

Tutorial: Python for Programmers (new to Python) 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: review of programming basics for new people to practice and experienced people to learn the syntax --plus constructs important for the Data Science class.

Outline: Today's Class

- About Python
- Getting Started
- Basics and Control Structures
- Data Structures
- Advanced: Functions and Classes

About Python

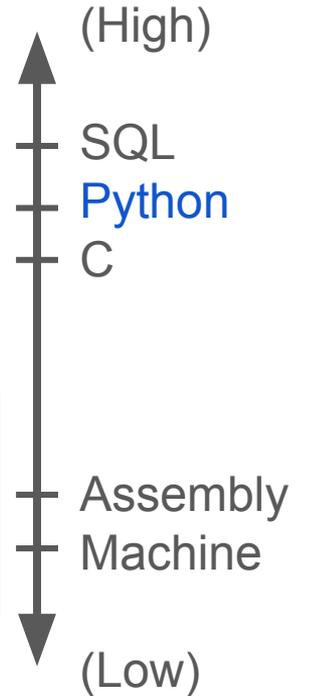


What is Python like?

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

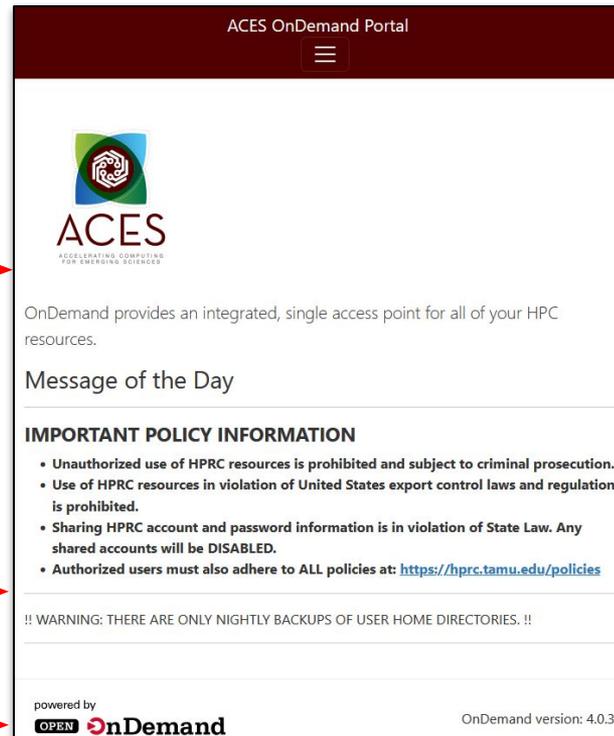
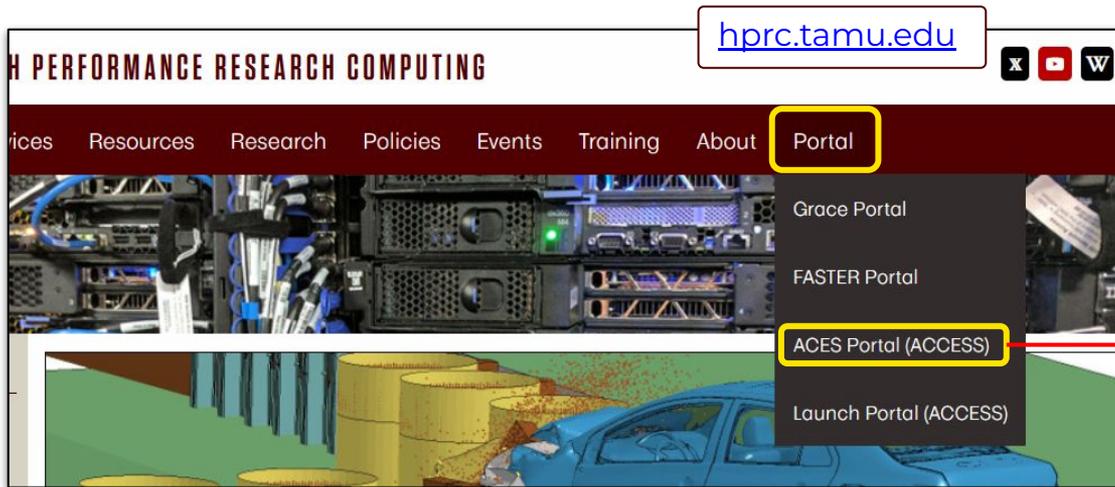
- Not the fastest
- Source code style is mandatory

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

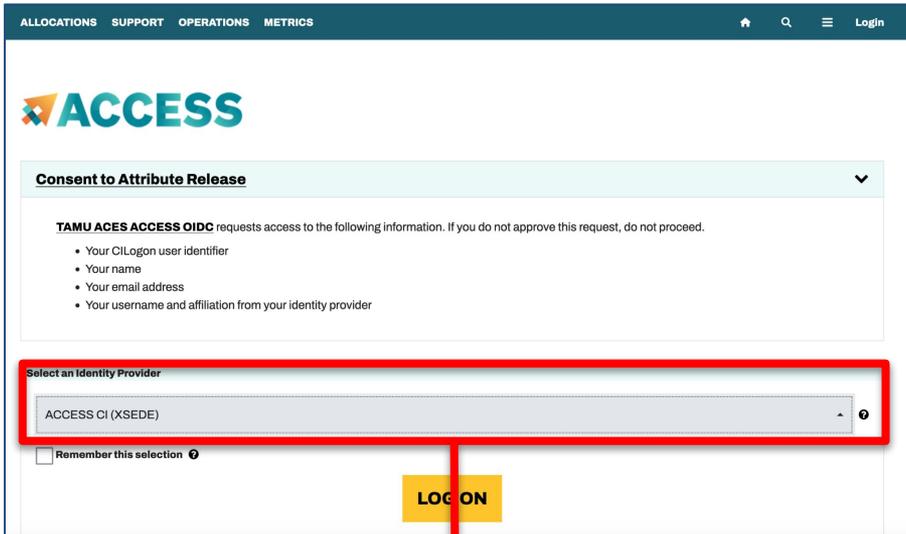


(You will have to log in with ACCESS if you haven't already)

ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

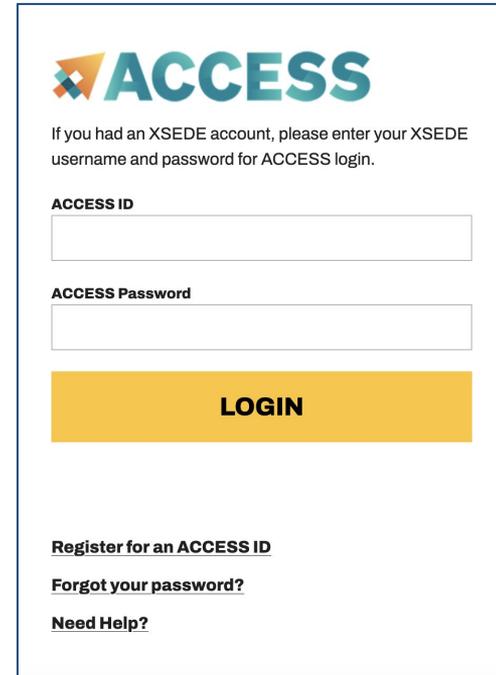
Open OnDemand (OOD) is an advanced web-based
graphical interface framework for HPC users

Accessing ACES via the Portal (ACCESS)



The screenshot shows the ACCESS portal interface. At the top, 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 and a list of requested information: CILogon user identifier, name, email address, and username/affiliation. Below this is a "Select an Identity Provider" dropdown menu with "ACCESS CI (XSEDE)" selected. A red box highlights this dropdown and the "LOG ON" button below it. A red line connects the "LOG ON" button to the text below.

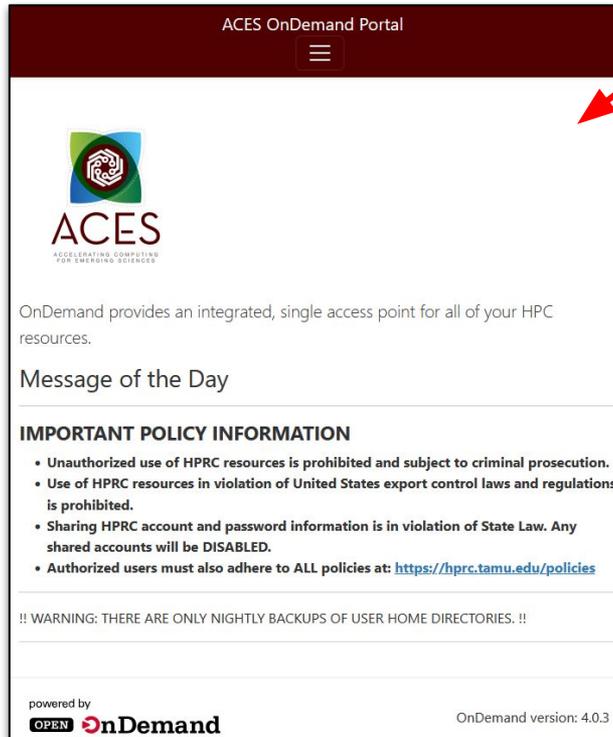
Select the Identity Provider appropriate for your account.



The screenshot shows the ACCESS portal login form. It features the ACCESS logo at the top, followed by a message: "If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login." Below this are two input fields: "ACCESS ID" and "ACCESS Password". A large yellow "LOGIN" button is positioned below the password field. At the bottom, there are links for "Register for an ACCESS ID", "Forgot your password?", and "Need Help?".

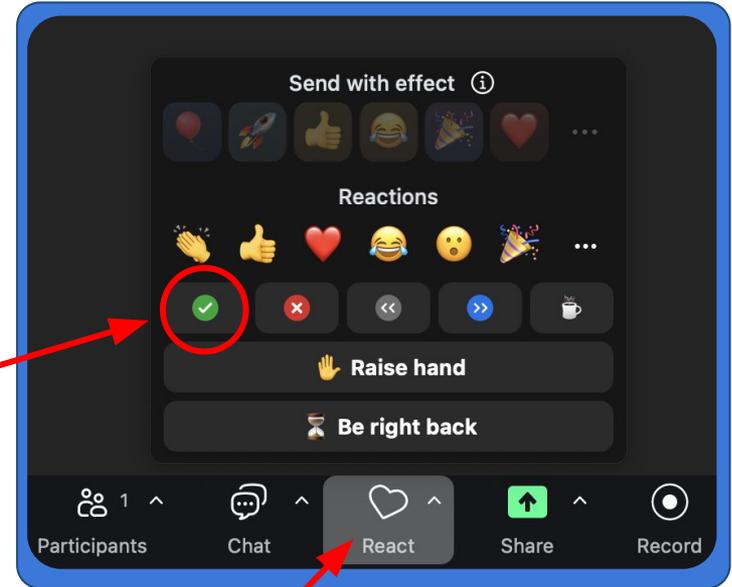
Log-in using your ACCESS or institutional credentials.

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. At the top, a dark red navigation bar contains the following items: "ACES OnDemand Portal", "Files", "Jobs", "Clusters", "Interactive Apps" (highlighted with a red box), "Affinity Groups", and "Chat". Below the navigation bar, the main content area features the ACES logo (a stylized green and blue square with a white circuit-like pattern) and the text "ACES ACCELERATING COMPUTING FOR EMERGING SCIENCES". Below the logo, there is a section titled "OnDemand provides an integrated, single access point" and another titled "Message of the Day". The "Message of the Day" section contains two entries: "ACES Status, January 27" and "ACES Accounting, January 13". The "ACES Status, January 27" entry includes the text "The pvc queue is now available with many nodes with PVCs composed of fabrics." The "ACES Accounting, January 13" entry includes the text "NOTICE: Accounting on ACES will be activated on Monday, January 13, 2025". On the right side of the page, a dropdown menu is open under the "Interactive Apps" header. The menu lists several applications: "GUI", "VNC", "NextSilicon VNC", "Imaging", "CryoSPARC", "ImageJ", "Jmol", "Paraview", "cisTEM", "Servers", "Jupyter Notebook", "Jupyter Notebook for Python Training" (highlighted with a red box), "JupyterLab", "RStudio", "TensorBoard", and "Tutorials OnDemand".

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

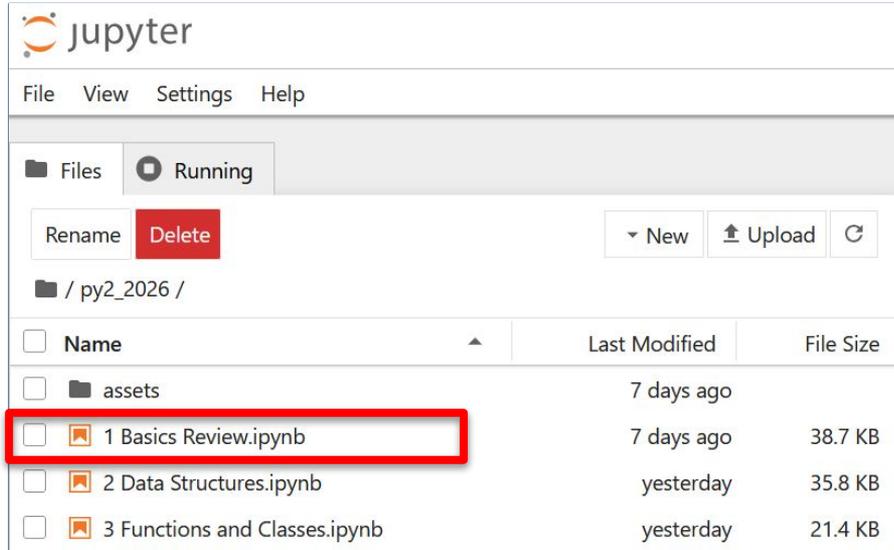
Created at: 2025-01-28 09:19:34 CST

Time Remaining: 7 hours and 9 minutes

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

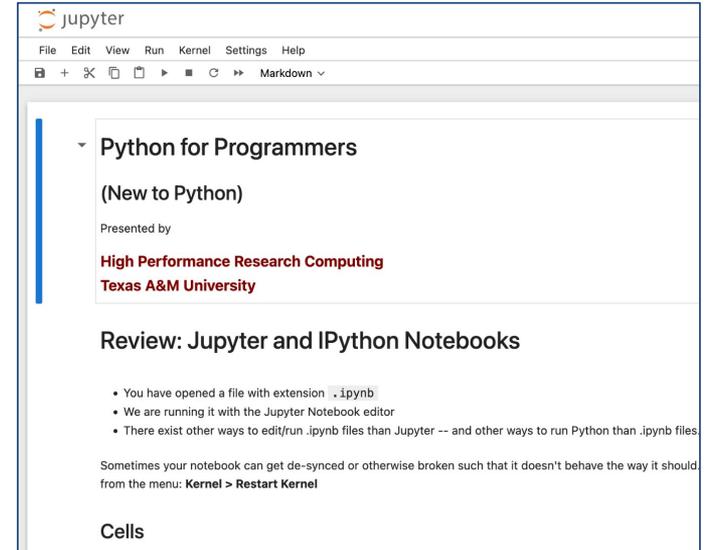
Connect to Jupyter

Jupyter Notebook for Python Training



The screenshot shows the Jupyter file browser interface. At the top, there is a navigation bar with 'File', 'View', 'Settings', and 'Help'. Below this, there are tabs for 'Files' and 'Running'. A toolbar contains 'Rename', 'Delete', 'New', 'Upload', and a refresh icon. The current directory is '/ py2_2026 /'. A table lists the files in the directory:

<input type="checkbox"/>	Name	Last Modified	File Size
<input type="checkbox"/>	assets	7 days ago	
<input type="checkbox"/>	1 Basics Review.ipynb	7 days ago	38.7 KB
<input type="checkbox"/>	2 Data Structures.ipynb	yesterday	35.8 KB
<input type="checkbox"/>	3 Functions and Classes.ipynb	yesterday	21.4 KB



The screenshot shows the Jupyter notebook editor interface. At the top, there is a navigation bar with 'File', 'Edit', 'View', 'Run', 'Kernel', 'Settings', and 'Help'. Below this, there is a toolbar with various icons. The notebook content is displayed in a scrollable area. The title is 'Python for Programmers' and the subtitle is '(New to Python)'. The presenter is 'High Performance Research Computing, Texas A&M University'. The section title is 'Review: Jupyter and IPython Notebooks'. The content includes a list of bullet points:

- 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.

Below the list, there is a note: '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**'.



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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.

