

# HIGH PERFORMANCE RESEARCH COMPUTING

Data science meets Geoscience: a case study in rock weathering calculations

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TEXAS A&M UNIVERSITY  
Oceanography



High Performance  
Research Computing  
DIVISION OF RESEARCH



TEXAS A&M  
Institute of  
Data Science



# Accessing Files

All materials are written in R and compiled in Jupyter Notebook files, which are available on the HPRC systems.

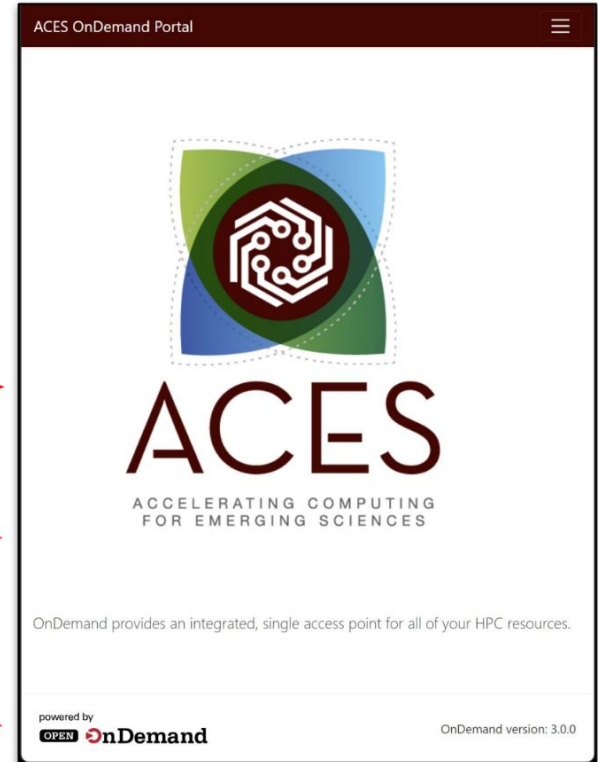
Now, let's log in to the ACES portal to retrieve the files!

# ACES Portal

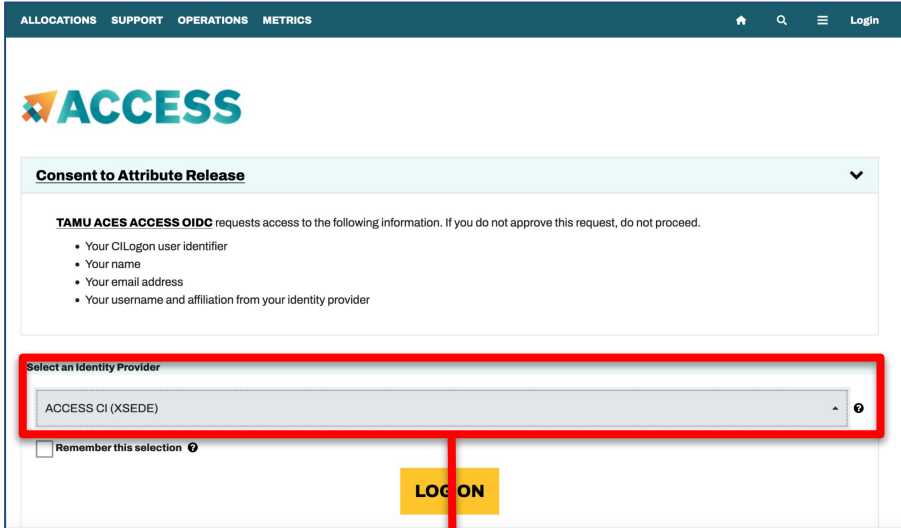


ACES Portal [portal-aces.hprc.tamu.edu](http://portal-aces.hprc.tamu.edu)  
is the web-based user interface for the ACES cluster

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" contains a message from TAMU ACES ACCESS OIDC and a list of requested information: CI/Logon 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. Below the dropdown is a "Remember this selection" checkbox and a yellow "LOG ON" button. A red line points from the "LOG ON" button to the text below.

ALLOCATIONS SUPPORT OPERATIONS METRICS Login

**ACCESS**

**Consent to Attribute Release**

**TAMU ACES ACCESS OIDC** requests access to the following information. If you do not approve this request, do not proceed.

- Your CI/Logon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

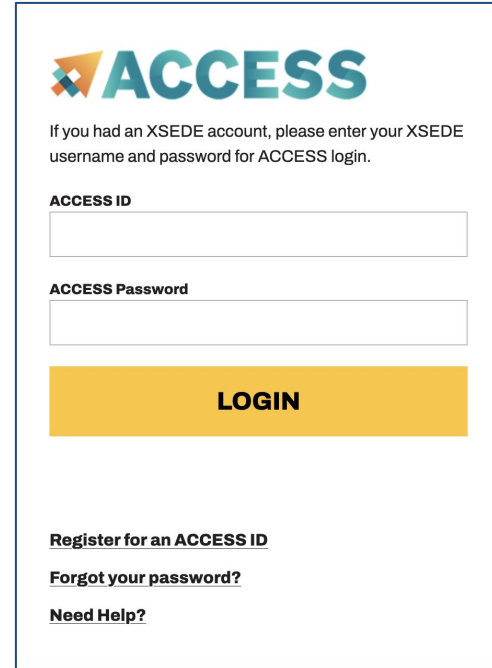
Select an Identity Provider

ACCESS CI (XSEDE)

☐ Remember this selection

**LOG ON**

Select the Identity Provider appropriate for your account.



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

**ACCESS**

If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login.

**ACCESS ID**

**ACCESS Password**

**LOGIN**

[Register for an ACCESS ID](#)

[Forgot your password?](#)

[Need Help?](#)

Log-in using your ACCESS or institutional credentials.

Home Directory

/scratch/user/u.sl170446  
/scratch/user/u.sl170446

&gt; \_ Open in Terminal ▾

Refresh

+ New File

New Directory

Upload

Download

Copy

Home Directory

/scratch/user/u.sl170446



/ scratch / user / u.sl170446 /

Change directory

☐ Show Owner/Mode☐ Show DotfilesFilter: 

Showing 3 rc

<input type="checkbox"/>	Type ▲	Name		Size	Modified at
<input type="checkbox"/>	Folder	ondemand	⋮ ▾	-	3/13/2024 9:26:34 PM
<input type="checkbox"/>	Folder	PIP_CACHE	⋮ ▾	-	3/13/2024 6:02:06 PM
<input type="checkbox"/>	Folder	user	⋮ ▾	-	4/9/2024 2:10:00 PM

Type 'cp -r /scratch/training/2025-R-Carbon-Workshop \$SCRATCH' in the terminal interface.

```
Type 'showquota' to view these quotas again.
[u.sl170446@aces-login3 u.sl170446]$ cp -r /scratch/training/2025-R-Carbon-Workshop $SCRATCH
```

Home Directory

/scratch/user/u.sl170446



/ scratch / user / u.sl170446 /

Change directory

Copy path

☐ Show Owner/Mode

















☐ Show Dotfiles

Filter:

Showing 4 rows - 0 rows selected

<input type="checkbox"/>	Type ▲	Name		Size	Modified at
<input type="checkbox"/>	Folder	2025-R-Carbon-Workshop	⋮	-	3/26/2025 11:37:24 PM
<input type="checkbox"/>	Folder	ondemand	⋮	-	3/13/2024 9:26:34 PM
<input type="checkbox"/>	Folder	PIP_CACHE	⋮	-	3/13/2024 6:02:06 PM
<input type="checkbox"/>	Folder	user	⋮	-	4/9/2024 2:10:00 PM

Here it is!

<input type="checkbox"/>		data		-
<input type="checkbox"/>		img		-
<input type="checkbox"/>		installation		-
<input type="checkbox"/>		output		-
<input type="checkbox"/>		01-R_workshop_carbon_cycle_Basics.ipynb		4.29 MB
<input type="checkbox"/>		02-R_workshop_carbon_cycle_ML.ipynb		236.21 kB
<input type="checkbox"/>		03_R_workshop_carbon_cycle_ML.ipynb		4.13 MB
<input type="checkbox"/>		04-R_workshop_carbon_cycle_Summary.ipynb		2.50 kB



# Create the interactive sessions.

Files ▾Jobs ▾Clusters ▾Interactive Apps ▾Affinity Groups ▾Dashboard ▾

Home / My Interactive Sessions

Interactive Apps

GUI

VNC

Imaging

CryoSPARC

ImageJ

Jmol

Paraview

cisTEM

Servers

Jupyter Notebook

JupyterLab

**JupyterLab (GeoDS)**

RStudio

TensorBoard

Tutorials OnDemand

Tutorials OnDemand (short course)

JupyterLab

JupyterLab (GeoDS)

RStudio

TensorBoard

Tutorials OnDemand

Tutorials OnDemand (short course)

Number of hours (max 4)

4

Number of cores (max 4)

4

Total GB memory (max 20)

20

Account

This field is optional.

Email

This field is optional.

☐ I would like to receive an email when the session starts

Launch

\* The JupyterLab (GeoDS) session data for this session can be accessed under the [data root directory](#).

Alternatively:  
Optional environment:  
/sw/hprc/sw/Anaconda3/2022.10/envs/hprc\_2025\_carbon

Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ Affinity Groups ▾ Dashboard ▾ Utilities ▾ My Interactive Sessions

Home / My Interactive Sessions / JupyterLab

Interactive Apps

GUI

VNC

Imaging

CryoSPARC

ImageJ

Jmol

Paraview

cisTEM

Servers

Jupyter Notebook

**JupyterLab**

RStudio

TensorBoard

Tutorials OnDemand

Tutorials OnDemand (short course)

### JupyterLab

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

Module

Anaconda3/2022.10

Optional Environment to be activated

/sw/hprc/sw/Anaconda3/2022.10/envs/hprc\_2025\_carbon

Enter the full path and name of the environment to be activated.

Leave blank to use the [default](#) environment for the selected Module.

Your optional conda environment must have been previously built with one of the Anaconda or Python modules listed in the Module option above. See [instructions](#).

Node type

CPU only

- Select a GPU node for software that supports GPU processing.

Number of hours (max 168)

5

Number of cores (max 96)

20

Total GB memory (max 488)

20

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[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.