

April 15, 2021

# XSEDE New User Training @University of Central Florida

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## XSEDE

Extreme Science and Engineering  
Discovery Environment



Supported by OAC 15-48562.

# Housekeeping

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Introductions

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Code of Conduct

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Terminology Acknowledgement

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Materials Repository - <http://hpcuniversity.org/trainingMaterials/253/>

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Post session survey

# Code of Conduct

XSEDE has an external code of conduct for XSEDE sponsored events which represents XSEDE's commitment to providing an inclusive and harassment-free environment in all interactions regardless of gender, sexual orientation, disability, physical appearance, race, or religion. The code of conduct extends to all XSEDE-sponsored events, services, and interactions.

**Code of Conduct:** <https://www.xsede.org/codeofconduct>

## **Contact:**

- Event organizer: Linda Akli, [akli@sura.org](mailto:akli@sura.org) or 202-256-5148
- XSEDE ombudspersons:
  - Linda Akli, Southeastern Universities Research Association ([akli@sura.org](mailto:akli@sura.org))
  - Lizanne Destefano, Georgia Tech ([lizanne.destefano@ceismc.gatech.edu](mailto:lizanne.destefano@ceismc.gatech.edu))
  - Ken Hackworth, Pittsburgh Supercomputing Center ([hackworth@psc.edu](mailto:hackworth@psc.edu))
  - Bryan Snead, Texas Advanced Computing Center ([jbsnead@tacc.utexas.edu](mailto:jbsnead@tacc.utexas.edu))



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# Terminology Statement

In line with XSEDE's Code of Conduct, XSEDE is committed to providing training events that foster inclusion and show respect for all. This commitment applies not only to how we interact during the event; it also applies to the training materials and presentation. It is not XSEDE's position to use, condone, or promote offensive terminology.

XSEDE instructors strive to keep inclusive language at the forefront. In the event that we have included inappropriate materials, verbal or written, please let us know at [terminology@xsede.org](mailto:terminology@xsede.org)

While XSEDE has no control over external third-party documentation, we are taking steps to effect change by contacting the relevant organizations; we hope this will be addressed by all third parties soon.

*If you see any terminology concerns in the following presentation or slides, we want to know!  
Please contact the Terminology Task Force: [terminology@xsede.org](mailto:terminology@xsede.org)*

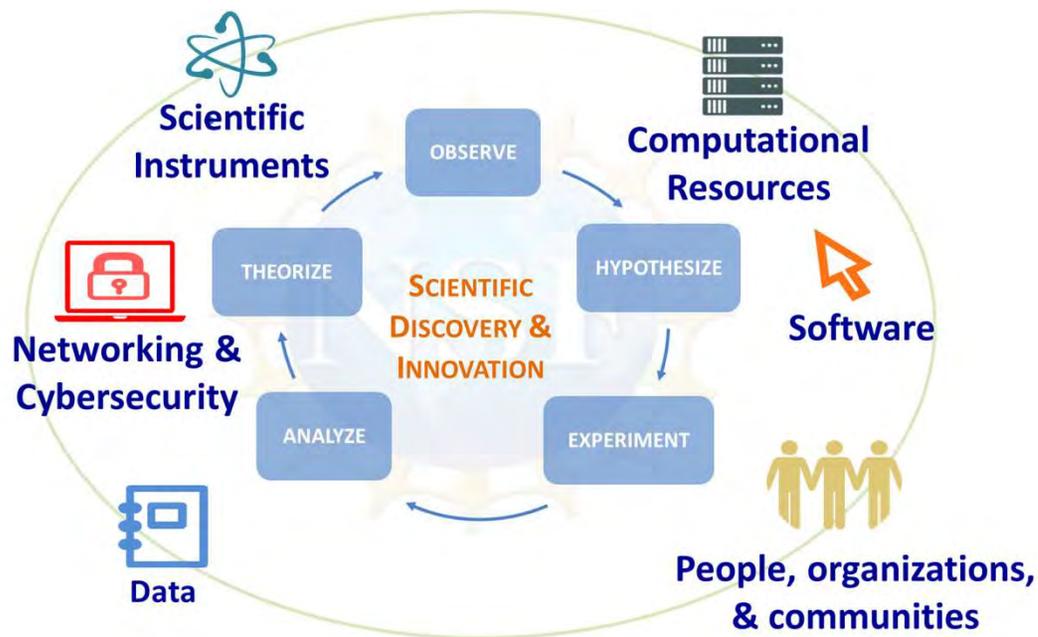


**XSEDE**

# What is Advanced Computing?

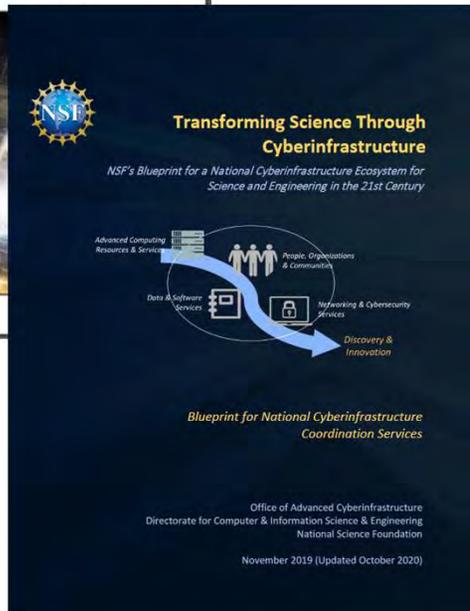
Resources and Services that support compute- and data-intensive research, which are too expensive to be purchased and operated by an individual research group, department and, in some cases, institutions.

- Cloud Computing
- Data Intensive Computing
- Parallel Computing
- High Performance Computing
- Supercomputing
- Data Analytics
- Data Mining
- Data Science
- Data Visualization
- Modeling and Simulation



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# What is XSEDE?



## Foundation for a National CI Ecosystem

- Comprehensive suite of advanced digital services that federates with other high-end facilities and campus-based resources



## Unprecedented Integration of Diverse Advanced Computing Resources

- Innovative, open architecture making possible the continuous addition of new technology capabilities and services



**XSEDE**

# XSEDE – accelerating scientific discovery

## XSEDE's Vision:

- *a world of digitally enabled scholars, researchers, and engineers participating in multidisciplinary collaborations while seamlessly accessing advanced computing resources and sharing data to tackle society's grand challenges.*

## XSEDE's Mission:

- *to enhance the productivity of a growing community of scholars, researchers, and engineers through access to advanced digital services that support open research by coordinating and adding value to the leading cyberinfrastructure resources funded by the NSF and other agencies.*

# XSEDE Supports a Breadth of Research

COVID-19 Modeling and Policy

Leveraging Twitter as an Epidemiological Tool to Understand Health Behaviors

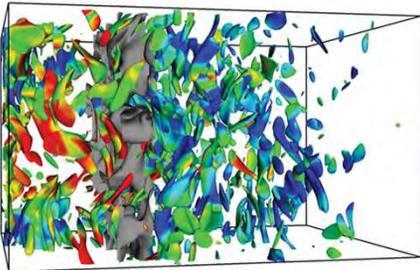
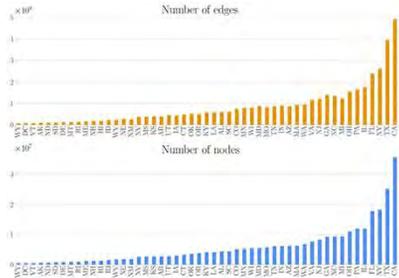
Understanding Shock-Turbulence Interactions

LED's Bright Early Light

Interactive Adaptation and Collaboration Tools for managing Water, Energy and Land

Simulations for Natural Disaster Case Studies

AI Classifying Galaxies



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# Upcoming Opportunities

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Monday, June 7 – Tuesday, June 15, 2021, Computational Chemistry for Chemistry Educators (CCCE) workshop <https://portal.xsede.org/course-calendar/-/training-user/class/2038/session/3995>

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June 17 – 18, 2021 Advanced Computing for Social Change Curriculum Workshop – contact [akli@sura.org](mailto:akli@sura.org)

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Summer 2022, International HPC Summer School – contact [alameda@illinois.edu](mailto:alameda@illinois.edu)

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EMPOWER ( Expert Mentoring Producing Opportunities for Work, Education, and Research ) – undergraduate student participants and faculty/research staff with projects – contact

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Spring 2022 Advanced Computing for Social Change Regional Student Workshops

April 15, 2021

# XSEDE New User Training @University of Central Florida

*Jay Alameda, NCSA  
Senior Technical Program Manager  
Manager, XSEDE Extended Support for Training Education & Outreach*

## XSEDE

Extreme Science and Engineering  
Discovery Environment



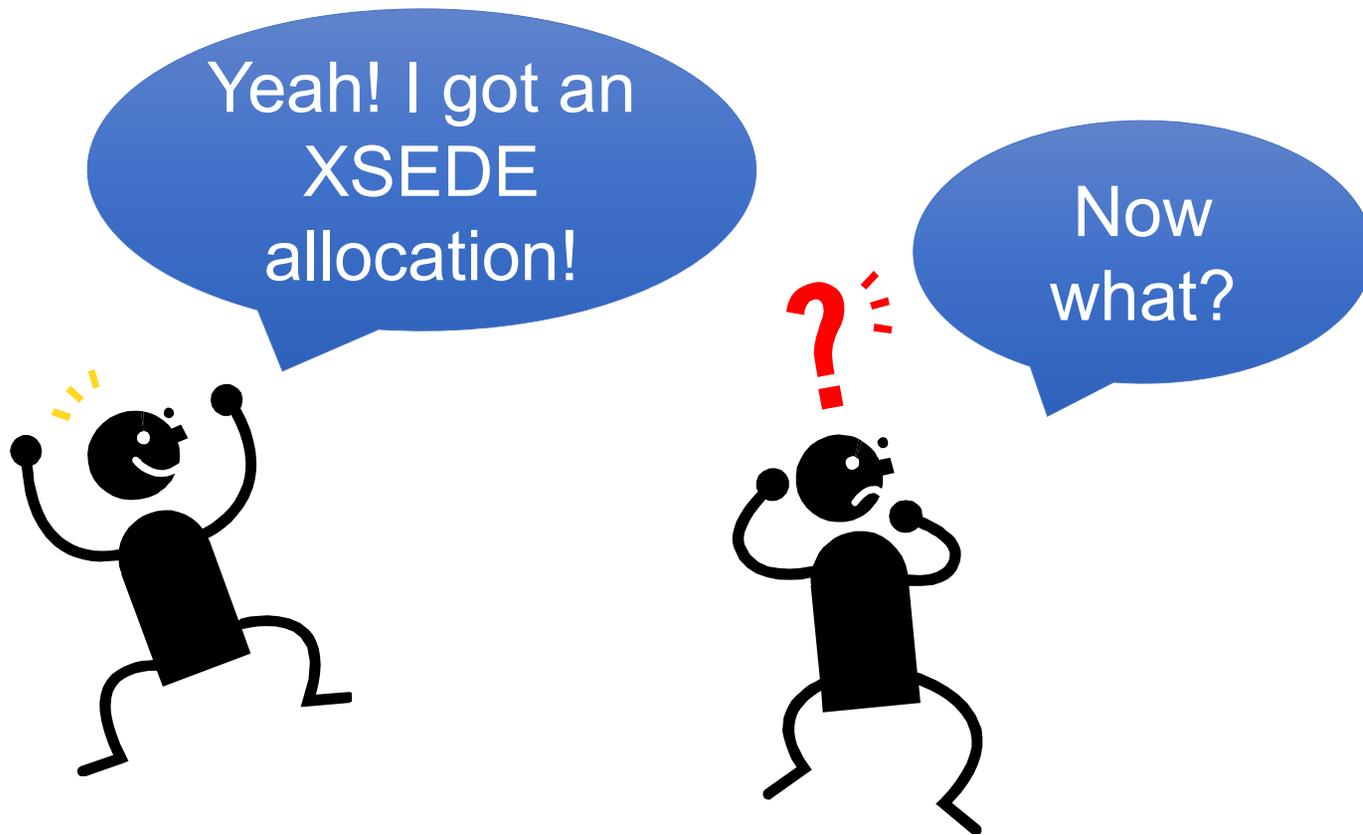
Supported by OAC 15-48562.

# Housekeeping

Materials Repository -

<http://hpcuniversity.org/trainingMaterials/253/>

Post session and post workshop survey



# Learning Outcomes

After completing this tutorial, you will be able to:

- Use the XSEDE User Portal
- Access your XSEDE resources
- Manage files
- Run jobs
- Get help



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# XSEDE User Portal (XUP)

- URL: [portal.xsede.org](https://portal.xsede.org)
- Single point-of-entry to information about XSEDE services and utilities for using them
- Anyone can create an XUP user account and access non-project features
- Only XSEDE allocation project members can access project features



**XSEDE**

## Using the XUP

- Create and login to your XUP Account
- Use XSEDE resources responsibly
- Get added to your XSEDE project
- Navigate your personal My XSEDE webpage
- Navigate the information in the XUP



**XSEDE**

# Create and login to your XUP account

portal.xsede.org

Enter the Portal

USER NAME

PASSWORD

Sign In  REMEMBER ME

Other Sign In Options

CREATE ACCOUNT VERIFY ACCOUNT FORGOT PASSWORD FORGOT USERNAME

1. From the XUP homepage, click CREATE ACCOUNT
2. Complete the User Account Form
3. Verify your account request
4. Select your username and password
5. Login to the XUP

Click the CREATE ACCOUNT link to access the XUP User Account Form



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# XSEDE Acceptable Use Policy

- Must accept the [User Responsibilities Form](#) after creating your XUP account and again at the beginning of each allocation you receive.
  - Available on the portal – Documentation, Usage Policy - <https://portal.xsede.org/web/xup/usage-policy>
- Choose a strong password and protect it.
- Close SSH terminals and log out of the User Portal when you are finished with your session.
- Report Suspicious Activity : email [help@xsede.org](mailto:help@xsede.org) or call 1-866-907-2383 immediately, regardless of the time of day.

XSEDE Cybersecurity Tutorial  
<https://portal.xsede.org/web/xup/online-training>



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## Get Added to Your XSEDE project

- PIs automatically have full access to their project's account.
- The PI is responsible for managing users on their account.
- Ask the PI, or their allocation manager, to add your XUP username to the project.



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# Your My XSEDE webpage

MY XSEDE | RESOURCES | DOCUMENTATION | ALLOCATIONS | TRAINING | USER FORUMS | HELP | ECSS | ABOUT

Summary | Allocations/Usage | Accounts | Jobs | Profile | Publications | Tickets | Change Password | Add User | Community Accounts | SSH Terminal

Share your feedback on XSEDE Training Services with a quick 5 question survey!

Share the impact of XSEDE!

- For all publications, please acknowledge your use of XSEDE and allocated resources and add publications your User Profile.
- Tell us about your achievements with XSEDE
- Help us improve our reporting by keeping your XSEDE User Profile up to date and completing the demographic information.

Welcome, Jay!  
Last login: Fri 03/31/17 at 06:44:01 AM CST

Profile | Allocations | Accounts | Training

NEW! Share your XSEDE Science Achievements

Publications: [View My Pubs]  
You have entered 3 publication(s)  
Add a Publication

Tickets: [Full List]  
New 0

In The Past 7 Days

XD SUs Charged, Total: by field of Science

Field of Science	Count
Computer and Information Science and Engineering	11,001,908.0
Materials Research	11,203,918.0
Biochemistry and Molecular Structures and Families	10,788,858.0
Biophysics	10,367,818.0
Astronomical Sciences	8,514,084.0
Gravitational Physics	2,004,872.0
Chemistry	1,827,896.0
Nuclear Physics	3,984,232.0
Extraterrestrial, Astronomical and Cosmology	6,209,082.0
Fluid, Particulate, and Hydraulic Systems	4,911,548.0
All 82 others	20,291,898.0

My XSEDE Resources (3) | System Monitor

Resource	Status	Load	Username	My Jobs
Stampede   UT Austin	Healthy	95%	tg455677	R: 0 Q: 0 O: 0

(1)

## Welcome to the XUP

- Quick access to commonly used features.

(2)

## Latest updates

- Latest information specific to your user account.

(3)

## My Resources and Allocations

- Summary of the active projects for which you are either a PI or member.

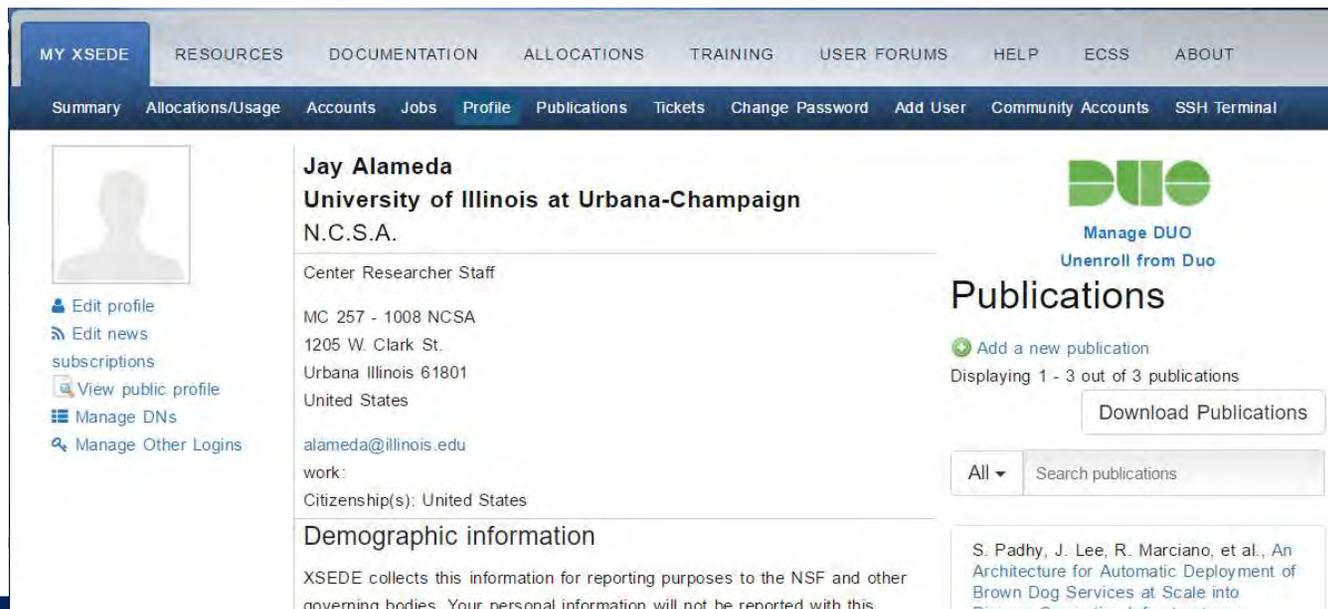


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# Update your XUP User Profile

## MY XSEDE → Profile

- View and or change your user information (organization, address).
- Make sure your email address is correct. XSEDE staff will use it to communicate with you regarding your allocation.



The screenshot shows the XSEDE user profile page for Jay Alameda. The page has a navigation bar at the top with links: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and ABOUT. Below the navigation bar is a sub-menu with links: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH Terminal. The profile information is displayed in a two-column layout. On the left, there is a placeholder for a profile picture and a list of actions: Edit profile, Edit news subscriptions, View public profile, Manage DNSs, and Manage Other Logins. The main profile section includes the name Jay Alameda, affiliation University of Illinois at Urbana-Champaign N.C.S.A., and job title Center Researcher Staff. Contact information includes address (MC 257 - 1008 NCSA, 1205 W. Clark St., Urbana Illinois 61801, United States) and email (alameda@illinois.edu). A section for Demographic information states that XSEDE collects this information for reporting purposes to the NSF and other governing bodies. On the right, there is a DUO logo with links to Manage DUO and Unenroll from Duo, a Publications section with an Add a new publication button, a Download Publications button, and a search bar for publications. A partial publication entry is visible: S. Padhy, J. Lee, R. Marciano, et al., An Architecture for Automatic Deployment of Brown Dog Services at Scale into Diverse Computing Infrastructures.



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# Navigating the XUP



- My XSEDE
- Resources
- Documentation
- Allocations
- Training
- Help
- About

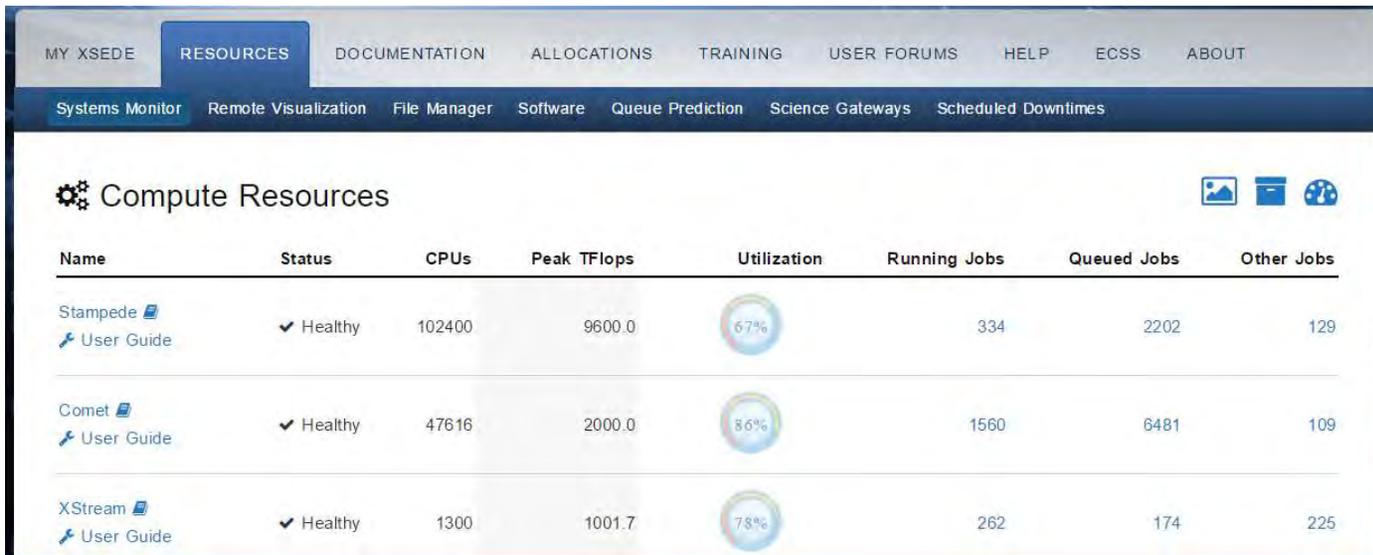


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# View the XSEDE Systems Monitor

- **Resources -> Systems Monitor**

- Provides technical and status information for all of XSEDE's resources.
- The STATUS column indicates whether the system is up or down. If down, can click on status to find when the machine is expected to come back up.



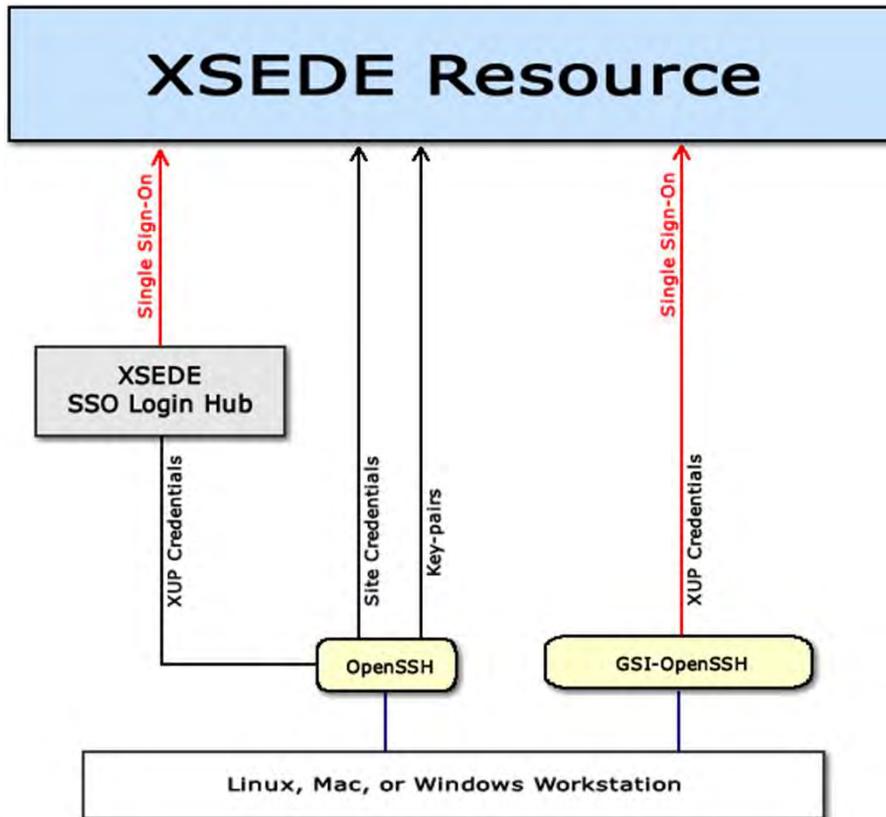
The screenshot shows the XSEDE Systems Monitor interface. The top navigation bar includes links for MY XSEDE, RESOURCES (selected), DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and ABOUT. Below this is a secondary navigation bar with links for Systems Monitor, Remote Visualization, File Manager, Software, Queue Prediction, Science Gateways, and Scheduled Downtimes. The main content area is titled "Compute Resources" and contains a table with the following data:

Name	Status	CPUs	Peak TFlops	Utilization	Running Jobs	Queued Jobs	Other Jobs
Stampede  <a href="#">User Guide</a>	✓ Healthy	102400	9600.0		334	2202	129
Comet  <a href="#">User Guide</a>	✓ Healthy	47616	2000.0		1560	6481	109
XStream  <a href="#">User Guide</a>	✓ Healthy	1300	1001.7		262	174	225



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# Accessing XSEDE Resources



## Authentication Methods

1. Password
  - XUP credentials
  - Site-password
  - One-time password
2. Key-based

## Single Sign-On

- Enables logging in once to access all of your allocated resources

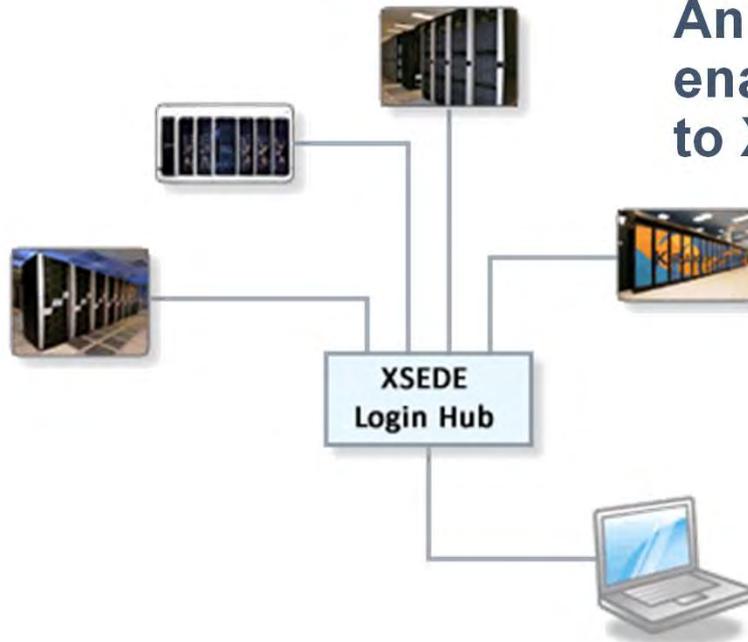
## Connection Methods

1. GSI-OpenSSH
2. OpenSSH



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# XSEDE SSO Login Hub



An Single Sign On (SSO) enabled connection point to XSEDE resources

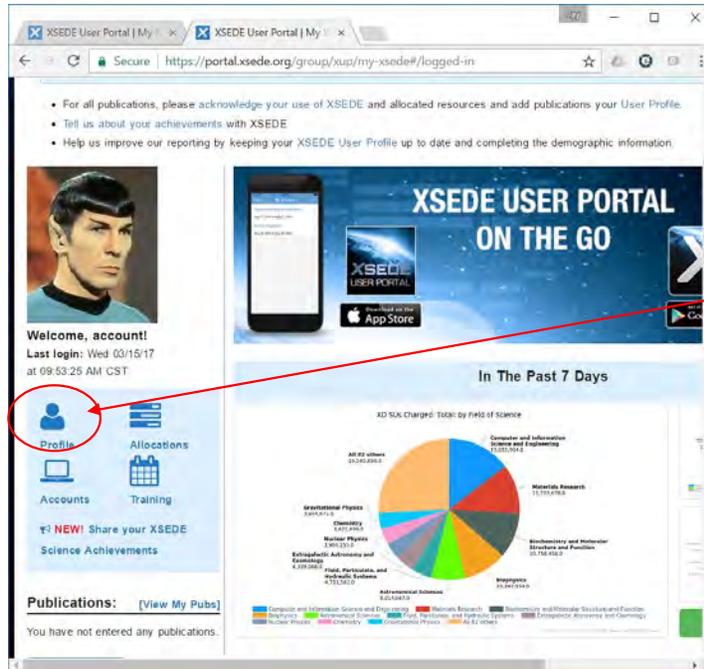
➤ Move among resources using **gssissh** command

➤ SSH to **login.xsede.org** using your XUP credentials with 2 Factor Authentication



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# Set up 2 Factor Authentication

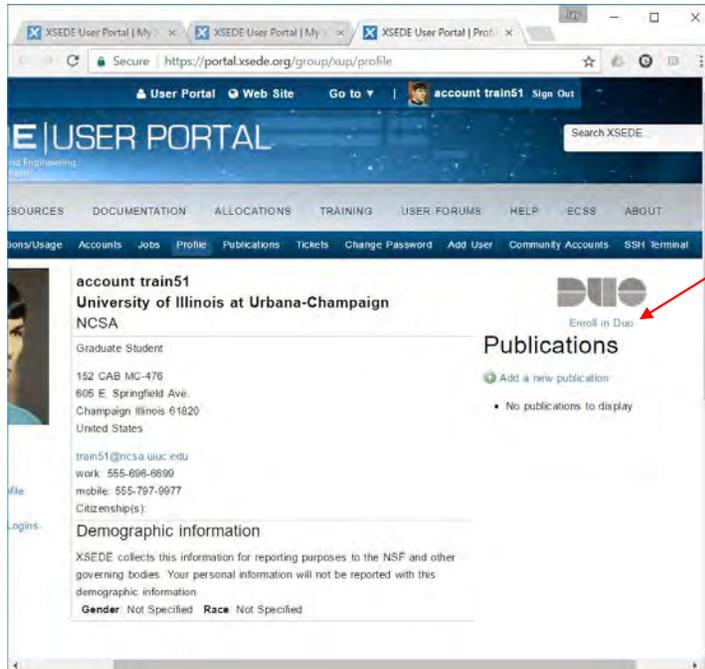


- After logging into the XSEDE User Portal, select your profile



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# Adding 2 Factor Authentication

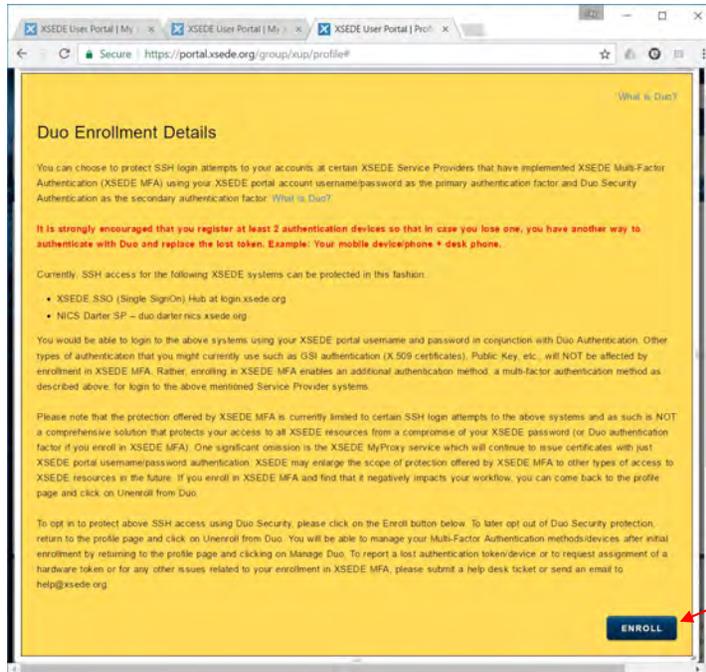


- Enroll in Duo



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# What is Duo?



- Note that DUO 2 Factor Authentication is required for access to the XSEDE Single Signon Hub
  - Select enroll



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# Duo Enrollment:



XSEDE USER PORTAL

Science and Engineering Research Communities

RESOURCES DOCUMENTATION ALLOCATIONS TRAINING USER FORUMS HELP ECSS

Allocations/Usage Accounts Jobs Profile Publications Tickets Change Password Add User Community Accounts

« Back

### Duo Enrollment

To proceed, please verify your XSEDE User Portal password

Password

**SUBMIT**

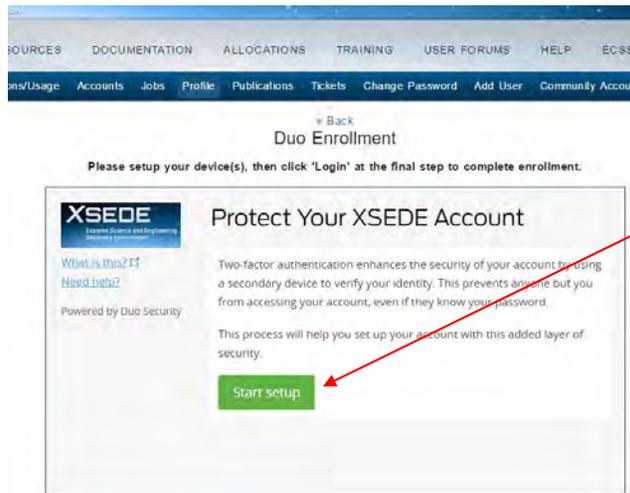
- To verify your identity in your current session, you will need to enter your XSEDE User Portal password



**XSEDE**

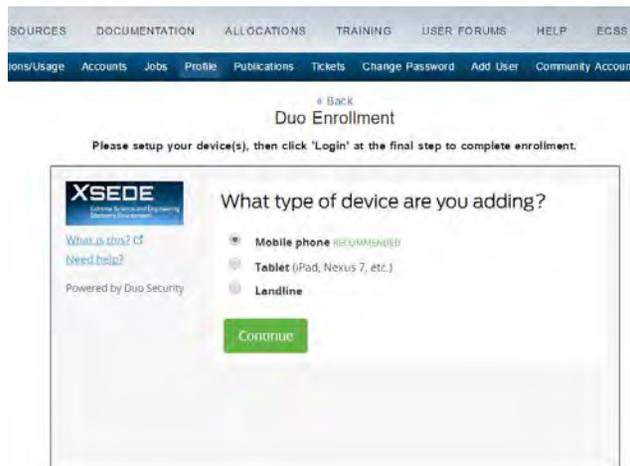
# Setup Duo

- Start the process of setting up 2 factor authentication



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# Choose the device for 2 Factor Auth



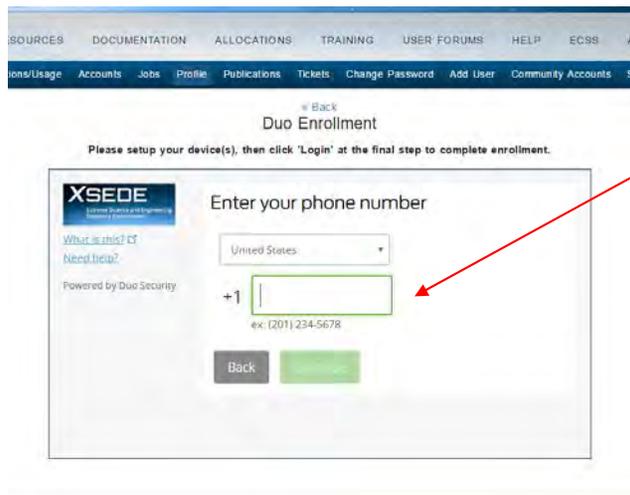
The screenshot shows a web interface for Duo Enrollment. At the top, there is a navigation bar with links: SOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ECSS. Below this is a secondary navigation bar with links: Home/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, and Community Account. The main content area is titled "Duo Enrollment" with a "Back" link. Below the title, it says "Please setup your device(s), then click 'Login' at the final step to complete enrollment." The main form area has the XSEDE logo and the text "What type of device are you adding?". There are three radio button options: "Mobile phone" (RECOMMENDED), "Tablet (Pad, Nexus 7, etc.)", and "Landline". A green "Continue" button is at the bottom. On the left side of the form, there are links for "What is this?", "Need help?", and "Powered by Duo Security".

- Mobile Phone is recommended
  - Tablet, Landline also OK (though not preferred)



# Connect Duo to your phone

- Add phone number
- Continue

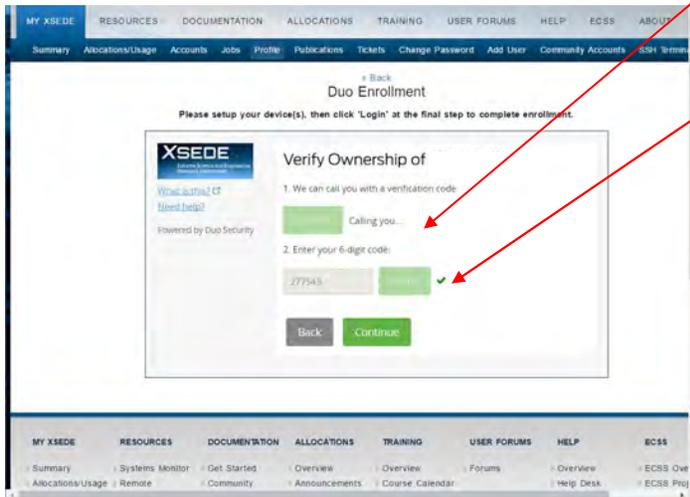


The screenshot shows the XSEDE Duo Enrollment page. At the top, there is a navigation bar with links: SOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and another partially visible link. Below this is a secondary navigation bar with links: Home/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, and Community Accounts. The main heading is "Duo Enrollment" with a "Back" link above it. Below the heading is the instruction: "Please setup your device(s), then click 'Login' at the final step to complete enrollment." The main content area is titled "Enter your phone number" and features the XSEDE logo on the left. To the right of the logo are links for "What is this? CT" and "Need help?". Below these links is the text "Powered by Duo Security". The phone number input section includes a dropdown menu for "United States", a text input field with a green border and a red arrow pointing to it, and a "Back" button. Below the input field is an example: "ex: (201) 234-5678".



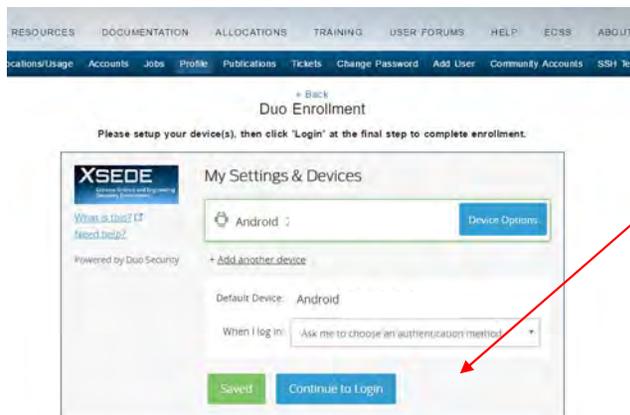
# Verifying phone number ownership

- Duo calls your phone
- Enter code from Duo call to your phone

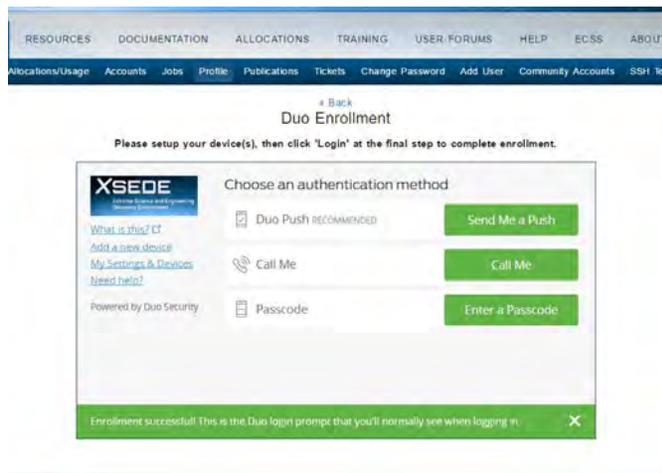


# Download Duo app (if desired)

- Set authentication method (push, text, call)
  - And continue to login



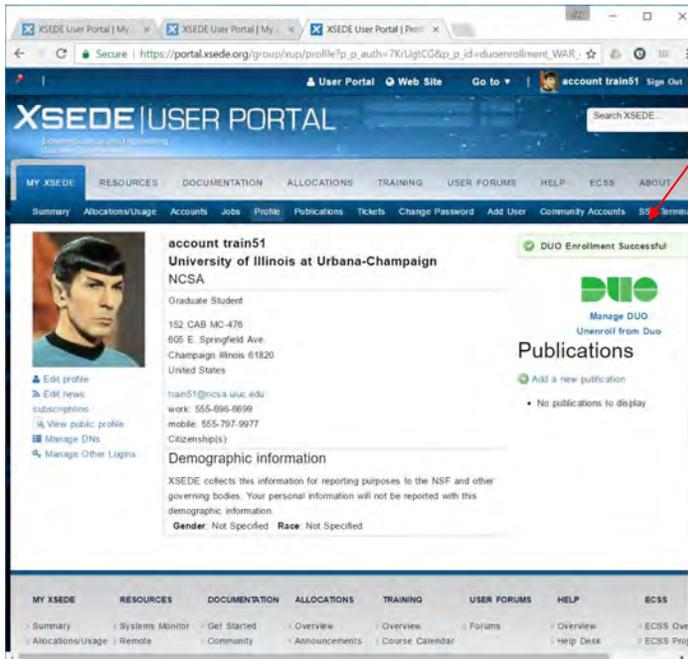
# Choose authentication method



- Duo push (to app)
- Call phone
- Text passcode



# Success!



- Indication of successful setup



# XSEDE

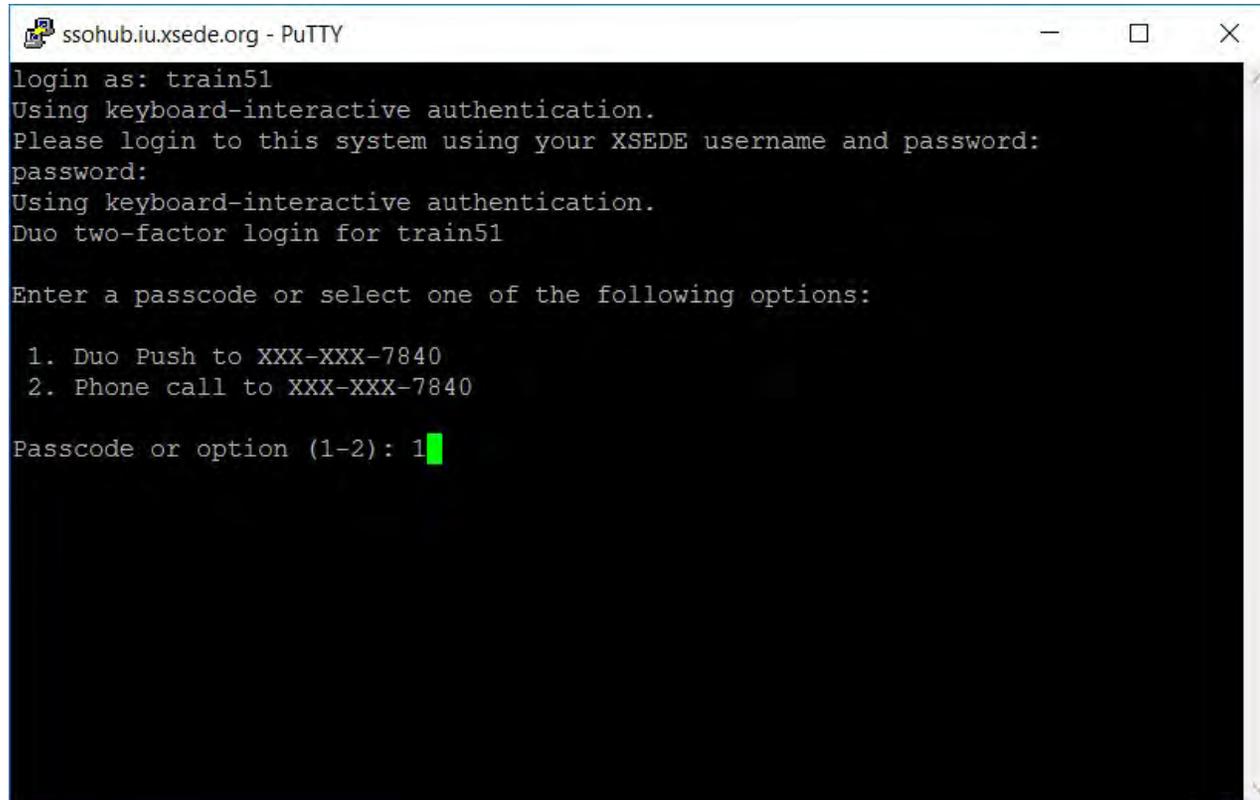
## Following along with today's tutorial:

- Verify that everyone has an ssh client on their laptop!
- For ssh to XSEDE SSO login hub (**today!**)  
*ssh `username@login.xsede.org`*  
*username is your XSEDE User Portal username*
- And from there go to your XSEDE resource, for example:  
*gssh `expance.sdsc.edu`*



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## 2 factor authentication



```
ssohub.iu.xsede.org - PuTTY
login as: train51
Using keyboard-interactive authentication.
Please login to this system using your XSEDE username and password:
password:
Using keyboard-interactive authentication.
Duo two-factor login for train51

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-7840
2. Phone call to XXX-XXX-7840

Passcode or option (1-2): 1
```



# Managing your XSEDE files

## 1. Where to store files

- Home directory
- Scratch directory
- Archival storage

## 2. How to move files

- Command line using globus-url-copy, uberftp, scp, or sftp
- **Globus Online**



# XSEDE File Systems

- **Home directory**

- Location specified in the environment variable \$HOME.
- Use to store project files you want to keep long term such as source code, scripts, and input data sets.
- Not backed up regularly and not purged.
- Quotas typically set to limit amount of disk space available.

- **Scratch directory**

- Location specified in environment variable varies among resources but will include the term SCRATCH, e.g. \$SCRATCH\_DIR.
- Use to temporarily store files produced during application runs.
- Not backed up and routinely purged.
- No quotas. Available space depends on cumulative use by all users.

- **Archival storage**

- Must request through allocation process



# Your XSEDE Compute Environment

- Your default XSEDE compute environment provides access to the compilers, directories, and software you will need to efficiently use your XSEDE resources.
  - Environment: *An area of a computer's memory used by the operating system and some programs to store certain variables to which they need frequent access*
- Customize environment using **Modules**

XSEDE Customizing Environment Tutorial  
<https://portal.xsede.org/web/xup/online-training>



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# Modules Package

- A command line interface used to configure the shell for an application. Two components:
  1. Modulefiles - contain configuration information
  2. **Module command** - interprets modulefiles
- Pre-written modulefiles available for compilers, mpi implementations
- Pre-written modulefiles available for common software, e.g. NAMD, GAMESS



# Module Commands

Module command	Description
<b>module avail [path...]</b>	List all modulefiles available on the system.
<b>module list</b>	List the modulefiles currently loaded in the shell environment.
<b>module help modulefile</b>	Print help information for the <b>modulefile</b> specified in the argument.
<b>module display modulefile</b>	Display the changes made to the environment when the specified modulefile is loaded.
<b>module load modulefile</b>	Interpret the commands contained within the specified modulefile.
<b>module swap modulefile1 modulefile2</b>	Remove the environment changes made by <b>modulefile1</b> and make the changes specified in <b>modulefile2</b> .
<b>module unload modulefile</b>	Remove the environment changes made by <b>modulefile</b> .



# Module Commands Example

```
% module list
```

```
Currently Loaded Modulefiles:
```

```
1) torque/2.3.13_psc  4) icc/14.0.0        7) globus/5.2.2
2) mpt/2.04           5) imkl/10.3.3      8) xdusage/1.0-r7
3) ifort/14.0.0      6) psc_path/1.0
```

```
% module avail gcc
```

```
----- /usr/local/opt/modulefiles -----
gcc/4.3.5 gcc/4.4.6 gcc/4.5.3 gcc/4.6.0 gcc/4.7.2 gcc/4.8.0 gcc/4.8.1
```

```
% module load gcc/4.8.1
```

```
% module list
```

```
Currently Loaded Modulefiles:
```

```
1) torque/2.3.13_psc  5) imkl/10.3.3      9) mpfr/3.1.0
2) mpt/2.04           6) psc_path/1.0    10) gmp/5.0.5
3) ifort/14.0.0      7) globus/5.2.2   11) mpc/0.8.2
4) icc/14.0.0        8) xdusage/1.0-r7  12) gcc/4.8.1
```

```
% module unload gcc
```

```
% module list
```

```
Currently Loaded Modulefiles:
```

```
1) torque/2.3.13_psc  4) icc/14.0.0        7) globus/5.2.2
2) mpt/2.04           5) imkl/10.3.3      8) xdusage/1.0-r7
3) ifort/14.0.0      6) psc path/1.0
```



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## Moving Files - Globus

- A fast, reliable, and secure file transfer service geared to the big data needs of the research community.
- Moves terabytes of data in thousands of files
- Automatic fault recovery
- Easy to use
- No client software installation
- Consolidated support and troubleshooting
- Supports file transfer to any machine
- Accounts are free - <https://www.globus.org/>



# Globus Dashboard

The screenshot shows the Globus website dashboard. At the top left is the Globus logo. To its right is a navigation menu with links: "I Want To...", "Pricing", "Resources", "Support", "About", and a "Log In" button. The main content area features a dark blue background with a network diagram. On the left, there are four icons representing data types: "HIPAA (with BAA)", "PHI", "PII", and "CONTROLLED UNCLASSIFIED". Each icon is a blue cylinder with a green padlock, indicating protection. To the right of these icons, the text reads: "Protected Data Support", "Working with PHI, PII, or CUI?", "Need to manage HIPAA-regulated data?", and "Globus has you covered!". Below this text are two buttons: "LEARN MORE" and "REQUEST PRICING". At the bottom of the dashboard, the text "Research data management simplified." is displayed above four icons and labels: "TRANSFER", "SHARE", "PUBLISH", and "BUILD".



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# Login to use Globus Web App

Log In using Globus

https://auth.globus.org/p/login?redirect\_uri=%2Fv2%2Foauth2%2Fauthorize%3Fclient\_id%3D89ba3e72...

globus Globus Account Log In

## Log in to use Globus Web App

Use your existing organizational login

e.g., university, national lab, facility, project

XSEDE

Didn't find your organization? Then use **Globus ID** to sign in. (What's this?)

Continue

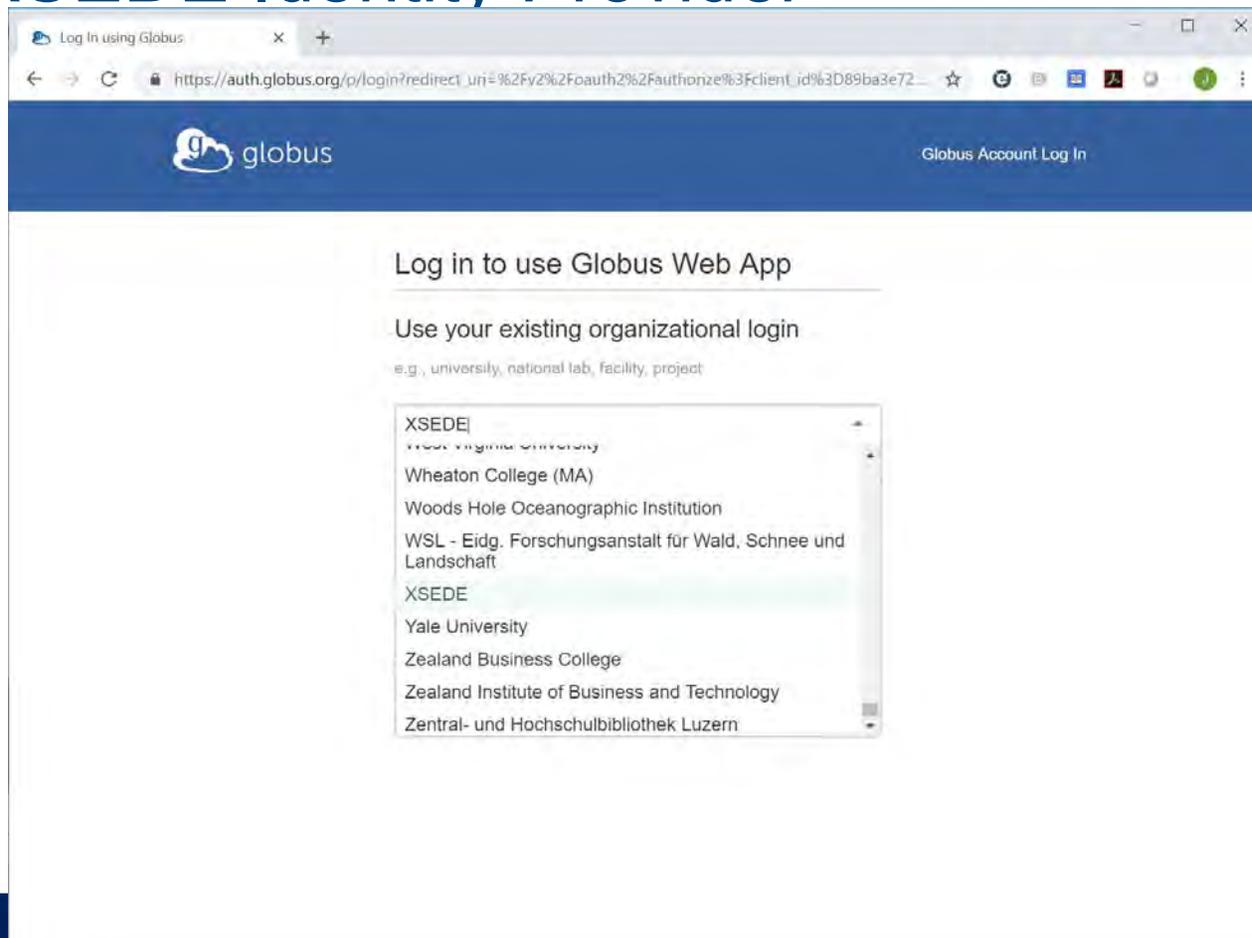
Or

Sign in with Google Sign in with ORCID.ID



XSEDE

# Use XSEDE Identity Provider



XSEDE

# Sign in with XSEDE credentials

XSEDE  
Extreme Science and Engineering  
Discovery Environment

Welcome to the XSEDE's Client Authorization Page

Science Gateway Access  
The XSEDE Science Gateway or Service below is requesting access to your XSEDE account. If you approve, please sign in with your XSEDE username and password.

Note: Only members of active XSEDE project allocations will be able to sign in on this page.

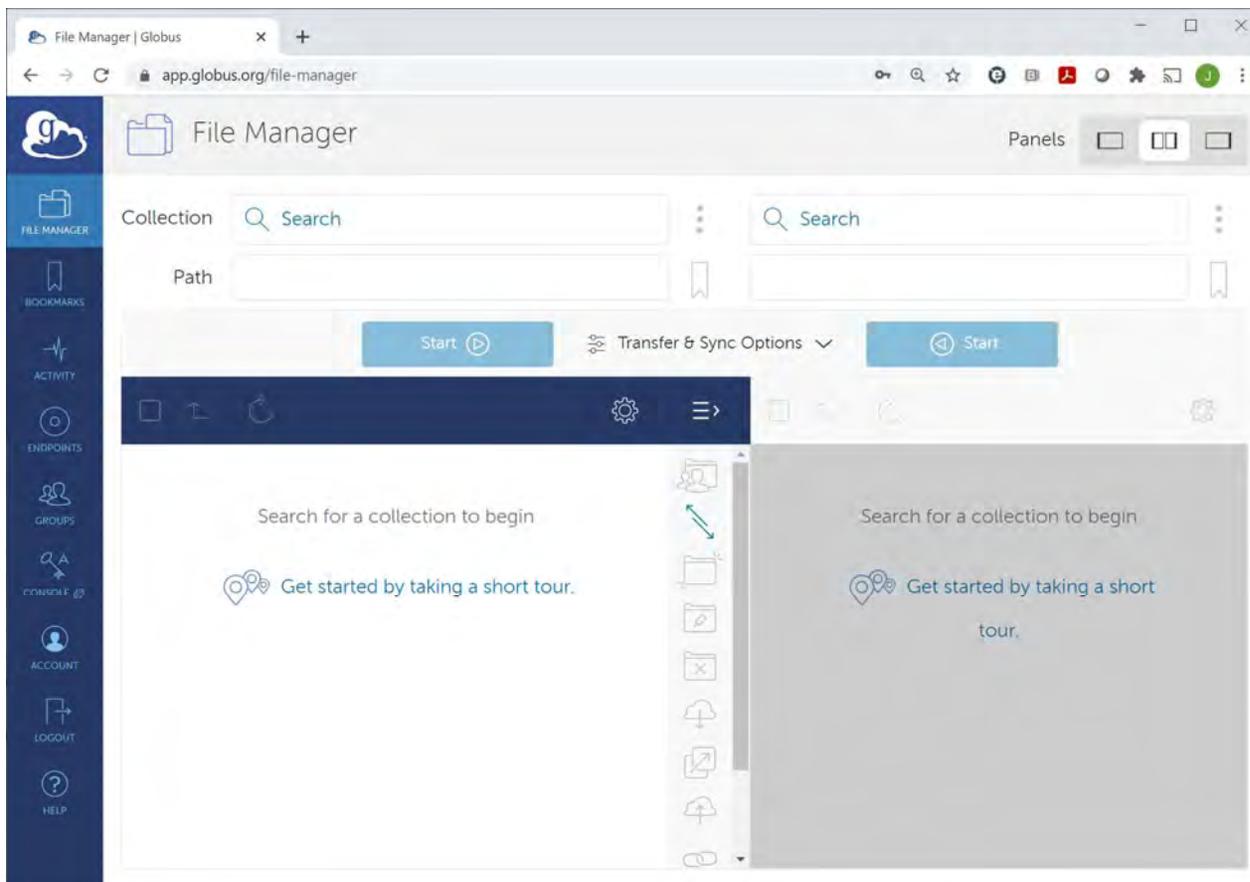
SCIENCE GATEWAY INFORMATION	SIGN IN
The XSEDE Science Gateway listed below is requesting access to your XSEDE account. If you approve, please sign in.  <i>Name:</i> Globus <i>URL:</i> <a href="http://www.globus.org/">http://www.globus.org/</a>	Username <input type="text"/> Password <input type="password"/>
	<input type="button" value="SIGN IN"/> <input type="button" value="CANCEL"/>

Please send any questions or comments about this site to [help@xsede.org](mailto:help@xsede.org)



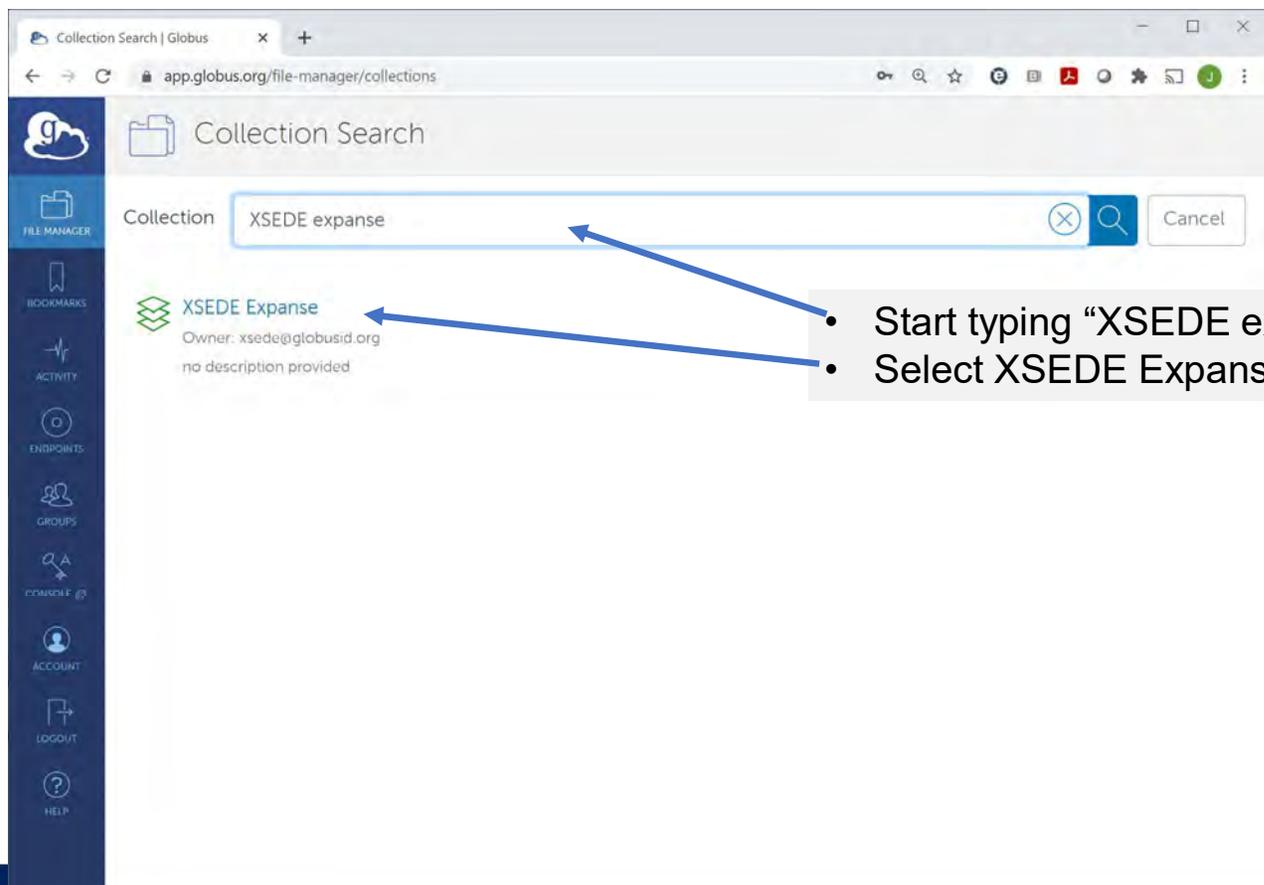
XSEDE

# Globus Online File Transfer



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# Start by typing one endpoint



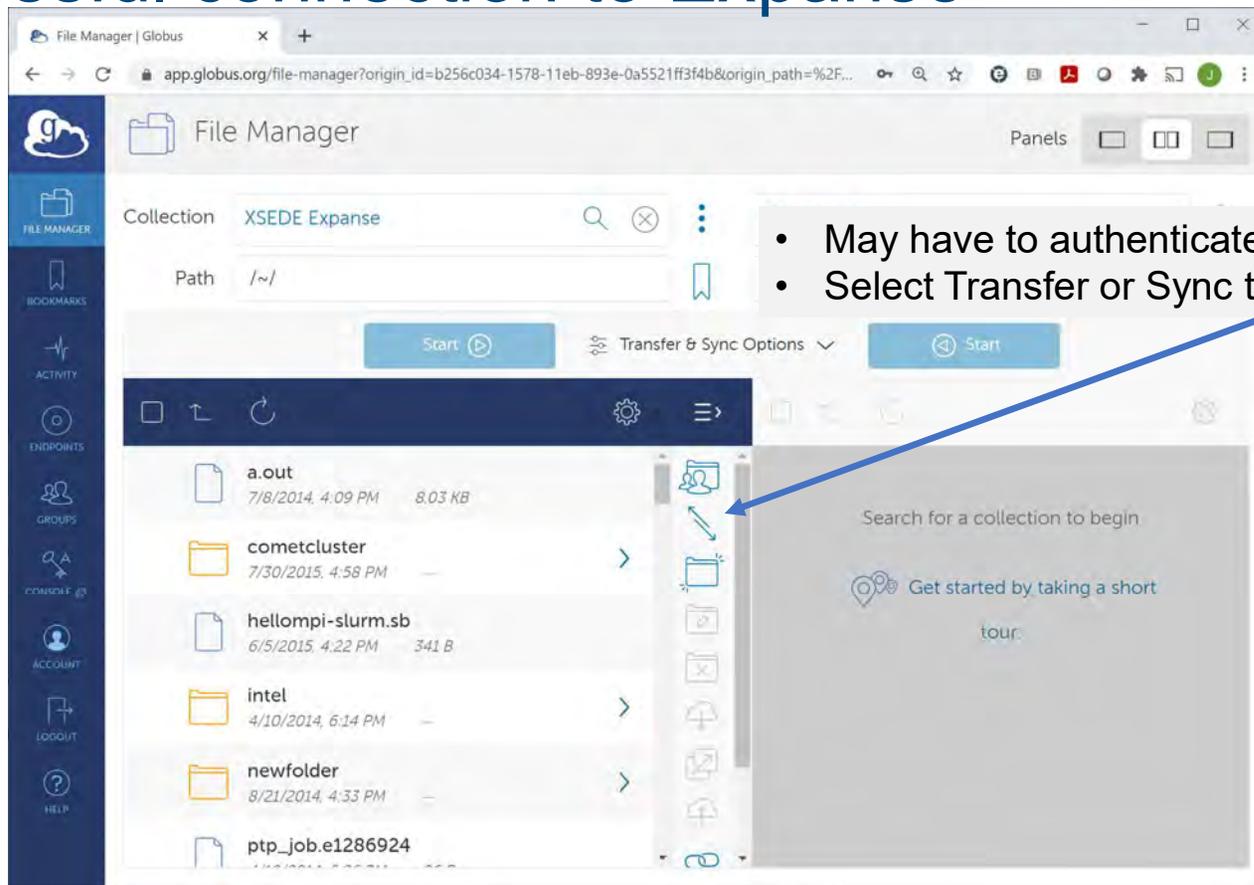
The screenshot shows a web browser window with the URL `app.globus.org/file-manager/collections`. The page title is "Collection Search | Globus". The main content area shows a search bar with the text "XSEDE expanse" and a search button. Below the search bar, a result is displayed: "XSEDE Expanse" with the owner "xsede@globusid.org" and "no description provided". A vertical sidebar on the left contains navigation icons for FILE MANAGER, BOOKMARKS, ACTIVITY, ENDPOINTS, GROUPS, CONSOLE, ACCOUNT, LOGOUT, and HELP. A callout box on the right contains two bullet points: "Start typing 'XSEDE expanse'" and "Select XSEDE Expanse". Blue arrows point from the callout box to the search input and the search result.

- Start typing "XSEDE expanse"
- Select XSEDE Expanse



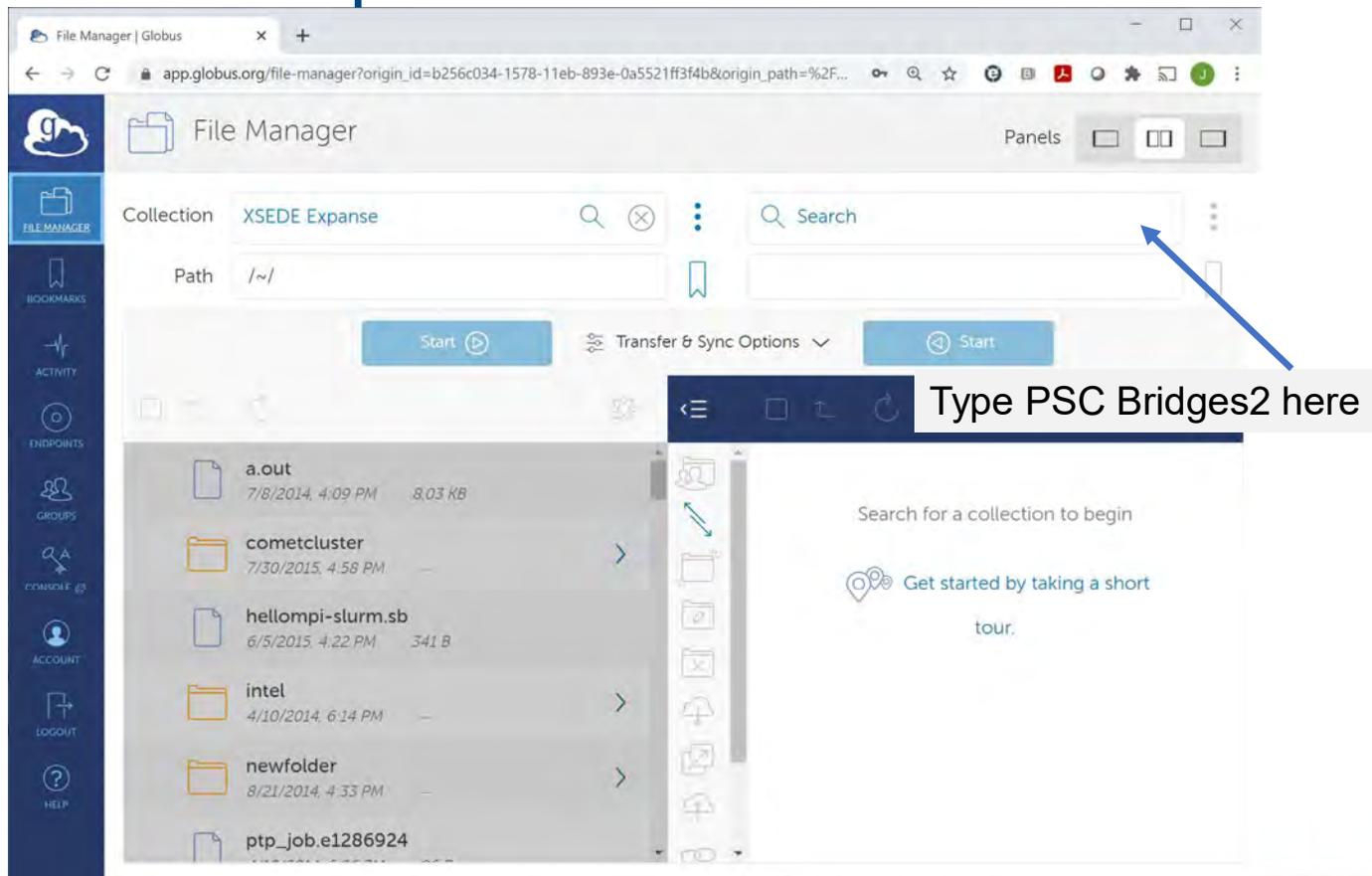
XSEDE

# Successful connection to Expanse



XSEDE

# Add second endpoint

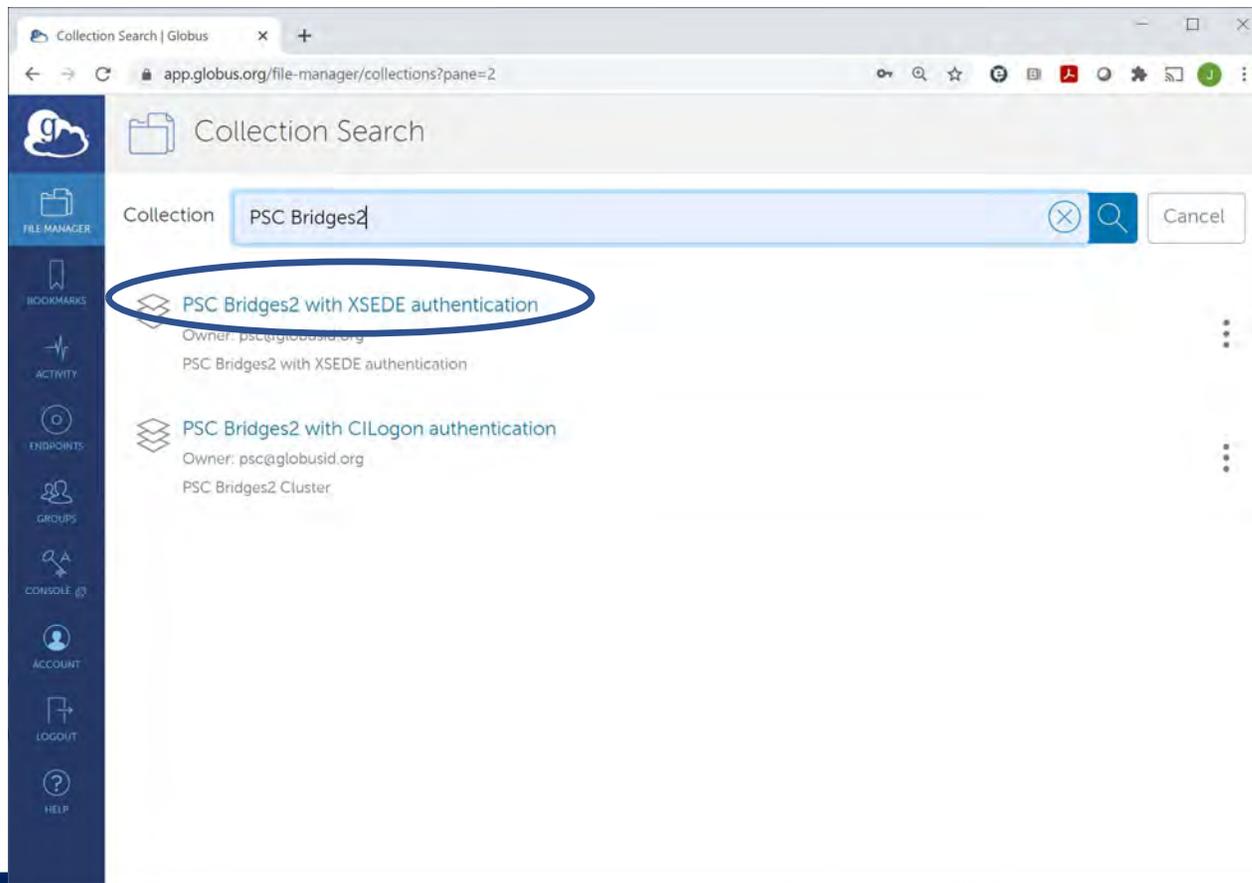


The screenshot shows the Globus File Manager interface. The browser address bar displays the URL: `app.globus.org/file-manager?origin_id=b256c034-1578-11eb-893e-0a5521ff3f4b&origin_path=%2F...`. The main interface includes a sidebar with navigation options like FILE MANAGER, BOOKMARKS, ACTIVITY, ENDPOINTS, GROUPS, COMMONLY @, ACCOUNT, LOGOUT, and HELP. The main content area shows the 'Collection' set to 'XSEDE Expanse' and the 'Path' as '/~/'. A search bar is visible with the text 'Search'. A blue arrow points to the search bar with a text box that says 'Type PSC Bridges2 here'. Below the search bar, there are 'Start' buttons and a 'Transfer & Sync Options' dropdown. A list of files and folders is displayed, including 'a.out', 'cometcluster', 'hellompi-slurm.sb', 'intel', 'newfolder', and 'ptp\_job.e1286924'. A modal window is open on the right, prompting the user to 'Search for a collection to begin' and 'Get started by taking a short tour.'



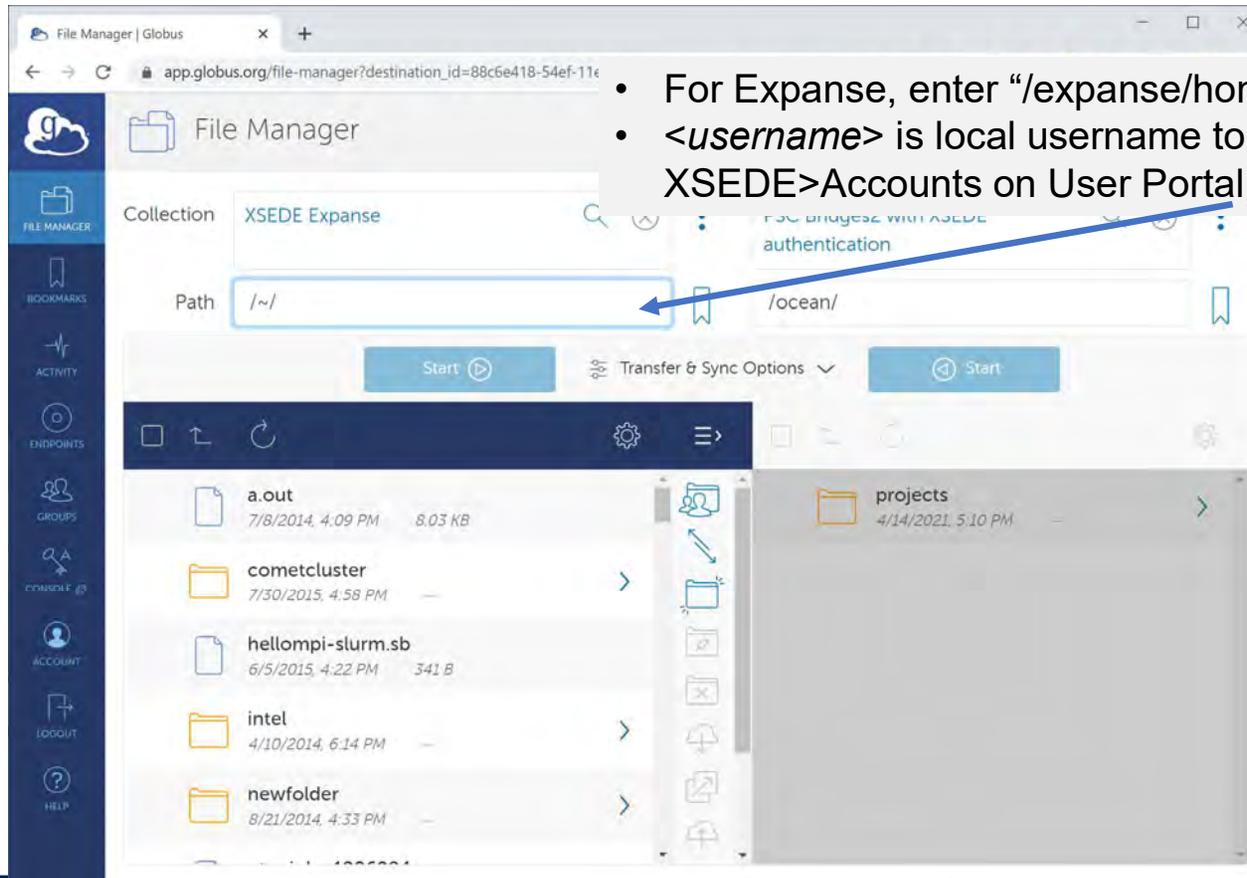
XSEDE

# Select Bridges2, XSEDE Authentication



XSEDE

# Need to get to your home directory on both systems



The screenshot shows the Globus File Manager interface. The 'Path' field is highlighted with a blue box and contains the text '/~/'. A blue arrow points from the text in the callout box to this field. The interface displays a list of files and folders, including 'a.out', 'cometcluster', 'hellompi-slurm.sb', 'intel', and 'newfolder'. A 'projects' folder is also visible on the right side of the interface.

- For Expanse, enter “/expanse/home/<username>” here
- <username> is local username to expanse (recall My XSEDE>Accounts on User Portal)

# Need to get to your home directory on both systems

File Manager | Globus

app.globus.org/file-manager?destination\_id=88c6e418-54ef-11e...

• For Bridges2, enter “/~/>” here

File Manager

Collection XSEDE Expand PSC Bridges2 with XSEDE authentication

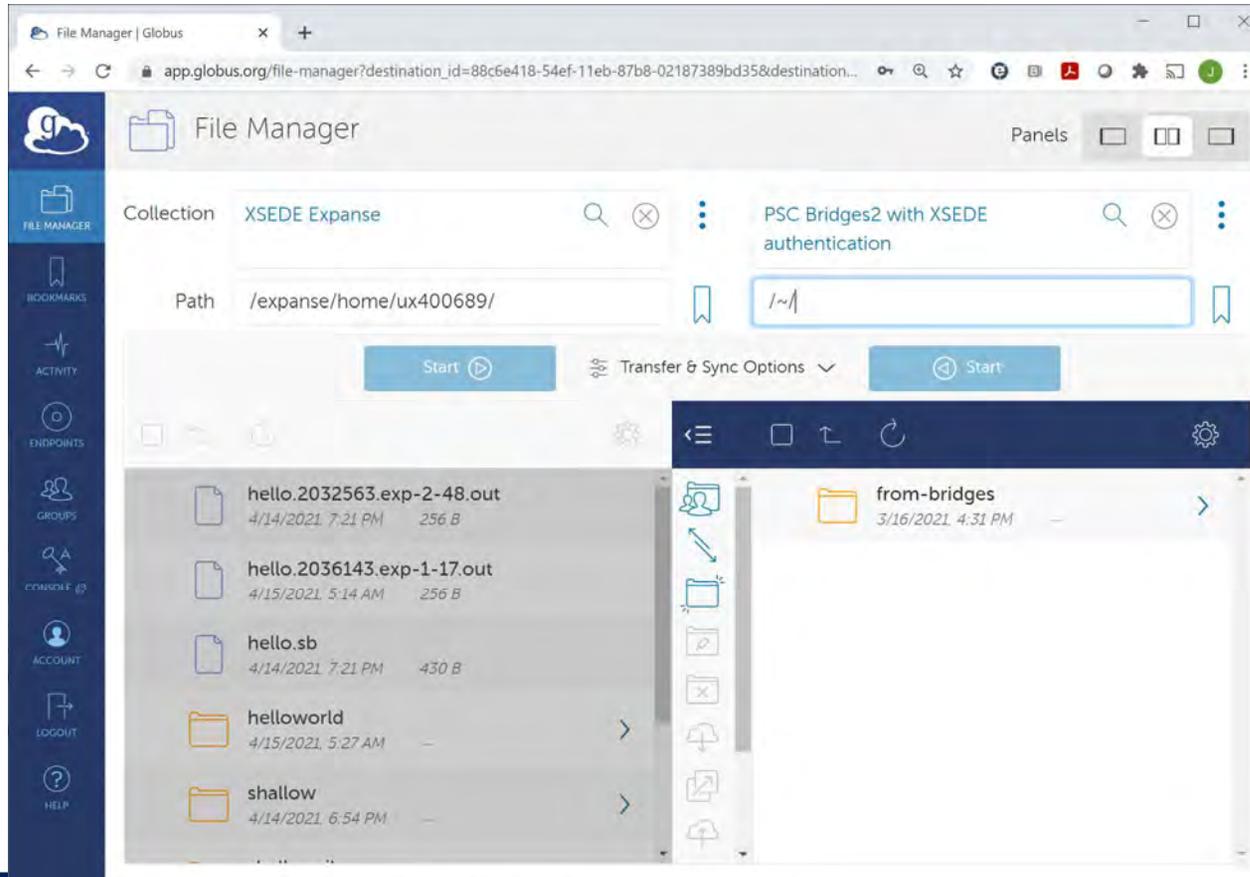
Path /~/ /ocean/

Start Transfer & Sync Options Start

Name	Created	Size
a.out	7/8/2014, 4:09 PM	8.03 KB
cometcluster	7/30/2015, 4:58 PM	—
hellompi-slurm.sb	6/5/2015, 4:22 PM	341 B
intel	4/10/2014, 6:14 PM	—
newfolder	8/21/2014, 4:33 PM	—

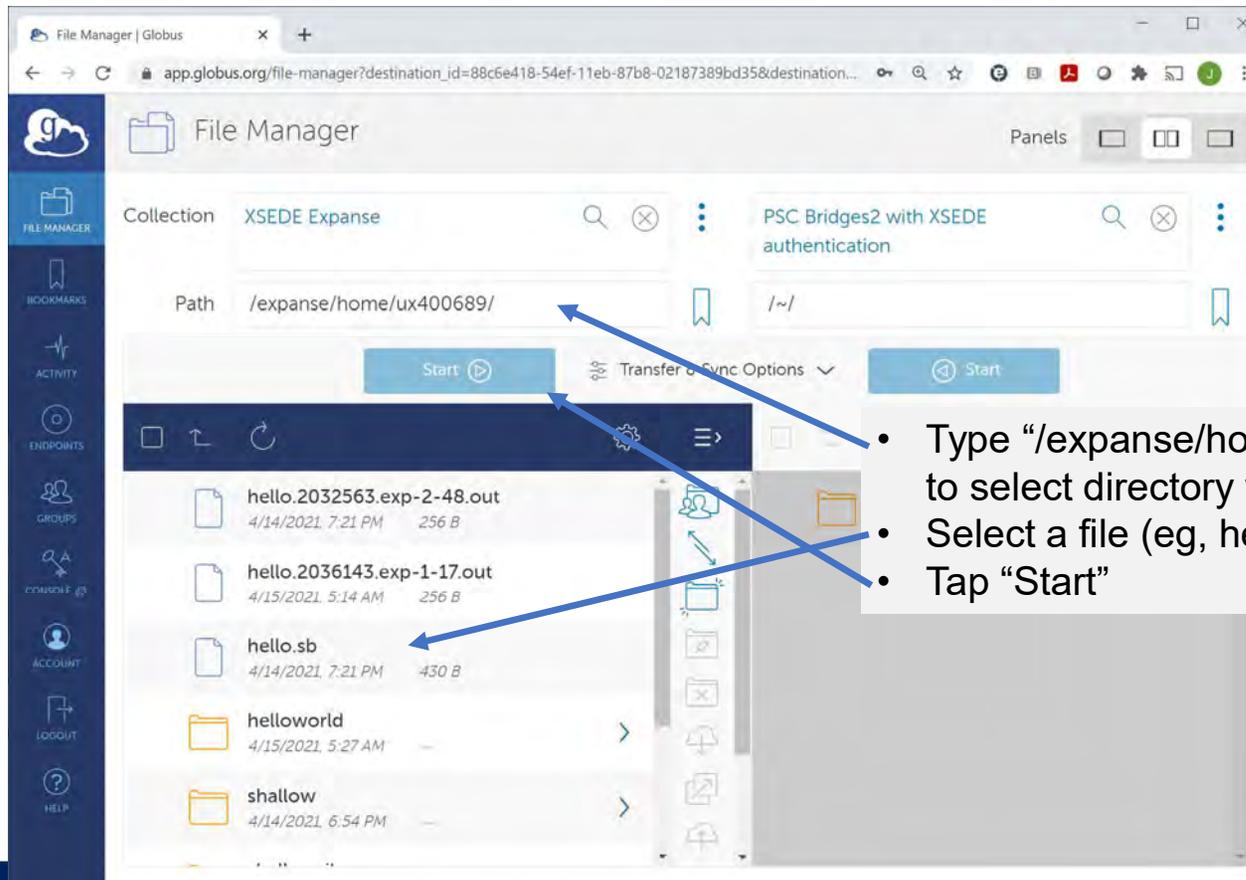
projects  
4/14/2021, 5:10 PM

# Now have directory listings for both systems



XSEDE

# Select file to move

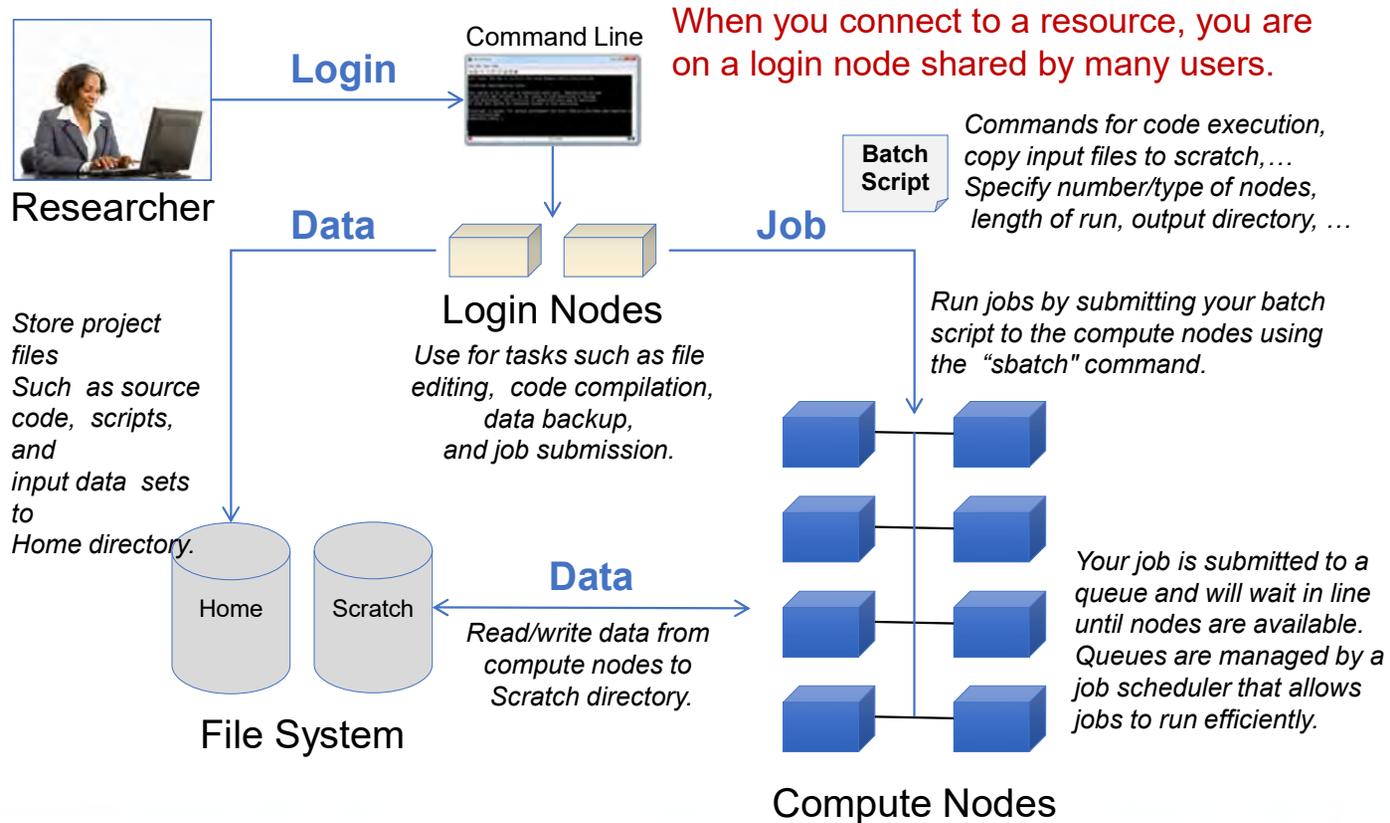


- Type `"/expance/home/ux400689"` to select directory with files
- Select a file (eg, hello.sb)
- Tap "Start"



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# Running Jobs Overview



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# Login Nodes

- When you login to an XSEDE resource, you connect to a login node.
- Use login nodes for basic tasks such as file editing, code compilation, data backup, and job submission.
- Do not run compute jobs on the login nodes.

Where do I run  
compute jobs?



**XSEDE**

# Running Compute Jobs

- Jobs are run on the **compute nodes** by submitting a **batch script** on a login node
- All jobs are placed in a **batch queue** after they are submitted.
- All XSEDE compute resources use a **batch scheduler** for running jobs.
- Resource User Guides on the XUP have details on your system's scheduler.



# Batch Schedulers

- Attempt to balance queue wait times of competing jobs with efficient system utilization.
  - Job prioritization influenced by number of cores and wall clock time requested
  - FIFO queues with fair use mechanisms to keep a single user from dominating the queue
  - Backfilling unused nodes with smaller jobs
- Will not start jobs if they will not finish before scheduled system maintenance.



# Batch Scripts

- Batch scripts include scheduler specific directives, comments, and executable commands, e.g.:
  - Number and type of nodes needed
  - Time needed to run the job
  - Where to write output files
- Script commands are system specific – see the resource’s User Guide on the XUP for details



## Running batch jobs on XSEDE resources

- XSEDE compute resources use a batch scheduler to submit, monitor and cancel jobs
- Although there are several widely used schedulers (LSF, Torque, Slurm) all XSEDE compute resources now use Slurm
- Configuration details vary from site to site (see User Portal Resource Guides), but basic functionality is consistent
  - **sbatch** to submit jobs
  - **squeue** to view information about jobs
  - **scancel** to cancel jobs
  - **sinfo** to view information about nodes and partitions
- See [slurm.schedmd.com/](http://slurm.schedmd.com/) for more details



## sbatch – submit a batch script to Slurm

- Arguments are generally specified in a batch script, but can also be set on command line

```
$ sbatch myjobscript
```

- Key parameters include
  - Number of nodes
  - Number of tasks/node or total number of tasks
  - Partition (queue)
  - Job duration
  - Job name
  - Account
- See [slurm.schedmd.com/sbatch.html](http://slurm.schedmd.com/sbatch.html) for more details



## SBATCH – basic job script

```
#!/bin/bash
#SBATCH --job-name="hellompi"
#SBATCH --nodes=8
#SBATCH --ntasks-per-node=24
#SBATCH --time=1:00:00

srun -n 192 ./hellompi.exe
```

} Job specification

} Executable statements



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## sbatch – basic job script

```
#!/bin/bash
#SBATCH -J "hellompi"
#SBATCH -N 8
#SBATCH --ntasks-per-node=24
#SBATCH -t 1:00:00

srun -n 192 ./hellompi.exe
```

} Job specification

} Executable statements

In the previous slide, we used the long form for the options. Slurm also provides abbreviations for some (not all) options



**XSEDE**

## SBATCH – selecting an account

- As a new user, you will probably have access to a single account (allocation)
- If you are on multiple allocations, be sure to explicitly specify the account that you want to charge to – the default won't necessarily be what you expect
- **This is mandatory on [expansion.sdsc.edu](https://expansion.sdsc.edu) (new!)**

```
#SBATCH --account=<account>  
-- or --  
#SBATCH -A <account>
```



## sbatch – improving your turnaround time

- Try to be as accurate as possible in estimating the wall time for your jobs
- But don't underestimate the time since your job will be killed if you exceed the time limit and any results that have not been checkpointed will be lost
- Note that the default wall time is normally set to the maximum wall time
- Slurm uses a strategy call backfill to improve throughput
- The scheduler can “loan out” nodes that are being held for a pending parallel job as long as the duration of the loan is less than time remaining until all nodes are available



## queue – monitor jobs

- With queue, you can monitor the state of jobs that had been submitted to the queues.
- Without any arguments, queue returns information on the job status for all users. In most cases you will probably want to restrict to yourself using the -u option
- Many options for formatting output and restricting to particular job states, partitions or job ids
- See [slurm.schedmd.com/queue.html](http://slurm.schedmd.com/queue.html) for more details



## queue – monitor jobs

```
$ queue
JOBID PARTITION      NAME      USER  ST      TIME  NODES NODELIST(REASON)
18912381 gpu-share      bash     rynlm PD      0:00      1 (Resources)
18941470 gpu-share      efe      rbnjko PD      0:00      1 (Priority)
18937286 gpu-share      aout     xyzj   PD      0:00      1 (Dependency)
18915882  compute      dask     willc97 PD      0:00      8 (Dependency)
18911406  compute  NGBW-JOB  cipres  R  3-17:30:45      2 comet-26-[01-02]
18918197  shared  NGBW-JOB  cipres  R  1-06:30:41      1 comet-08-16
```

- For running jobs (state R), queue lists the nodes being used
- For pending jobs (state PD), queue states why job is not running
- Other job states include Completing (CG), Failed (F) and Cancelled (CA). See queue documentation for full list
- **Helpful Tip: queue -u *username* lists only your jobs!**



## scancel – cancel jobs

- Slurm allows you to cancel jobs that are running or queued
- Use `squeue` to find jobid
- Comes in handy if you realize job is not progressing as expected, wrong input files were used, etc.

```
$ scancel jobid [jobid] [jobid]  
$ scancel -u username # cancel all my jobs
```

- See [slurm.schedmd.com/scancel.html/](http://slurm.schedmd.com/scancel.html/) for more details



## Site specific batch scheduling details

We touched briefly on batch scheduling and the generic Slurm command, but many of the details are site specific

- Partition names
- Maximum job sizes and wall times
- Scheduler tuning (e.g. optimized for throughput vs. large jobs)
- Ability to run shared jobs (e.g. use less than all core on node)

See the Stampede2, Expanse, Bridges2 and other user guides for more information



**XSEDE**

## Common problems encountered when running jobs:

- Invalid number of cores were requested
- Job runs out of CPU time
- Files can't be found
- Inadequate software permissions



# Managing Your Environment: **Modules**

Allows you to manipulate your environment.

- **'module list'** shows currently loaded modules.
- **'module avail'** shows available modules.
- **'module load'** <name> loads desired module
- **'module swap'** <name1> <name2> unloads <name1> and loads <name2>
- **'module show'** <name> describes module.

Full documentation:

<https://buildmedia.readthedocs.org/media/pdf/lmod/latest/lmod.pdf>



**XSEDE**

# Quick module demo

```
[ux400689@login02 ~]$ module list
```

Currently Loaded Modules:

1) shared 2) cpu/0.15.4 3) DefaultModules 4) gcc/10.2.0 5) slurm/expense/20.02.3

```
[ux400689@login02 ~]$ which gcc
```

```
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1/gcc-10.2.0-n7su7jf54rc7l2ozegds5xksy6qhrjin/bin/gcc
```

```
[ux400689@login02 ~]$ module swap gcc/10.2.0 gcc/9.2.0
```

The following have been reloaded with a version change:

1) gcc/10.2.0 => gcc/9.2.0

```
[ux400689@login02 ~]$ which gcc
```

```
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1/gcc-9.2.0-w7xm5ba2an66khz7wjkjnocbdhmou2qb/bin/gcc
```

```
[ux400689@login02 ~]$ module unload gcc
```

```
[ux400689@login02 ~]$ which gcc
```

```
/usr/bin/gcc
```

## And which gcc is /usr/bin/gcc?

- Operating system default gcc:

```
[ux400689@login02 ~]$ gcc -v
```

```
Using built-in specs.
```

```
COLLECT_GCC=gcc
```

```
COLLECT_LTO_WRAPPER=/usr/libexec/gcc/x86_64-redhat-linux/8/lto-wrapper
```

```
OFFLOAD_TARGET_NAMES=nvptx-none
```

```
OFFLOAD_TARGET_DEFAULT=1
```

```
Target: x86_64-redhat-linux
```

```
Configured with: ../configure --enable-bootstrap --enable-languages=c,c++,fortran,lto --  
prefix=/usr --mandir=/usr/share/man --infodir=/usr/share/info --with-  
bugurl=http://bugzilla.redhat.com/bugzilla --enable-shared --enable-threads=posix --enable-  
checking=release --enable-multilib --with-system-zlib --enable-__cxa_atexit --disable-  
libunwind-exceptions --enable-gnu-unique-object --enable-linker-build-id --with-gcc-major-  
version-only --with-linker-hash-style=gnu --enable-plugin --enable-initfini-array --with-isl  
--disable-libmpx --enable-offload-targets=nvptx-none --without-cuda-driver --enable-gnu-  
indirect-function --enable-cet --with-tune=generic --with-arch_32=x86-64 --build=x86_64-  
redhat-linux
```

```
Thread model: posix
```

```
gcc version 8.3.1 20190507 (Red Hat 8.3.1-4) (GCC)
```

## For the following exercise (same steps as before):

- Check to see if connection is still live, if not:
- For ssh to XSEDE SSO login hub (**today!**)  
*ssh `username@login.xsede.org`*  
*username is XSEDE User Portal username*
- And from there go to your XSEDE resource, for example:  
*gssh `expanse`*



**XSEDE**

# SDSC Expanse Cluster & Modules

- Default environment gcc compilers, no MPI implementation
- We will add openmpi library (issue the commands below)

```
module load openmpi  
which mpicc
```



# SDSC Expanse Cluster & Modules

- Default environment gcc compilers, no MPI implementation
- We will add openmpi library (issue the commands below)

```
module load openmpi  
which mpicc
```

```
[ux400689@login02 ~]$ module load openmpi  
[ux400689@login02 ~]$ which mpicc  
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-  
10.2.0/openmpi-4.0.4-  
g62qv7hwmzegprnzni6cjbvombwxu3cu6/bin/mpicc
```



# Module demo on expanse

```
[ux400689@login02 ~]$ module list
```

Currently Loaded Modules:

```
1) shared 2) cpu/0.15.4 3) DefaultModules 4) gcc/10.2.0 5)
slurm/expanse/20.02.3
```

```
[ux400689@login02 ~]$ module load openmpi
```

```
[ux400689@login02 ~]$ which mpicc
```

```
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-10.2.0/openmpi-4.0.4-
g62qv7hwmzegprnzni6cjevombwxu3cu6/bin/mpicc
```

```
[ux400689@login02 ~]$ module list
```

Currently Loaded Modules:

```
1) shared 2) cpu/0.15.4 3) DefaultModules 4) gcc/10.2.0 5)
slurm/expanse/20.02.3 6) openmpi/4.0.4
```



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## Exercise

- Make sure you are on `expanse.sdsc.edu`
- Run the `hello_world` sample code provided
- No input file needed
- Copy batch script from my home directory:  

```
cp ~ux400689/hello.sb .
```
- *Note the period at the end of the command, this means “my current directory”*



# Job script

```
#!/bin/bash
#SBATCH --job-name="hello"
#SBATCH --output="hello.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=4
#SBATCH --mem=4G
#SBATCH --account=uic410
#SBATCH --export=ALL
#SBATCH -t 00:05:00
```

```
#This job runs with 1 nodes, 4 cores per node for a total of 4 cores
module purge
module load cpu
module load gcc
module load openmpi
module load slurm
srun -n 4 ~ux400689/helloworld/mpi_hello_world
```



## Exercise:

- Submit the job  
`sbatch hello.sb`
- Monitor the job (`squeue -u username`)
- Make sure you have the output files at job completion

```
[ux400689@login02 ~]$ ls
hello.2032563.exp-2-48.out  hello.sb      shallow      shallow-ihpcss.sb
hello.2036143.exp-1-17.out helloworld  shallow-ihpcss shallow-slurm.sb
[ux400689@login02 ~]$
```

`more hello*.out` (for this case, yours will be different!)



## Output files: need to show successful completion

```
[ux400689@login02 ~]$ more hello.2036143.exp-1-17.out
Hello world from processor exp-1-17, rank 2 out of 4 processors
Hello world from processor exp-1-17, rank 0 out of 4 processors
Hello world from processor exp-1-17, rank 1 out of 4 processors
Hello world from processor exp-1-17, rank 3 out of 4 processors
```

This example shows that we ran on node exp-1-17,  
using 4 processor (cores) on that node



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## More “helpful” resources

xsede.org → User Services

- Resources available at each Service Provider
  - User Guides describing memory, number of CPUs, file systems, etc.
  - Storage facilities
  - Software (Comprehensive Search)
- Training: [portal.xsede.org](http://portal.xsede.org) → Training
  - Course Calendar
  - On-line training
- Get face-to-face help from XSEDE experts at your institution; contact your local Campus Champions.
- Extended Collaborative Support



**XSEDE**

## Need help? Reporting and Tracking Issues

- [portal.xsede.org](https://portal.xsede.org) → Help  
Submit ticket
- [portal.xsede.org](https://portal.xsede.org) → My XSEDE → Tickets
  - Submit ticket
  - View past tickets (both open and closed)
- Can also email [help@xsede.org](mailto:help@xsede.org) or call 1-866-907-2383, at any hour (24/7)



**XSEDE**

# XSEDE Training Survey

- After the end of this training, you will receive a link to a survey by email. Please complete this survey, *we value your feedback*, and will use your input to help improve our training offerings.
- Slides from this workshop will be available at <http://hpcuniversity.org/trainingMaterials/253/>



**XSEDE**

**Thanks for listening and  
welcome to XSEDE!**

**XSEDE**

Extreme Science and Engineering  
Discovery Environment



Supported by OAC 15-48562.

Additional slides to set up Globus Connect for transfers to your laptop

# Globus Dashboard

The screenshot shows the Globus website dashboard. At the top left is the Globus logo. To its right is a navigation menu with links: "I Want To...", "Pricing", "Resources", "Support", "About", and a "Log In" button. The main content area features a dark blue background with a network diagram. On the left, there are four icons representing data types: "HIPAA (with BAA)", "PHI", "PII", and "CONTROLLED UNCLASSIFIED". Each icon is a blue cylinder with a green checkmark and a lock symbol. To the right of these icons, the text reads: "Protected Data Support", "Working with PHI, PII, or CUI?", "Need to manage HIPAA-regulated data?", and "Globus has you covered!". Below this text are two buttons: "LEARN MORE" and "REQUEST PRICING". At the bottom of the dashboard, the text "Research data management simplified." is displayed above four icons with labels: "TRANSFER", "SHARE", "PUBLISH", and "BUILD".



**XSEDE**

# Login to use Globus Web App

Log In using Globus

https://auth.globus.org/p/login?redirect\_uri=%2Fv2%2Foauth2%2Fauthorize%3Fclient\_id%3D89ba3e72...

globus Globus Account Log In

### Log in to use Globus Web App

Use your existing organizational login

e.g., university, national lab, facility, project

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Didn't find your organization? Then use **Globus ID** to sign in. (What's this?)

Continue

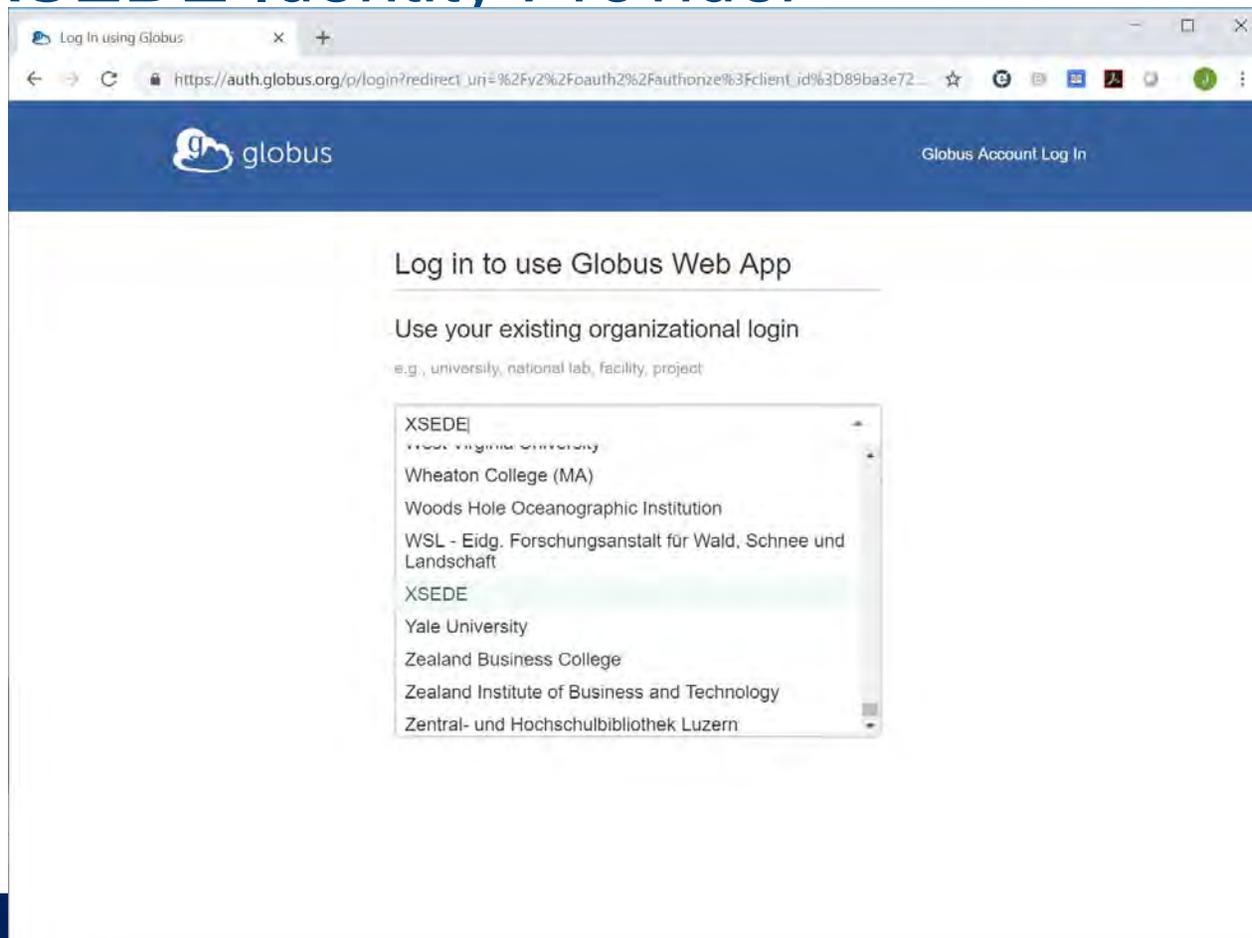
Or

Sign in with Google Sign in with ORCID.ID



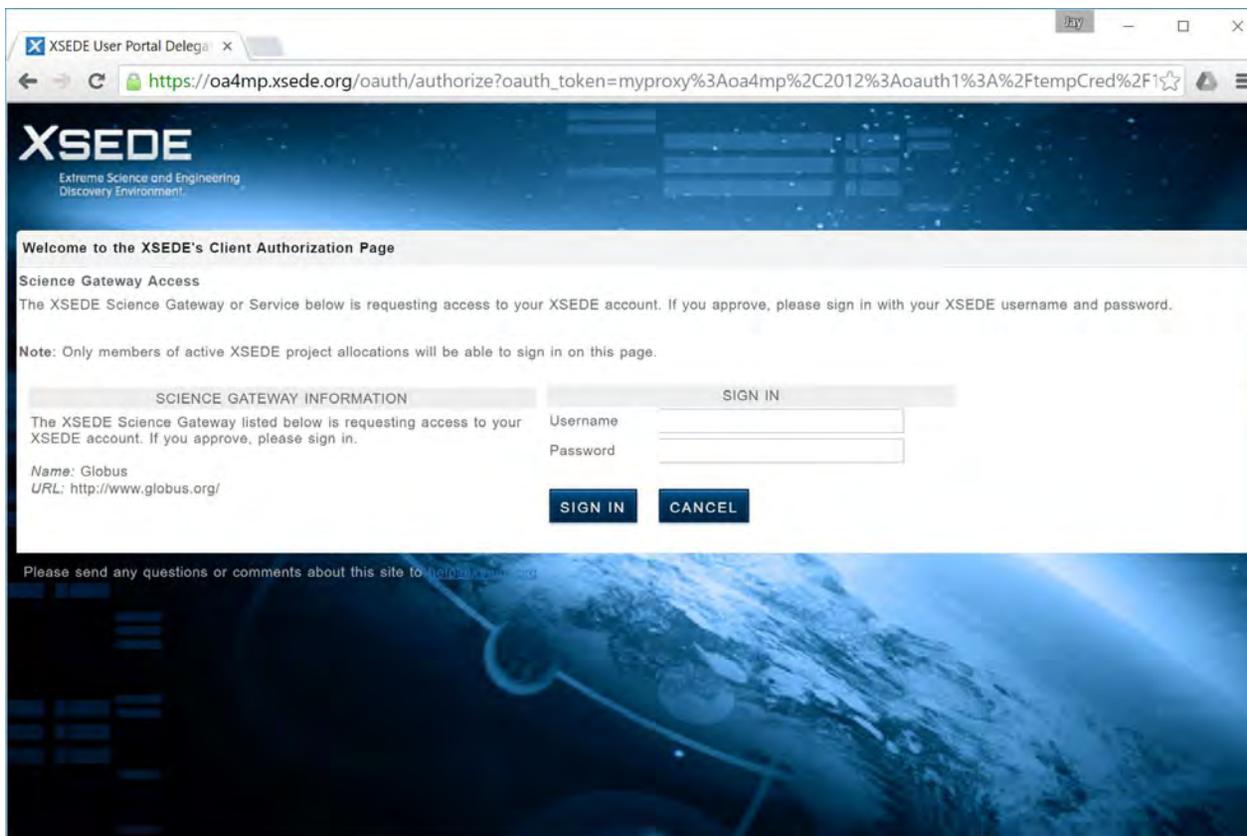
XSEDE

# Use XSEDE Identity Provider



XSEDE

# Sign in with XSEDE credentials



The screenshot shows a browser window with the URL `https://oa4mp.xsede.org/oauth/authorize?oauth_token=myprox%3Aoa4mp%2C2012%3Aauth1%3A%2FtempCred%2F1`. The page header features the XSEDE logo and the tagline "Extreme Science and Engineering Discovery Environment".

**Welcome to the XSEDE's Client Authorization Page**

**Science Gateway Access**  
The XSEDE Science Gateway or Service below is requesting access to your XSEDE account. If you approve, please sign in with your XSEDE username and password.

**Note:** Only members of active XSEDE project allocations will be able to sign in on this page.

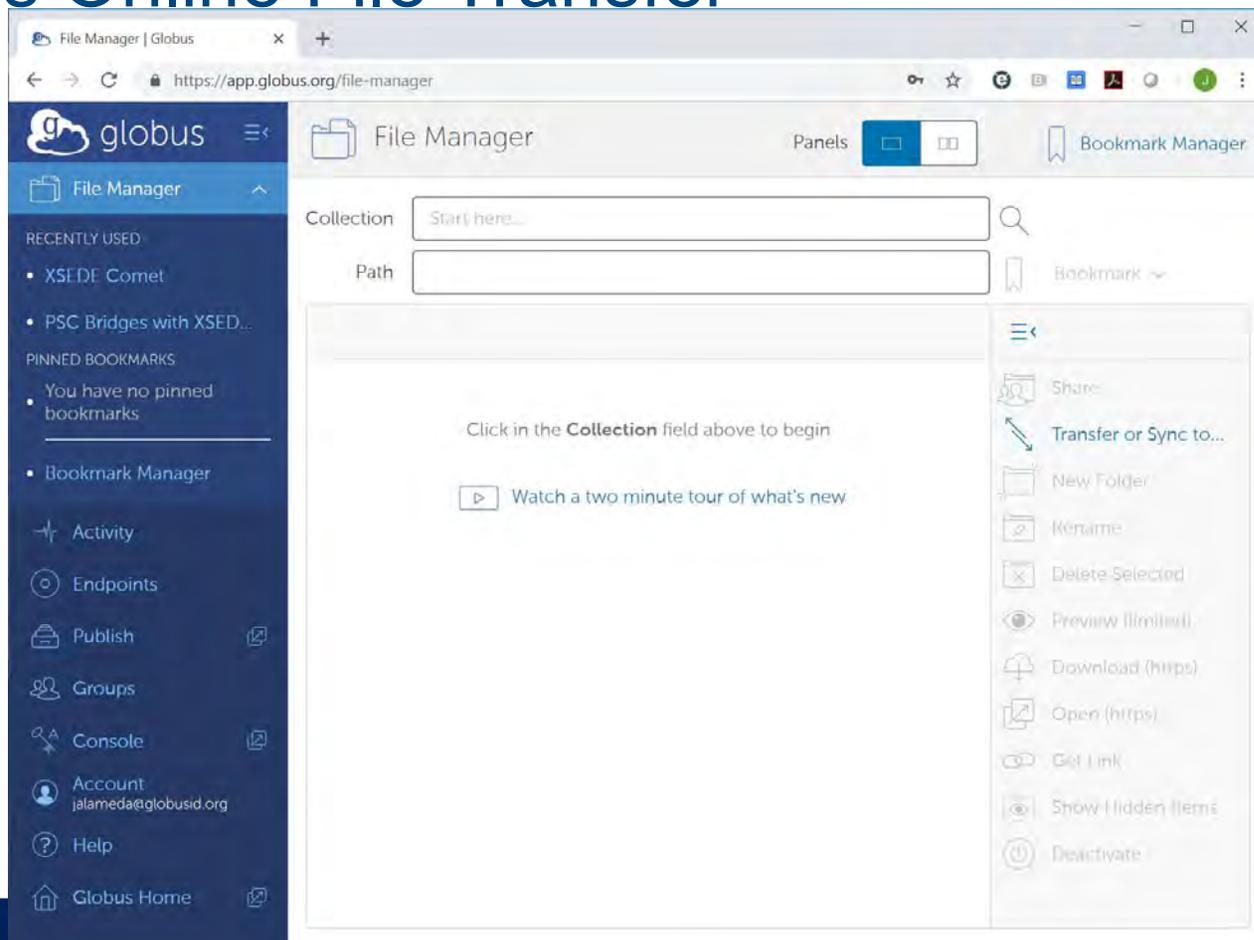
SCIENCE GATEWAY INFORMATION	SIGN IN
The XSEDE Science Gateway listed below is requesting access to your XSEDE account. If you approve, please sign in. <i>Name:</i> Globus <i>URL:</i> <a href="http://www.globus.org/">http://www.globus.org/</a>	Username <input type="text"/> Password <input type="password"/>
	<input type="button" value="SIGN IN"/> <input type="button" value="CANCEL"/>

Please send any questions or comments about this site to [help@xsede.org](mailto:help@xsede.org)



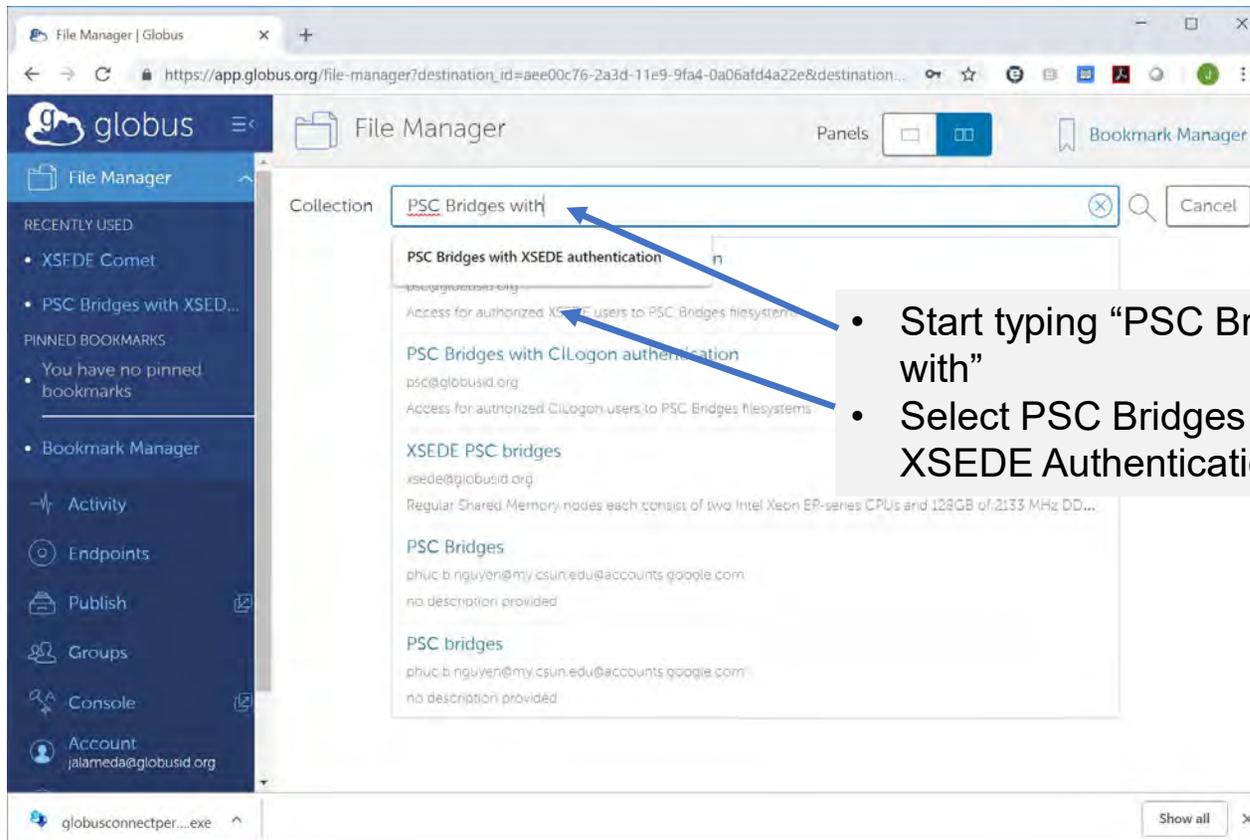
**XSEDE**

# Globus Online File Transfer



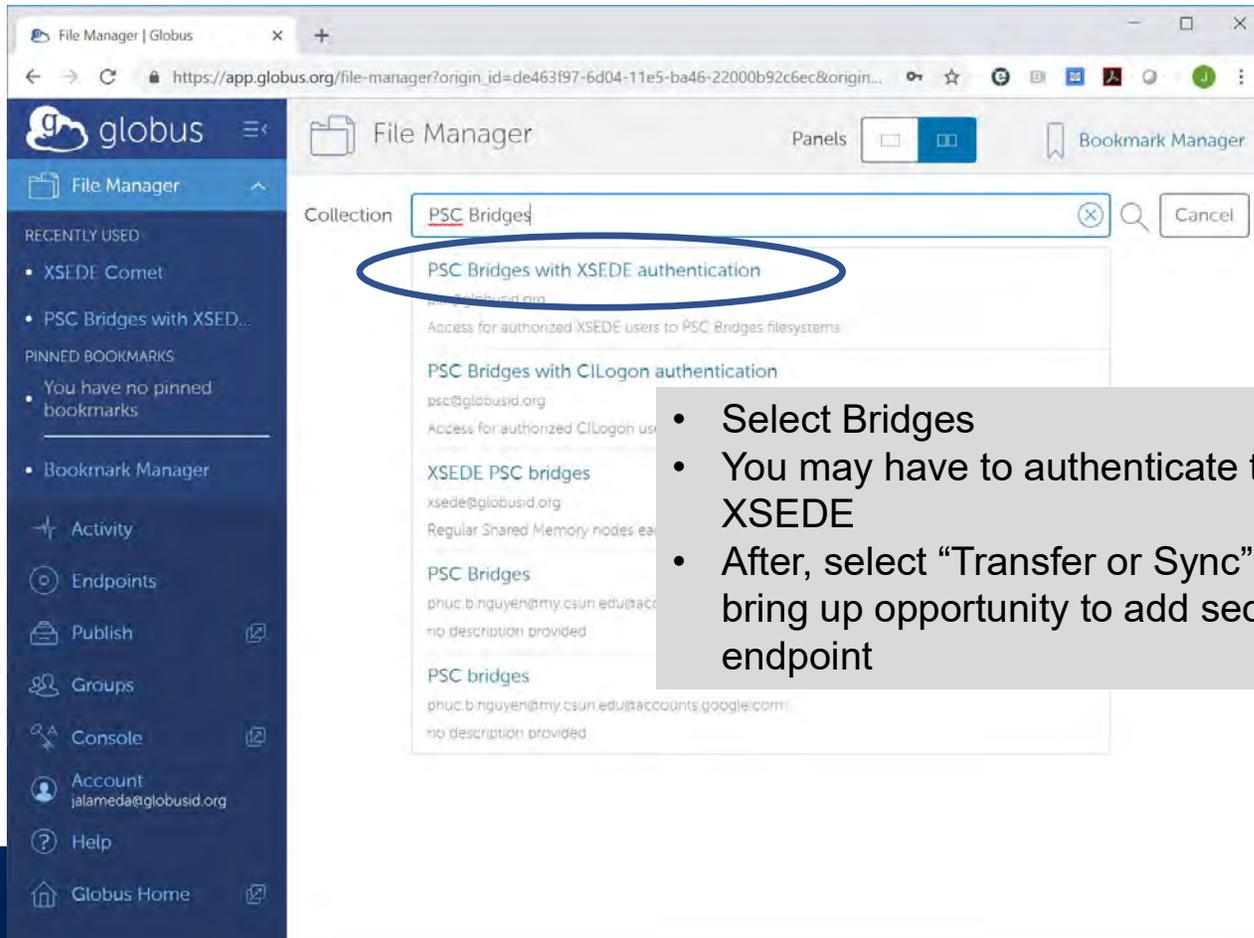
XSEDE

# Start by typing one endpoint



XSEDE

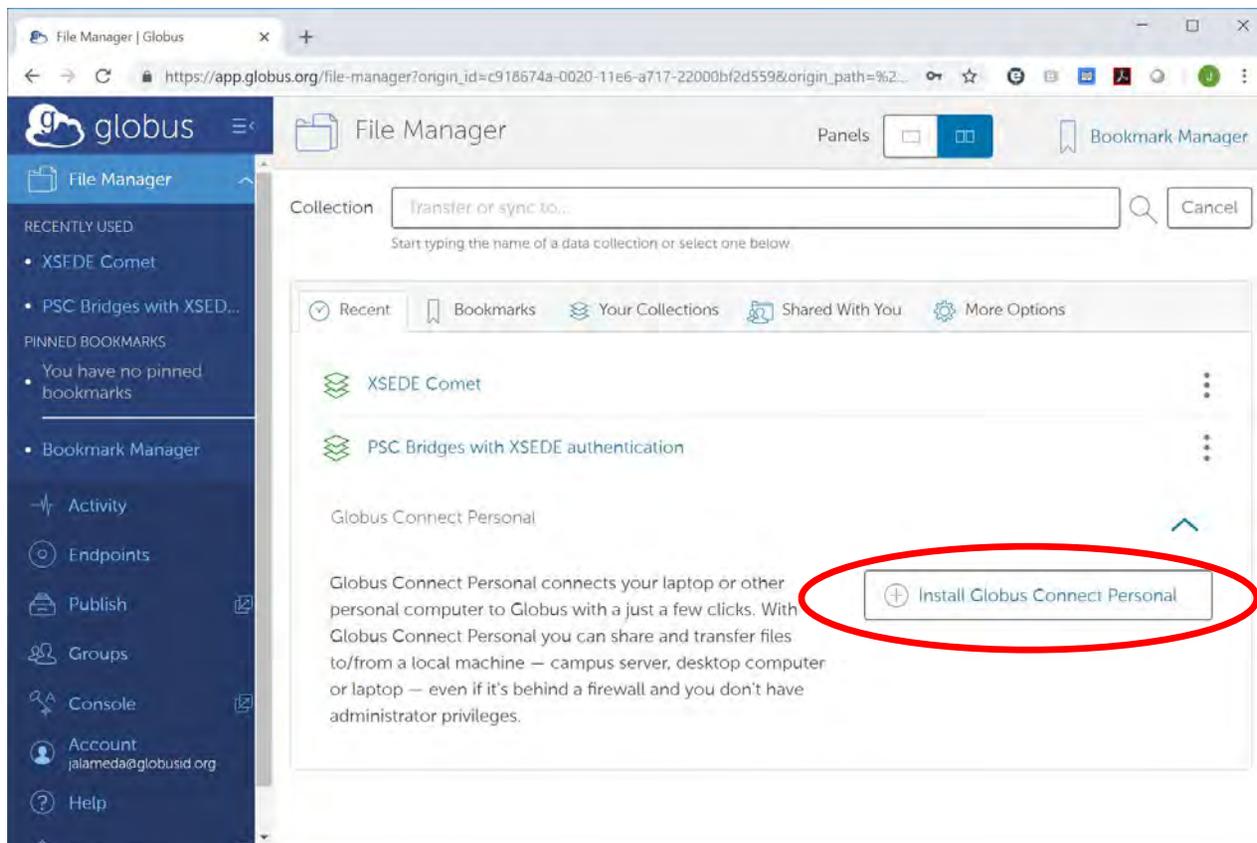
# Select Bridges, XSEDE Authentication



The screenshot shows the Globus File Manager interface. The search bar contains the text "PSC Bridges". Below the search bar, a dropdown menu displays search results. The first result, "PSC Bridges with XSEDE authentication", is circled in blue. Other results include "PSC Bridges with CILogon authentication", "XSEDE PSC bridges", and "PSC Bridges".

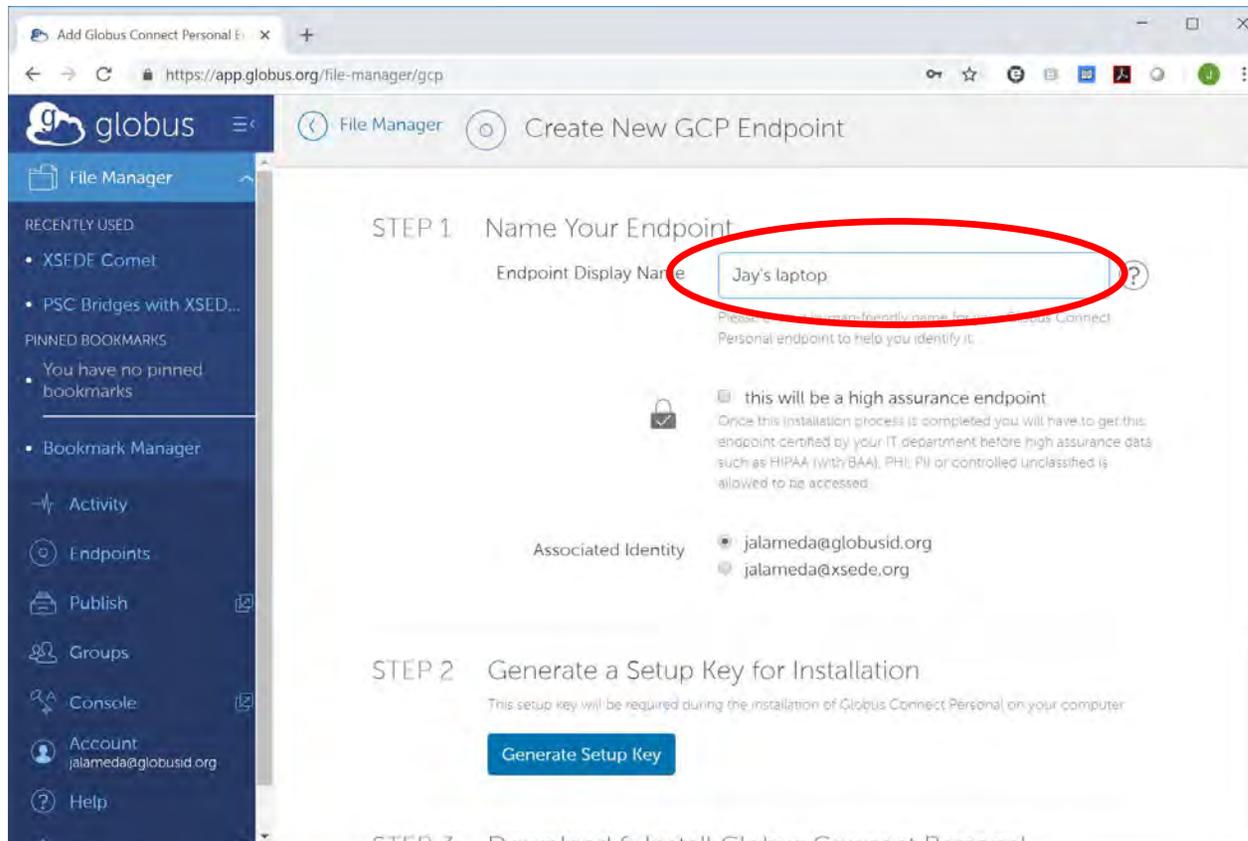
- Select Bridges
- You may have to authenticate to XSEDE
- After, select "Transfer or Sync" to bring up opportunity to add second endpoint

# Install Globus Connect Personal



XSEDE

# Name your endpoint



The screenshot shows a web browser window at <https://app.globus.org/file-manager/gcp>. The page title is "Create New GCP Endpoint". The main content area is titled "STEP 1: Name Your Endpoint". A text input field labeled "Endpoint Display Name" contains the text "Jay's laptop" and is circled in red. Below the input field, there is a checkbox labeled "this will be a high assurance endpoint" which is checked. Underneath, a note states: "Once this installation process is completed you will have to get this endpoint certified by your IT department before high assurance data such as HIPAA (With BAA), PHI, PII or controlled unclassified is allowed to be accessed." Below this, the "Associated Identity" section lists two email addresses: "jalameda@globusid.org" and "jalameda@xsede.org". The next step, "STEP 2: Generate a Setup Key for Installation", includes a sub-note: "This setup key will be required during the installation of Globus Connect Personal on your computer." and a blue button labeled "Generate Setup Key".



XSEDE

# Associate with your XSEDE identity

The screenshot shows the 'Create New GCP Endpoint' page in the Globus Connect Personal web interface. The page is divided into three steps:

- STEP 1: Name Your Endpoint**
  - Endpoint Display Name:** A text input field containing 'Jay's laptop'.
  - Associated Identity:** A section with two radio button options: 'jalameda@globusid.org' (unselected) and 'jalameda@xsede.org' (selected). A red arrow points to this section.
- STEP 2: Generate a Setup Key for Installation**
  - A blue button labeled 'Generate Setup Key'.
- STEP 3: Download & Install Globus Connect Personal**

The left sidebar contains navigation options: File Manager, RECENTLY USED (XSEDE Comet, PSC Bridges with XSED...), PINNED BOOKMARKS (You have no pinned bookmarks), Bookmark Manager, Activity, Endpoints, Publish, Groups, Console, Account (jalameda@globusid.org), and Help.



XSEDE

# Generate Setup Key

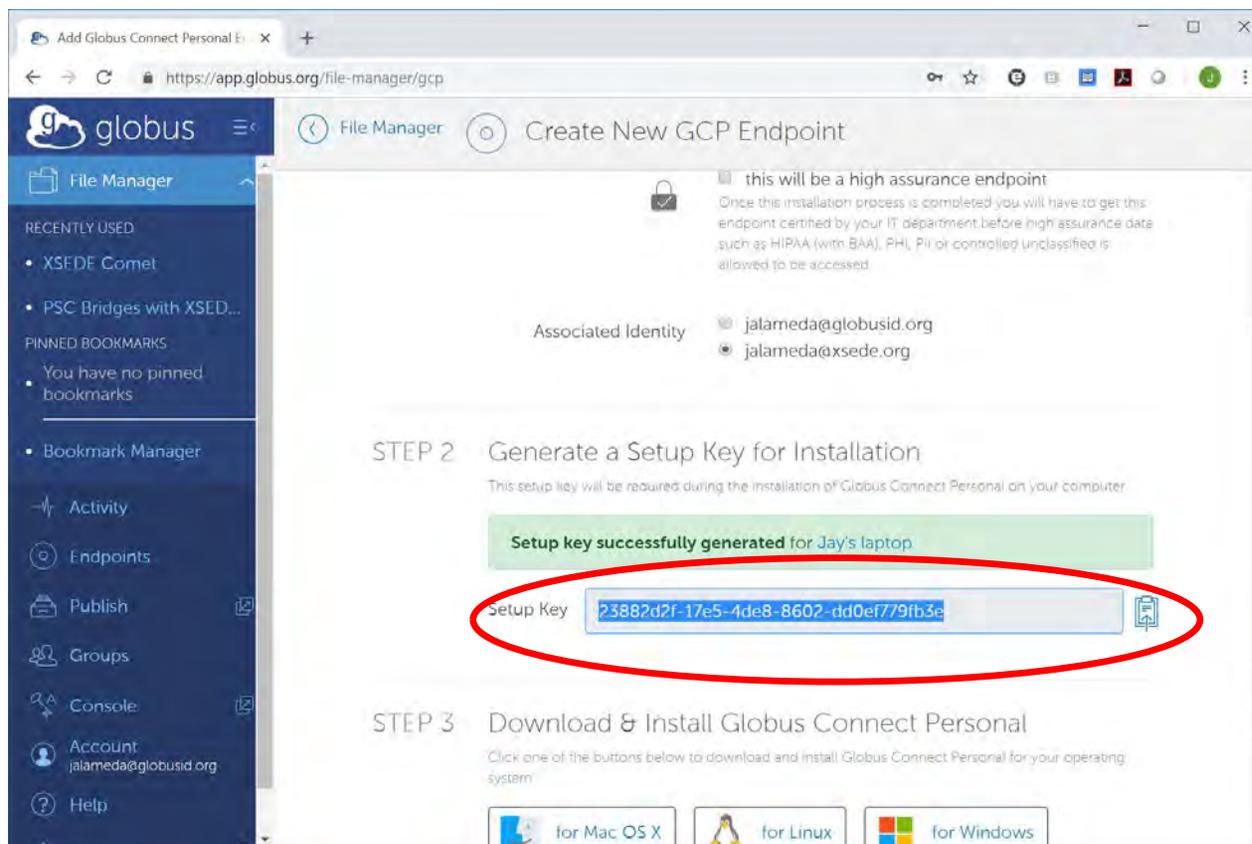
The screenshot shows a web browser window at <https://app.globus.org/file-manager/gcp>. The page title is "Create New GCP Endpoint". A warning message states: "this will be a high assurance endpoint. Once this installation process is completed you will have to get this endpoint certified by your IT department before high assurance data such as HIPAA (with BAA), PHI, PII or controlled unclassified is allowed to be accessed." Below this, the "Associated Identity" section lists two email addresses: `jalameda@globusid.org` and `jalameda@xsede.org`. The main content area is divided into three steps:

- STEP 2: Generate a Setup Key for Installation**  
This setup key will be required during the installation of Globus Connect Personal on your computer.  
**Generate Setup Key** (button highlighted with a red circle)
- STEP 3: Download & Install Globus Connect Personal**  
Click one of the buttons below to download and install Globus Connect Personal for your operating system.  
Buttons: **for Mac OS X**, **for Linux**, **for Windows**

Below the download buttons, it says: "Once downloaded, run the installer. When prompted, paste in the Setup Key to complete the installation."



# Copy Setup Key into your clipboard



The screenshot shows the 'Create New GCP Endpoint' page in the Globus Connect Personal web interface. The page is titled 'File Manager' and 'Create New GCP Endpoint'. It displays the associated identity as 'jalameda@globusid.org' and 'jalameda@xsede.org'. The main content area is divided into three steps:

- STEP 1:** A warning message states 'this will be a high assurance endpoint' and notes that the endpoint will require certification by the IT department before high assurance data (such as HIPAA, PHI, or controlled unclassified) is allowed to be accessed.
- STEP 2: Generate a Setup Key for Installation**  
This step includes a green notification box: 'Setup key successfully generated for Jay's laptop.' Below this, the 'Setup Key' is displayed in a text field: `23882d2f-17e5-4de8-8602-dd0ef779fb3e`. This key and its label are circled in red.
- STEP 3: Download & Install Globus Connect Personal**  
This step instructs the user to click one of the buttons below to download and install Globus Connect Personal for their operating system. Three buttons are visible: 'for Mac OS X', 'for Linux', and 'for Windows'.



g globus

File Manager

RECENTLY USED

- XSEDE Comet
- PSC Bridges with XSED...

PINNED BOOKMARKS

- You have no pinned bookmarks

Bookmark Manager

Activity

Endpoints

Publish

Groups

Console

Account  
jalameda@globusid.org

Help

File Manager

### Create New GCP Endpoint

Associated Identity

- jalameda@globusid.org
- jalameda@xsede.org

#### STEP 2 Generate a Setup Key for Installation

This setup key will be required during the installation of Globus Connect Personal on your computer.

**Setup key successfully generated for Jay's laptop**

Setup Key

#### STEP 3 Download & Install Globus Connect Personal

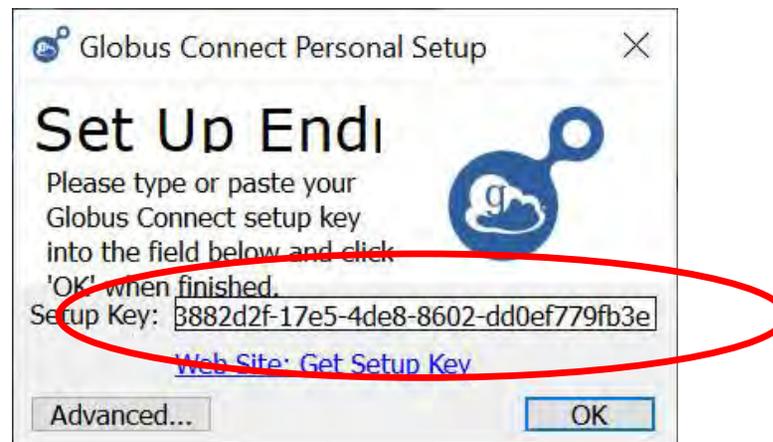
Click one of the buttons below to download and install Globus Connect Personal for your operating system.

[for Mac OS X](#) [for Linux](#) [for Windows](#)

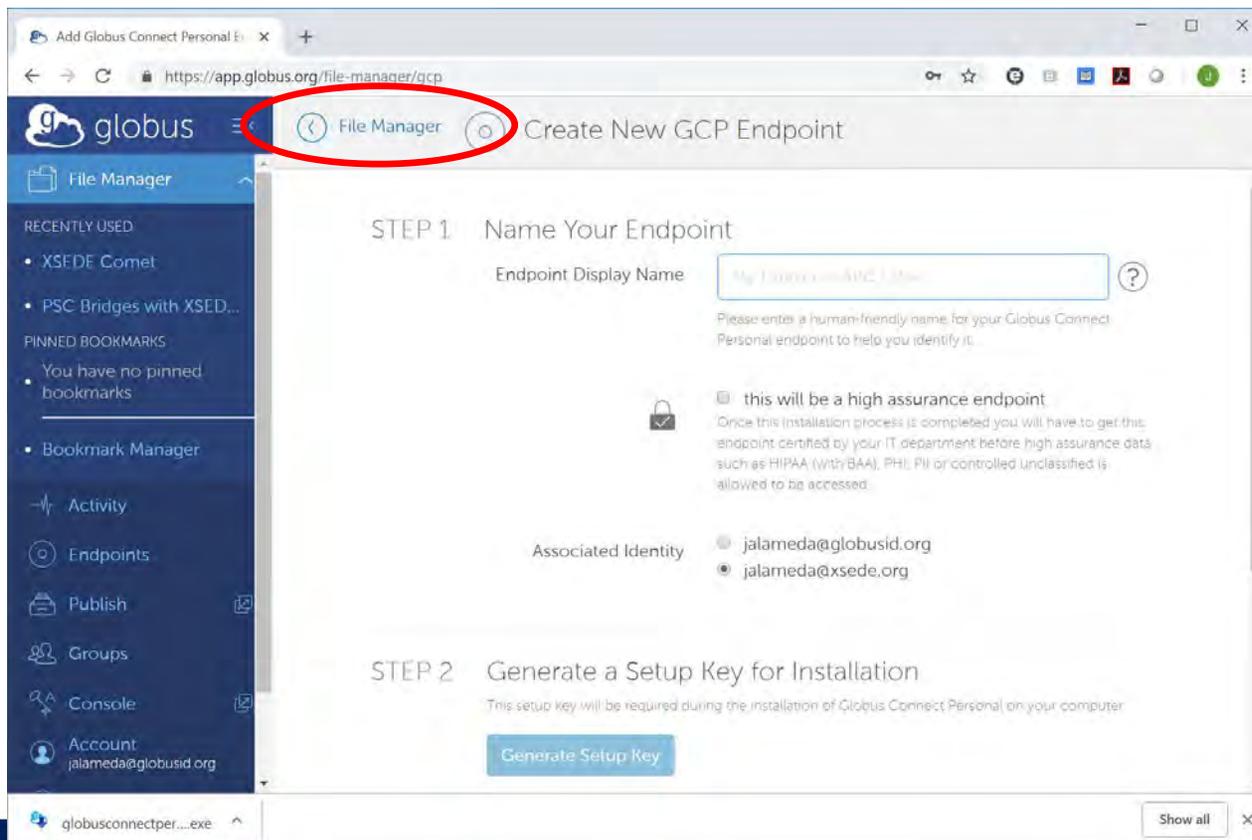
Once downloaded, run the installer. When prompted, paste in the Setup Key to complete the installation.



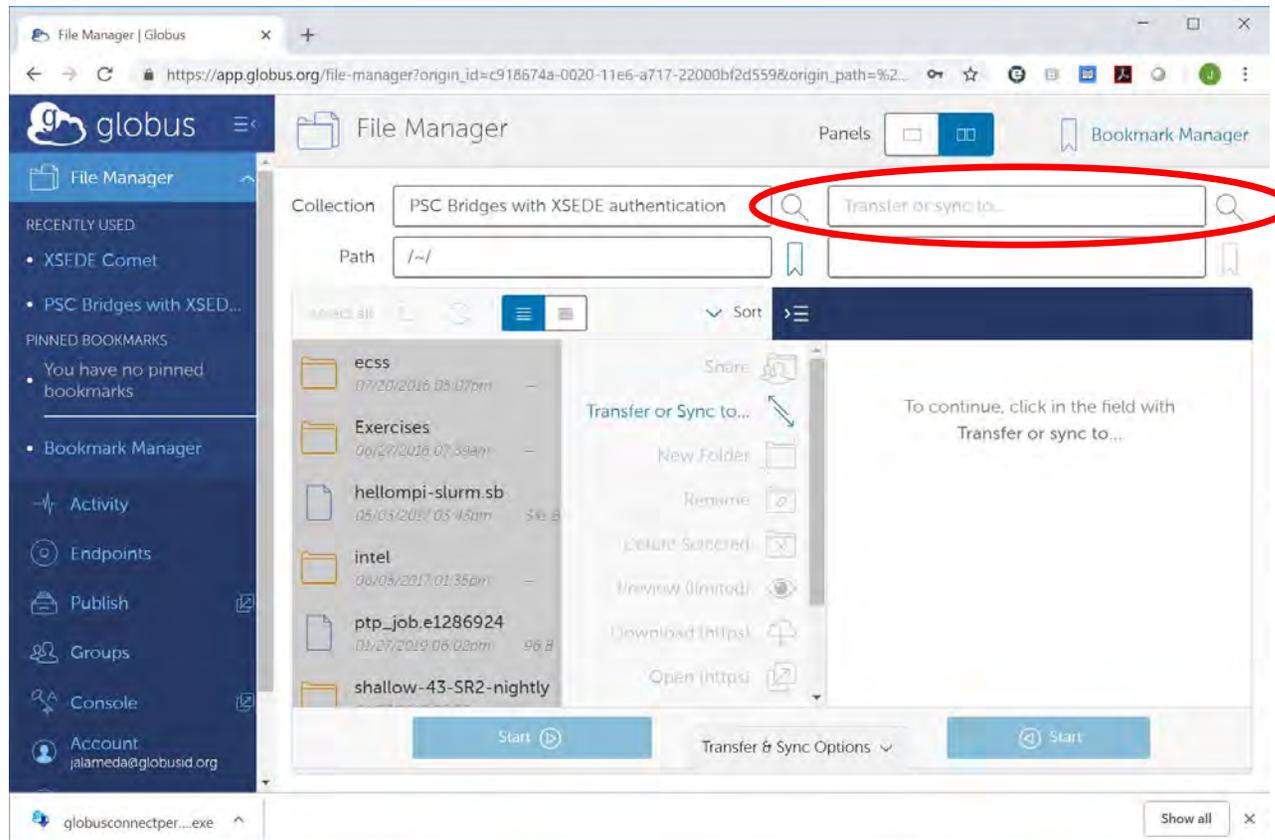
# Paste Setup Key after installing Globus Connect Personal



# Return to the File Manager to access your new endpoint

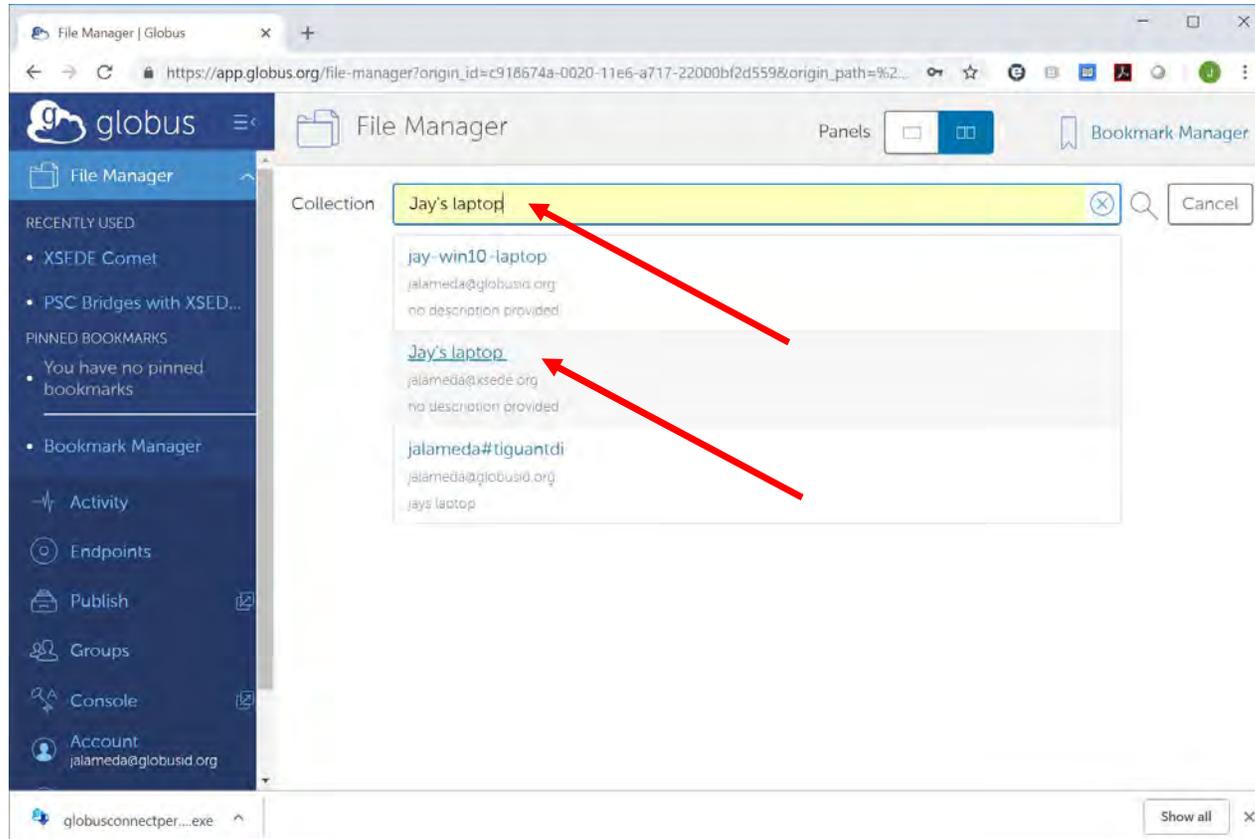


# Select new endpoint in second collection bar



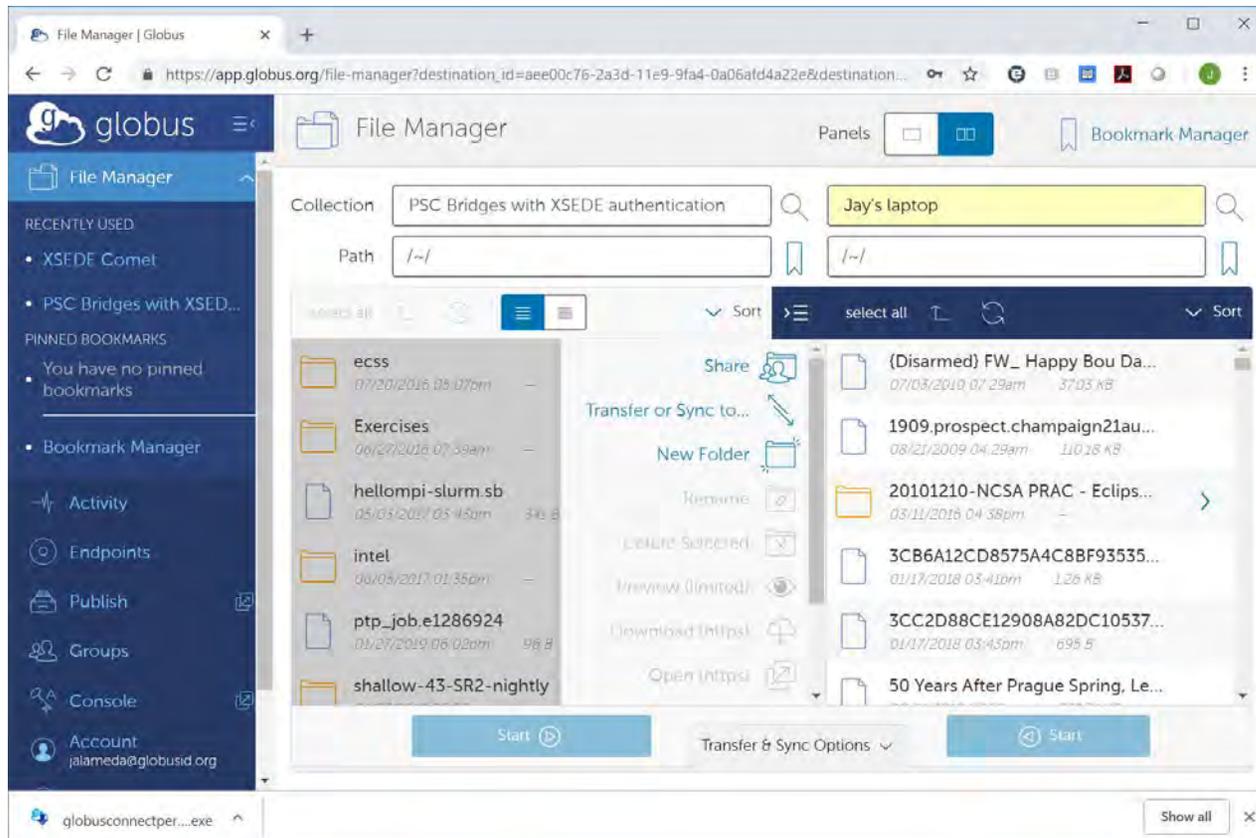
XSEDE

Start typing the endpoint name, and select your endpoint



XSEDE

# Now have directory listings for both systems



XSEDE

# Select file to move

File Manager | Globus

https://app.globus.org/file-manager?destination\_id=ae00c76-2a3d-11e9-9fa4-0a06afd4a22e&destination...

globus File Manager

Collection: PSC Bridges with XSEDE authentication Jay's laptop

Path: /~/ /~/

- Select a file on either directory
- Tap "Start"

ecss (Disarmed) FW\_ Happy Bou Da... 07/03/2010 07:29am 3705 KB

1909.prospect.champaign21au... 08/21/2009 04:29am 11028 KB

20101210-NCSA PRAC - Eclips... 03/11/2016 04:38pm

3CB6A12CD8575A4C8BF93535... 01/17/2018 05:41pm 1.26 KB

3CC2D88CE12908A82DC10537... 01/17/2018 03:45pm 695 B

50 Years After Prague Spring, Le...

Start Transfer & Sync Options Start

globusconnectper...exe Show all



XSEDE