

May 13, 2016

XSEDE New User Tutorial

XSEDE

Extreme Science and Engineering
Discovery Environment

Jay Alameda
National Center for
Supercomputing Applications

XSEDE Training Survey

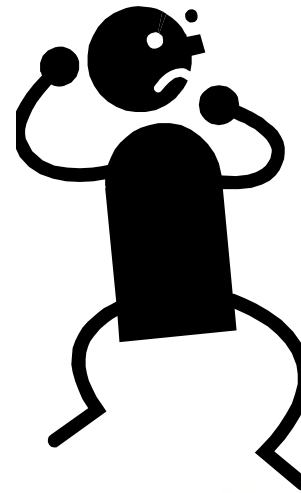
- Please complete a short on-line survey about this module at <http://bit.ly/hamptonxsede>. We value your feedback, and will use your feedback to help improve our training offerings.
- Slides from this workshop are available at <http://hpcuniversity.org/trainingMaterials/219>

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)

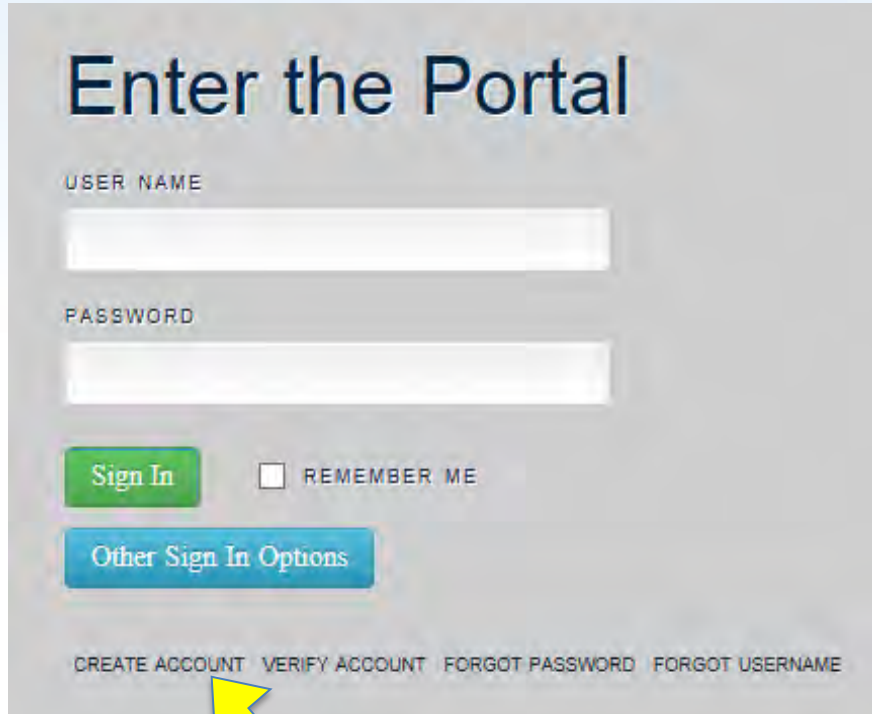
- URL: portal.xsede.org
- Single point-of-entry to information about XSEDE services and utilities for using them
- Anyone can create an XUP user account and access non-project features
- Only XSEDE allocation project members can access project features

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

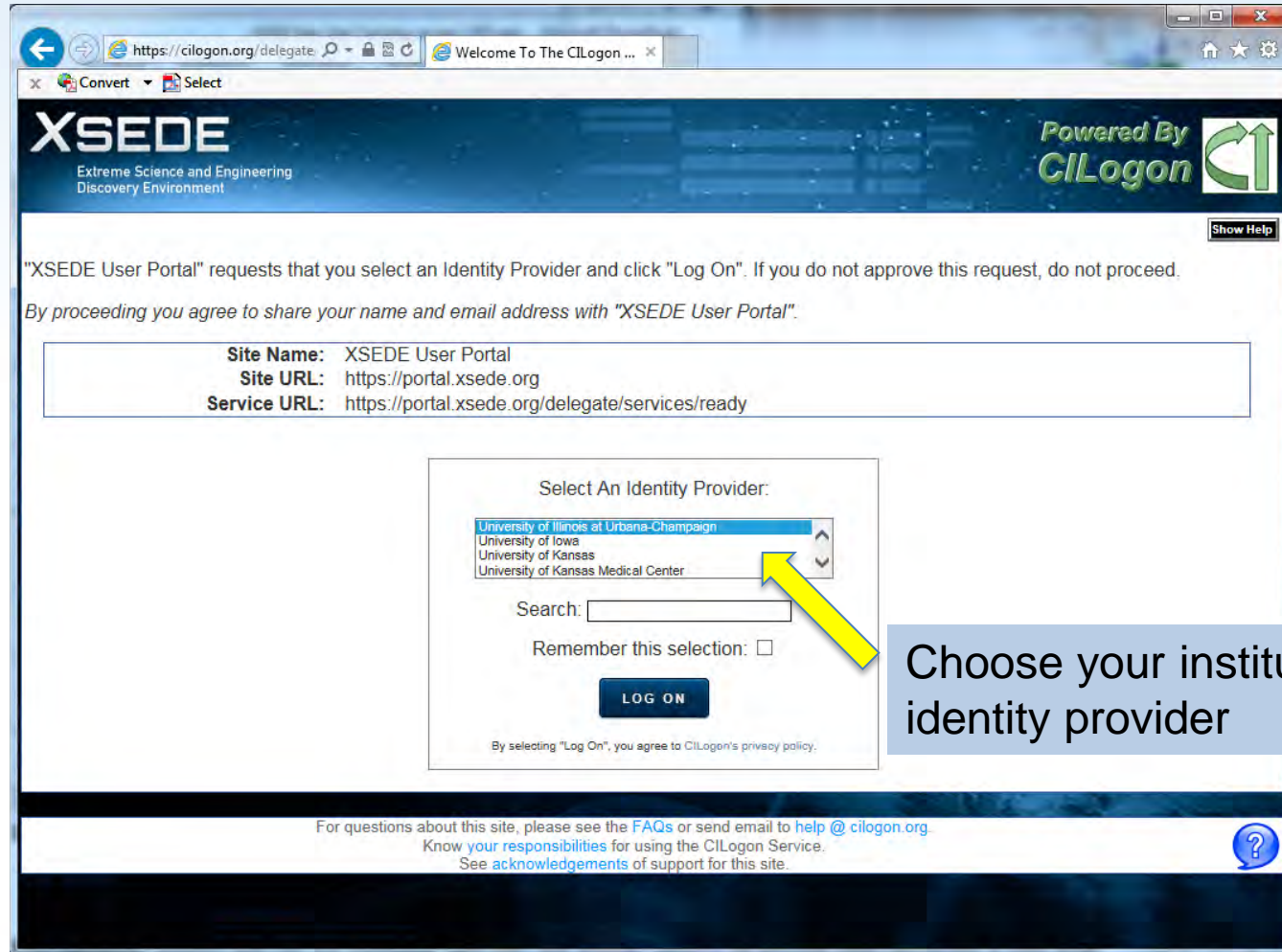


The screenshot shows the 'Enter the Portal' login interface. It features two input fields for 'USER NAME' and 'PASSWORD'. Below these is a green 'Sign In' button, a checkbox for 'REMEMBER ME', and a blue 'Other Sign In Options' button. At the bottom, there are four links: 'CREATE ACCOUNT', 'VERIFY ACCOUNT', 'FORGOT PASSWORD', and 'FORGOT USERNAME'. A yellow arrow points to the 'CREATE ACCOUNT' link.

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

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

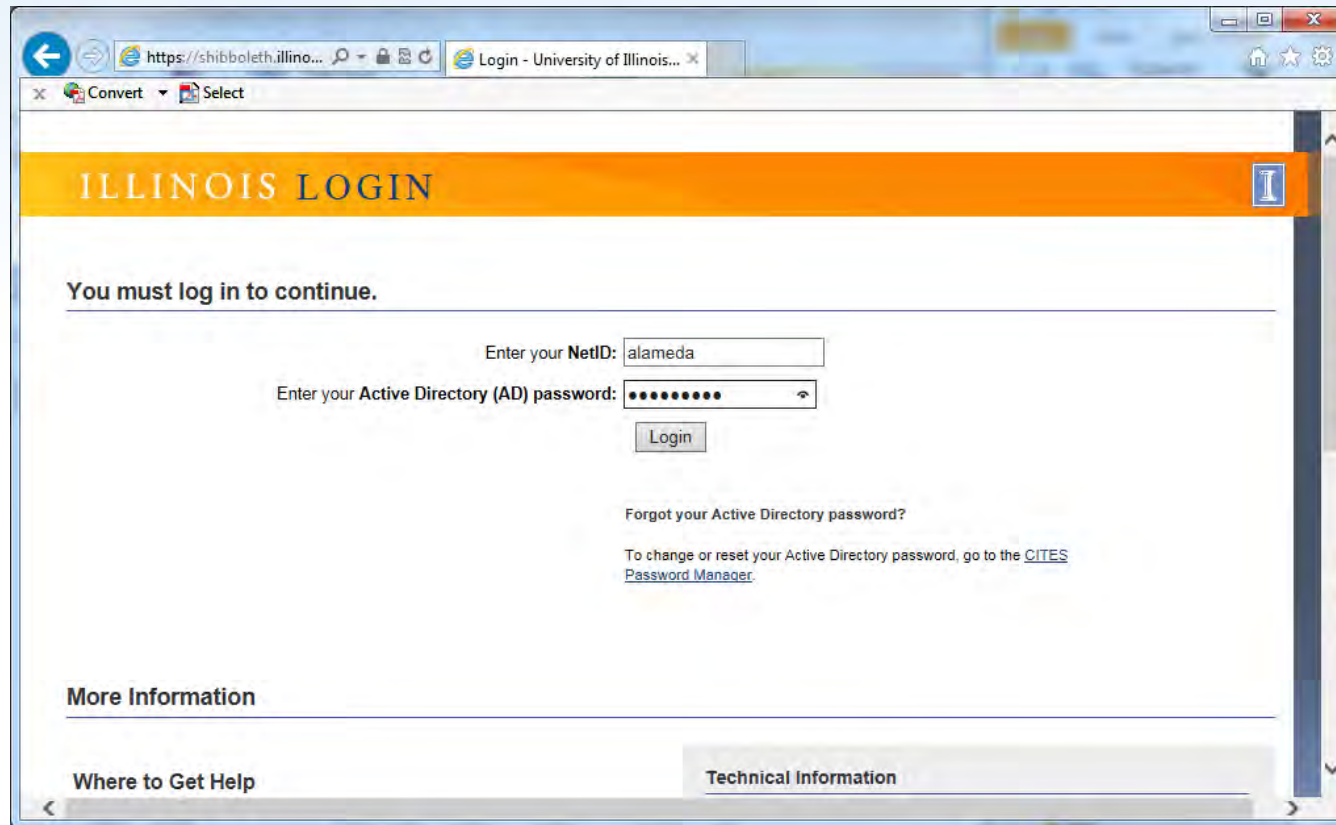
By selecting "Log On", you agree to CILogon's privacy policy.

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.

Choose your institutions's
identity provider

XSEDE

Example: Logging in with Illinois credentials



The screenshot shows a web browser window with the URL <https://shibboleth.illinois...> and a tab titled "Login - University of Illinois...". The page features an orange header with the text "ILLINOIS LOGIN" and a small "I" logo. Below the header, a message states "You must log in to continue." The login form includes 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. A link for "Forgot your Active Directory password?" is provided, along with a note to go to the "CITES Password Manager" for password changes. At the bottom, there are links for "More Information", "Where to Get Help", and "Technical Information".

ILLINOIS LOGIN

You must log in to continue.

Enter your NetID: alameda

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 displays the XSEDE User Portal interface. At the top, the browser address bar shows the URL <https://portal.xsede.org/web/>. The page header features the XSEDE logo and the text "Extreme Science and Engineering Discovery Environment". A search bar labeled "Search XSEDE" is located in the top right corner, along with a "SIGN IN" link. Below the header, a navigation menu includes links for MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ABOUT. A secondary menu below this lists various user actions: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH Terminal. The main content area is titled "Please select a method to connect your Federated Identity to your XSEDE account". It provides instructions for existing users (select "Connect") and new users (select "Create"). Two buttons, "Connect" (green) and "Create" (blue), are prominently displayed. A vertical "FEEDBACK" button is on the right side. The footer contains a detailed grid of links organized by category: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ABOUT.

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 select a method to connect your Federated Identity to your XSEDE account

If you have an XSEDE account, please select the Connect option. This will prompt you to log in with your credentials

If you do not have an XSEDE account, please select the Create option and come back to connect your accounts

[Connect](#) [Create](#)

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

XSEDE

Login to the portal to link identities

https://portal.xsede.org/cilogic

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

https://portal.xsede.org/group

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

Jay Alameda
University of Illinois at Urbana-Champaign
N.C.S.A.

Center Researcher Staff

MC 257 - 1008 NCSA
1205 W. Clark St.
Urbana Illinois 61801
United States

jalameda@ncsa.illinois.edu
work: 217-244-4696

Publications
Add a new publication
No publications to display

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 demographic information.
Gender: Not Specified Race: Not Specified

Other XSEDE Login Identities
To add a new identity please login to portal.xsede.org and select 'Other Login Options':

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.
- 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>



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

The screenshot shows the My XSEDE User Portal (XUP) interface. At the top is a navigation bar with links: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ABOUT. Below this is a sub-navigation bar with links: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH Terminal.

The main content area is divided into three sections:

- WELCOME TO XUP (1)**: A welcome message to Sandra, stating that the XUP is the home for XSEDE users to view and manage their accounts and allocations. It also provides a link to the Getting Started Guide.
- LATEST UPDATES (2)**: A section showing the user's profile information, including their last login, open tickets, jobs, publications, and training status. It includes a "Update profile" and "Submit a ticket" link.
- MY ACTIVE ALLOCATIONS (3)**: A section showing the user's active allocations. It includes a table with columns: RESOURCE, % LEFT, END DATE [DAYS LEFT], and BURN RATE. The table shows a single allocation for "Staff Resources" with 100% left, 300,000 SUs remaining, and an end date of 2014-09-20 (326 days left). A "Burn Rate" gauge is also displayed.

On the left side of the page, there is a sidebar with links for "New to XSEDE?" (Read the Getting Started Guide), "Find your Campus Champion" (Find your Campus Champion your local source of knowledge about high-performance computing opportunities and resources), and "Now that you are logged in you can:" (Manage Your Allocations, Login to your XSEDE Accounts, View and monitor systems and jobs, Manage your files, Find and register for training classes, and NEW! Share your XSEDE Science Achievements).

(1)

WELCOME TO XUP

- Quick access to commonly used features.

(2)

LATEST UPDATES

- Latest information specific to your user account.

(3)

MY ACTIVE 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 Portal interface. The header includes the XSEDE logo and the text "USER PORTAL" and "Extreme Science and Engineering Discovery Environment". A navigation bar contains links: HOME, MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, CONSULTING, and USER FORUMS. Below this is a secondary navigation bar with links: Allocations/Usage, Accounts, My Jobs, Profile (highlighted), Tickets, Registered DNs, Change Portal Password, Add/Remove User, Community Accounts, and SSH Terminal. The main content area displays a profile form with the following fields:

Name	
Email	
NSF Status	
Organization	Pittsburgh Supercomputing Center
Address	

XSEDE

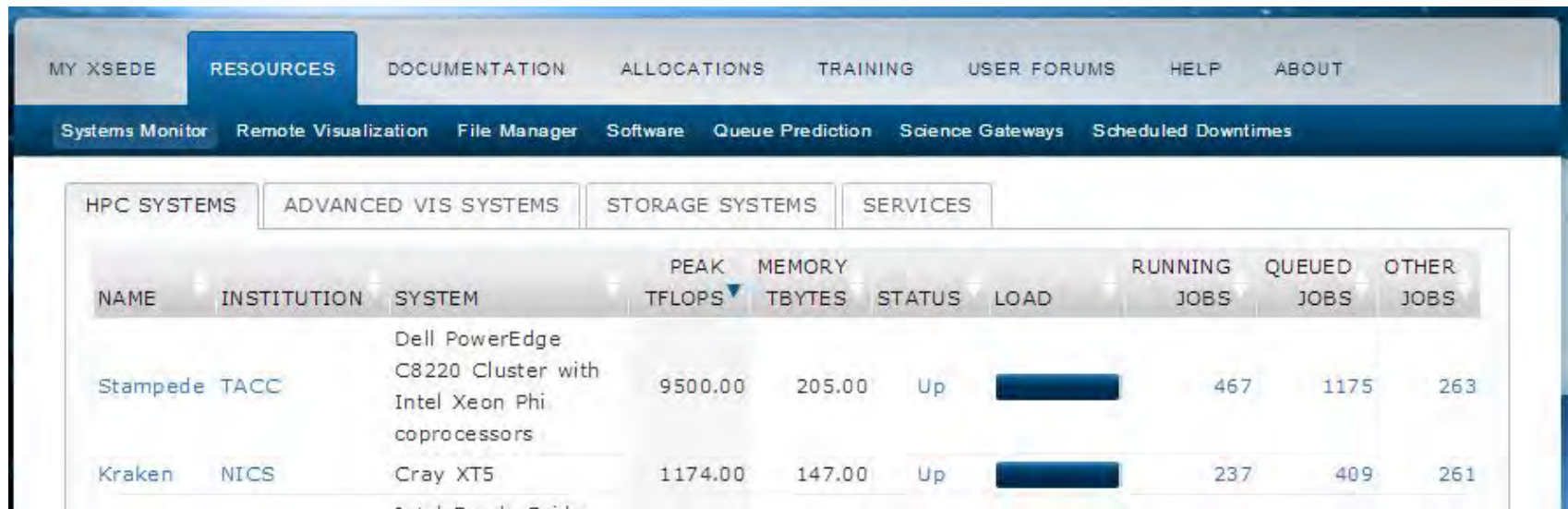
Navigating the XUP



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

View the XSEDE Systems Monitor

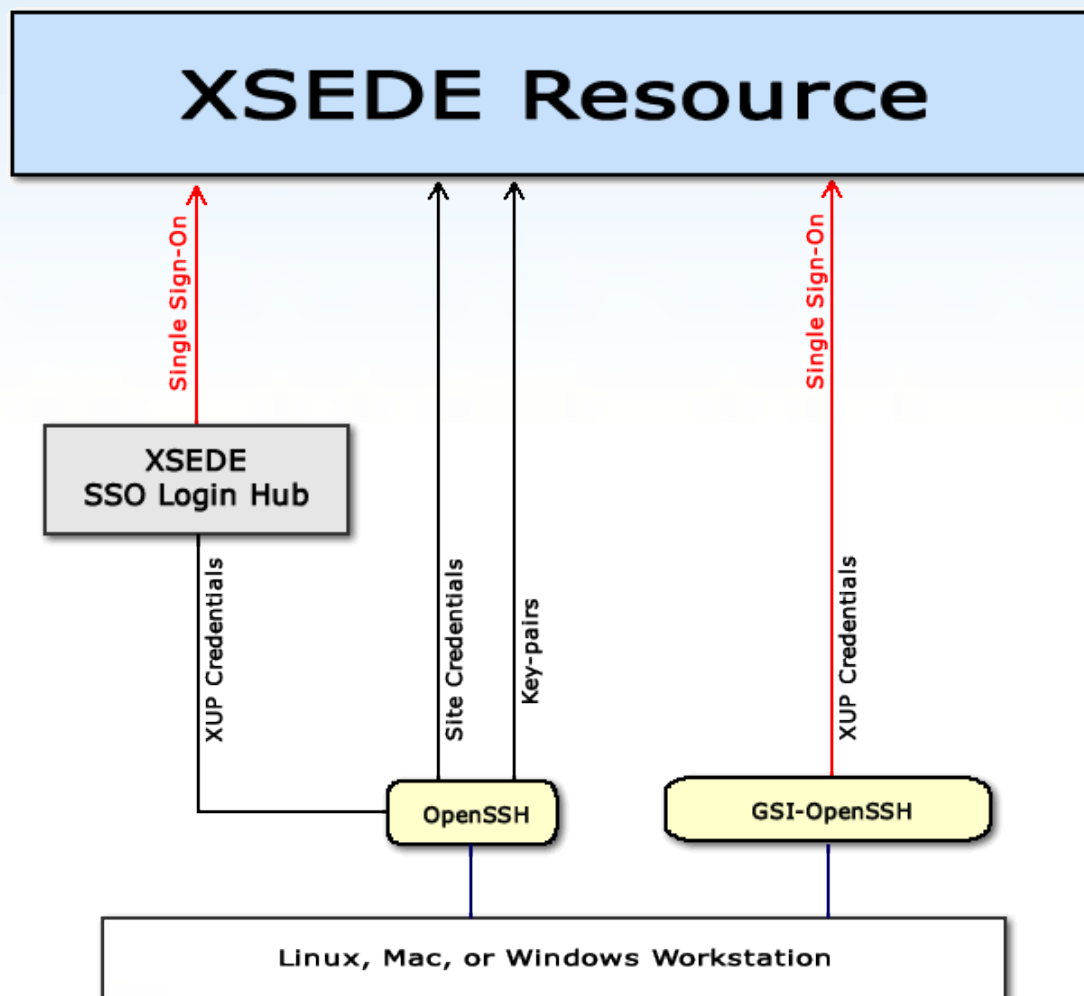
- **Resources -> Systems Monitor**
 - Provides technical and status information for all of XSEDE's resources.
 - The STATUS column indicates whether the system is up or down. If down, can click on status to find when the machine is expected to come back up.



The screenshot shows 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, 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 has tabs for HPC SYSTEMS, ADVANCED VIS SYSTEMS, STORAGE SYSTEMS, and SERVICES. The HPC SYSTEMS tab is active, displaying a table of systems.

NAME	INSTITUTION	SYSTEM	PEAK TFLOPS	MEMORY TBYTES	STATUS	LOAD	RUNNING JOBS	QUEUED JOBS	OTHER JOBS
Stampede	TACC	Dell PowerEdge C8220 Cluster with Intel Xeon Phi coprocessors	9500.00	205.00	Up	<div></div>	467	1175	263
Kraken	NICS	Cray XT5	1174.00	147.00	Up	<div></div>	237	409	261

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

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

Managing your XSEDE files

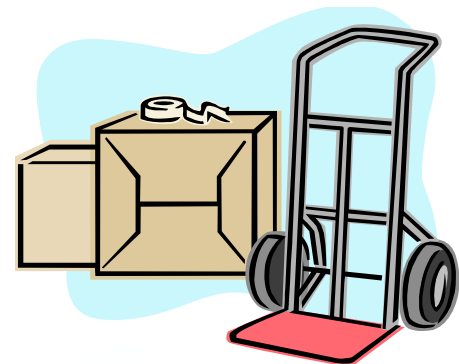
1. Where to store files

- 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 faint grid pattern and a stylized image of a planet or celestial body on the left side. The overall aesthetic is high-tech and scientific.

XSEDE

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 digital counter displays '41,023,758,737 MB TRANSFERRED'. The page is divided into three columns: 'Researchers', 'Resource Providers', and 'How It Works'. Each column contains a brief description of the service, a 'LEARN MORE' link with a right-pointing arrow, and a 'GET GLOBUS PLUS' link with a right-pointing arrow. Small headshots of three individuals are placed at the bottom of each column.

Firefox | Home | globus

<https://www.globus.org>

globus

Products - News - About - Support - Log In Sign Up

share move sync

BIG DATA

Your research data where you need it.

41,023,758,737 MB TRANSFERRED

Researchers

Focus on your research, not IT problems. We make it easy to move, manage, and share big data.

[LEARN MORE](#)

[GET GLOBUS PLUS](#)

Resource Providers

Globus gives you more control over your data infrastructure, while providing excellent ease-of-use for your researchers.

[LEARN MORE](#)

[GLOBUS PROVIDER PLANS](#)

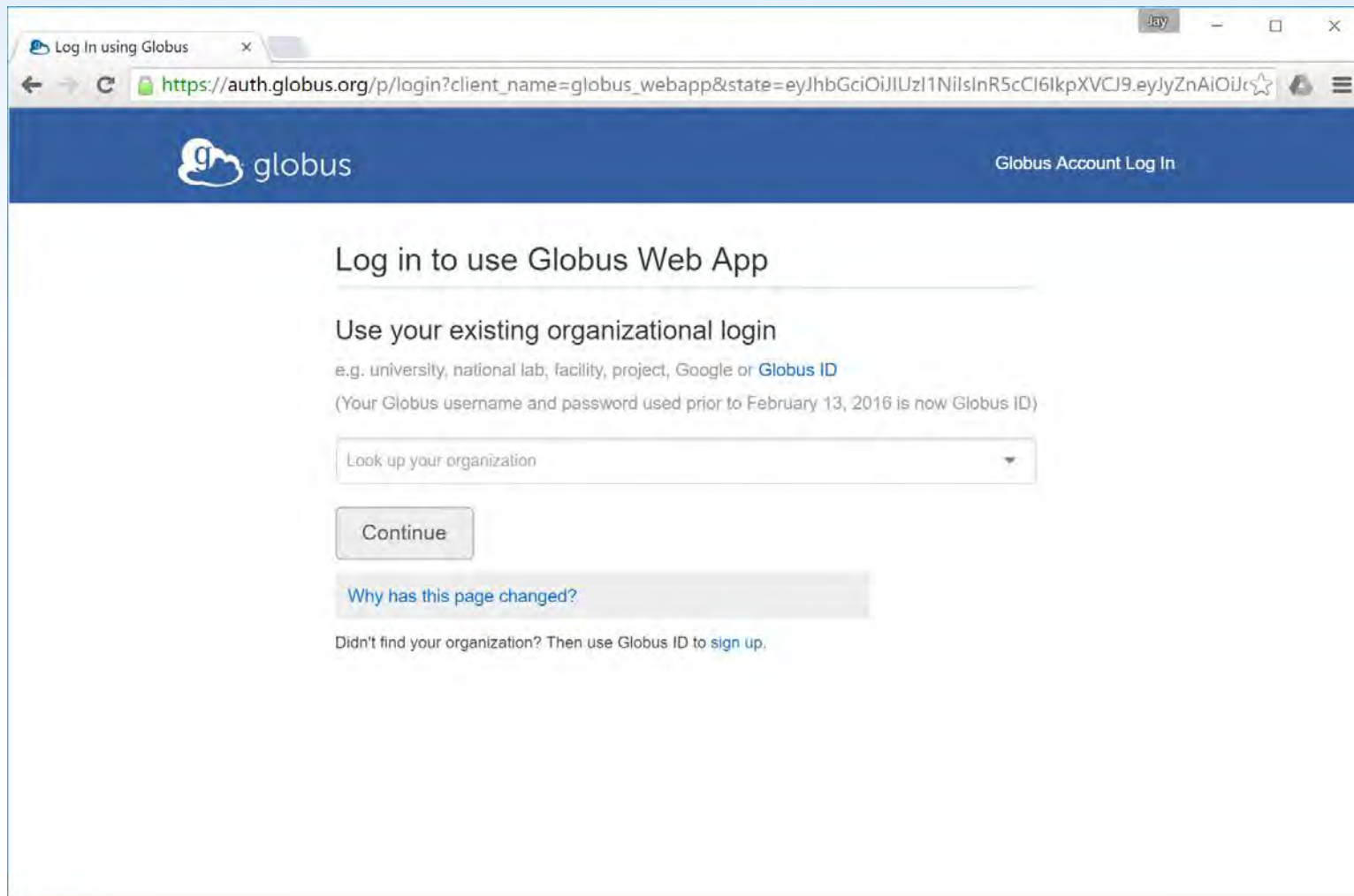
How It Works

Globus' tools and services help connect people and HPC resources, so that no researcher is an island.

[LEARN MORE](#)

XSEDE

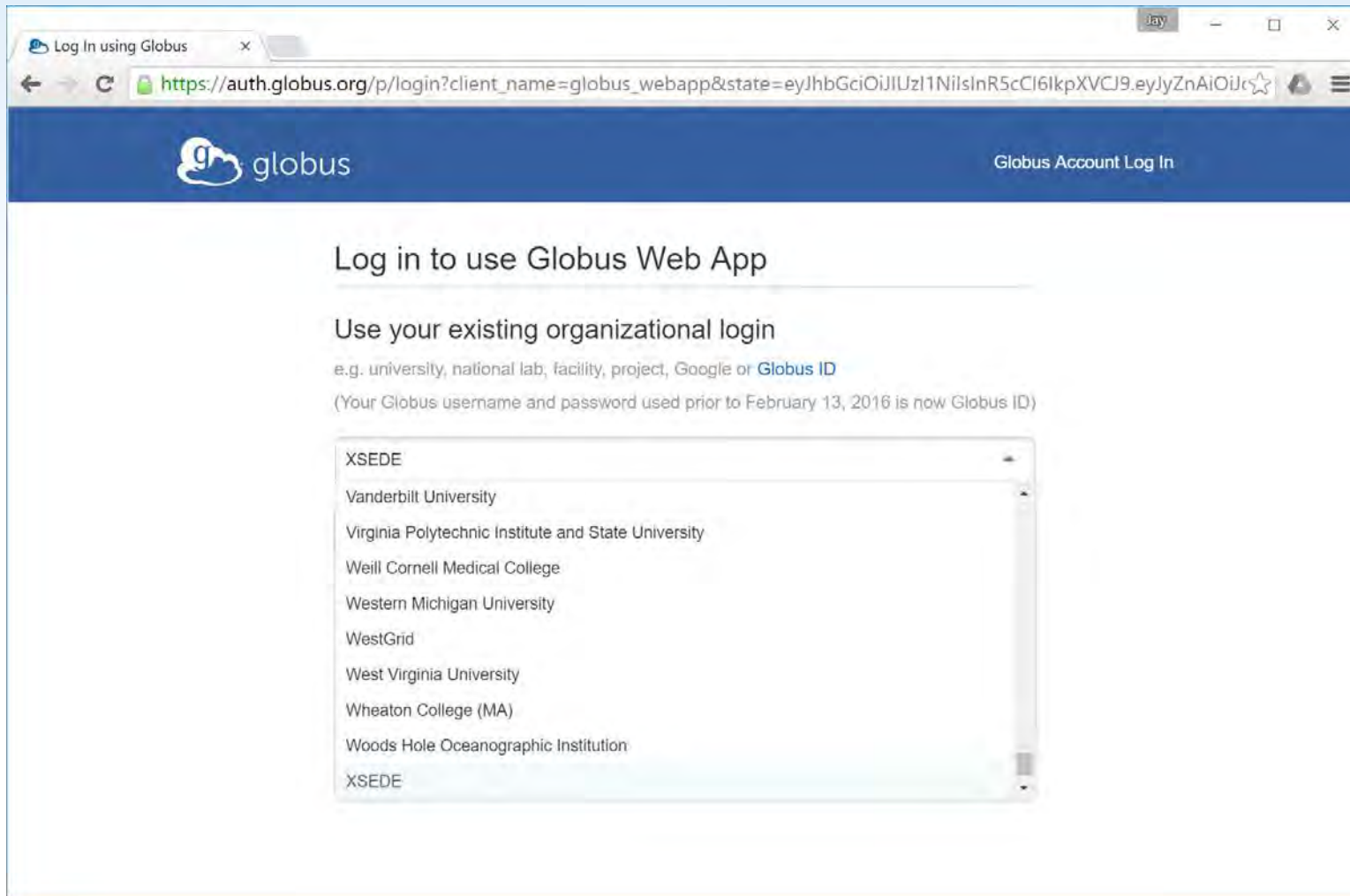
Login to use Globus Web App



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.eyJyZnAiOiJc. 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 is white and contains the following text and elements:

- ## 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)
-
-
- [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 address bar displaying `https://auth.globus.org/p/login?client_name=globus_webapp&state=eyJhbGciOiJIUzI1NiIsInR5cCI6IkpXVCJ9.eyJyZnAiOiJr...`. 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)". Below this, a dropdown menu is open, showing a list of organizations. The first two entries are "XSEDE" and "Vanderbilt University". Other visible entries include "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

Log in to use Globus Web App

Use your existing organizational login

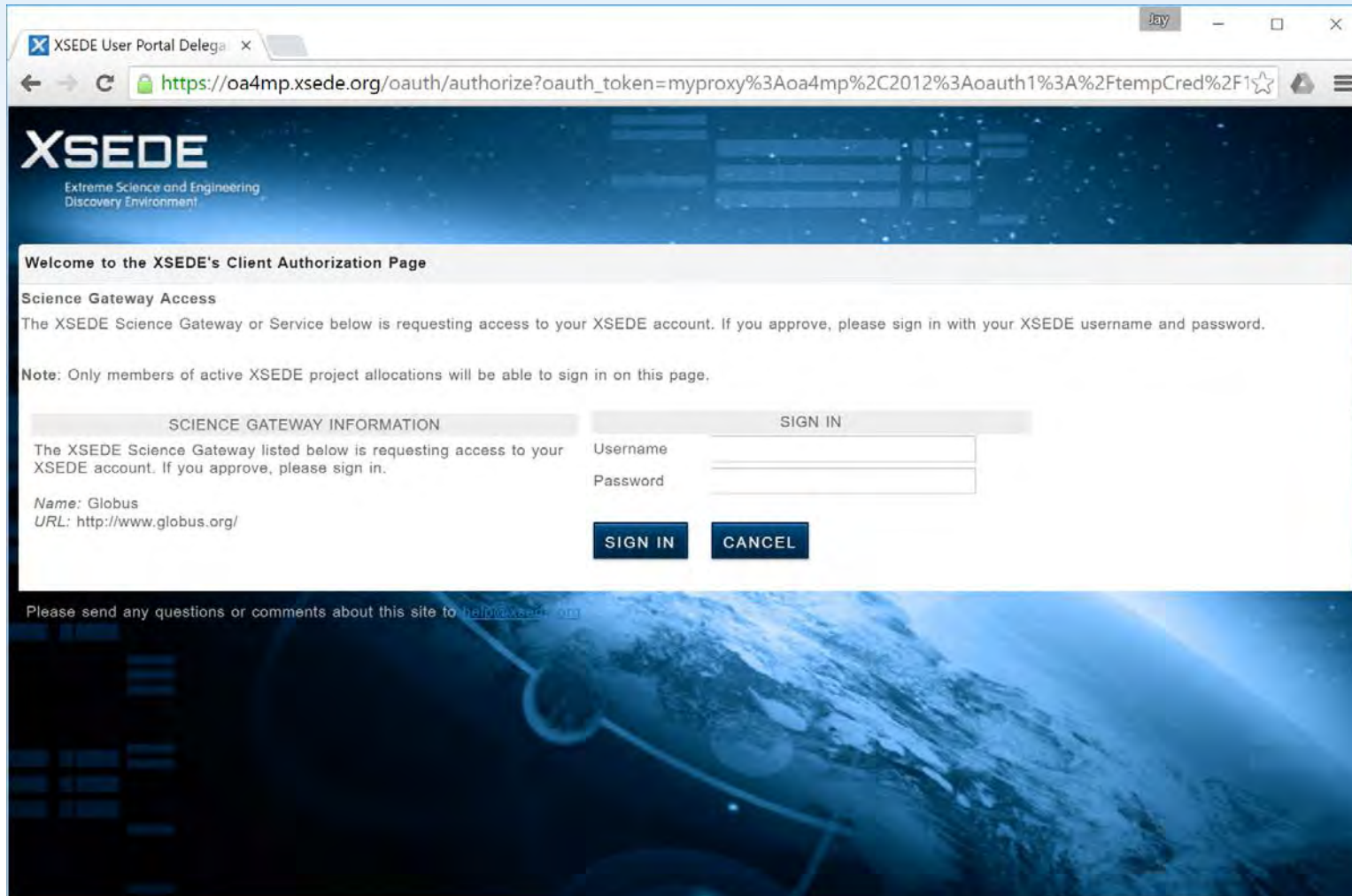
e.g. university, national lab, facility, project, Google or [Globus ID](#)

(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 text "Extreme Science and Engineering Discovery Environment". The main content area is titled "Welcome to the XSEDE's Client Authorization Page" and includes a section for "Science Gateway Access". This section explains that the XSEDE Science Gateway is requesting access to the user's XSEDE account and provides a note about active project allocations. Below this, there are two columns: "SCIENCE GATEWAY INFORMATION" and "SIGN IN". The "SCIENCE GATEWAY INFORMATION" column lists the gateway name as "Globus" and the URL as "http://www.globus.org/". The "SIGN IN" column contains input fields for "Username" and "Password", along with "SIGN IN" and "CANCEL" buttons. At the bottom of the page, 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"/>
<i>Name:</i> Globus <i>URL:</i> http://www.globus.org/	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

XSEDE

Globus Online File Transfer

The screenshot displays the Globus Online File Transfer web 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 the path '/~/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 the path '/~/'. It contains a folder named 'project-files'.

At the bottom of the interface, 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...

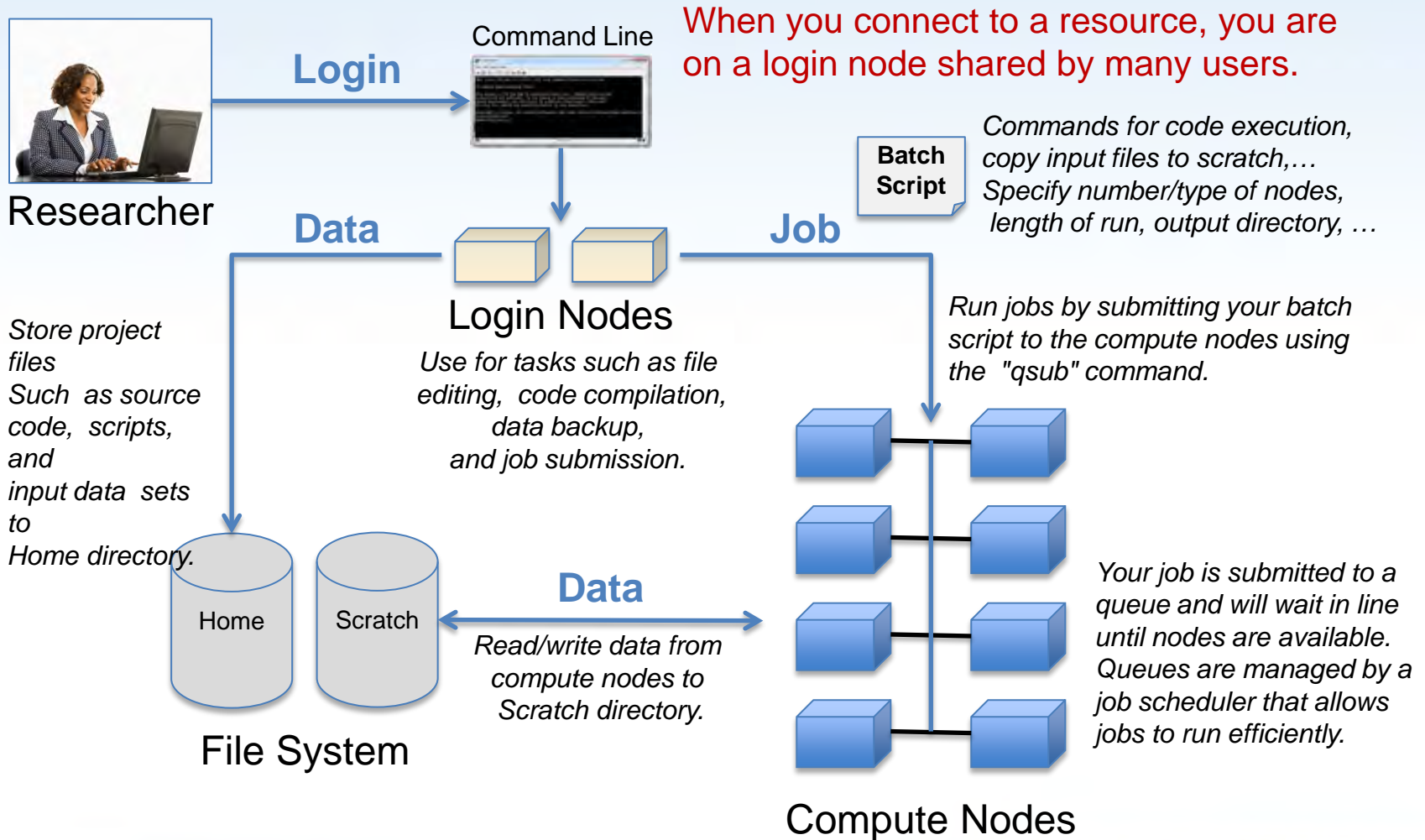
The screenshot shows the Globus Transfer Files web interface. The browser address bar displays `https://www.globus.org/xfer/StartTransfer#...`. The page header includes the Globus logo, navigation links (Manage Data, Groups, Support, jalameda), and a secondary navigation bar (Transfer Files, Activity, Manage Endpoints, Dashboard). The main heading is "Transfer Files", with a sub-header "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. Each panel has an "Endpoint" field (e.g., `xsede#comet` and `xsede#blacklight`), a "Path" field (e.g., `/lux400689/` and `/`), and a "Go" button.

Below the input fields are two file lists. The left list shows a directory structure with folders like `intel`, `newfolder`, `shallow`, and `shallow-12jun2014`, and files like `a.out`, `hellompi-slurm.sb`, `ptp_job.e1286924`, and `ptp_job.e1286961`. The right list shows folders like `PweTest`, `shallow-sr1-kepler-jan2014`, `shallow-trestles-icc`, `shallow_43_SR2_SEA`, and `trainingSC12_C`, and a file `ptp_job.e1286924`.

At the bottom, 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?



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$
```


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 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.o CVS 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))

XSEDE Training Survey

- Please complete a short on-line survey about this module at <http://bit.ly/hamptonxsede>. 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/219>

May 13, 2016

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

XSEDE

Extreme Science and Engineering
Discovery Environment