

October 20, 2016

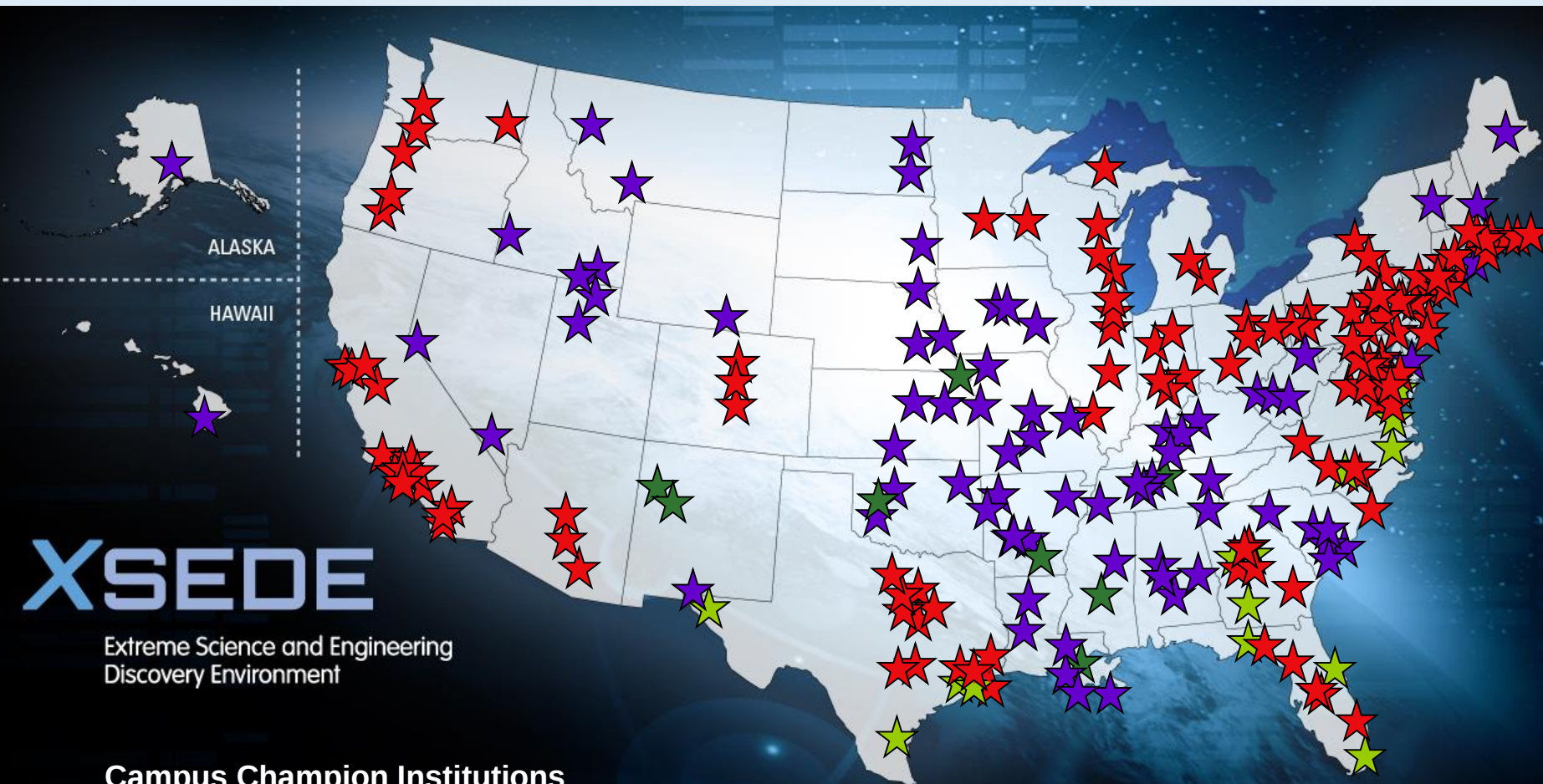
XSEDE Resource Support at CHPC

Campus Champion: Anita Orendt
anita.orendt@utah.edu

XSEDE

Extreme Science and Engineering
Discovery Environment





XSEDE

Extreme Science and Engineering
Discovery Environment

Campus Champion Institutions

- ★ Standard – 119
- ★ EPSCoR States – 73
- ★ Minority Serving Institutions – 15
- ★ EPSCoR States and Minority Serving Institutions – 10

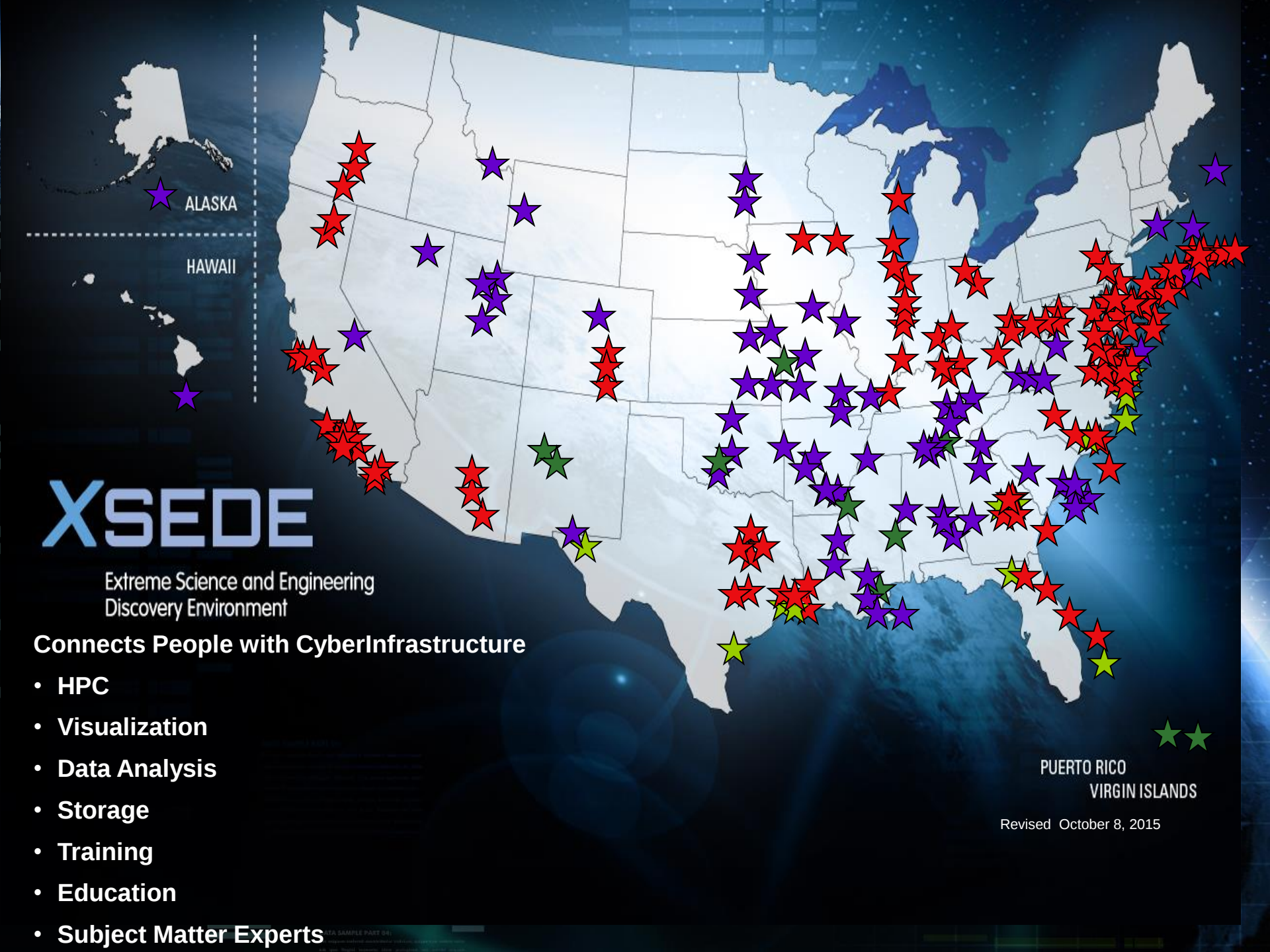
Total Campus Champion Institutions – 217

PUERTO RICO
VIRGIN ISLANDS

Revised June 29, 2016



XSEDE

A map of the United States, including Alaska and Hawaii, with numerous colored stars (red, purple, green, and yellow) indicating the locations of XSEDE sites. The stars are distributed across all states, with a higher concentration in the Northeast and Midwest. The background of the map is a dark blue space-themed image with a faint grid pattern.

XSEDE

Extreme Science and Engineering
Discovery Environment

Connects People with CyberInfrastructure

- HPC
- Visualization
- Data Analysis
- Storage
- Training
- Education
- Subject Matter Experts

PUERTO RICO
VIRGIN ISLANDS

Revised October 8, 2015

NSF Funded program that connects People with CyberInfrastructure:

- HPC
- Visualization
- Data Analysis
- Storage
- Training
- Education
- Subject Matter Experts



Overview

- Current XSEDE Resources
- Signing up for an XSEDE User Portal (XUP) account
- Short Review of User Responsibility and Security
- Requesting an Allocation on XSEDE Resources
- Short review of the XSEDE Computing Environment
- Signing up for XSEDE Training
- Where to Get Help on XSEDE



XSEDE HPC Computing Resources

<https://www.xsede.org/resources/overview>

TACC Stampede Debut of Intel's new MIC technology on a massive scale. With 6400 16 core Intel sandybridge nodes (10PFlops) it is designed for large scale computing needs. Some nodes with GPUs and some with larger memory; Xeon Phi systems

SDSC Comet About 1950 Intel Haswell nodes, SSD local scratch. It is intended for moderately scalable parallel applications with an emphasis on improving productivity for a broad spectrum of users. Additional nodes with four NVIDIA GPUs; others have 1.5TB RAM

XStream Stanford, GPU cluster

LSU SuperMIC Intel Ivybridge nodes with MIC coprocessors; 40% cycles to XSEDE

SDSC Gordon 1024 Intel Sandybride nodes; data-intensive, high-performance computing resource for computing spanning many domains

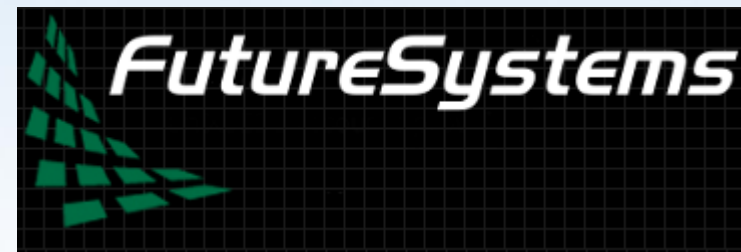
IU Jetstream Cloud Computing resource

PSC Bridges A connected set of interacting systems offering a flexible mix of gateways (web portals), Hadoop and Spark ecosystems, batch processing (large shared memory and GPU nodes) and interactivity. Regular and large memory resources



Other Computing Resources

- [Open Science Grid](#)
- [FutureSystems](#)
- [Blue Waters \(NCSA\)](#)
- [Titan \(OakRidge\)](#)
- [ALCF \(Argonne\)](#)
- [Edison \(NERSC\)](#)



Other Services

- [Visualization](#)
- Storage – at [TACC](#), [PSC](#), [SDSC](#), [NICS](#), [Indiana](#)
- [Science Gateways](#)
- [Extended Support](#)

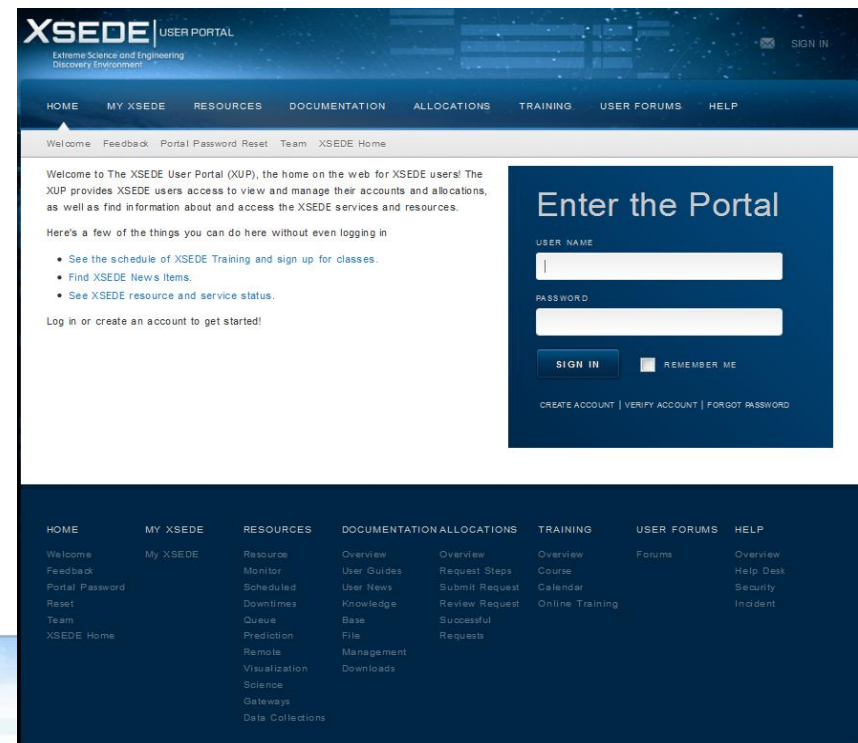
<http://portal.xsede.org>

The Portal provides a single location for information on and access to XSEDE resources

- Continually updated information about your allocations
- Access to your XSEDE accounts and allocated resources
- Interfaces for data management, data collections, and other user tasks and resources

- Access to:

- Help Desk
- Allocation and queue stats
- User management
- Documentation/training

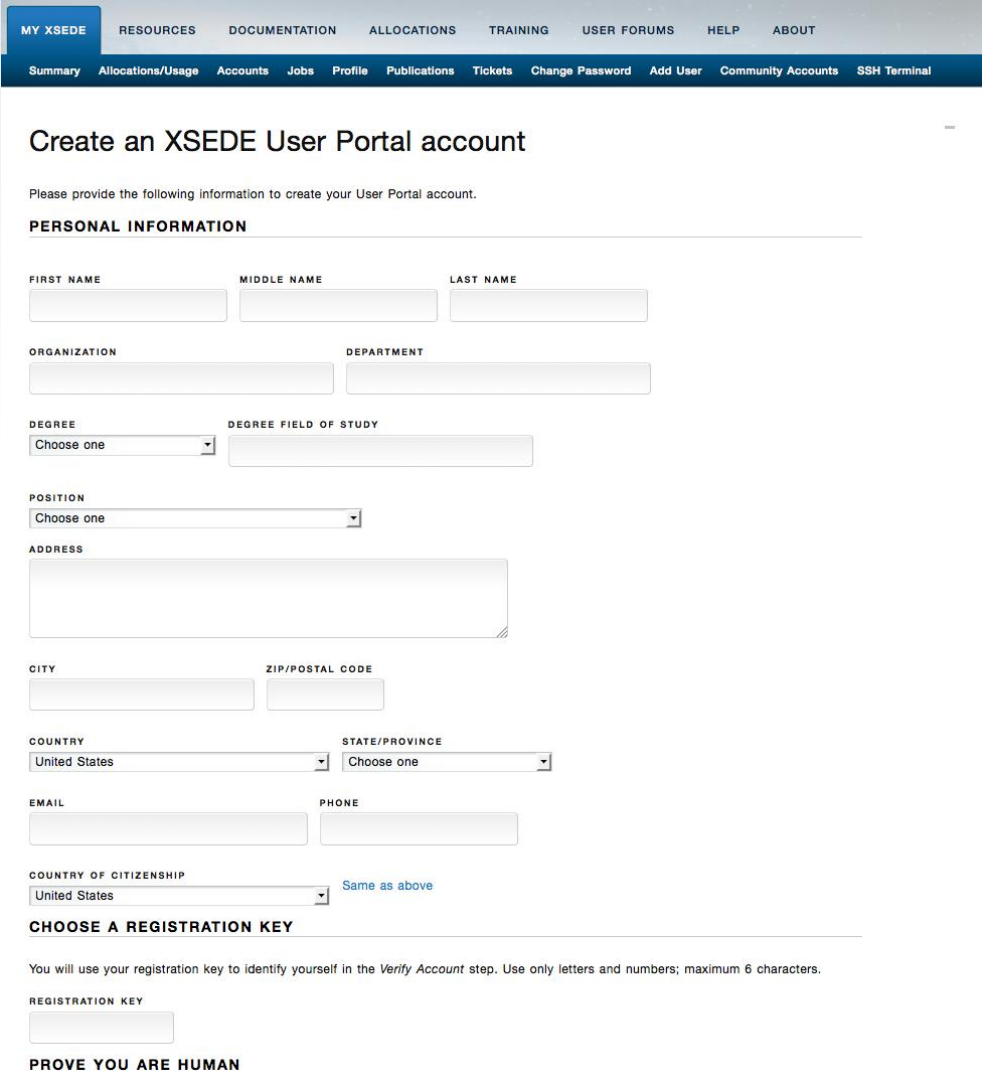


The screenshot shows the XSEDE User Portal homepage. The header features the XSEDE logo and 'USER PORTAL' text, with a tagline 'Extreme Science and Engineering Discovery Environment'. A navigation bar includes links for HOME, MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, and HELP. Below the navigation bar, a welcome message states: 'Welcome to The XSEDE User Portal (XUP), the home on the web for XSEDE users! The XUP provides XSEDE users access to view and manage their accounts and allocations, as well as find information about and access the XSEDE services and resources.' It lists several actions users can take without logging in: seeing the XSEDE Training schedule, finding XSEDE News items, and seeing XSEDE resource and service status. A 'Log in or create an account to get started!' prompt is also present. On the right side, there is a 'Enter the Portal' login box with fields for USER NAME and PASSWORD, a SIGN IN button, and a REMEMBER ME checkbox. Below the login box are links for CREATE ACCOUNT, VERIFY ACCOUNT, and FORGOT PASSWORD. The footer contains a detailed grid of links organized by category: HOME (Welcome, Feedback, Portal Password Reset, Team, XSEDE Home), MY XSEDE (My XSEDE), RESOURCES (Resource Monitor, Scheduled Downtimes, Queue Prediction, Remote Visualization Science Gateways, Data Collections), DOCUMENTATION (Overview, User Guides, User News, Knowledge Base, File Management, Downloads), ALLOCATIONS (Overview, Request Steps, Submit Request, Review Request, Successful Requests), TRAINING (Overview, Course, Calendar, Online Training), USER FORUMS (Forums), and HELP (Overview, Help Desk, Security, Incident).



Creating an XSEDE portal account (XUP)

- Fill in personal information
- Choose a registration key
- System will send you email with a confirmation number
- You will use the confirmation number together with passkey to verify your account



The screenshot shows the XSEDE User Portal account creation 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 secondary navigation bar with links: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, Add User, Community Accounts, and SSH Terminal. The main heading is "Create an XSEDE User Portal account". Below the heading is a note: "Please provide the following information to create your User Portal account." The form is divided into two sections: "PERSONAL INFORMATION" and "CHOOSE A REGISTRATION KEY". The "PERSONAL INFORMATION" section includes fields for FIRST NAME, MIDDLE NAME, LAST NAME, ORGANIZATION, DEPARTMENT, DEGREE (a dropdown menu with "Choose one" selected), DEGREE FIELD OF STUDY, POSITION (a dropdown menu with "Choose one" selected), ADDRESS (a large text area), CITY, ZIP/POSTAL CODE, COUNTRY (a dropdown menu with "United States" selected), STATE/PROVINCE (a dropdown menu with "Choose one" selected), EMAIL, PHONE, and COUNTRY OF CITIZENSHIP (a dropdown menu with "United States" selected and a "Same as above" link). The "CHOOSE A REGISTRATION KEY" section includes a note: "You will use your registration key to identify yourself in the Verify Account step. Use only letters and numbers; maximum 6 characters." and a field for the REGISTRATION KEY. At the bottom is a section labeled "PROVE YOU ARE HUMAN".

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

Create an XSEDE User Portal account

Please provide the following information to create your User Portal account.

PERSONAL INFORMATION

FIRST NAME MIDDLE NAME LAST NAME

ORGANIZATION DEPARTMENT

DEGREE DEGREE FIELD OF STUDY

Choose one

POSITION

Choose one

ADDRESS

CITY ZIP/POSTAL CODE

COUNTRY STATE/PROVINCE

United States Choose one

EMAIL PHONE

COUNTRY OF CITIZENSHIP Same as above

United States

CHOOSE A REGISTRATION KEY

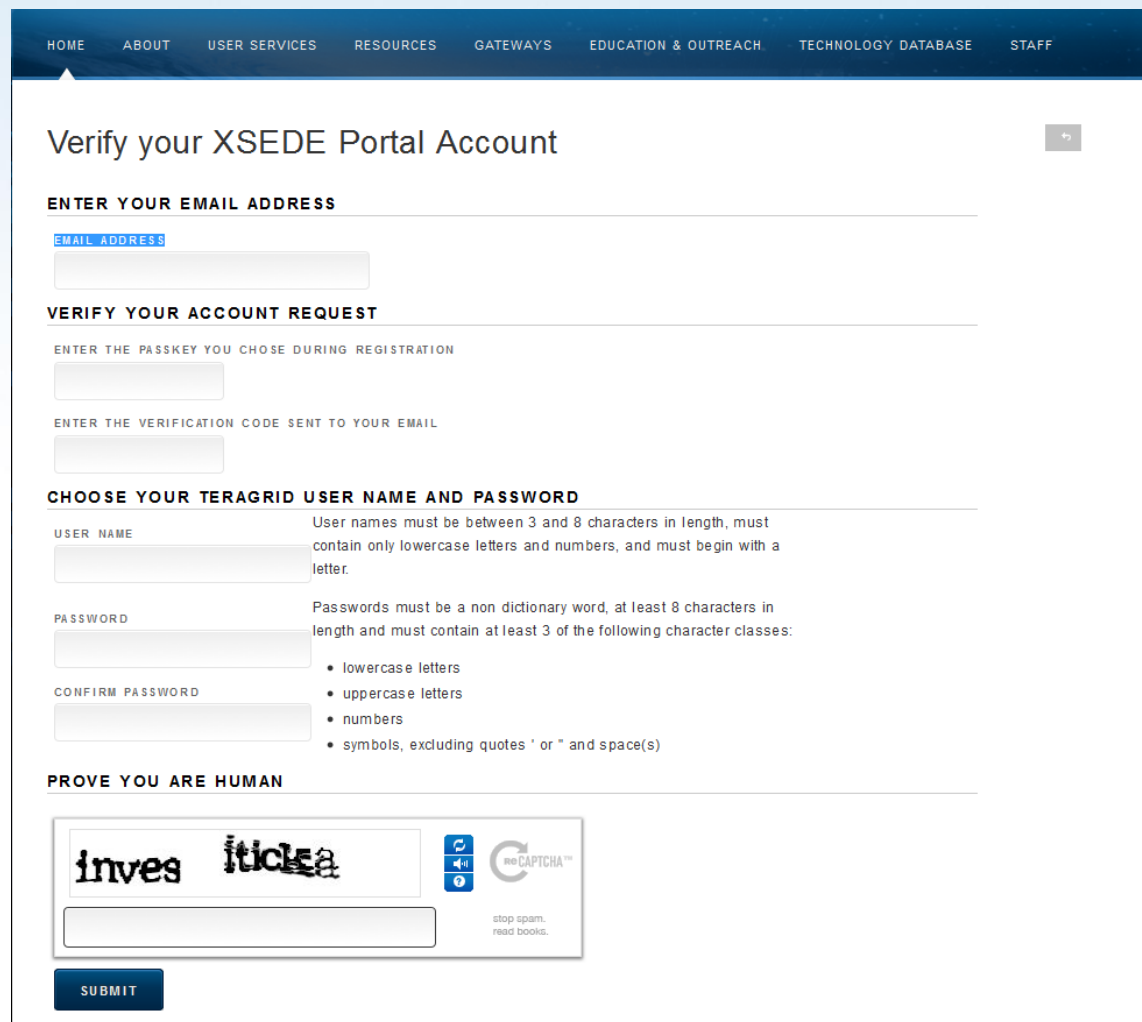
You will use your registration key to identify yourself in the Verify Account step. Use only letters and numbers; maximum 6 characters.

REGISTRATION KEY

PROVE YOU ARE HUMAN

Creating an XSEDE portal account (2)

- Verify your account
 - email address
 - passkey
 - verification code
- Choose username
- Choose password
 - Must comply with password rules



The screenshot shows the 'Verify your XSEDE Portal Account' page. At the top is a navigation bar with links: HOME, ABOUT, USER SERVICES, RESOURCES, GATEWAYS, EDUCATION & OUTREACH, TECHNOLOGY DATABASE, and STAFF. The main heading is 'Verify your XSEDE Portal Account'. Below it are four sections:

- ENTER YOUR EMAIL ADDRESS**: A form with a label 'EMAIL ADDRESS' and a text input field.
- VERIFY YOUR ACCOUNT REQUEST**: Two form fields. The first is labeled 'ENTER THE PASKEY YOU CHOSE DURING REGISTRATION'. The second is labeled 'ENTER THE VERIFICATION CODE SENT TO YOUR EMAIL'.
- CHOOSE YOUR TERAGRID USER NAME AND PASSWORD**:
 - USER NAME**: A text input field. To its right, instructions state: 'User names must be between 3 and 8 characters in length, must contain only lowercase letters and numbers, and must begin with a letter.'
 - PASSWORD**: A text input field. To its right, instructions state: 'Passwords must be a non dictionary word, at least 8 characters in length and must contain at least 3 of the following character classes:'
 - lowercase letters
 - uppercase letters
 - numbers
 - symbols, excluding quotes ' or " and space(s)
 - CONFIRM PASSWORD**: A text input field.
- PROVE YOU ARE HUMAN**: A reCAPTCHA widget showing the text 'inves iticlea' and a checkbox. Below the widget is a 'SUBMIT' button.

Your XSEDE portal account

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 Extended Collaborative Support Services with a quick 5 question survey!



Welcome, Anita !
Last login: Thu 09/24/15
at 11:05:45 AM CST

Profile

Accounts

All ocations

Training

NEW! Share your XSEDE Science Achievements

Publications: [\[Full List\]](#)

You have not entered any publications.

You can review 3 publication(s).

[Add a Publication](#)

Tickets: [\[Full List\]](#)

New:

0

Open:

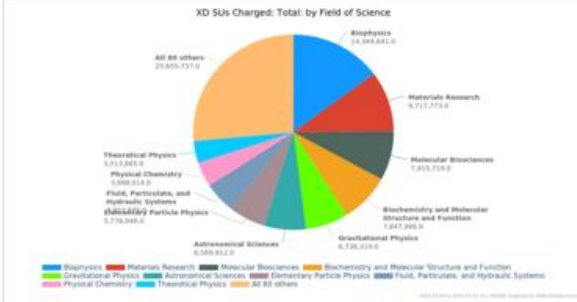
0

XSEDE USER PORTAL ON THE GO




In The Past 7 Days

XO SLUs Charged: Total: by Field of Science



Biophysics 14,064,841.0
Materials Research 9,717,779.8
Molecular Biosciences 7,803,719.9
Biochemistry and Molecular Structure and Function 7,847,299.0
Gravitational Physics 6,719,319.0
Astrochemical Sciences 6,568,912.0
Fund, Particulate, and Hydraulic Systems 6,568,912.0
Elementary Particle Physics 6,568,912.0
Physical Chemistry 5,000,219.0
Theoretical Physics 3,113,249.0
All 80 others 25,855,737.0



[View Gallery](#)

My XSEDE Resources [System Monitor](#)

Resource	Status	Load	Username	My Jobs
Stampede TACC	✓ Healthy	99%	amorednt	R: 0 Q: 0 O: 0
Comet SDSC	✓ Healthy	92%	amorednt	R: 0 Q: 0 O: 0
SuperMIC LSU CCT	✓ Healthy		amorednt	R: 0 Q: 0 O: 0

User Responsibility and Security

- You are responsible for your account and for protecting your passwords.
- First time you login, you will be asked to accept User Responsibilities
 - Do not share passwords, do not write passwords down where they can be easily found, and do not use tools that expose passwords on the network. This includes private keys: make sure they are password-protected.
 - Close SSH terminals and log out of the User Portal when finished
 - Report Suspicious Activity. If you have **any** suspicion that your account or personal computer has been compromised, email help@xsede.org or call, 24/7, 1-866-907-2383 immediately.



Get an Allocation: Types of Allocations

- Campus Champion
 - Get your feet wet with XSEDE
 - < 10k core-hours
 - 2 day lead time
- Start-Up
 - Benchmark and gain experience with resources
 - Different limits per resource
- Education
 - 2 week lead time
- Research
 - Class and workshop support
 - Short term (1 week to 6 months)
- Research
 - No Limit
 - 10 page request, 4 month lead time

<https://portal.xsede.org/allocations-overview>
<https://portal.xsede.org/allocation-policies>



Campus Champion Allocation

FREE

- Log onto the portal and get an account
 - <http://portal.xsede.org>
- Send anita.orendt@utah.edu
 - your portal account ID
 - What you want to do with XSEDE (brief!)
 - Email address
- 1-2 day lead time before you can access systems
- Up to 10K cpu-hours



Start Up and Education Allocations

FREE

- For investigators new to XSEDE
- Use the new XRAS (XSEDE Resource Allocation Service) system to submit request – anytime throughout the year
- Documents Required
 - PI CV
 - Additional information helpful
 - Education also requires course syllabus
- Takes up to two weeks for approval
- Max 200k cpu-hours (total on all resources)
- Can share it with colleagues/collaborators



Research Allocation

FREE

- Use the new XRAS system to submit request
- <https://portal.xsede.org/allocations-overview> for details
- Review occurs four times a year by XSEDE Resource Allocation Committee (XRAC)

Submit Requests during	for the Allocation Starting
Dec 15 through Jan 15	Apr 1
Mar 15 through Apr 15	Jul 1
Jun 15 through Jul 15	Oct 1
Sep 15 through Oct 15	Jan 1

- Documents required: PI CV, Main Document and Code Performance and Scaling
- Look at sample requests provided!



Submit Allocation Requests: XRAS

- Go to XSEDE portal and login:
 - <http://portal.xsede.org>
- Go to “Allocations”, then “Submit/Review Request”
- For a step-by-step walkthrough of the allocation process see:
 - <https://portal.xsede.org/group/xup/allocation-request-steps>



Accessing XSEDE Systems

- Go to XSEDE portal and login:
 - <http://portal.xsede.org>
- Multifactor authentication required as of Sept 27, 2016
- Go to “My XSEDE”, then “Accounts”
- Notice your usernames and the login hostname for each system
 - May be different from your XSEDE portal username!
- Click on “Login” for the system you want to access
- **NOTE:** Some sites (e.g. TACC) may email you to do account activation – check your inbox!



XSEDE Accounts

[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](#)

XSEDE Single Sign on Login Hub

You can SSH into any XSEDE system with your PORTAL username and PORTAL password from the convenience of your desktop.

XSEDE recommends you use the XSEDE Single Sign on Login Hub to login to XSEDE resources with your local username and password. Use a local SSH client on your desktop to SSH to login.xsede.org with your portal username and password then easily `gsi-ssh` to any XSEDE system you have an account on with no additional username or passwords. For more information please visit the [XSEDE Single Sign on Login Hub](#) documentation page.

RESOURCE NAME	GSI-SSH LOGIN HOST	INSTITUTION	LOCAL USERNAME
Gordon ION	<code>gordon.sdsc.xsede.org</code>	SDSC	
Maverick	<code>maverick.tacc.xsede.org</code>	TACC	<code>amorendt</code>
Mason	<code>mason.iu.xsede.org</code>	IU	
SuperMIC	not available	LSU CCT	<code>amorendt</code>
<code>greenfield.psc.xsede</code>	<code>greenfield.psc.xsede</code>	PSC	
OSG	<code>submit-1.osg.xsede.org</code>	OSG	<code>amorendt</code>
Comet	<code>comet.sdsc.xsede.org</code>	SDSC	<code>amorendt</code>
Wrangler	<code>wrangler.tacc.xsede.org</code>	TACC	
Gordon	<code>gordon.sdsc.xsede.org</code>	SDSC	<code>amorendt</code>
Stampede	<code>stampede.tacc.xsede.org</code>	TACC	<code>amorendt</code>
Darter	<code>gsissh.darter.nics.utk.edu</code>	NICS	
Nautilus	<code>gsissh.nautilus.nics.xsede.org</code>	NICS	



XSEDE

Single Sign On (SSO) Login Hub

- `ssh`
`<XUPlogin>@login.xsede.org`
- `>gsissh <machine-name>`
- Easy to setup host alias file
- <https://portal.xsede.org/web/xup/single-sign-on-hub>

```
[u0028729@ash1 ~]$ ssh amrendt@login.xsede.org
Please login to this system using your XSEDE username and password:
password:
Last login: Mon Jul 11 11:33:12 2016 from 155.101.26.21

# Welcome to the XSEDE Single Sign-On (SSO) Hub!
#
# This system is for use by authorized users only, and is subject to the XSEDE
# Acceptable Use Policy, described at https://www.xsede.org/usage-policies.
# All activities on this system may be monitored and logged.
#
# Your storage on this system is limited to 100MB. Backup is not provided.
#
# From this system, you may login to other XSEDE system login hosts on which
# you currently have an active account. To see a list of your accounts, visit:
# https://portal.xsede.org/group/xup/accounts
#
# To login to an XSEDE system login host, enter: gsissh <login-host>
# where <login-host> is the hostname, alias or IP address of the login host.
# The following default gsissh host aliases have been defined:
#
# bridges comet darter gordon greenfield mason maverick nautilus
#   osg stampede supermic wrangler-iu wrangler-tacc xstream
#
# For example, to login to the Comet system at SDSC, enter: gsissh comet
#
# E-mail help@xsede.org if you require assistance in the use of this system.
```

Direct login access via command line

- Traditional way of accessing supercomputing resources
- Must submit a help ticket requesting a password to that resource in order to login directly.
- `ssh <username>@<machine-name>`

Examples:

- `ssh amorendt@gordon.sdsc.xsede.org`

Data Storage and File Transfer

- Easy data transfer
 - In-browser SFTP or SCP clients through Portal SSH
- Standard data transfer
 - scp to move data in/out of XSEDE systems
 - Requires SSH key setup
 - rsync to move data in
- High performance data transfer
 - Globus Online: <https://www.globusonline.org/>

Computing Environment: File Systems

Where your data resides on XSEDE and the appropriate storage is your responsibility. XSEDE users have access to three types of storage:

- **Stand-alone Storage:** Allows storage allocations independent of compute/visualization allocation
- **Archival Storage:** (large scale persistent storage) Long term storage of large amounts of data (often tape); slower access, accessible from all sites
- **Resource File System Storage:** All allocations include access to limited disk and scratch file systems
- For more info: <https://www.xsede.org/storage>

Computing Environment: Modules

- Environment management package
- Command line interface for modifying environment variables, like PATH.
- Makes it easier to manage collections of software packages and versions.
- **Syntax:** `module <command>`
- **A few Commands:** `avail, list, load <module>, unload, help <`

Computing Environment: Modules

- Simple Modules Commands
 - module avail - lists available modules
 - module list - lists currently loaded modules
 - module help foo - help on module foo
 - module whatis foo - brief description of module foo
 - module display foo - displays the changes that are made to the environment by loading module foo without actually loading it.
 - module load foo - load module foo
 - module unload foo - unloads module foo and removes all changes that it made in the environment

Computing Environment – Running Jobs

- All XSEDE systems use some type job scheduler (batch)
 - Request number/type of nodes
 - How long to run
 - What to do with output files
 - Submit job script with these specifications
- Most XSEDE systems use either SLURM or PBS/TORQUE
- <https://www.xsede.org/web/guest/user-guides>



Sign up for training

- XSEDE has a large set of online and in person training (programming, visualization & code improvement)
 - <https://www.xsede.org/web/xup/online-training>
 - <https://www.xsede.org/web/xup/course-calendar>

CHPC offers some of the in person offerings – watch for announcements

Support Resources

- Local Campus Champions:
 - anita.orendt@utah.edu
- Centralized XSEDE help: help@xsede.org
- Extended one-on-one help (ECSS) – can request along with allocation:
 - <https://www.xsede.org/ecss>
- Training
 - <http://www.xsede.org/training>



Gateways

- <https://www.xsede.org/web/guest/gateways-listing> for list
- Most are domain specific
- Way to use select XSEDE resources without allocation or need to login
- Portal or interface to prepare inputs, select resources, submit jobs, get results
- Will present more next semester





Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.

XSEDE

Extreme Science and Engineering
Discovery Environment