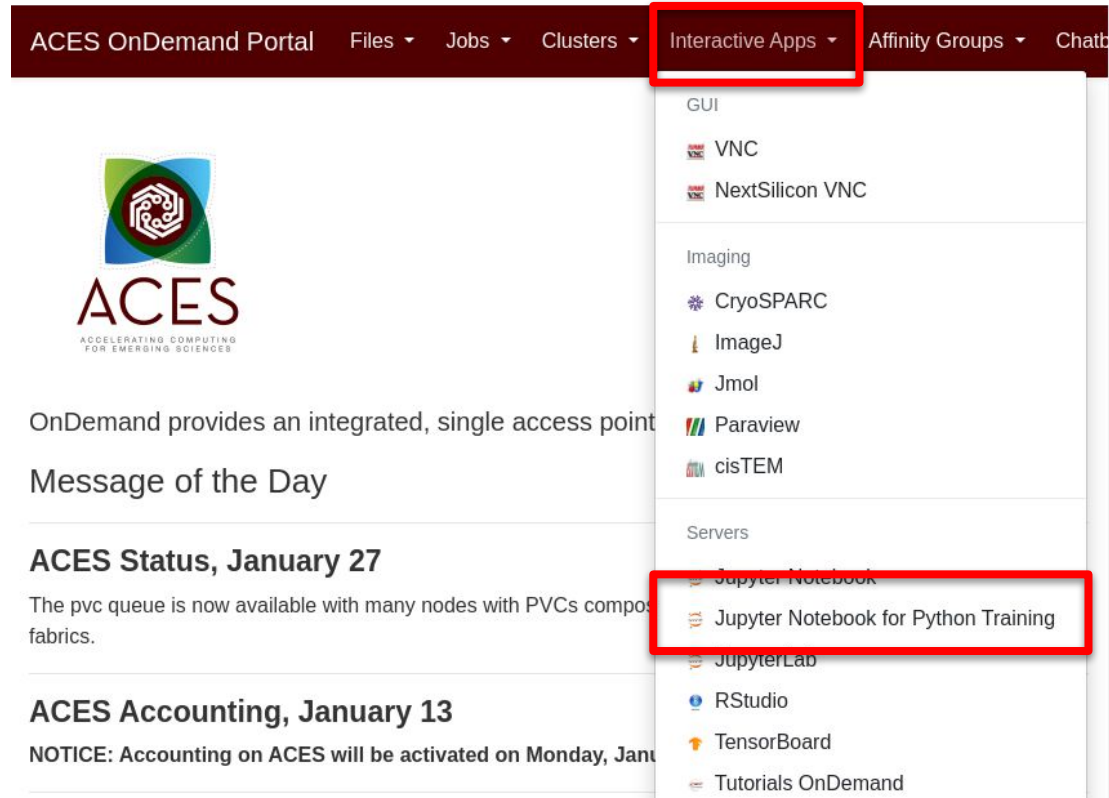
Once you're on this screen...

...Click the  
green  
checkmark  
reaction in  
Zoom



(find it here)

# Jupyter Notebook for Python Training



The screenshot shows the ACES OnDemand Portal interface. The top navigation bar is dark blue with white text for 'ACES OnDemand Portal', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'Affinity Groups', and 'Chat'. The 'Interactive Apps' menu is open, displaying a list of applications categorized by function: GUI (VNC, NextSilicon VNC), Imaging (CryoSPARC, ImageJ, Jmol, Paraview, cisTEM), Servers (Jupyter Notebook, Jupyter Notebook for Python Training, JupyterLab, RStudio, TensorBoard, Tutorials OnDemand), and Visualization (VNC, NextSilicon VNC). The 'Jupyter Notebook for Python Training' option is highlighted with a red box. The main content area on the left features the ACES logo (Accelerating Computing for Emerging Sciences) and several news items: 'OnDemand provides an integrated, single access point', 'Message of the Day', 'ACES Status, January 27' (noting PVC queue availability), and 'ACES Accounting, January 13' (noting activation on Monday).

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

**GUI**

- VNC
- NextSilicon VNC

**Imaging**

- CryoSPARC
- ImageJ
- Jmol
- Paraview
- cisTEM

**Servers**

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

**Visualization**

- VNC
- NextSilicon VNC

**ACES**  
ACCELERATING COMPUTING  
FOR EMERGING SCIENCES

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, January 13, 2025.

# 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

Create

Time

Session

Your session

take a

Jupyter Notebook for Python Training (636884)

1 node | 1 core | Running

Host: >\_ ac058

Delete

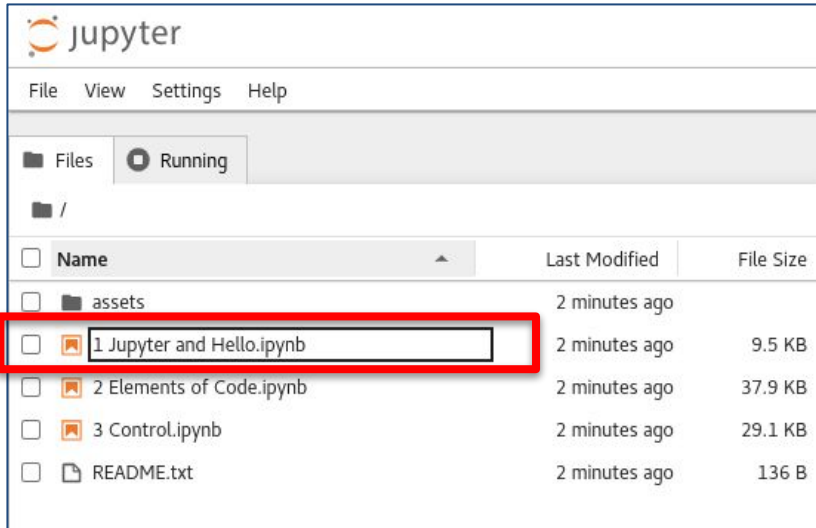
Created at: 2025-01-28 09:19:34 CST

Time Remaining: 7 hours and 9 minutes

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

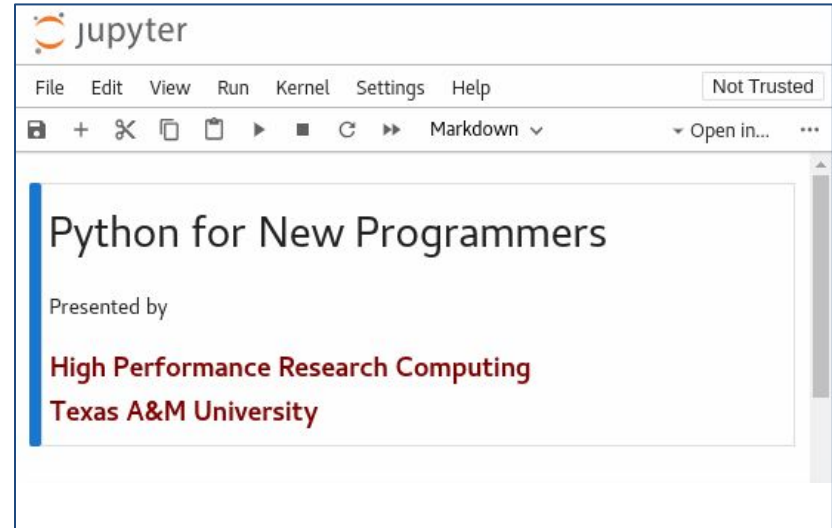
Connect to Jupyter

# Jupyter Notebook for Python Training



The Jupyter File Browser interface shows a list of files in the current directory. The file '1 Jupyter and Hello.ipynb' is highlighted with a red box. The interface includes a 'Files' tab, a 'Running' button, and a table of files with columns for Name, Last Modified, and File Size.

<input type="checkbox"/>	Name	Last Modified	File Size
<input type="checkbox"/>	assets	2 minutes ago	
<input type="checkbox"/>	1 Jupyter and Hello.ipynb	2 minutes ago	9.5 KB
<input type="checkbox"/>	2 Elements of Code.ipynb	2 minutes ago	37.9 KB
<input type="checkbox"/>	3 Control.ipynb	2 minutes ago	29.1 KB
<input type="checkbox"/>	README.txt	2 minutes ago	136 B



The Jupyter Notebook Editor interface shows a notebook titled 'Python for New Programmers'. The notebook content includes the title, a presenter 'Presented by', and the affiliation 'High Performance Research Computing, Texas A&M University'. The interface includes a 'Not Trusted' warning, a toolbar with icons for file operations, and a 'Markdown' dropdown menu.

Python for New Programmers

Presented by

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



**HIGH PERFORMANCE  
RESEARCH COMPUTING**  
TEXAS A&M UNIVERSITY

<https://hprc.tamu.edu>

HPRC Helpdesk:

[help@hprc.tamu.edu](mailto:help@hprc.tamu.edu)

Phone: 979-845-0219

*Take our short course 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.

