

March 5, 2014

# XSEDE New User Tutorial

# XSEDE

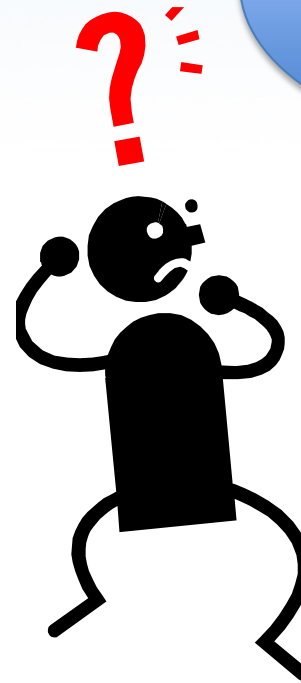
Extreme Science and Engineering  
Discovery Environment

Jay Alameda  
National Center for  
Supercomputing Applications

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](http://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

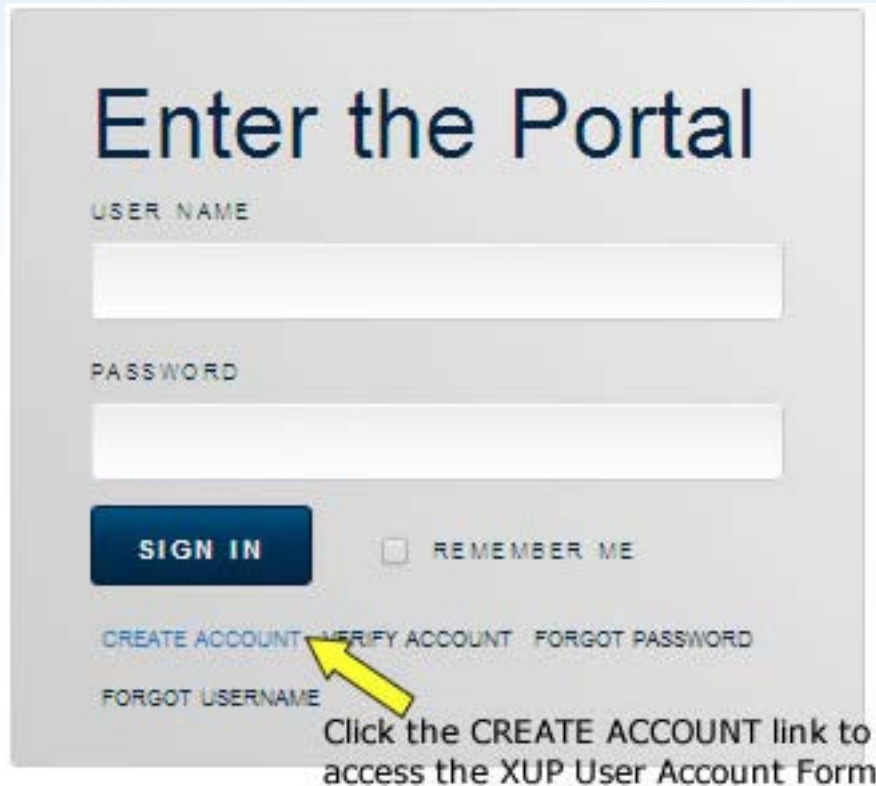
# Using the XUP

- 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

[CREATE ACCOUNT](#) [VERIFY ACCOUNT](#) [FORGOT PASSWORD](#)  
[FORGOT USERNAME](#)

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

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

# 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](mailto:help@xsede.org) or call 1-866-907-2383 immediately, regardless of the time of day.

## XSEDE Cybersecurity Tutorial

<http://www.citutor.org>

The background of the slide features a space-themed image with a view of Earth from space, showing clouds and the horizon. In the foreground, there are several spherical objects, possibly planets or moons, and a network of lines connecting them, suggesting a global or interconnected theme. The XSEDE logo is prominently displayed in the bottom right corner, rendered in a large, bold, white font with a slight shadow effect.

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# Get Added to Your XSEDE project

- If you are not the project PI, you will need to be added to your project's account in the XUP.
- Contact your project's PI or Allocation Manager and request that you be added to the project. You will need to provide them with your XSEDE User Portal user name.



# Your My XSEDE webpage

The screenshot shows the My XSEDE User Portal (XUP) homepage. 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, explaining that the XUP is the home for XSEDE users to manage accounts and allocations. It includes a link to "Read the Getting Started Guide" and a "Find your Campus Champion" section.
- LATEST UPDATES (2)**: A section for Sandra's profile updates. It shows her last login (Mon 10/28/13 at 04:13:25 PM -0500), open tickets (None), jobs (0 running, 0 queued, 0 other), publications (New! Add publications to your Profile), and training (You are not registered for any upcoming classes).
- MY ACTIVE ALLOCATIONS (3)**: A section showing active projects. It includes a table for "ACTIVE PROJECTS SUMMARY" and a "Burn Rate" gauge.

RESOURCE	% LEFT	END DATE [DAYS LEFT]	BURN RATE
Staff Resources	100%   300,000 SUs remaining	2014-09-20 [326d]	

(1)

## WELCOME TO XUP

- Quick access to commonly used features.

(2)

## LATEST UPDATES

- Latest information specific to your user account.

(3)

## MY ACTIVE ALLOCATIONS

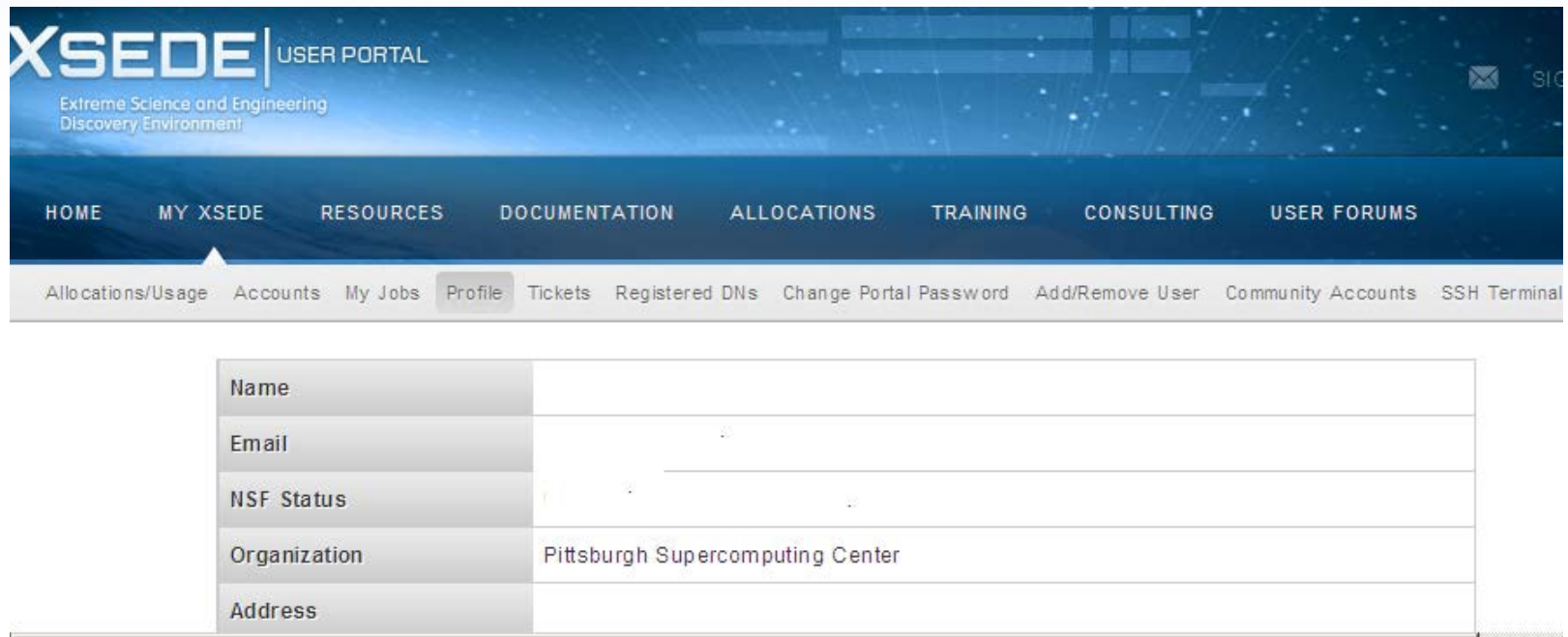
- Summary of the active projects for which you are either a PI or member.

# 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	

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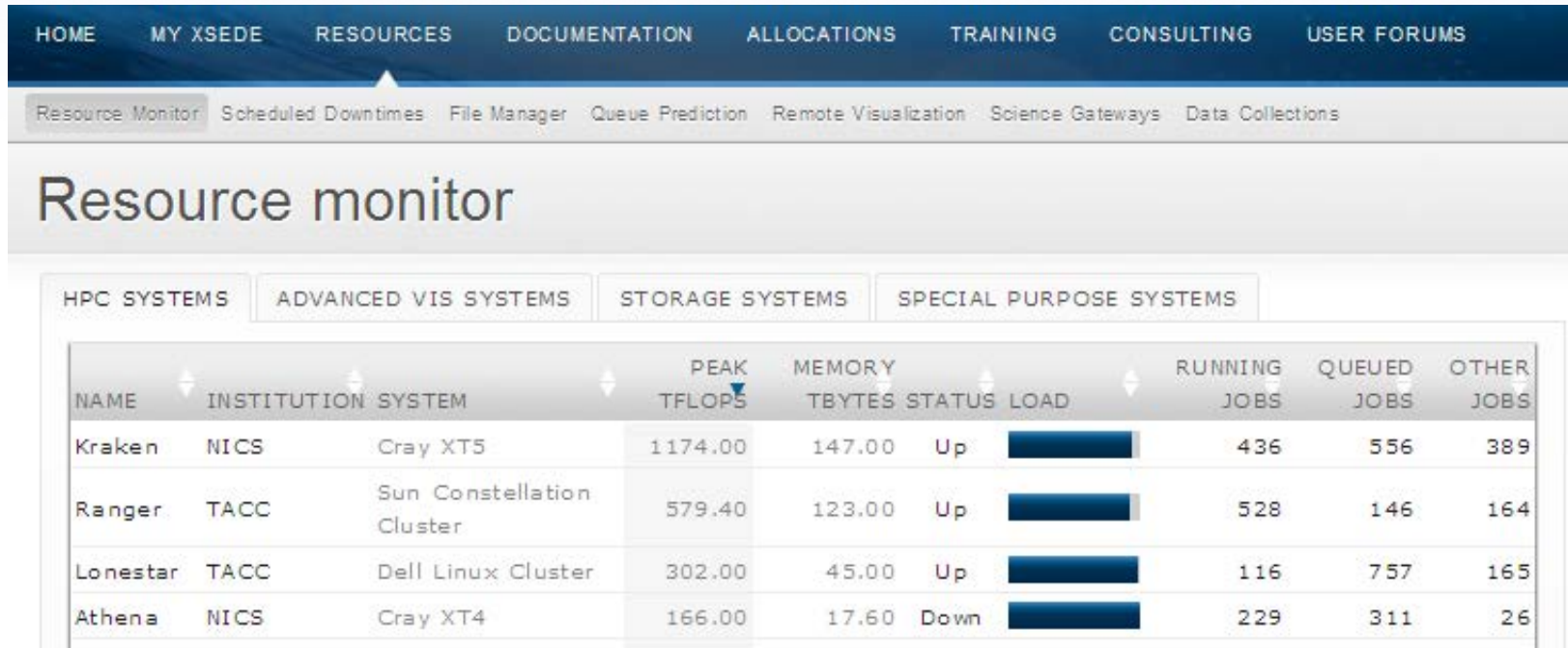
# Navigating the XUP



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

# View the XSEDE Resource 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.



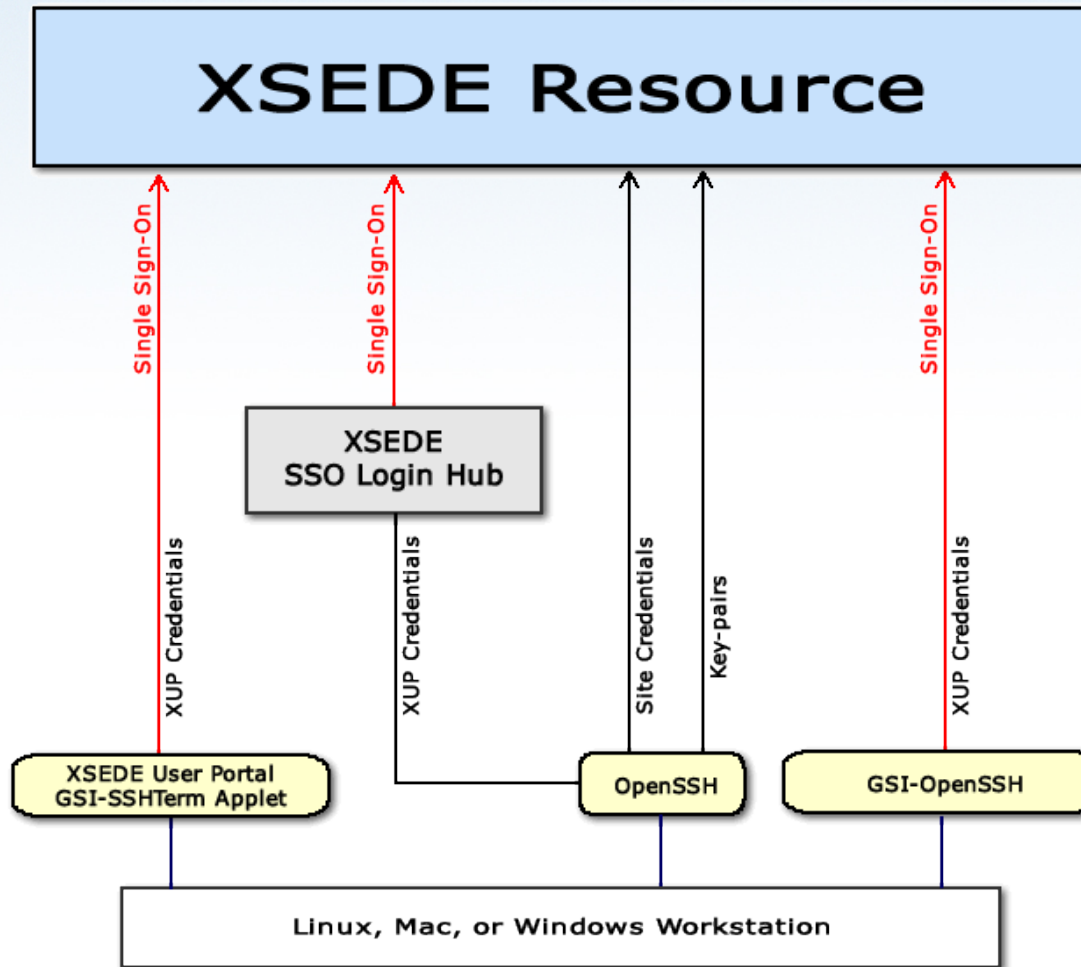
Resource monitor									
HPC SYSTEMS   ADVANCED VIS SYSTEMS   STORAGE SYSTEMS   SPECIAL PURPOSE SYSTEMS									
NAME	INSTITUTION	SYSTEM	PEAK TFLOPS	MEMORY TBYTES	STATUS	LOAD	RUNNING JOBS	QUEUED JOBS	OTHER JOBS
Kraken	NICS	Cray XT5	1174.00	147.00	Up	<div></div>	436	556	389
Ranger	TACC	Sun Constellation Cluster	579.40	123.00	Up	<div></div>	528	146	164
Lonestar	TACC	Dell Linux Cluster	302.00	45.00	Up	<div></div>	116	757	165
Athena	NICS	Cray XT4	166.00	17.60	Down	<div></div>	229	311	26



XSEDE



# 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. XUP GSI-SSHTerm
2. GSI-OpenSSH
3. OpenSSH

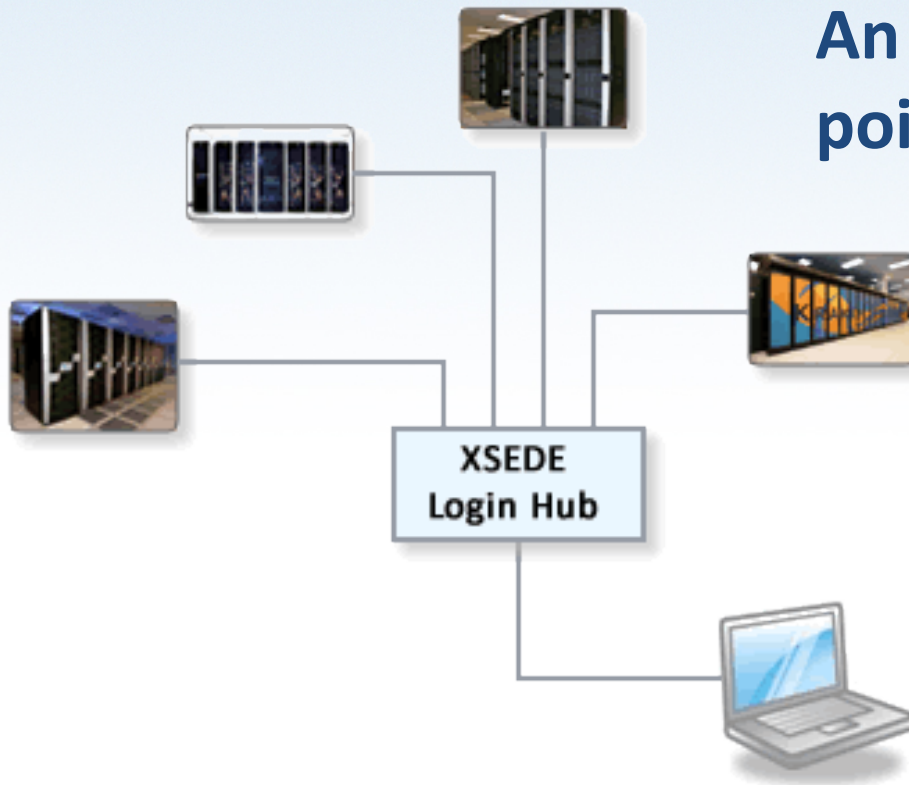
# XSEDE User Account Mapping

- Portal logins do not necessarily match local logins
- Can access mapping from My XSEDE > Accounts
- (only needed for site passwords, or one-time passwords)

RESOURCE NAME ▲	LOGIN NAME ◆	INSTITUTION ◆	USERNAME ◆	CONNECT ◆
Blacklight	<a href="http://blacklight.psc.teragrid.org">blacklight.psc.teragrid.org</a>	PSC	skappes	<a href="#">Login</a>
Condor	<a href="http://tg-condor.purdue.teragrid.org">tg-condor.purdue.teragrid.org</a>	Purdue	skappes	<a href="#">Login</a>
Gordon Compute Cluster	<a href="http://gordon.sdsc.edu">gordon.sdsc.edu</a>	SDSC	skappes	<a href="#">Login</a>
Gordon ION	<a href="http://gordon.sdsc.edu">gordon.sdsc.edu</a>	SDSC		



# 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

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# Managing your XSEDE files

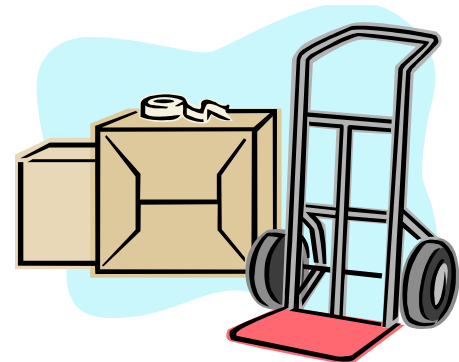
## 1. Where to store files

- 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.
- Customize it using **Modules**



# 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 switch 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
```

# Moving Files - **Globus Online**

- 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 - [www.globusonline.org](http://www.globusonline.org)



# Globus Online Dashboard

[Manage Transfers](#)[Groups](#)[Support](#)[skappes](#)[start transfer](#) | [view activity](#) | [manage endpoints](#) | [dashboard](#)

## Transfer Summary

### Requested Today

0 active transfers.  
0 transfers completed successfully.  
0 inactive transfers.  
0 transfers failed.

### Requested This Week

0 active transfers.  
0 transfers completed successfully.  
0 inactive transfers.  
0 transfers failed.

### Lifetime

0 active transfers.  
3 transfers completed successfully.  
0 inactive transfers.  
0 transfers failed.



## File Transfer

Use your browser to move data securely and reliably.

[Start Transfer](#)[View Activity](#)

## Browse Groups

Browse and join groups that fit your interests



## My Profile

View and change your account settings, including contact information and security credentials



## Globus Connect

Use Globus Connect to transfer files between your computer and any Globus Online endpoint.

## In the Spotlight

2013 IEEE International Conference on Cluster Computing (CLUSTER)

2013 IEEE International Conference on Cluster Computing (CLUSTER) 649 88 2013 IEEE International More ...

Big Data Management for Science - Joint ESnet and Globus Online webinar  
Big Data Management for Science - Joint ESnet and Globus Online webinar 650 88 Big Data More ...


Front Range High Performance Computing Symposium  
Front Range High Performance Computing Symposium 651 88 Front Range High Performance Computing More ...

OLCF Workshop on Processing and Analysis of Very Large Data Sets  
OLCF Workshop on Processing and Analysis of Very Large Data Sets 644 88 OLCF Workshop on More ...

[More News](#)

# XSEDE

# Globus Online File Transfer

 globus

Manage TransfersGroupsSupportskappes

start transfer | view activity | manage endpoints | dashboard

Transfer Files

Get Globus Connect  
Turn your computer into an endpoint.

Endpoint  Go

Path  Go

select all | none | up one folder | refresh list

Process Colors - Copy.c2.77 kB

Process Colors.c2.77 kB

Endpoint  Go

Path  Go

select all | none | up one folder | refresh list

project-filesFolder

more options

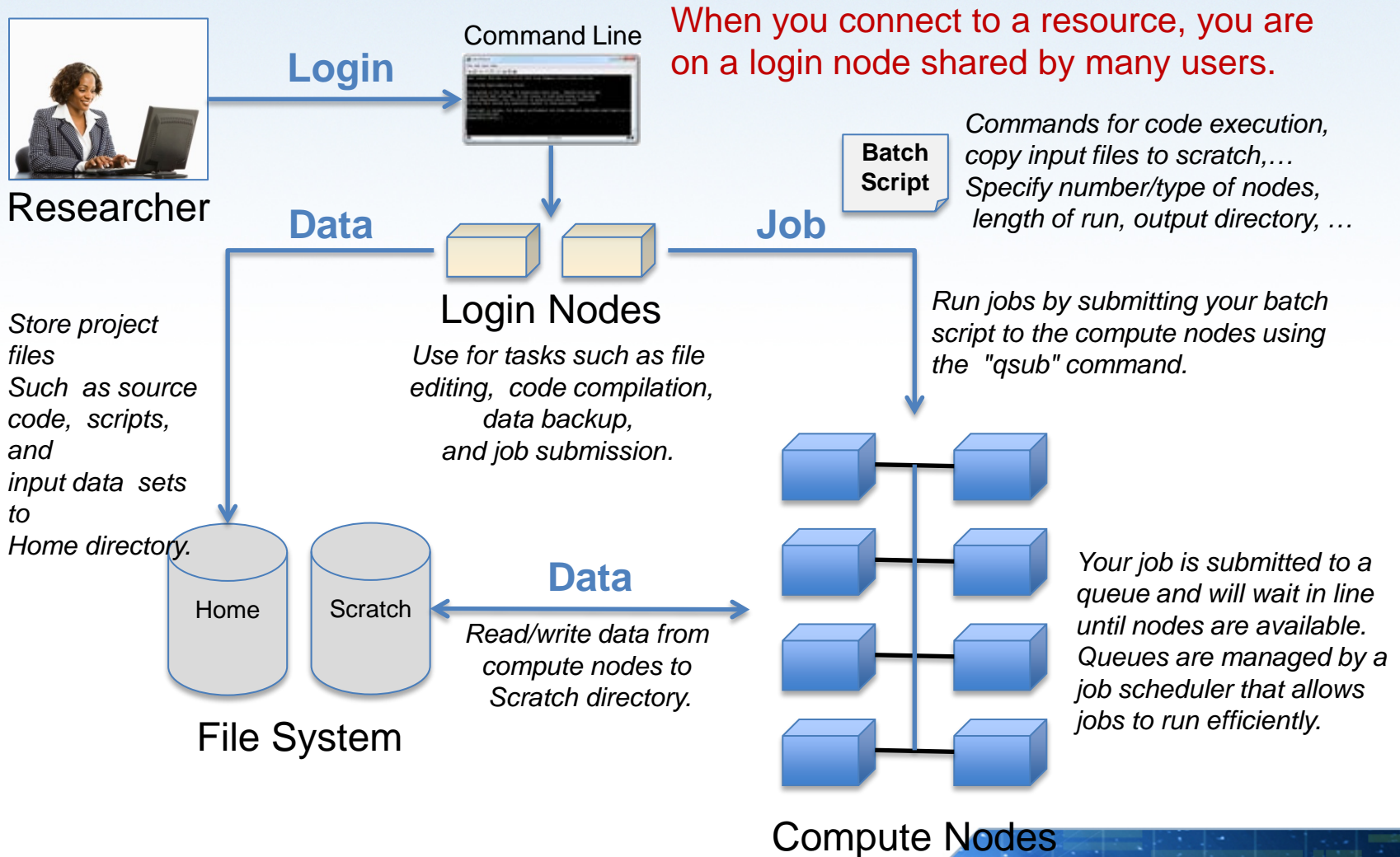
Label This Transfer

This will be displayed in your transfer activity.

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# Running Jobs Overview



# Login nodes

- When you login, you are in the login node.
- Login nodes should only be used for basic tasks such as file editing, code compilation, data backup, and job submission.
- Login nodes should not be used to run production simulations. Production work should be performed on the system's compute resources.



# Batch Jobs

- Compute jobs \*cannot\* be run on the login nodes.
- All XSEDE compute resources use some form of batch scheduler.
- There are several batch systems in use, but all work basically the same way. Create a job script specifying:
  - Number/type of nodes you need.
  - How long you need to run.
  - Where your output files should be written to.

# Create a script

```
#!/bin/csh
#PBS -l ncpus=16
#ncpus must be a multiple of 16
#PBS -l walltime=5:00
#PBS -j oe
#PBS -q batch

set echo

ja

#move to my $SCRATCH directory
cd $SCRATCH

#copy executable to $SCRATCH
cp $HOME/mympi .

#run my executable
mpirun -np $PBS_NCPUS ./mympi

ja -chlst
```

Example script for running an MPI job on Blacklight at PSC.

Actual commands are site and machine specific, but they follow general principles.

Needs to be modified to run on other XSEDE machines.

The XSEDE logo is displayed in a large, bold, white sans-serif font against a dark blue background. The background features a grid of small white dots and a faint, stylized image of a globe or planet with a blue and white horizon line.



# Submitting/Manipulating Batch jobs

- Batch system should be used to run your job.
- Do not run on the login nodes.
- Submit the script that you have created:

Actual commands are machine specific, but they follow general principles.

`qsub jobname`

`qstat -a`

`qstat -u username`

`qdel jobid`

`man qsub`

# Batch command examples

- **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)**



# Why has my job not run?

- Never made it to the queue:

- Job not accepted by the queue:

Core requests on Kraken must be a multiple of twelve. You have requested an invalid number of cores ( 8 ). Please resubmit the job requesting an appropriate number of cores.

- Solution: Change the job script to request correct number of cores or memory for the resource.

# My job did not complete

- Check the log files created `job.e.89890`  
`job.o.89890`
- One common problem: job run out of CPU time.
- Check the job script: time and memory requested, directory where you are writing files to.
- Do the input files exist in the directory where you specified?
- Do you have permission to use software?
- Waiting a very long time in the queue...
- If all fails... submit a ticket



# Queue structure: job priority

- Job priority in the batch queues is based on the number of cores and wall clock time requested. Differs by site. Examples:
- Blacklight: *approx.* FIFO system. (Mechanisms in place to prevent a single user from dominating the batch queue and to prevent idle time on the machine).
- *Flexible time request* can improve your turnaround. *Packing small jobs.*
- Kraken: Priority to jobs that request large number of cores (over 32K processors) (except capability and dedicated jobs). Jobs with smaller core counts run on other systems (Trestles). However, they can run effectively on Kraken as *backfill*.
- *Backfill*: While the scheduler is collecting nodes for larger jobs, those with short wall clock limits and small core counts may use those nodes without delaying the start time of the larger job.

# Queue structure: Backfill, Flexible time

- *Backfill*: While the scheduler is collecting nodes for larger jobs, those with short wall clock limits and small core counts may use those nodes without delaying the start time of the larger job.
- The system will not start a job that will not finish before the system maintenance time begins. Ex. Will run a 512 core jobs next. Waiting to finish a 256 core job that will take 4 more hours. Can run jobs that add up to 256 cores and will finish in 4 hours.
- To take advantage of this, request flexible walltime in your job script. A flexible walltime request can improve your job's turnaround in several circumstances.



# Improving job turnaround

- Try to be as accurate as possible in estimating the walltime request for your job. Asking for more time than your job will actually need will almost certainly result in poorer turnaround for your job: Asking for the maximum walltime you can ask for a job will almost always result in poorer turnaround.
- Use flexible walltime

# Improving job turnaround: Flexible time

-l walltime\_min=HH:MM:SS

-l walltime\_max=HH:MM:SS

- Using flexible walltime limits increases the opportunity for your job to run on backfill blades.

- **Example:** if your job requests 64 cores and a range of walltime between 2 and 4 hours and a 64-core slot is available for 3 hours, your job could run in this slot with a walltime request of 3 hours. If your job had asked for a fixed walltime request of 4 hours it would not have been started.



# Flexible time

- If the system starts one of your jobs with a flexible walltime request, it selects a walltime within the two specified limits. This walltime will not change during your job's execution. Can determine the walltime your job was assigned by

```
qstat -f $PBS_JOBID | grep Resource_List.walltime
```

- Your program should begin writing checkpoint files sufficiently in advance of the walltime so that the file writing is completed when the limit is reached. ***Save time to allow your job to transfer files after your program ends but before your job ends.***

```
timeout --timeout=$PROGRAM_TIME -- mpirun -np 32 ./mympi
```

# Packing your jobs

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



# Packing your jobs

Run each program execution in the background and place a wait command after each execution. Sample job to pack serial executions:

```
#!/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 your jobs, serial or MPI:

```
dplace -c 0 ./myserial1 < serial1.dat &  
dplace -c 32 ./myserial2 < serial2.dat &  
dplace -c 64 ./myserial3 < serial3.dat &  
wait
```

- The dplace command insures that each execution will run on its own set of 32 cores. The executions will run concurrently.
- Same approach using the dplace command can be used to pack MPI executables.

•



# Packing your jobs: OpenMP

- 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`

# Need help? Reporting and Tracking Issues

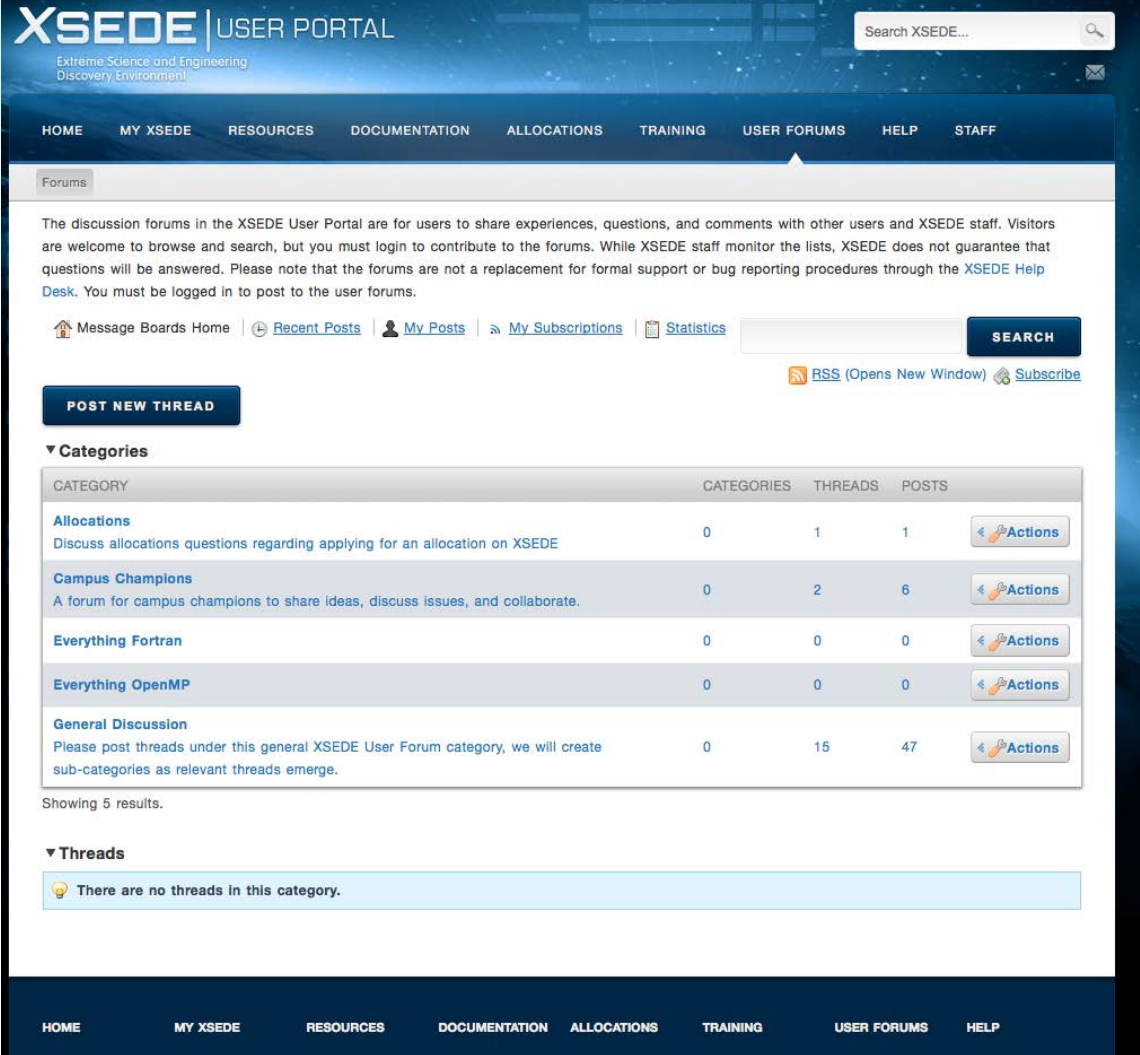
- [portal.xsede.org](https://portal.xsede.org) → Help  
Submit ticket
- [portal.xsede.org](https://portal.xsede.org) → My XSEDE → Tickets
  - Submit ticket
  - View past tickets (both open and closed)
- Can also email [help@xsede.org](mailto:help@xsede.org) or call 1-866-907-2383, at any hour (24/7)



# Discussing your problems...

## User Portal: User Forums

- The User Forums are a great place to ask questions, get help, or discuss ideas about XSEDE.



The screenshot shows the XSEDE User Portal interface. At the top, the XSEDE logo is followed by "USER PORTAL" and the tagline "Extreme Science and Engineering Discovery Environment". A search bar is in the top right. A navigation menu includes links for HOME, MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS (which is highlighted), HELP, and STAFF.

Below the navigation menu, there's a "Forums" tab. A paragraph explains that the forums are for users to share experiences, questions, and comments, but visitors must login to contribute. It also mentions that XSEDE staff monitor the lists but does not guarantee answers, and that the forums are not a replacement for formal support or bug reporting through the XSEDE Help Desk. A note states that users must be logged in to post.

Below this text are links for "Message Boards Home", "Recent Posts", "My Posts", "My Subscriptions", and "Statistics". A "SEARCH" button is also present. There are also links for "RSS (Opens New Window)" and "Subscribe".

A "POST NEW THREAD" button is located below the search area.

The "Categories" section is expanded, showing a table with the following data:

CATEGORY	CATEGORIES	THREADS	POSTS	
<b>Allocations</b> Discuss allocations questions regarding applying for an allocation on XSEDE	0	1	1	<a href="#">Actions</a>
<b>Campus Champions</b> A forum for campus champions to share ideas, discuss issues, and collaborate.	0	2	6	<a href="#">Actions</a>
<b>Everything Fortran</b>	0	0	0	<a href="#">Actions</a>
<b>Everything OpenMP</b>	0	0	0	<a href="#">Actions</a>
<b>General Discussion</b> Please post threads under this general XSEDE User Forum category, we will create sub-categories as relevant threads emerge.	0	15	47	<a href="#">Actions</a>

Below the table, it says "Showing 5 results."

The "Threads" section is expanded, showing a message: "There are no threads in this category."

At the bottom, there is another navigation menu with links for HOME, MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, and HELP.

# XSEDE

# More “helpful” resources

[xsede.org](https://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](https://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 bright light source on the right side, creating a high-tech or scientific atmosphere.

XSEDE



March 5, 2014

# Thanks for listening and welcome to XSEDE!

# XSEDE

Extreme Science and Engineering  
Discovery Environment