

Tutorial: Python for Programmers (new to Python) on **ACES**

Josh Winchell
2025/09/30



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: review of programming basics, control structures, and introduction to Python data structures

Outline: Today's Class

- About Python
- Getting Started
- Basics and Control Structures
- Data Structures

About Python

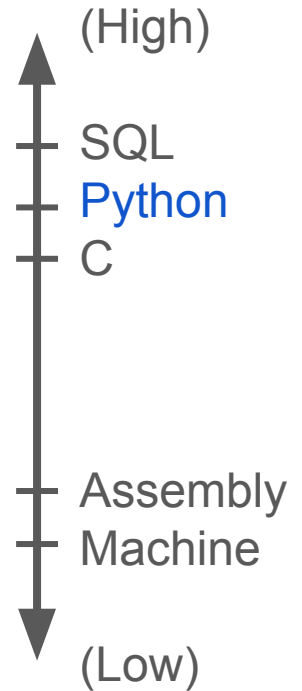


What is Python like?

Python is a High-level language, which means:

- Syntax is similar to human language syntax
- Supports abstract concepts
- Takes care of mundane hardware tasks for you

Python is designed to simplify the development process so you can focus on what matters.



Is Python right for me?

No programming language is perfect for every task.

Python is best for research and rapid development.

Pros

- Easy to use
- Modules are readily available
- Portable

Cons

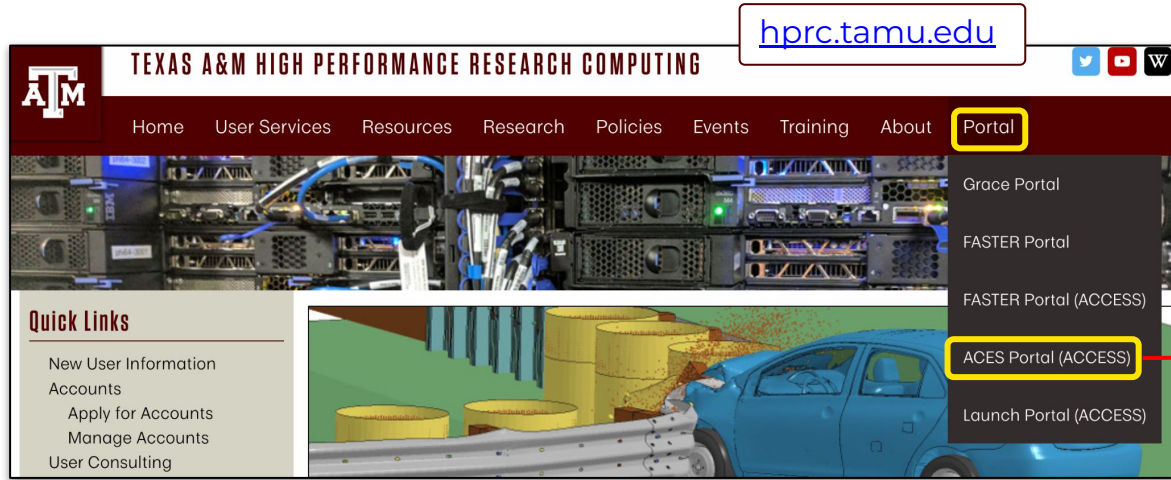
- Not the fastest
- Source code style is mandatory

Learning Resources

- Slides on the course web page
https://hprc.tamu.edu/training/aces_python4programmers.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

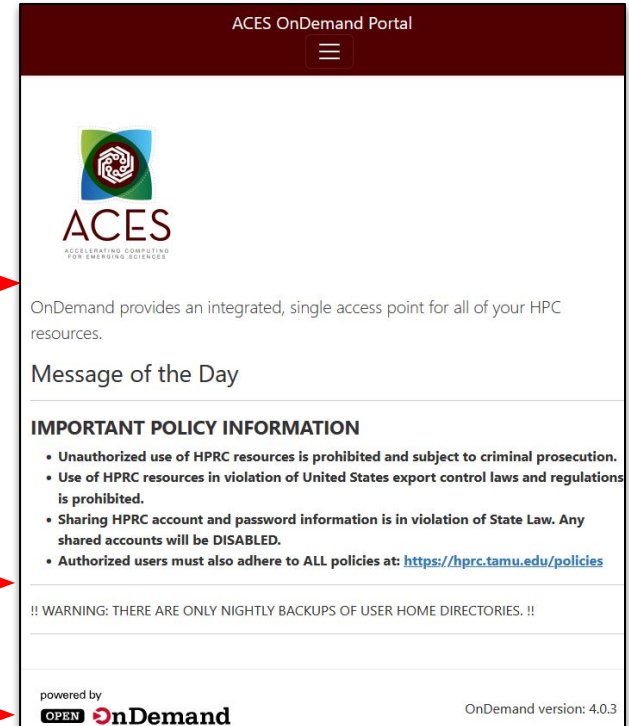
Login to ACES Portal



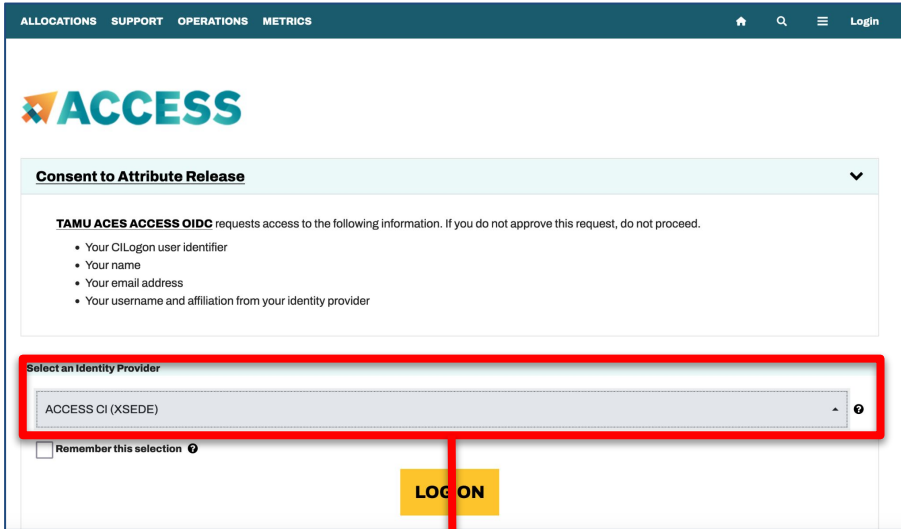
(You'll have to log in with ACCESS if you haven't already)

ACES Portal 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

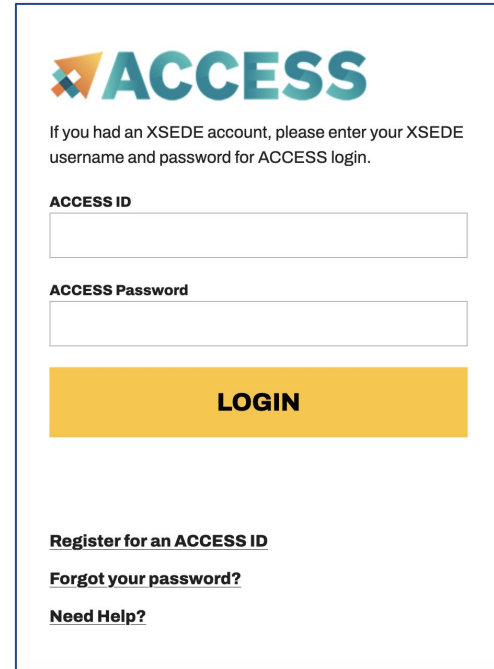


Accessing ACES via the Portal (ACCESS)



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 message from TAMU ACES ACCESS OIDC requesting access to user information. Below this is a "Select an Identity Provider" dropdown menu, which is highlighted with a red rectangle. The dropdown shows "ACCESS CI (XSEDE)" as the selected option. Below the dropdown is a checkbox labeled "Remember this selection". A yellow "LOG ON" button is positioned below the dropdown menu.

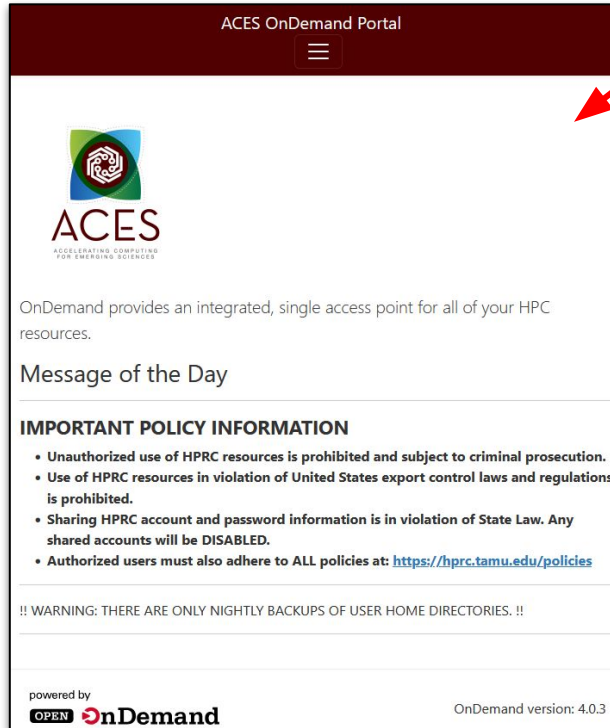
Select the Identity Provider appropriate for your account.



The screenshot shows the ACCESS portal login form. 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 large yellow "LOGIN" button. At the bottom of the form are three links: "Register for an ACCESS ID", "Forgot your password?", and "Need Help?".

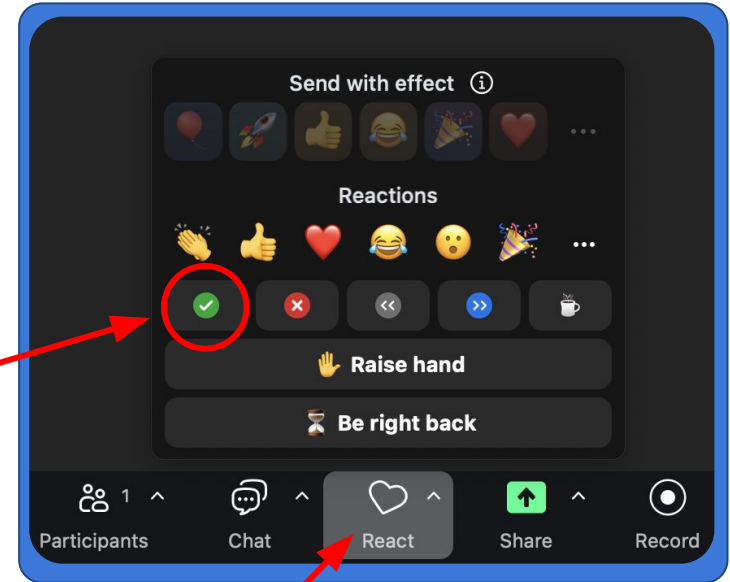
Log-in using your ACCESS or institutional credentials.

Login to ACES Portal



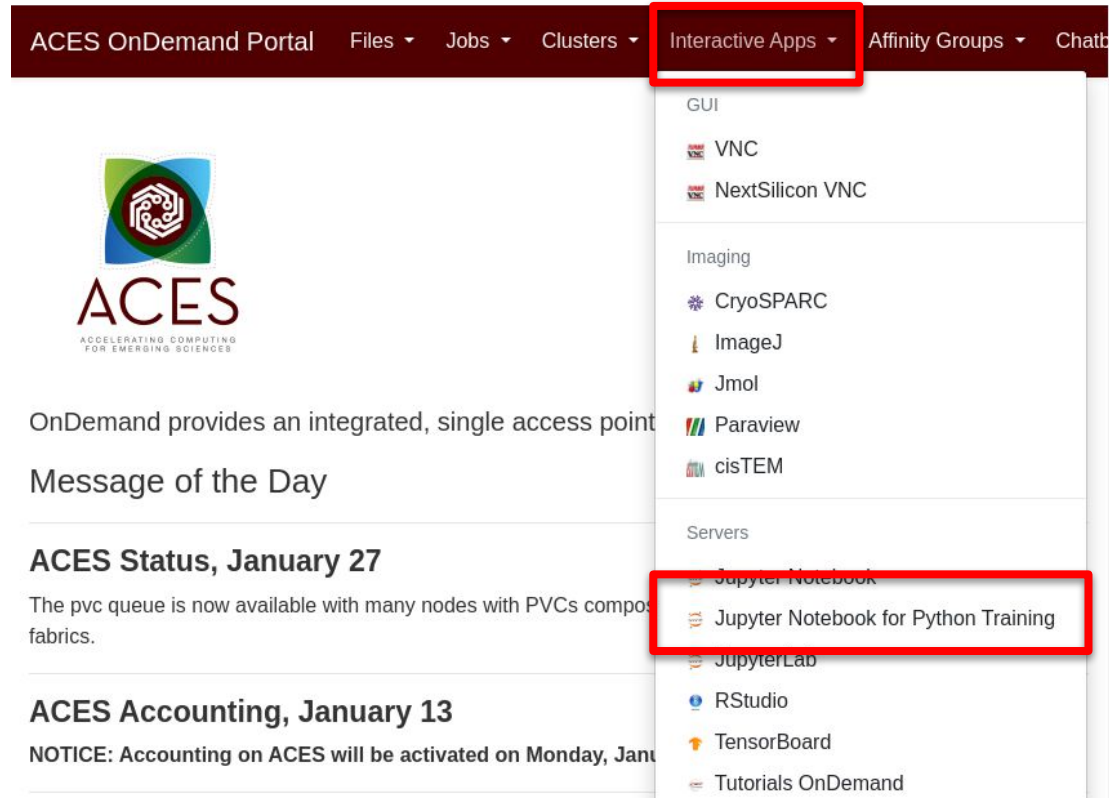
Once you're on this screen...

...Click the
green
checkmark
reaction in
Zoom



(find it here)

Jupyter Notebook for Python Training



The screenshot displays the ACES OnDemand Portal interface. The top navigation bar includes links for 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'Affinity Groups', and 'Chat'. The 'Interactive Apps' menu is open, showing a list of applications categorized under 'GUI', 'Imaging', and 'Servers'. The 'Jupyter Notebook for Python Training' option is highlighted with a red box. The main content area on the left features the ACES logo, a message about the OnDemand portal, and status updates for January 27 and January 13.

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

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, 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

Create

Time

Session

Your session

take a

Jupyter Notebook for Python Training (636884)

1 node | 1 core | Running

Host: >_ ac058

Delete

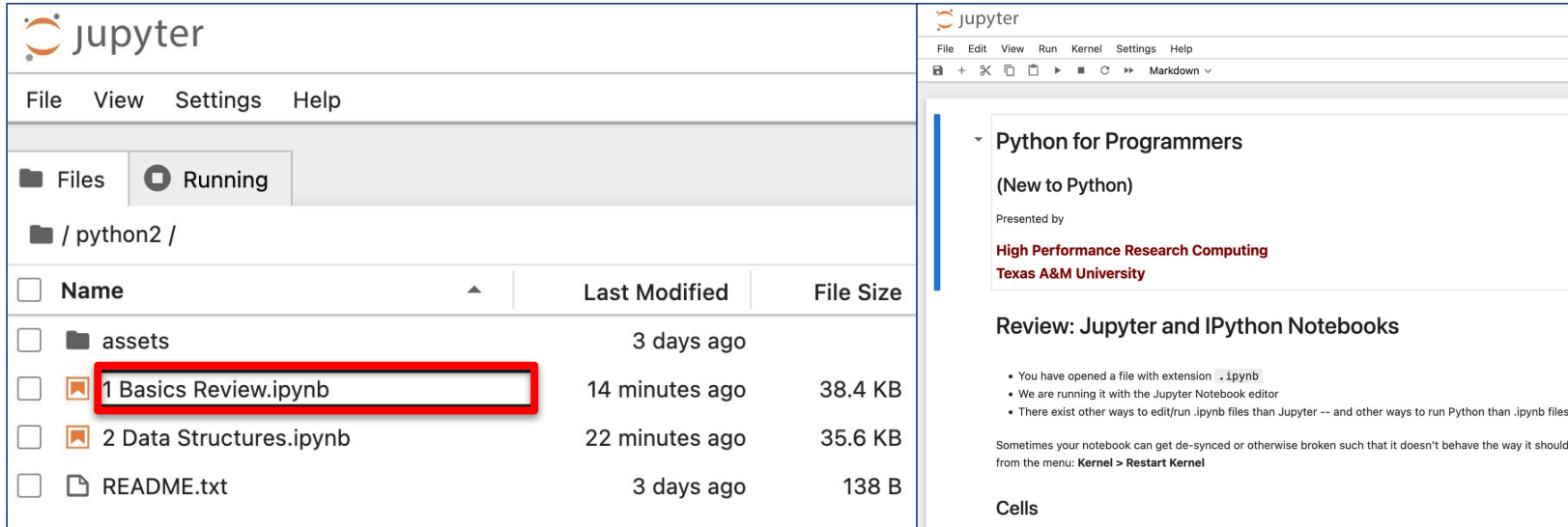
Created at: 2025-01-28 09:19:34 CST

Time Remaining: 7 hours and 9 minutes

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

Connect to Jupyter

Jupyter Notebook for Python Training



The screenshot displays the Jupyter Notebook interface. On the left, the file browser shows a directory structure with a 'python2' folder. Inside this folder, there is a table of files. The file '1 Basics Review.ipynb' is highlighted with a red rectangle. The right pane shows the content of the selected notebook, which includes a title 'Python for Programmers', a subtitle '(New to Python)', and a section titled 'Review: Jupyter and IPython Notebooks' with a list of bullet points.

Name	Last Modified	File Size
assets	3 days ago	
1 Basics Review.ipynb	14 minutes ago	38.4 KB
2 Data Structures.ipynb	22 minutes ago	35.6 KB
README.txt	3 days ago	138 B

Python for Programmers
(New to Python)
Presented by
High Performance Research Computing
Texas A&M University

Review: Jupyter and IPython Notebooks

- You have opened a file with extension `.ipynb`
- We are running it with the Jupyter Notebook editor
- There exist other ways to edit/run `.ipynb` files than Jupyter -- and other ways to run Python than `.ipynb` files.

Sometimes your notebook can get de-synced or otherwise broken such that it doesn't behave the way it should, from the menu: **Kernel > Restart Kernel**

Cells



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<https://hprc.tamu.edu>

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

Take our short course survey!



HPRC 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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