

May 3, 2017

XSEDE New User Tutorial

XSEDE

Extreme Science and Engineering
Discovery Environment

Jay Alameda
National Center for
Supercomputing Applications

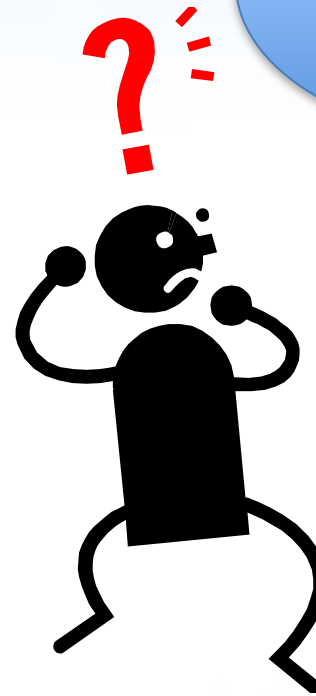
XSEDE Training Survey

- Please complete a short on-line survey about this module at <http://bit.ly/xsedejackson>. We value your feedback, and will use your feedback to help improve our training offerings.
- Slides from this workshop are available at <http://hpcuniversity.org/trainingMaterials/238/>

Yeah! I got an
XSEDE
allocation!



Now
what?



XSEDE

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

XSEDE User Portal (XUP)

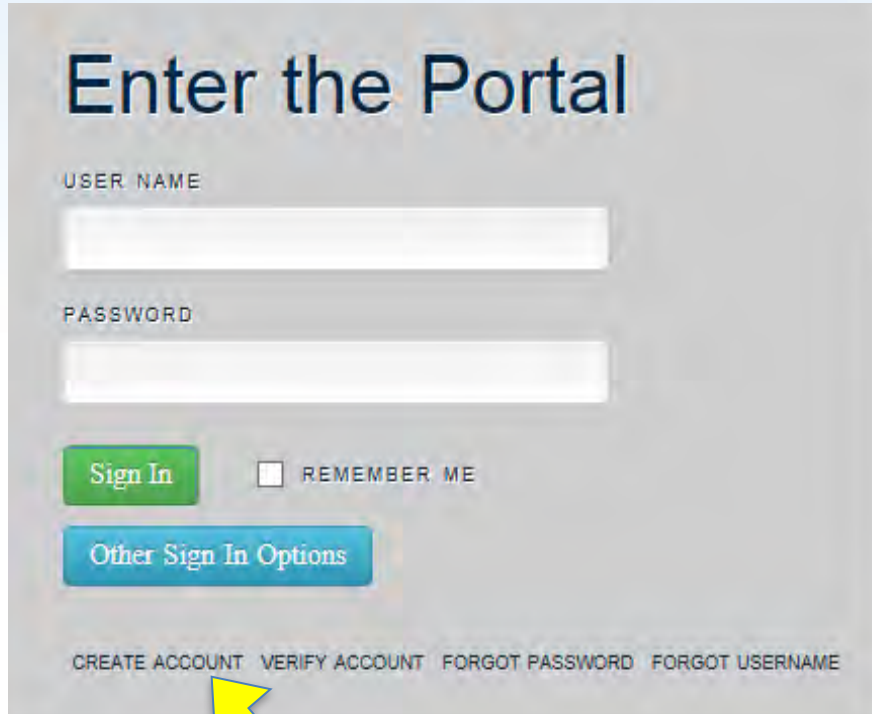
- URL: portal.xsede.org
- Single point-of-entry to information about XSEDE services and utilities for using them
- Anyone can create an XUP user account and access non-project features
- Only XSEDE allocation project members can access project features

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

Create and login to your XUP account

portal.xsede.org



Enter the Portal

USER NAME

PASSWORD

Sign In ☐ REMEMBER ME

Other Sign In Options

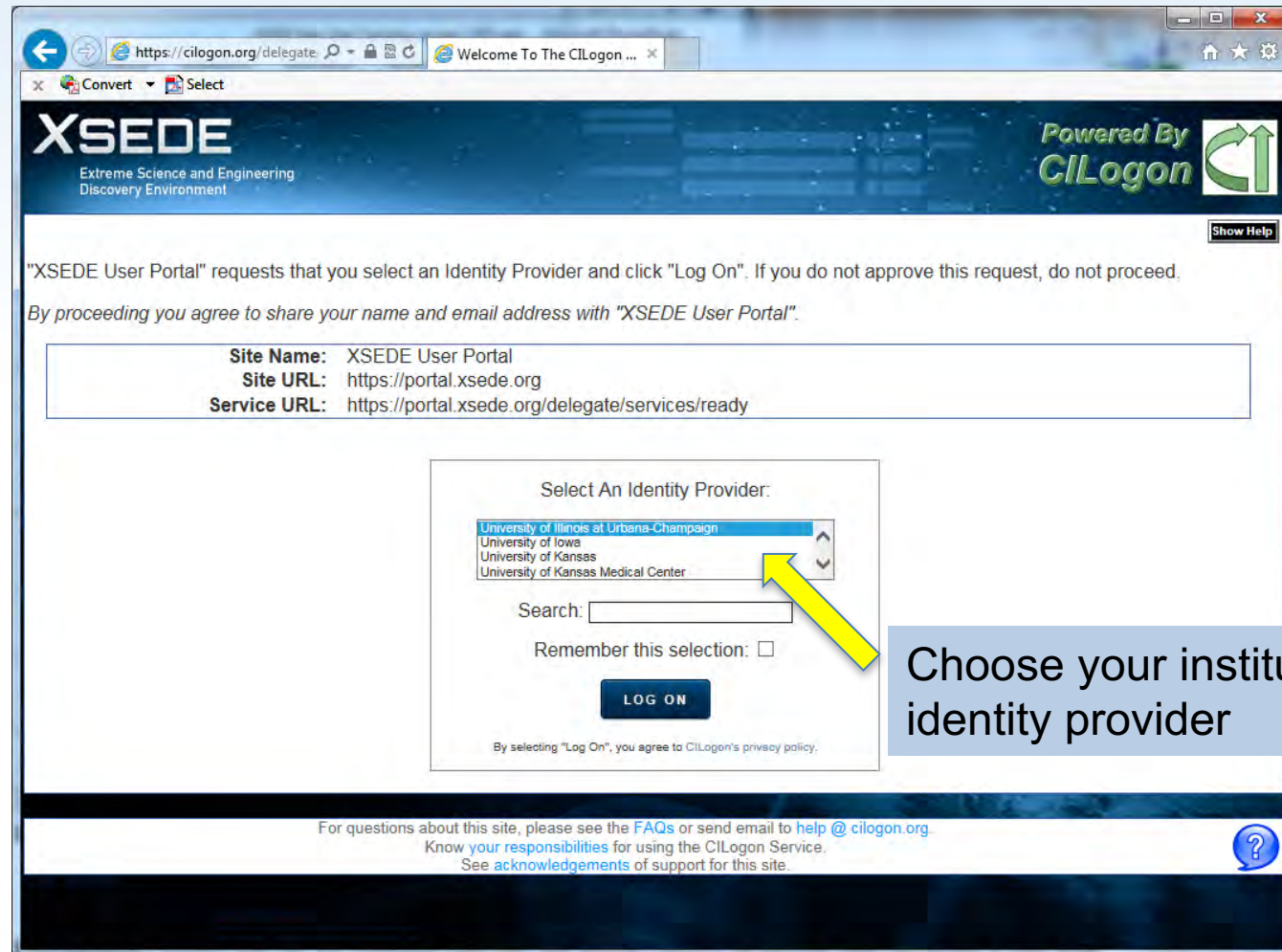
CREATE ACCOUNT VERIFY ACCOUNT FORGOT PASSWORD FORGOT USERNAME

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

XSEDE

Other Sign In Options



https://cilogon.org/delegate Welcome To The CILogon ...

XSEDE
Extreme Science and Engineering
Discovery Environment

Powered By **CILogon**

Show Help

"XSEDE User Portal" requests that you select an Identity Provider and click "Log On". If you do not approve this request, do not proceed.
By proceeding you agree to share your name and email address with "XSEDE User Portal".

Site Name: XSEDE User Portal
Site URL: https://portal.xsede.org
Service URL: https://portal.xsede.org/delegate/services/ready

Select An Identity Provider:

University of Illinois at Urbana-Champaign
University of Iowa
University of Kansas
University of Kansas Medical Center

Search:

Remember this selection: ☐

LOG ON

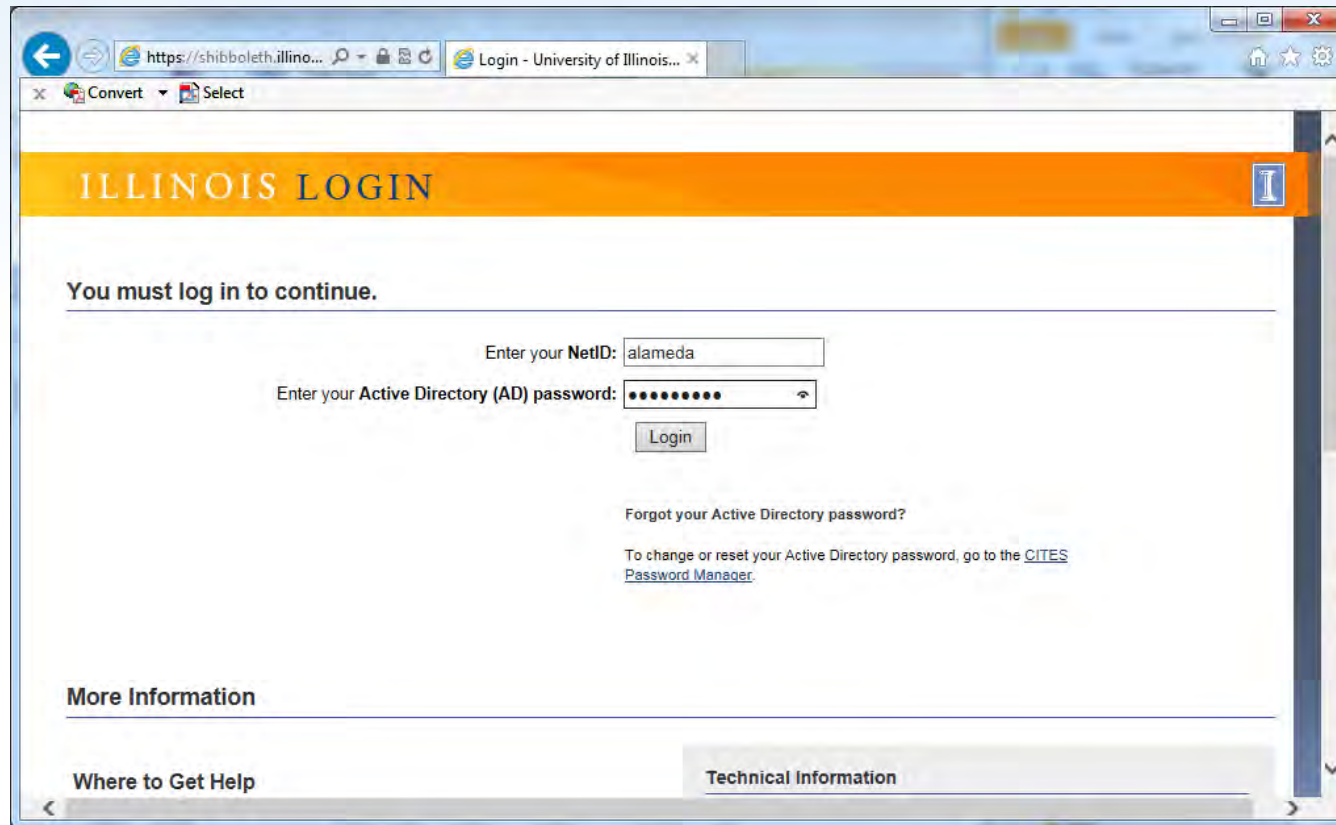
By selecting "Log On", you agree to CILogon's privacy policy.

Choose your institutions's identity provider

For questions about this site, please see the [FAQs](#) or send email to help@cilogon.org.
Know your [responsibilities](#) for using the CILogon Service.
See [acknowledgements](#) of support for this site.

XSEDE

Example: Logging in with Illinois credentials



The screenshot shows a web browser window with the address bar displaying `https://shibboleth.illino...` and a tab titled "Login - University of Illinois...". The page has an orange header with the text "ILLINOIS LOGIN" and a small "I" logo. Below the header, the text "You must log in to continue." is displayed. The login form consists of two input fields: "Enter your NetID:" with the value "alameda" and "Enter your Active Directory (AD) password:" with masked characters. A "Login" button is positioned below the password field. Below the login fields, there is a link for "Forgot your Active Directory password?" and a link to the "CITES Password Manager" for changing or resetting the password. At the bottom, there are two tabs: "Where to Get Help" and "Technical Information".

ILLINOIS LOGIN

You must log in to continue.

Enter your NetID:

Enter your Active Directory (AD) password:

Login

Forgot your Active Directory password?

To change or reset your Active Directory password, go to the [CITES Password Manager](#).

More Information

Where to Get Help Technical Information

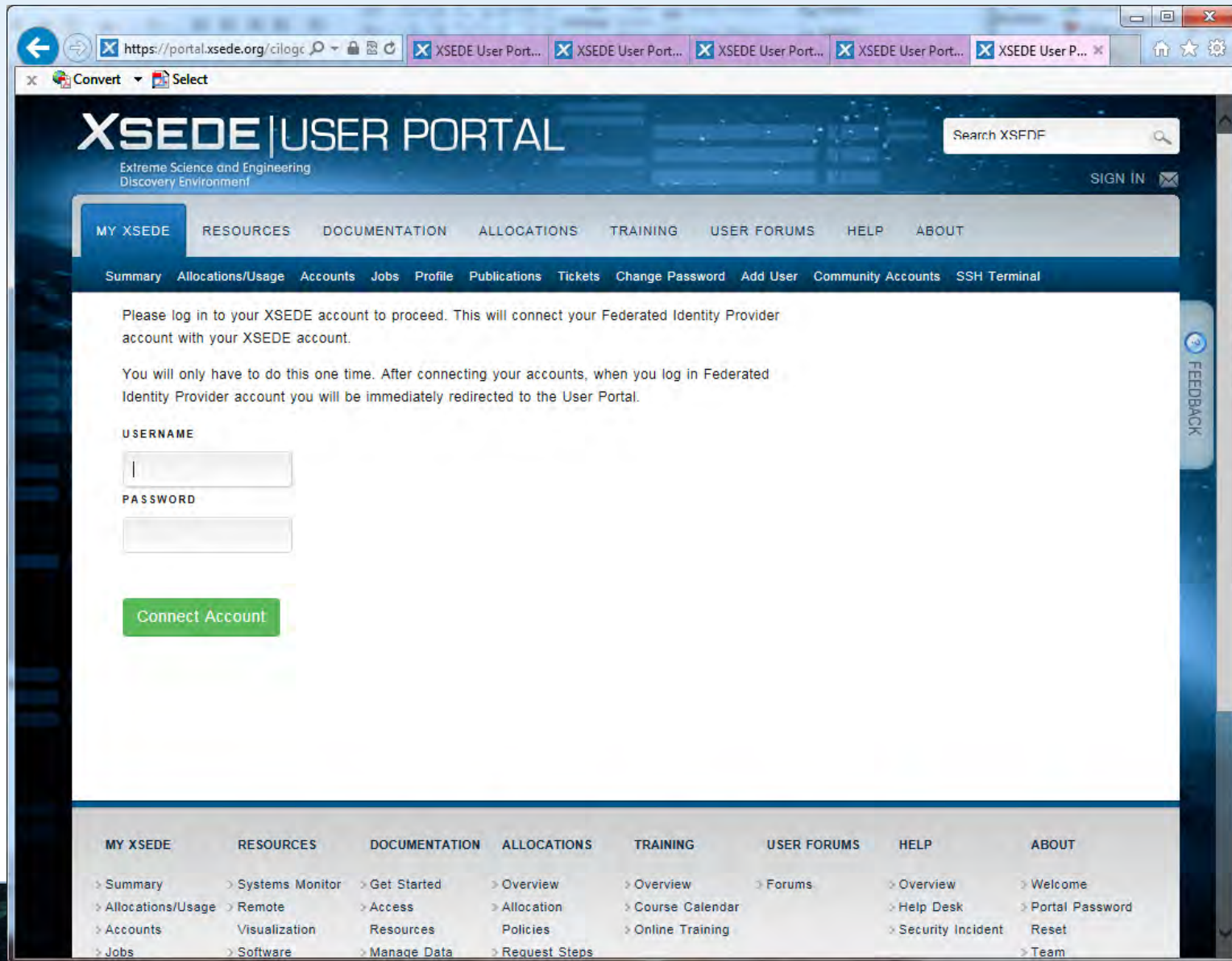
Link your campus identity and portal identity

The screenshot shows the XSEDE User Portal interface. The browser address bar displays <https://portal.xsede.org/web/>. The page title is "XSEDE | USER PORTAL" with the subtitle "Extreme Science and Engineering Discovery Environment". A search bar labeled "Search XSEDE" is in the top right, along with a "SIGN IN" link. The main navigation menu includes: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ABOUT. Below this, a secondary menu lists: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH Terminal. The central content area prompts the user to "Please select a method to connect your Federated Identity to your XSEDE account". It provides two options: "Connect" (for existing accounts) and "Create" (for new accounts). A vertical "FEEDBACK" button is on the right. The footer contains a detailed grid of links for all portal sections.

MY XSEDE	RESOURCES	DOCUMENTATION	ALLOCATIONS	TRAINING	USER FORUMS	HELP	ABOUT
> Summary	> Systems Monitor	> Get Started	> Overview	> Overview	> Forums	> Overview	> Welcome
> Allocations/Usage	> Remote	> Access	> Allocation	> Course Calendar		> Help Desk	> Portal Password
> Accounts	Visualization	Resources	Policies	> Online Training		> Security Incident	Reset
> Jobs	> Software	> Manage Data	> Request Steps				> Team

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Login to the portal to link identities



XSEDE USER PORTAL
Extreme Science and Engineering
Discovery Environment

Search XSEDE

SIGN IN

MY XSEDE RESOURCES DOCUMENTATION ALLOCATIONS TRAINING USER FORUMS HELP ABOUT

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

Please log in to your XSEDE account to proceed. This will connect your Federated Identity Provider account with your XSEDE account.

You will only have to do this one time. After connecting your accounts, when you log in Federated Identity Provider account you will be immediately redirected to the User Portal.

USERNAME

PASSWORD

Connect Account

FEEDBACK

MY XSEDE	RESOURCES	DOCUMENTATION	ALLOCATIONS	TRAINING	USER FORUMS	HELP	ABOUT
Summary	Systems Monitor	Get Started	Overview	Overview	Forums	Overview	Welcome
Allocations/Usage	Remote	Access	Allocation	Course Calendar		Help Desk	Portal Password
Accounts	Visualization	Resources	Policies	Online Training		Security Incident	Reset
Jobs	Software	Manage Data	Request Steps				Team

And inspect your new linked identity, via user profile

The screenshot shows the XSEDE user profile page for Jay Alameda. The page is titled "Jay Alameda" and "University of Illinois at Urbana-Champaign N.C.S.A.". It includes a profile picture placeholder, a list of links (Edit profile, Edit news, subscriptions, View public profile, Manage DNS, Manage Other Logins), and a "Publications" section. The "Demographic information" section states that XSEDE collects information for reporting purposes. The "Other XSEDE Login Identities" section is circled in red and contains a table of linked identities.

IDENTITY	STATUS
CN=Jay Alameda A7281, O=University of Illinois at Urbana-Champaign, C=US, DC=cilogon, DC=org	active

[Display Inactive Logins](#)

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 or call 1-866-907-2383 immediately, regardless of the time of day.

XSEDE Cybersecurity Tutorial

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

The XSEDE logo is displayed in a large, bold, white sans-serif font. It is positioned on a dark blue background that features a grid of glowing blue squares and a faint image of a planet's horizon with a bright light source. The logo itself is slightly transparent, allowing the background elements to be seen through it.

XSEDE

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.

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

XSEDE USER PORTAL ON THE GO

Download on the App Store

GET IT ON Google play

In The Past 7 Days

XD SUS Charged: Total: by Field of Science

Computer and Information Science and Engineering 15,055,364.0
Materials Research 11,750,678.0
Biochemistry and Molecular Structure and Function 10,756,458.0
Biophysics 10,242,934.0
Astronomical Sciences 8,024,067.0
Fluid, Particulate, and Hydraulic Systems 4,751,561.0
Extragalactic Astronomy and Cosmology 4,139,066.0
Nuclear Physics 3,961,220.0
Chemistry 3,857,890.0
Gravitational Physics 3,604,871.0
All 62 others 28,335,420.0

View Gallery

My XSEDE Resources [System Monitor]

Resource	Status	Load	Username	My Jobs
Stampede UT Austin	Healthy	66%	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.

XSEDE

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 top navigation bar with links: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and ABOUT. Below this is a sub-navigation bar with links: Summary, Allocations/Usage, Accounts, Jobs, Profile (highlighted), Publications, Tickets, Change Password, Add User, Community Accounts, and SSH Terminal.

Profile Information:

- Name:** Jay Alameda
- Organization:** University of Illinois at Urbana-Champaign
- Address:** N.C.S.A., Center Researcher Staff, MC 257 - 1008 NCSA, 1205 W. Clark St., Urbana Illinois 61801, United States
- Email:** alameda@illinois.edu
- Work:** work: Citizenship(s): United States

Demographic information:

XSEDE collects this information for reporting purposes to the NSF and other governing bodies. Your personal information will not be reported with this

DUO Security:

- Manage DUO
- Unenroll from Duo

Publications:

- Add a new publication
- Displaying 1 - 3 out of 3 publications
- Download Publications

Search:

All Search publications

Publication List:

- S. Padhy, J. Lee, R. Marciano, et al., An Architecture for Automatic Deployment of Brown Dog Services at Scale into Diverse Computing Infrastructures

XSEDE

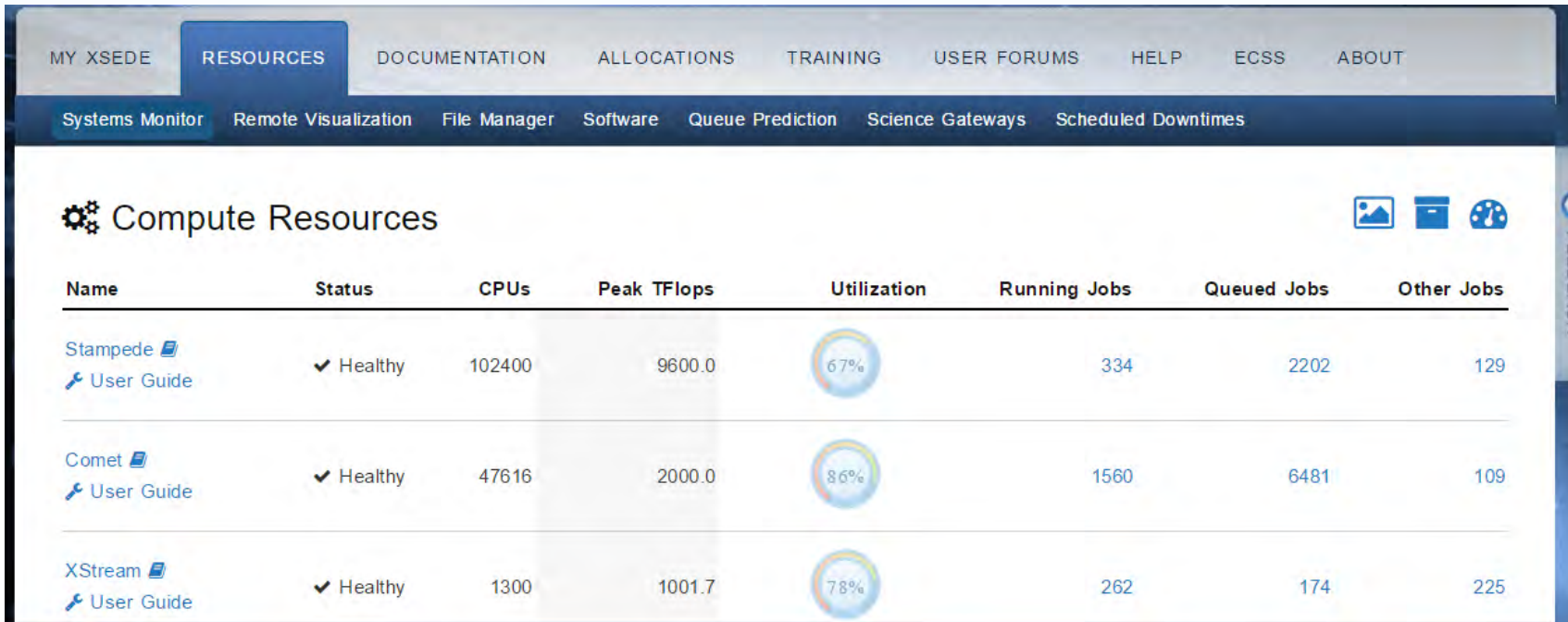
Navigating the XUP



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

View the XSEDE Systems Monitor

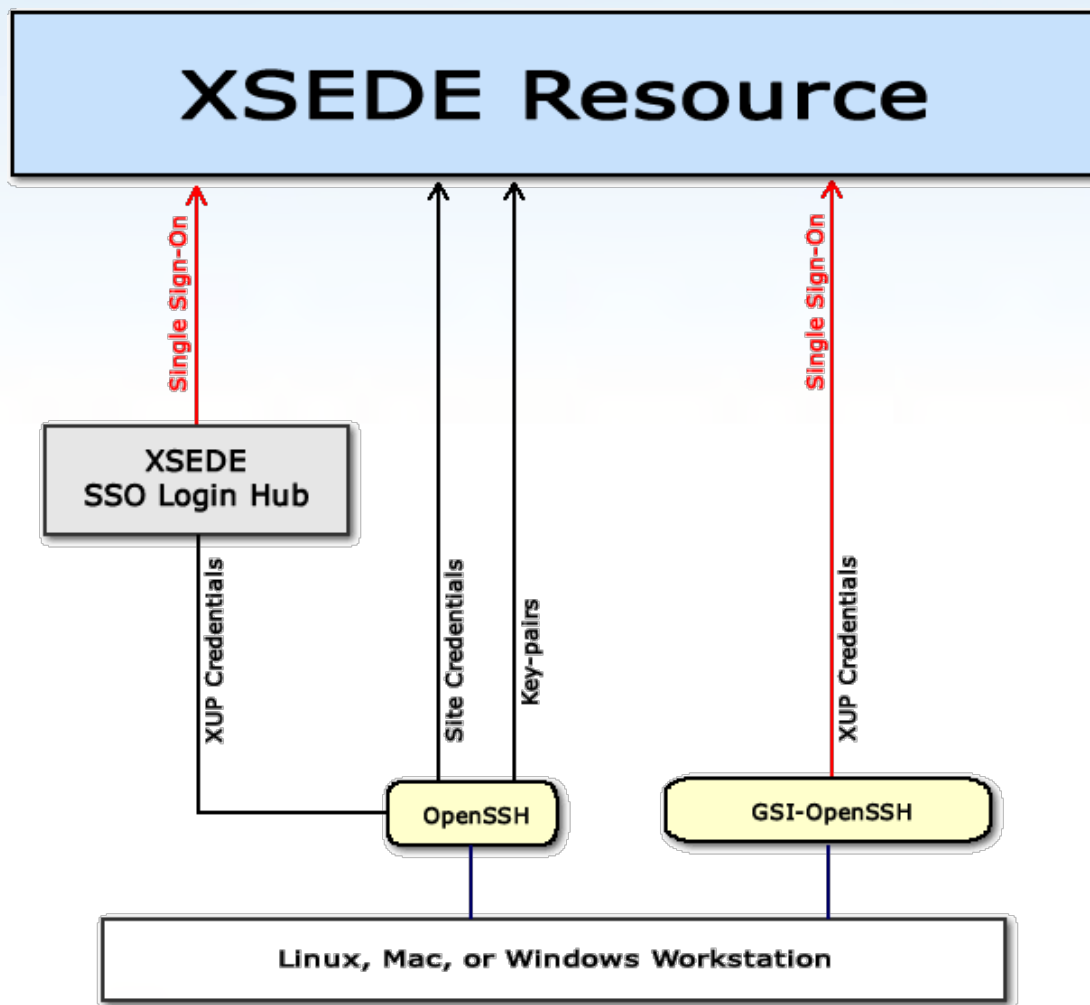
- **Resources -> Systems Monitor**
 - Provides technical and status information for all of XSEDE's resources.
 - The STATUS column indicates whether the system is up or down. If down, can click on status to find when the machine is expected to come back up.



The screenshot displays the XSEDE Systems Monitor interface. At the top, there is a navigation bar with links: MY XSEDE, RESOURCES (selected), DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and ABOUT. Below this is a secondary navigation bar with links: Systems Monitor (selected), Remote Visualization, File Manager, Software, Queue Prediction, Science Gateways, and Scheduled Downtimes. The main content area is titled "Compute Resources" and features a table of system information. The table has columns for Name, Status, CPUs, Peak TFlops, Utilization, Running Jobs, Queued Jobs, and Other Jobs. Three systems are listed: Stampede, Comet, and XStream, all with a status of "Healthy". Each system row includes a "User Guide" link and a circular utilization gauge.

Name	Status	CPUs	Peak TFlops	Utilization	Running Jobs	Queued Jobs	Other Jobs
Stampede User Guide	✓ Healthy	102400	9600.0	67%	334	2202	129
Comet User Guide	✓ Healthy	47616	2000.0	86%	1560	6481	109
XStream User Guide	✓ Healthy	1300	1001.7	78%	262	174	225

Accessing XSEDE Resources



Authentication Methods

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

Single Sign-On

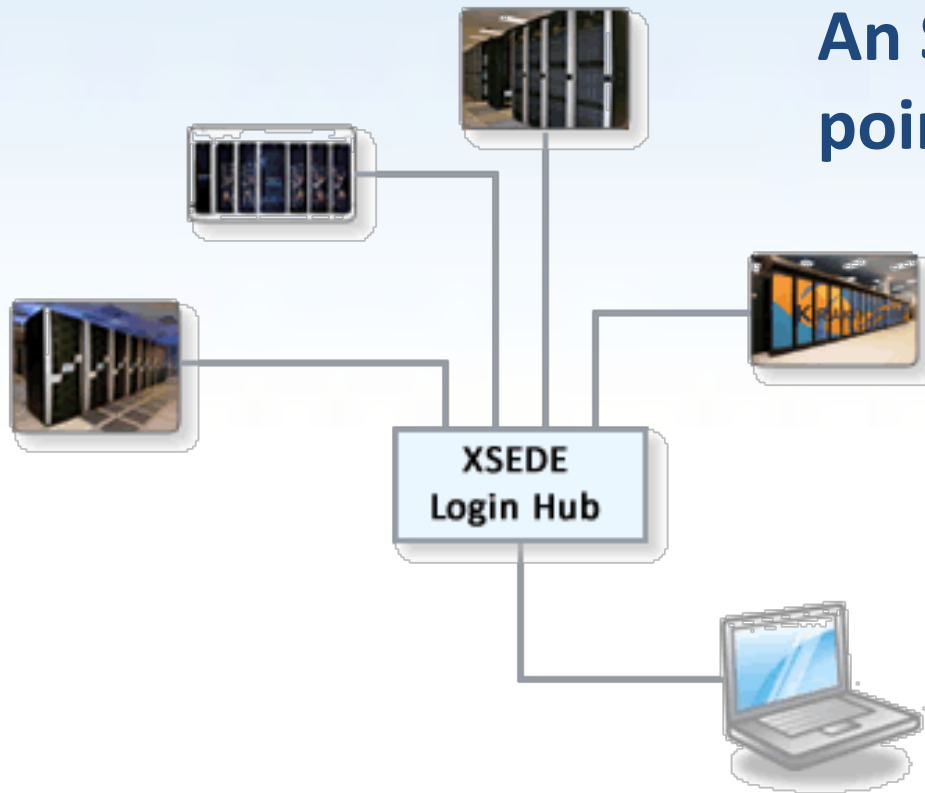
- Enables logging in once to access all of your allocated resources

Connection Methods

1. GSI-OpenSSH
2. OpenSSH

XSEDE SSO Login Hub

An SSO enabled connection point to XSEDE resources



➤ Move among resources using **gsissh** command

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

Set up 2 Factor Authentication

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

The screenshot shows the XSEDE User Portal interface. The left sidebar contains navigation links: Profile (circled in red), Allocations, Accounts, and Training. The main content area displays a welcome message, a 'XSEDE USER PORTAL ON THE GO' banner with app download links, and a pie chart titled 'XO SUs Charged - Total: By Field of Science'. Below the chart is a legend for various scientific fields.

For all publications, please acknowledge your use of XSEDE and allocated resources and add publications to 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, account!

Last login: Wed 03/15/17 at 09:53:25 AM CST

Profile (circled in red)

Allocations

Accounts

Training

NEW! Share your XSEDE Science Achievements

Publications: [View My Pubs]

You have not entered any publications.

XSEDE USER PORTAL ON THE GO

Download on the App Store

In The Past 7 Days

XO SUs Charged - Total: By Field of Science

Computer and Information Science and Engineering 11,800,504.0

Materials Research 11,755,674.0

Biochemistry and Molecular Structure and Function 10,716,408.0

Biophysics 10,747,318.0

Chemistry 9,822,800.0

Gravitational Physics 2,809,412.0

AD 82 others 20,380,000.0

Field, Particulate, and Hydraulic Systems 4,751,342.0

Astronomical Sciences 8,811,087.0

Extraterrestrial Astrobiology and Cosmology 4,070,040.0

Nuclear Physics 2,774,250.0

Computer and Information Science and Engineering 11,800,504.0

Biophysics 10,747,318.0

Astronomical Sciences 8,811,087.0

Chemistry 9,822,800.0

Gravitational Physics 2,809,412.0

AD 82 others 20,380,000.0

Field, Particulate, and Hydraulic Systems 4,751,342.0

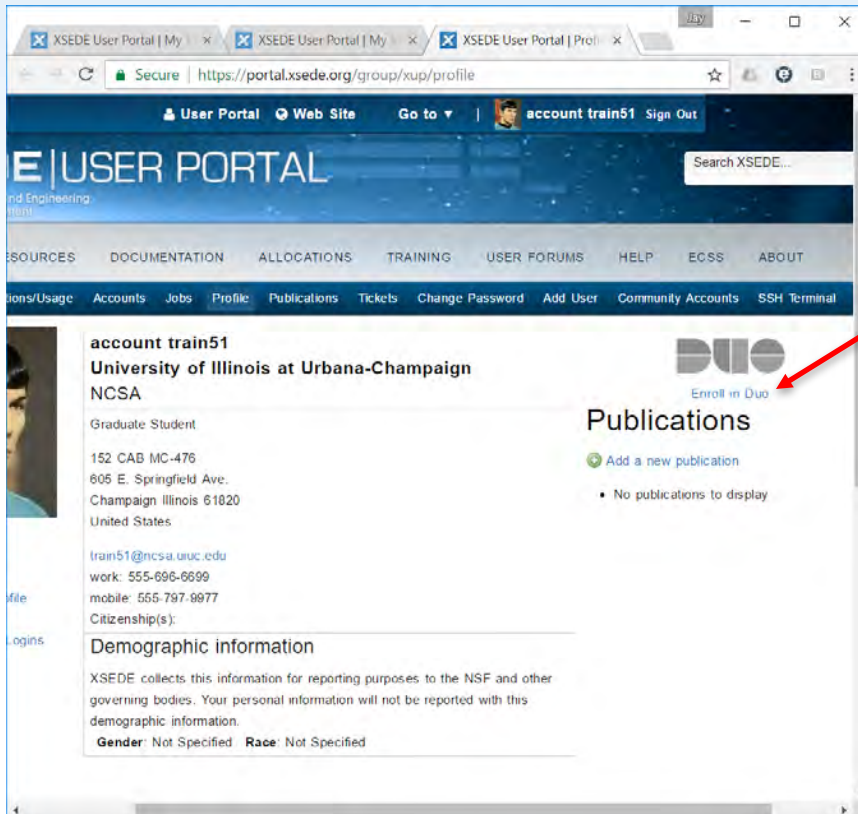
Extraterrestrial Astrobiology and Cosmology 4,070,040.0

Nuclear Physics 2,774,250.0

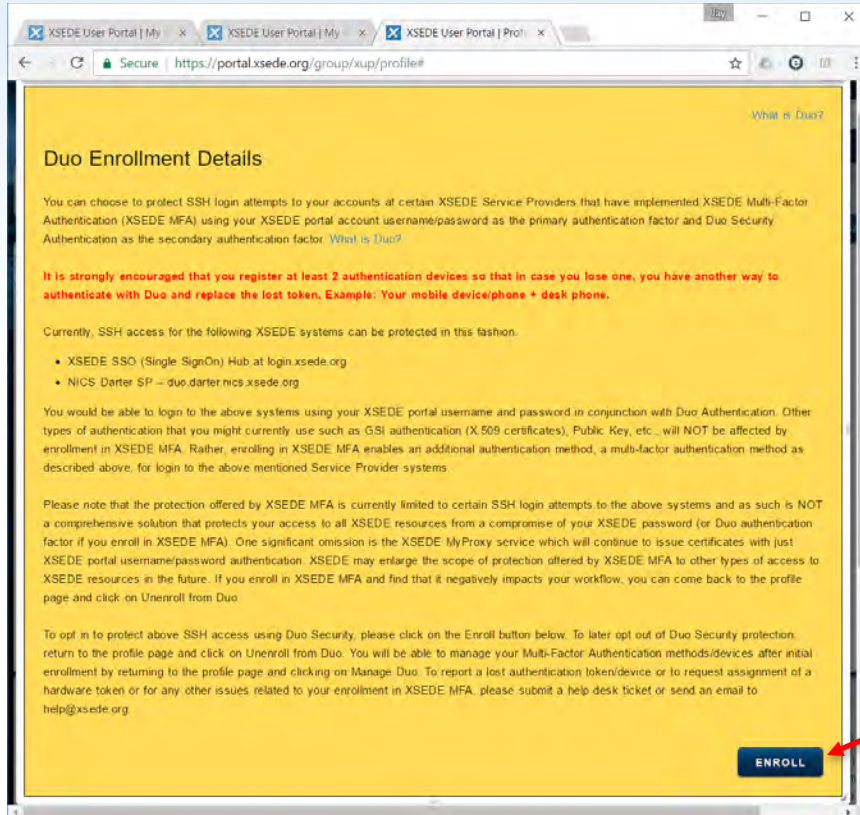
XSEDE

Adding 2 Factor Authentication

- Enroll in Duo

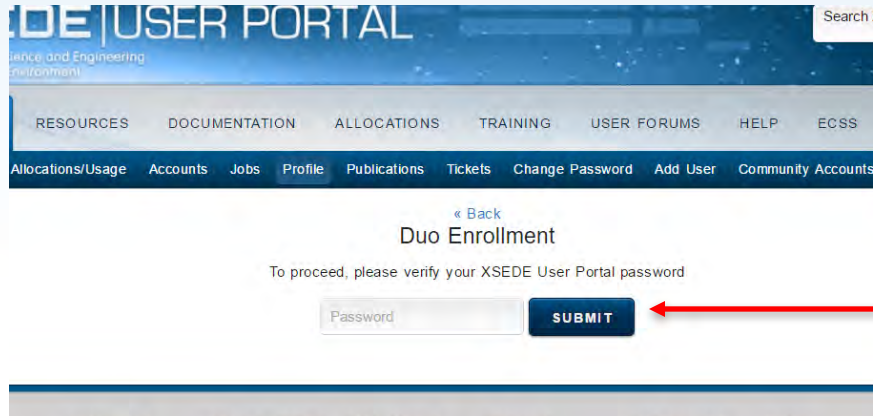


What is Duo?



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

Duo Enrollment:

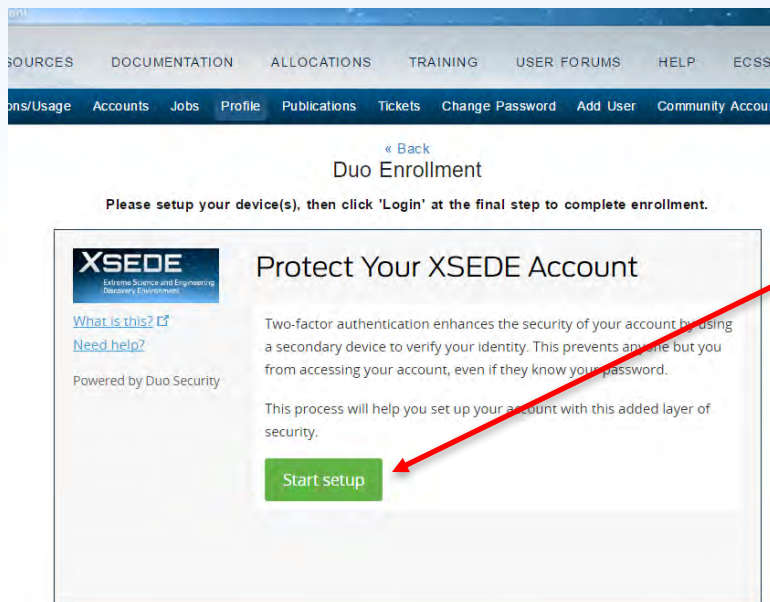


The screenshot shows the XSEDE User Portal interface. At the top, there's a header with the XSEDE logo and 'USER PORTAL' text. Below this is a navigation bar with links: RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ECSS. A secondary navigation bar contains links: Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, and Community Accounts. The main content area displays a 'Duo Enrollment' form. It includes a 'Back' link, the title 'Duo Enrollment', and the instruction 'To proceed, please verify your XSEDE User Portal password'. Below this is a text input field labeled 'Password' and a dark blue 'SUBMIT' button. A red arrow points from the text 'your XSEDE User Portal password' in the adjacent list item to the 'SUBMIT' button.

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

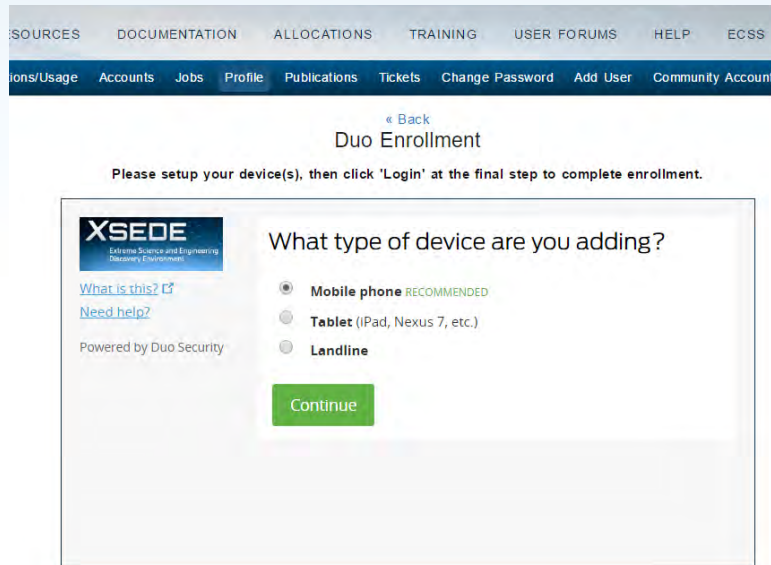
Setup Duo

- Start the process of setting up 2 factor authentication



Choose the device for 2 Factor Auth

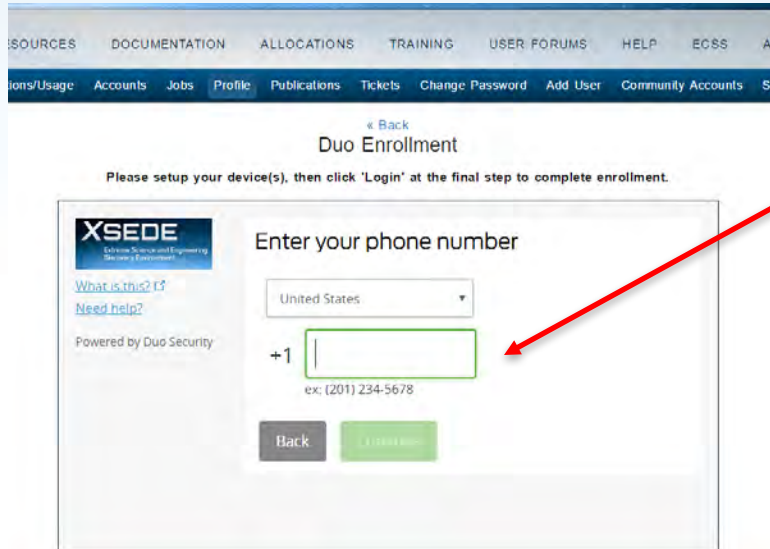
- Mobile Phone is recommended
 - Tablet, Landline also OK (though not preferred)



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

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 AE. Below this is a secondary navigation bar with links: Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SS. The main heading is "Duo Enrollment" with a "Back" link. Below the heading is a instruction: "Please setup your device(s), then click 'Login' at the final step to complete enrollment." The main form area is titled "Enter your phone number". It includes a dropdown menu for "United States", a text input field for the phone number (with a green border and a red arrow pointing to it), and a "Back" button. The text "+1" is displayed to the left of the input field, and "ex: (201) 234-5678" is shown below it. On the left side of the form, there is an XSEDE logo, a "What is this? I?" link, a "Need help?" link, and the text "Powered by Duo Security".

Verifying phone number ownership

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

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 Termination

« Back
Duo Enrollment

Please setup your device(s), then click 'Login' at the final step to complete enrollment.

What is this? [Need help?](#)

Powered by Duo Security

Verify Ownership of

1. We can call you with a verification code.

Calling you...

2. Enter your 6-digit code:

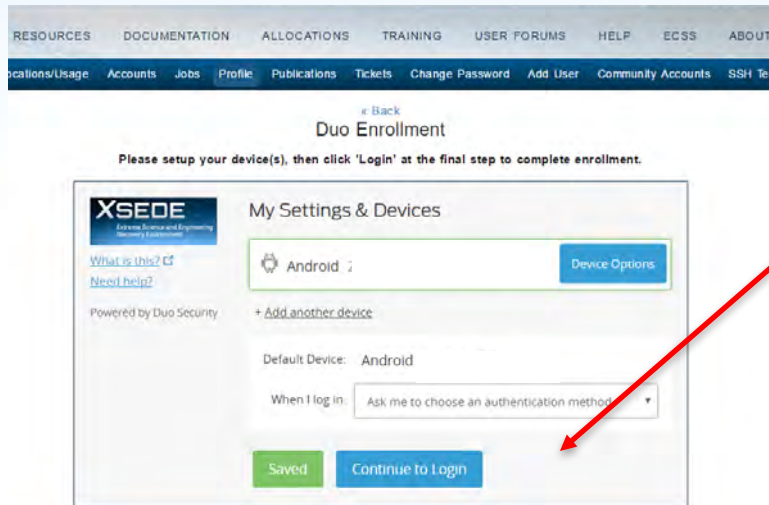
277543

MY XSEDE RESOURCES DOCUMENTATION ALLOCATIONS TRAINING USER FORUMS HELP ECSS

Summary Systems Monitor Get Started Overview Overview Forums Overview ECSS Overview
Allocations/Usage Remote Community Announcements Course Calendar Help Desk ECSS Project

Download Duo app (if desired)

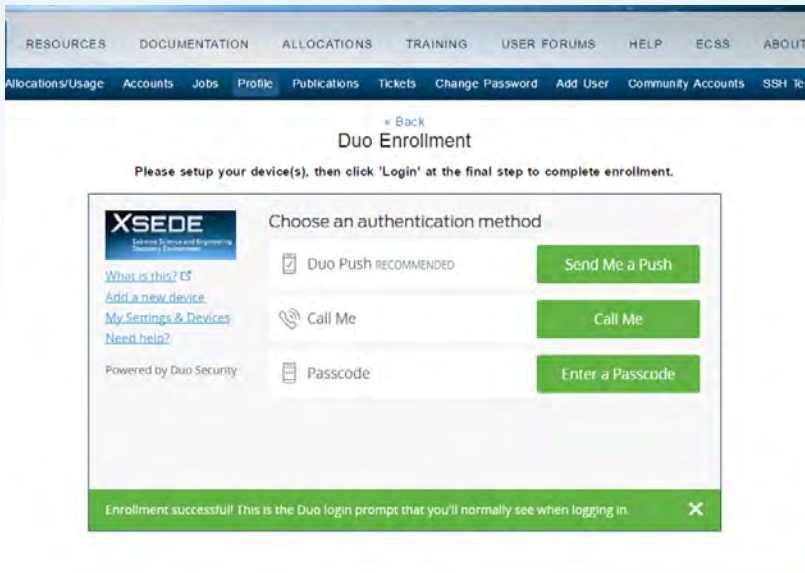
- Set authentication method (push, text, call)
 - And continue to login



The screenshot shows the XSEDE Duo Enrollment interface. At the top, there's a navigation bar with links like RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and ABOUT. Below this is a sub-navigation bar with links like Applications/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH. The main heading is 'Duo Enrollment' with a 'Back' link. A message says: 'Please setup your device(s), then click 'Login' at the final step to complete enrollment.' The 'My Settings & Devices' section shows a list of devices with 'Android' selected. There's a 'Device Options' button next to it. Below the device list, it says 'Default Device: Android' and 'When I log in: Ask me to choose an authentication method'. At the bottom, there are 'Saved' and 'Continue to Login' buttons. A red arrow points from the 'Continue to Login' button to the text 'And continue to login' in the list above.

Choose authentication method

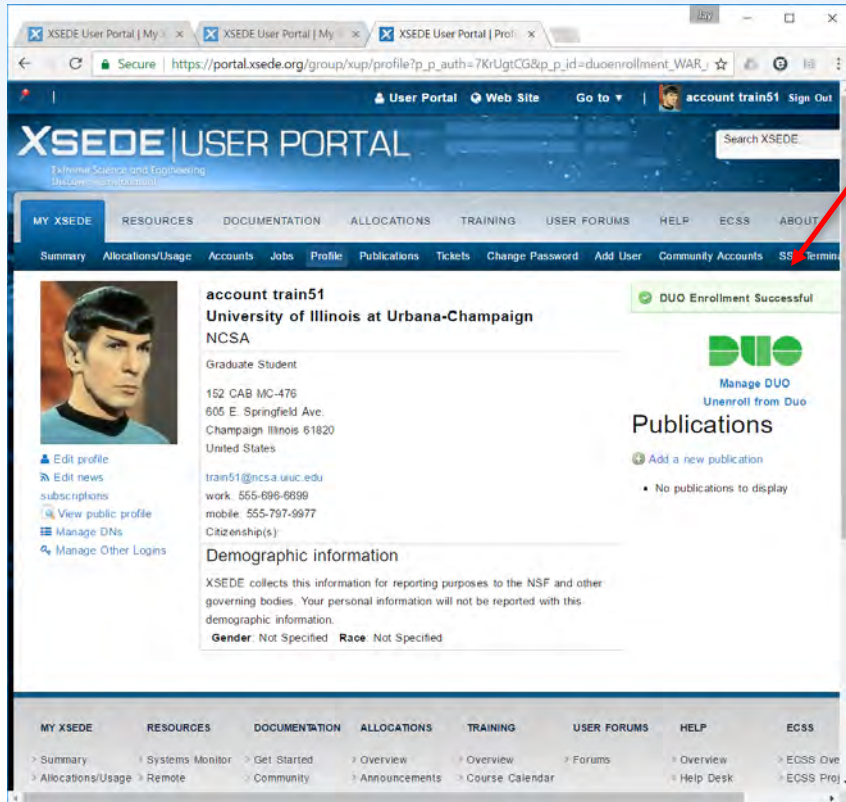
- Duo push (to app)
- Call phone
- Text passcode



The screenshot shows the XSEDE Duo Enrollment page. At the top, there is a navigation bar with links: RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, ECSS, and ABOUT. Below this is a secondary navigation bar with links: Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH. The main content area is titled "Duo Enrollment" with a "Back" link. Below the title is a message: "Please setup your device(s), then click 'Login' at the final step to complete enrollment." The main section is titled "Choose an authentication method" and contains three options: "Duo Push RECOMMENDED" with a "Send Me a Push" button, "Call Me" with a "Call Me" button, and "Passcode" with an "Enter a Passcode" button. On the left side of the main section, there is a sidebar with the XSEDE logo, links for "What is this?", "Add a new device", "My Settings & Devices", and "Need help?", and a note "Powered by Duo Security". At the bottom of the main section, there is a green banner that says "Enrollment successful! This is the Duo login prompt that you'll normally see when logging in." with a close button.

Success!

- Indication of successful setup

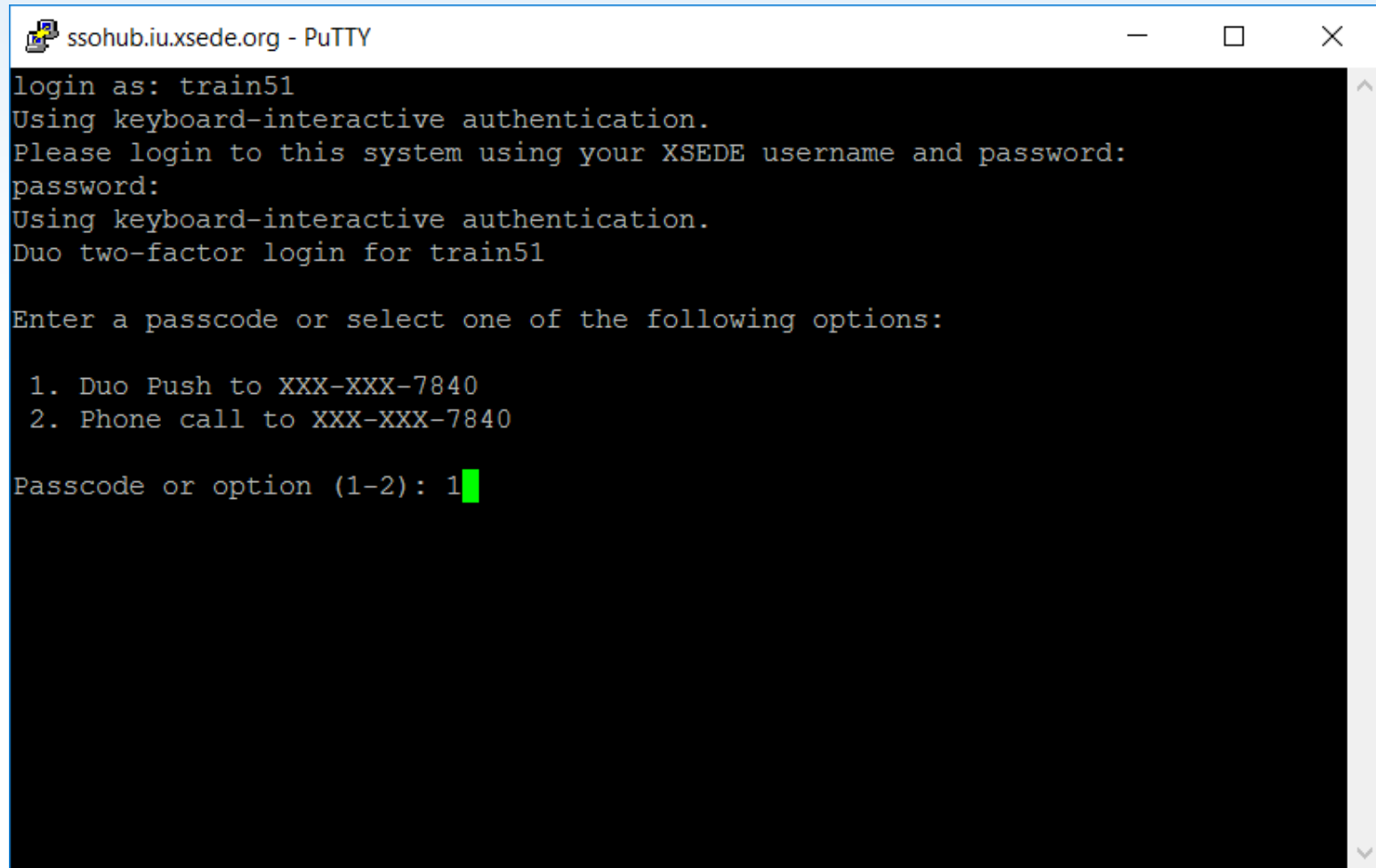


XSEDE

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 -l **username** login.xsede.org*
***username** on handout*
- And from there go to your XSEDE resource, for example:
gsissh comet.sdsc.edu

2 factor authentication



The screenshot shows a PuTTY terminal window titled "ssohub.iu.xsede.org - PuTTY". The terminal output is as follows:

```
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
```

The user has selected option 1, "Duo Push to XXX-XXX-7840".

Managing your XSEDE files

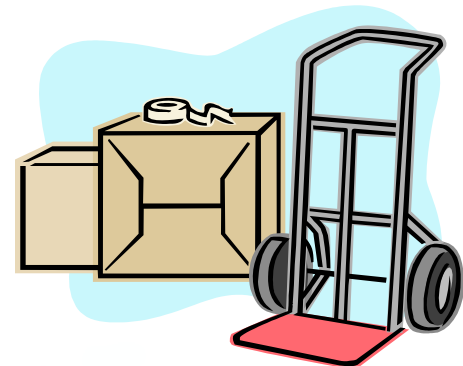
1. Where to store files

- 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>

The XSEDE logo is displayed in a large, bold, white sans-serif font. It is positioned on a dark blue background that features a grid of glowing blue squares and a faint image of a planet's horizon with a bright light source. The logo is partially overlaid by a dark blue banner that spans the width of the slide at the bottom.

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

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
```

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 Dashboard website in a Firefox browser window. The browser's address bar displays "https://www.globus.org". The website has a dark blue header with the Globus logo (a stylized 'g' in a cloud) and the word "globus". Navigation links include "Products", "News", "About", "Support", "Log In", and "Sign Up".

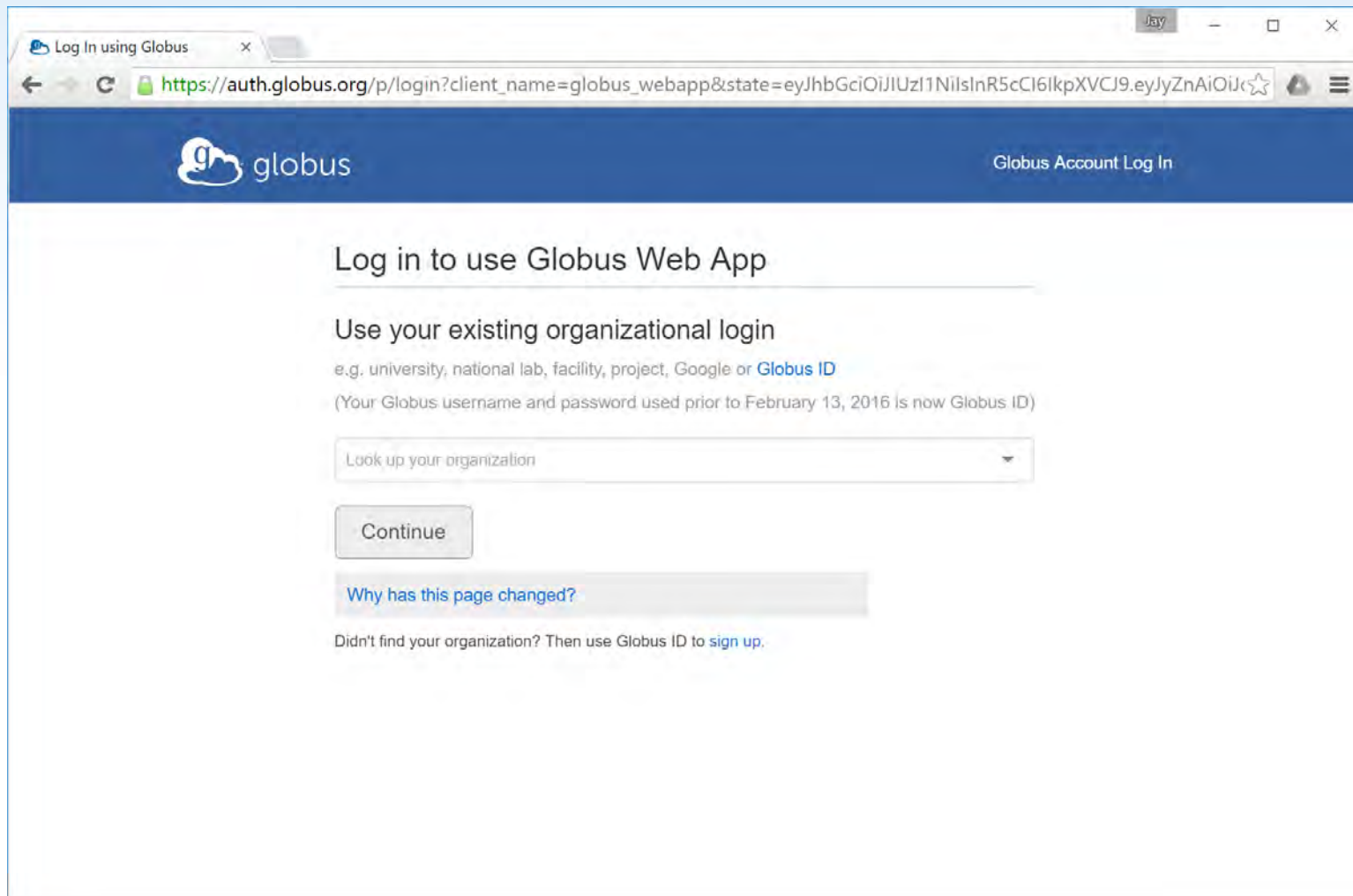
The main content area features a large graphic with three orange curved arrows labeled "share", "move", and "sync" surrounding a central circle that says "BIG DATA". To the right of this graphic, the text reads "Your research data where you need it." Below the graphic, a large counter displays "41,023,758,737 MB TRANSFERRED".

The page is divided into three columns:

- Researchers**: Focus on your research, not IT problems. We make it easy to move, manage, and share big data. Includes a "LEARN MORE" link with a right arrow and a "GET GLOBUS PLUS" link with a right arrow. A portrait of a woman is shown at the bottom.
- Resource Providers**: Globus gives you more control over your data infrastructure, while providing excellent ease-of-use for your researchers. Includes a "LEARN MORE" link with a right arrow and a "GLOBUS PROVIDER PLANS" link with a right arrow. A portrait of a man is shown at the bottom.
- How It Works**: Globus' tools and services help connect people and HPC resources, so that no researcher is an island. Includes a "LEARN MORE" link with a right arrow. A portrait of a woman is shown at the bottom.

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Login to use Globus Web App



The screenshot shows a web browser window with the title "Log In using Globus". The address bar displays the URL: https://auth.globus.org/p/login?client_name=globus_webapp&state=eyJhbGciOiJIUzI1NiIsInR5cCI6IkpXVCJ9.eyJyZnAiOiJk. The page features a blue header with the Globus logo on the left and "Globus Account Log In" on the right. The main content area has a heading "Log in to use Globus Web App" followed by the instruction "Use your existing organizational login". Below this, it provides examples of organizational logins: "e.g. university, national lab, facility, project, Google or [Globus ID](#)". A note states: "(Your Globus username and password used prior to February 13, 2016 is now Globus ID)". There is a text input field with the placeholder "Look up your organization" and a dropdown arrow. A "Continue" button is positioned below the input field. A link "[Why has this page changed?](#)" is shown in a light gray box. At the bottom, a message says: "Didn't find your organization? Then use Globus ID to [sign up](#)."

Log In using Globus

https://auth.globus.org/p/login?client_name=globus_webapp&state=eyJhbGciOiJIUzI1NiIsInR5cCI6IkpXVCJ9.eyJyZnAiOiJk

globus Globus Account Log In

Log in to use Globus Web App

Use your existing organizational login

e.g. university, national lab, facility, project, Google or [Globus ID](#)

(Your Globus username and password used prior to February 13, 2016 is now Globus ID)

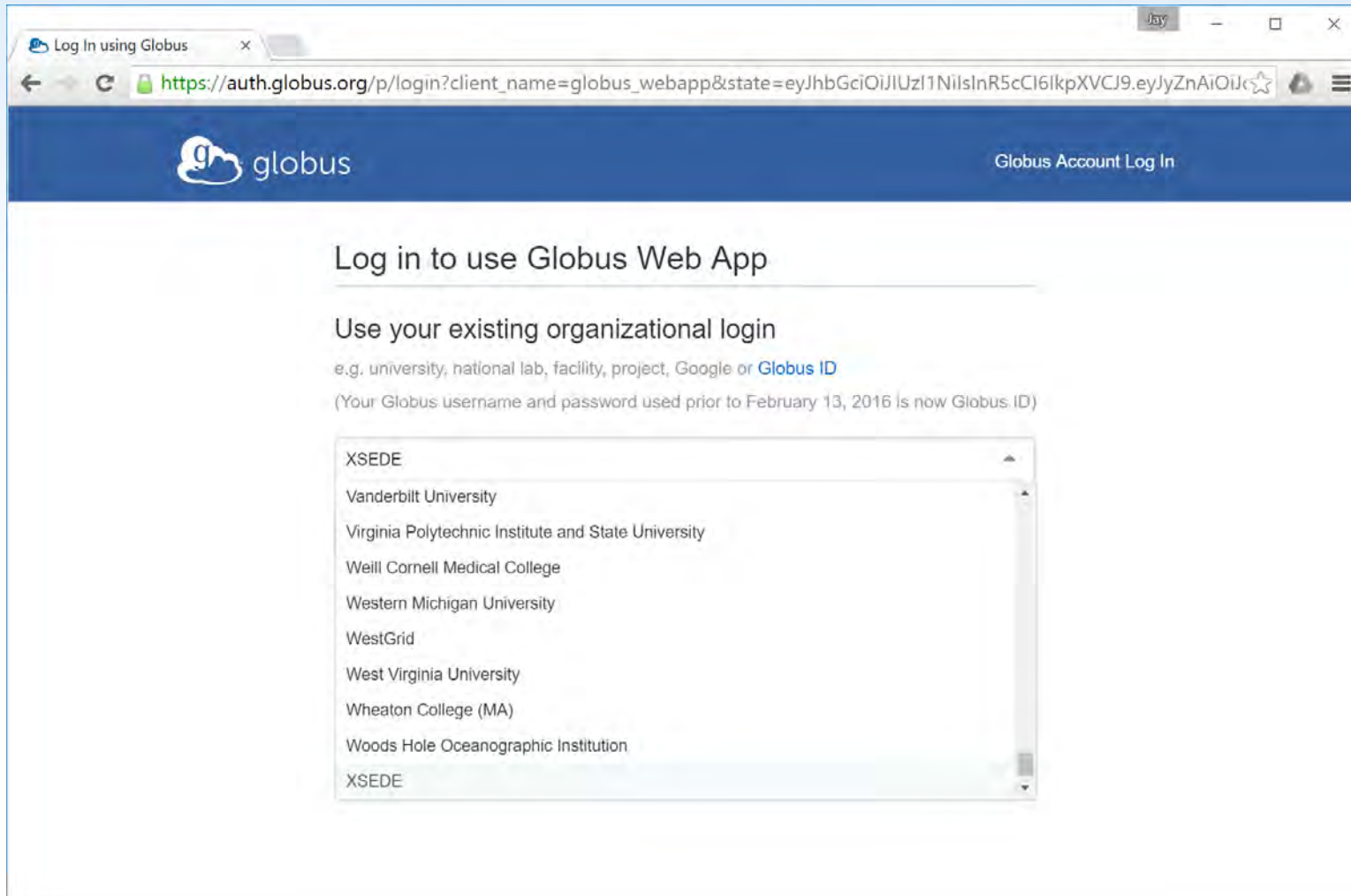
Look up your organization

Continue

[Why has this page changed?](#)

Didn't find your organization? Then use Globus ID to [sign up](#).

Use XSEDE Identity Provider



The screenshot shows a web browser window with the title "Log In using Globus". The address bar displays the URL: https://auth.globus.org/p/login?client_name=globus_webapp&state=eyJhbGciOiJIUzI1NiIsInR5cCI6IkpXVCJ9.eyJyZnAiOiJk. The page header features the Globus logo and a "Globus Account Log In" link. The main content area is titled "Log in to use Globus Web App" and instructs users to "Use your existing organizational login" with examples like university, national lab, facility, project, Google, or Globus ID. A note states: "(Your Globus username and password used prior to February 13, 2016 is now Globus ID)". A dropdown menu is open, showing a list of organizations. The first item is "XSEDE", which is highlighted. Other visible items include "Vanderbilt University", "Virginia Polytechnic Institute and State University", "Weill Cornell Medical College", "Western Michigan University", "WestGrid", "West Virginia University", "Wheaton College (MA)", "Woods Hole Oceanographic Institution", and another "XSEDE" entry at the bottom.

Log In using Globus

https://auth.globus.org/p/login?client_name=globus_webapp&state=eyJhbGciOiJIUzI1NiIsInR5cCI6IkpXVCJ9.eyJyZnAiOiJk

globus

Globus Account Log In

Log in to use Globus Web App

Use your existing organizational login

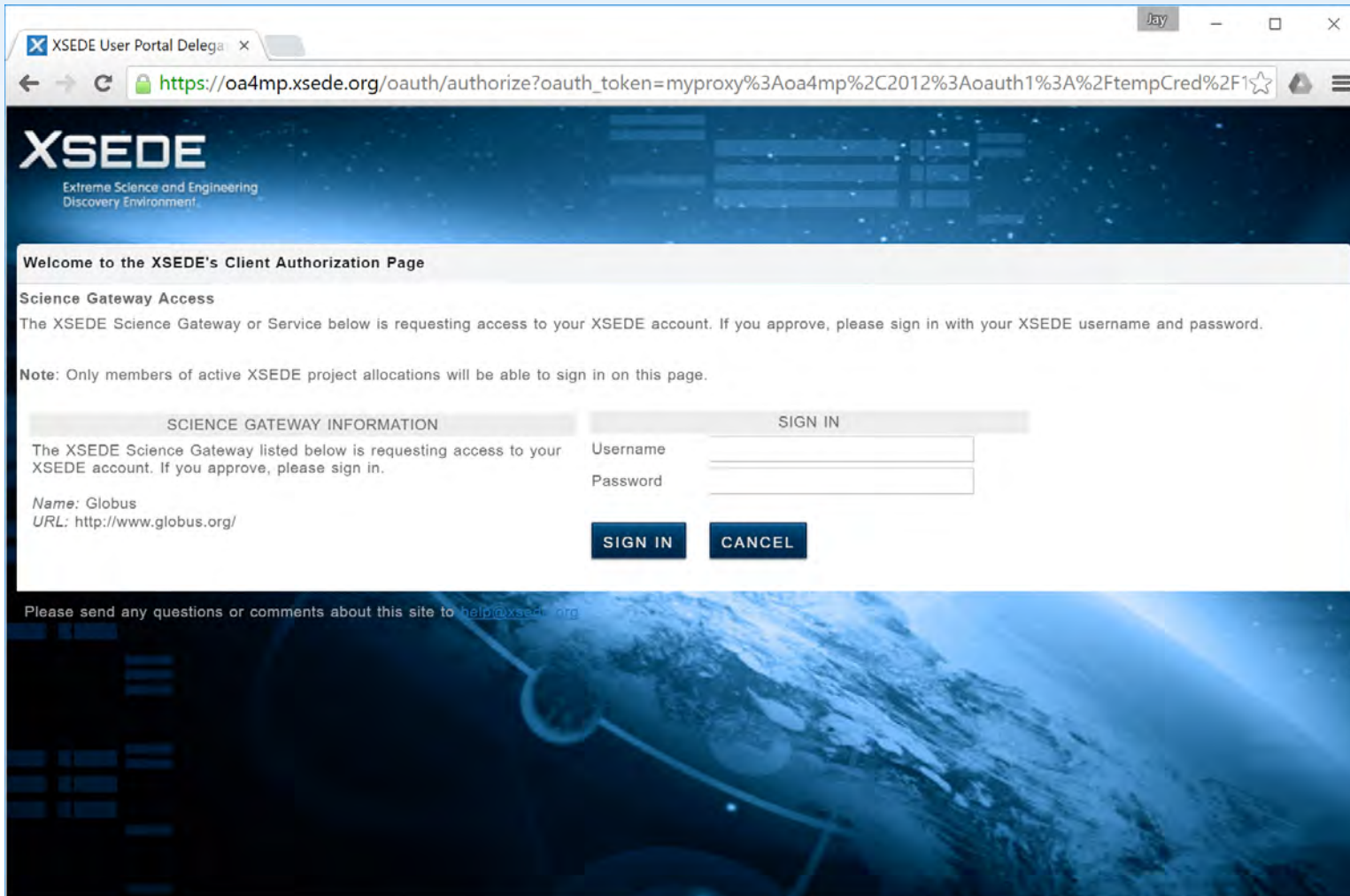
e.g. university, national lab, facility, project, Google or [Globus ID](#)

(Your Globus username and password used prior to February 13, 2016 is now Globus ID)

- XSEDE
- Vanderbilt University
- Virginia Polytechnic Institute and State University
- Weill Cornell Medical College
- Western Michigan University
- WestGrid
- West Virginia University
- Wheaton College (MA)
- Woods Hole Oceanographic Institution
- XSEDE

XSEDE

Sign in with XSEDE credentials



The screenshot shows a web browser window with the address bar displaying https://oa4mp.xsede.org/oauth/authorize?oauth_token=myproxy%3Aoa4mp%2C2012%3Aoauth1%3A%2FtempCred%2F1. The page header features the XSEDE logo and the tagline "Extreme Science and Engineering Discovery Environment". The main content area is titled "Welcome to the XSEDE's Client Authorization Page" and "Science Gateway Access". It explains that the XSEDE Science Gateway is requesting access to the user's XSEDE account and provides a note that only members of active XSEDE project allocations can sign in. The form is divided into two sections: "SCIENCE GATEWAY INFORMATION" and "SIGN IN". The "SCIENCE GATEWAY INFORMATION" section lists the gateway name as "Globus" and the URL as "http://www.globus.org/". The "SIGN IN" section contains input fields for "Username" and "Password", and two buttons: "SIGN IN" and "CANCEL". At the bottom, there is a link to help@xsede.org for questions or comments.

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.	Username <input type="text"/>
Name: Globus	Password <input type="password"/>
URL: http://www.globus.org/	<input type="button" value="SIGN IN"/> <input type="button" value="CANCEL"/>

Please send any questions or comments about this site to help@xsede.org

XSEDE

Globus Online File Transfer

The screenshot displays the Globus Online File Transfer interface. At the top, the Globus logo is on the left, and navigation links for "Manage Transfers", "Groups", "Support", and "skappes" are on the right. Below the navigation bar, there are links for "start transfer", "view activity", "manage endpoints", and "dashboard". A section titled "Transfer Files" includes a link to "Get Globus Connect" with the subtext "Turn your computer into an endpoint."

The main interface is divided into two panels for source and destination endpoints. The left panel shows the source endpoint "skappes#sandle" with a path of "/~/Project Files/". It contains a file list with two items: "Process Colors - Copy.c" and "Process Colors.c", both 2.77 kB in size. The right panel shows the destination endpoint "xsede#psodata" with a path of "/~/", containing a folder named "project-files".

At the bottom, there is a "Label This Transfer" section with a text input field and a note: "This will be displayed in your transfer activity."

XSEDE

Choosing a file to move...

The screenshot shows the Globus Transfer Files web interface. The browser address bar displays `https://www.globus.org/xfer/StartTransfer#c`. The page has a dark blue header with the Globus logo and navigation links: [Manage Data](#), [Groups](#), [Support](#), and [jalameda](#). Below the header, there are tabs for [Transfer Files](#), [Activity](#), [Manage Endpoints](#), and [Dashboard](#). The main heading is "Transfer Files".

On the right side, there is a link: "Get Globus Connect Personal Turn your computer into an endpoint."

The interface is divided into two main panels for file selection, separated by left and right arrow buttons.

Left Panel:

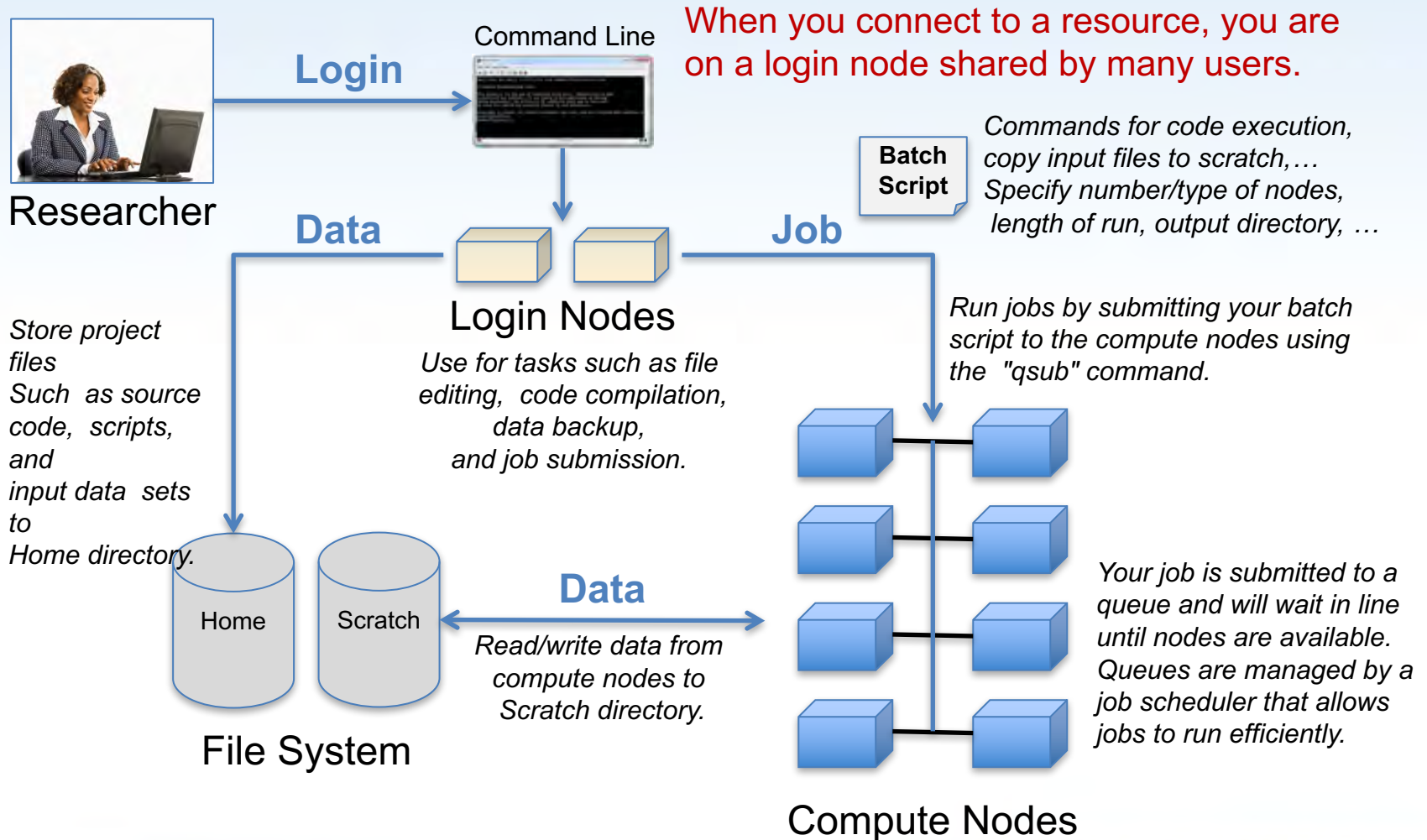
- Endpoint: `xsede#comet` (with a dropdown menu and a "Go" button)
- Path: `/ux400689/` (with a "Go" button)
- Actions: [select all](#), [none](#), [up one folder](#), [refresh list](#)
- File List:
 - intel Folder
 - newfolder Folder
 - shallow Folder
 - shallow-12jun2014 Folder
 - shallow-43-SR2-nightly Folder
 - shallow-SR1_kepler_try2 Folder
 - shallow-SR2-RC1-23jan2014 Folder
 - shallow-gordon-icc Folder
 - shallow-luna-SR1-RC4-candidate Folder
 - shallow-luna-sr1-rc1-candidate Folder
 - shallow-sr1-kepler-jan2014 Folder
 - shallow-trestles-icc Folder
 - shallow-trestles-icc-43SR2 Folder
 - shallow_43_SR2_SEA Folder
 - test-synch Folder
 - trainingSC12_C Folder
 - a.out 7.84 kB
 - hellompi-slurm.sb 341 b
 - ptp_job.e1286924 96 b
 - ptp_job.e1286961 837 b

Right Panel:

- Endpoint: `xsede#blacklight` (with a dropdown menu and a "Go" button)
- Path: `/` (with a "Go" button)
- Actions: [select all](#), [none](#), [up one folder](#), [refresh list](#)
- File List:
 - PweTest Folder
 - shallow-sr1-kepler-jan2014 Folder
 - shallow-trestles-icc Folder
 - shallow_43_SR2_SEA Folder
 - trainingSC12_C Folder
 - ptp_job.e1286924 96 b

At the bottom of the interface, there is a "more options" link, a "Label This Transfer" input field, and a note: "This will be displayed in your transfer activity."

Running Jobs Overview



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 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

Batch Script for PSC's Blacklight

```
1. #!/bin/csh
2. #PBS -l ncpus=16
3. #ncpus must be a multiple of 16
4. #PBS -l walltime=5:00
5. #PBS -j oe
6. #PBS -q batch
7. set echo
8. ja
9. #move to my $SCRATCH directory
10. cd $SCRATCH
11. #copy executable to $SCRATCH
12. cp $HOME/mympi
13. #run my executable
14. mpirun -np $PBS_NCPUS ./mympi
15. ja -chlst
```

Blacklight uses the Portable Batch System (PBS) scheduler. Lines 2,4,5, and 6 are PBS directives.

Submitting Batch Scripts

- Commands are machine specific, but follow general principles
- With PBS batch scripts, use the **qsub command**
`qsub myscript.job`
- Can also specify PBS directives as command-line options:

```
qsub -l ncpus=16 -l walltime=5:00 -j oe -q batch myscript.job
```
- Command-line directives override directives in your scripts.

More PBS commands

- `qstat` - displays the status of batch jobs.

<code>-a</code>	gives the status of all jobs on the system.
<code>qstat -n</code>	lists nodes allocated to a running job in addition to basic information.
<code>qstat -f PBS_JOBID</code>	gives detailed information on a particular job.
<code>-q</code>	provides summary information on all the queues.

- `qdel` – deletes a queued job or kills a running job.
- See the `qsub` manpage for more

Example Batch Command

```
qsub amber.job
```

```
qstat -a
```

Job ID	Username	Queue	Jobname	SessID	NDS	Tasks	Memory	Time	S	Time
29668	user1	batch	job2	21909	1	256	--	08:00	R	02:28
29894	user2	batch	run128	--	1	128	--	02:30	Q	--
29895	user3	batch	STDIN	15921	1	1	--	01:00	R	00:10
29896	user2	batch	jobL	21988	1	2048	--	01:00	R	00:09
29897	user4	batch	STDIN	22367	1	2	--	00:30	R	00:06
29898	user1	batch	amber	25188	1	1	--	01:10	R	00:00

```
qdel 29668
```

- After job 29898 runs: user1 should get file `amber.job.o29898` with output/errors (log file)

Job Scheduling

- All XSEDE compute resources use a **batch scheduler** for running jobs.
- All jobs are placed in a **batch queue** after they are submitted.
- 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.



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

Improving job turnaround

- Request accurate walltime
- Use flexible walltime
- Pack your job
 - Running many small jobs places a great burden on the scheduler and is also inconvenient for you.
 - Pack many executions into a single job, which you then submit to PBS with a single qsub command.

Requesting flexible walltime

```
-l walltime_min=HH:MM:SS  
-l walltime_max=HH:MM:SS
```

Example: Your job requests 64 cores and a walltime between 2 and 4 hours. If there is a 64 core slot available for 3 hours, your job could run in this slot. However, if your job had requested a fixed walltime of 4 hours it would not run until the larger time slot becomes available.

Packing Serial Jobs

Run each program execution in the background and place a wait command after each execution.

```
#!/bin/csh
#PBS -l ncpus=96
#PBS -l walltime=5:00
#PBS -q batch
dplace -c 0 ./myserial1 < serial1.dat &
dplace -c 32 ./myserial2 < serial2.dat &
dplace -c 64 ./myserial3 < serial3.dat &
wait
```

Packing OpenMP Jobs

To pack OpenMP executables, replace the dplace command with the omplace command. Sample job to pack OpenMP executables:

```
omplace -nt 32 -c 0 ./myopenmp1 < myopenmp1.dat &  
omplace -nt 32 -c 32 ./myopenmp2 < myopenmp2.dat &  
omplace -nt 32 -c 64 ./myopenmp3 < myopenmp3.dat &  
omplace -nt 32 -c 96 ./myopenmp4 < myopenmp4.dat &  
wait
```

Managing Your Environment: Modules

- Allows you to manipulate your environment.
- **'module list'** shows currently loaded modules.
- **'module avail'** shows available modules.
- **'module show' <name>** describes module.
<http://modules.sourceforge.net/>

```
% module load gcc/3.1.1
% which gcc
/usr/local/gcc/3.1.1/linux/bin/gcc
```

```
% module switch gcc/3.1.1 gcc/3.2.0
% which gcc
/usr/local/gcc/3.2.0/linux/bin/gcc
```

```
% module unload gcc
% which gcc
gcc not found
```


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 -l **username** login.xsede.org*
***username** on handout*
- And from there go to your XSEDE resource, for example:
gsissh comet.sdsc.edu

SDSC comet Cluster & Modules

- Default environment intel compilers, mvapich2 MPI implementation
- We will swap intel compilers with gnu compilers
 - module swap intel gnu
 - which gcc
- And then we'll load the openMPI library
 - module load openmpi_ib
 - which mpicc

Module demo on comet

```
-bash-4.1$ module swap intel gnu
Unloading compiler-dependent module tau/2.23
Need to load an mpi module before loading fftw/2.23
Unloading compiler-dependent module pdt/3.20
Unloading compiler-dependent module papi/5.4.1
Unloading compiler-dependent module tau/2.23
Need to load an mpi module before loading fftw/2.23
-bash-4.1$ module list
Currently Loaded Modulefiles:
  1) gnutools/2.69      2) globus/5.2.5      3) gnu/4.9.2         4) .intel/tau/2.23
-bash-4.1$ module load openmpi_ib
-bash-4.1$ which mpicc
/opt/openmpi/gnu/ib/bin/mpicc
-bash-4.1$
```


Using modules in your job script

- First,
`source /usr/share/Modules/init/shell-name`
`module load module-name`
- Check on-line documentation

Exercise

- Make sure you are on comet.sdsc.edu
- Run the shallow water model code provided
- No input file needed
- Copy batch script from my home directory:
`cp ~ux400689/shallow-slurm.sb .`

Job script

```
#!/bin/bash
#SBATCH --job-name="shallow"
#SBATCH --output="shallow.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=5
#SBATCH --export=ALL
#SBATCH -t 00:30:00
```

#This job runs with 1 nodes, 5 cores per node for a total of 5 cores.
#ibrun in verbose mode will give binding detail

```
ibrun -v ~ux400689/shallow/shallow
```

~

Exercise:

- Submit the job (`sbatch --res=JSUResDay2 shallow-slurm.sb`)
- Monitor the job (`squeue -u username`)
- Make sure you have the output files at job completion

```
-bash-4.1$ ls calc.c decs.h eclipse.inc Makefile shallow-batch.sh
tstep.f90 calc.o diag.c init.c shallow shallow-slurm.sb
tstep.ocopy.c diag.o init.o shallow.582135.comet-03-56.out time.c
worker.ccopy.o dump.c main.c shallow.591445.comet-04-66.out time.o
worker.oCVS dump.o main.o shallow.591474.comet-04-66.out tstep.c
-bash-4.1$
```

more shallow*out (for this case, yours will be different!)

Output files: need to show successful completion

```
Remote System Details Tasks Terminals Remote Environments
login.xsede.org
jstart=0, jend=7, next=2, prev=4
jstart=8, jend=15, next=3, prev=1
jstart=16, jend=23, next=4, prev=2
jstart=24, jend=31, next=1, prev=3

Shallow water weather model - Distributed Memory Version 0.6

Number of points in the X direction      32
Number of points in the Y direction      32
Grid spacing in the X direction          100000.00
Grid spacing in the Y direction          100000.00
Time step                                90.000
Time filter parameter                     0.001
Cycle number      1      Model time in days  0.00
    Potential energy      0.000      Kinetic Energy      48036.828
    Total Energy          48036.828      Pot. Enstrophy      0.000000e+00

Cycle number      50      Model time in days  0.05
    Potential energy      1256.284      Kinetic Energy      46526.969
    Total Energy          47783.254      Pot. Enstrophy      -nan

Cycle number      100      Model time in days  0.10
```

1,1 Top

Need help? Reporting and Tracking Issues

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

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 → 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 (formerly known as Advanced User Support (AUSS))

The XSEDE logo is displayed in a large, white, sans-serif font against a dark blue background. The background features a stylized representation of a globe with grid lines and a network of glowing blue lines, suggesting a global or networked environment.

XSEDE

XSEDE Training Survey

- Please complete a short on-line survey about this module at <http://bit.ly/xsedejackson>. We value your feedback, and will use your feedback to help improve our training offerings.
- Slides from this workshop are available at <http://hpcuniversity.org/trainingMaterials/238/>

May 3, 2017

Thanks for listening and welcome to
XSEDE!

XSEDE

Extreme Science and Engineering
Discovery Environment