October 20, 2016

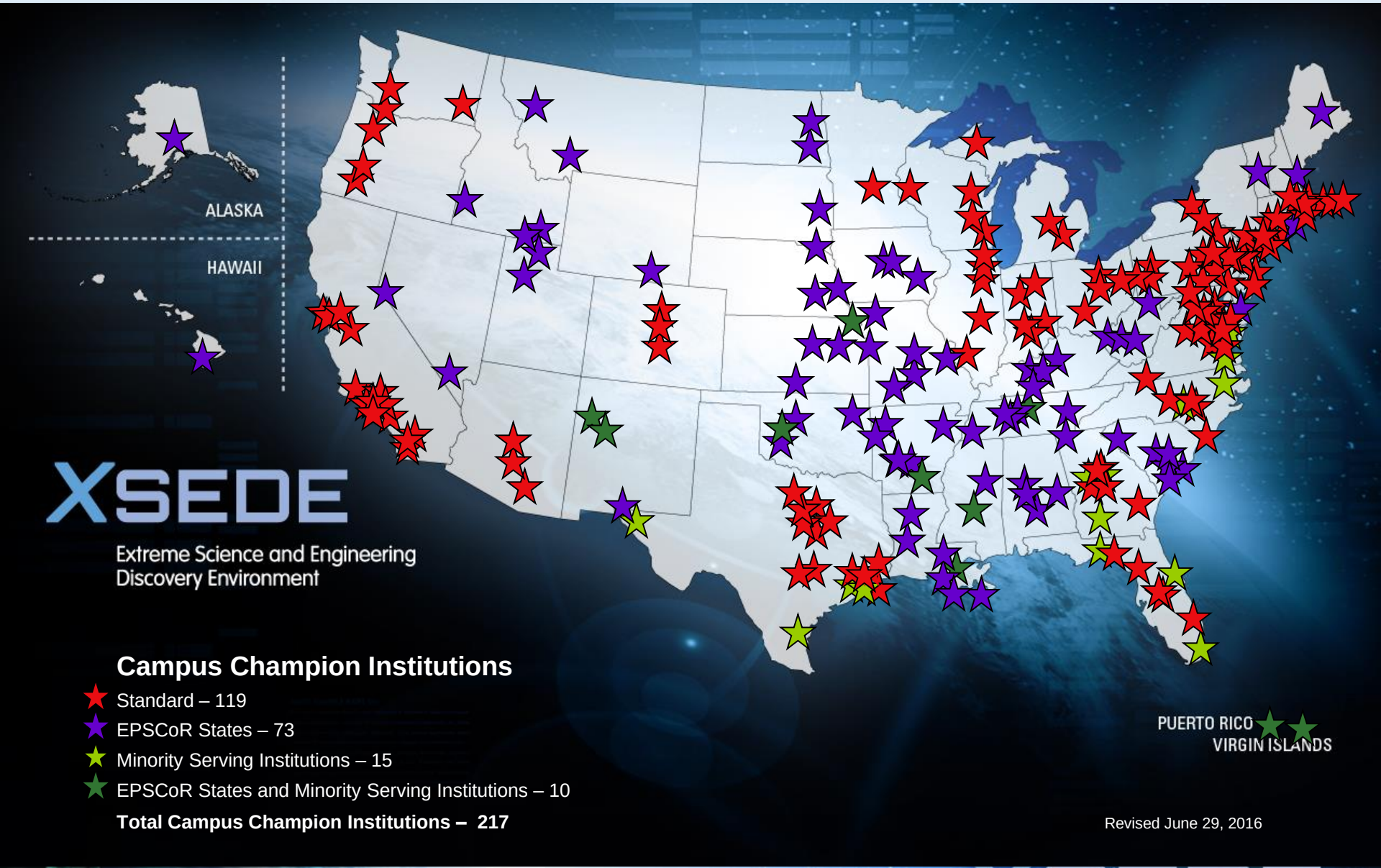
XSEDE Resource Support at CHPC

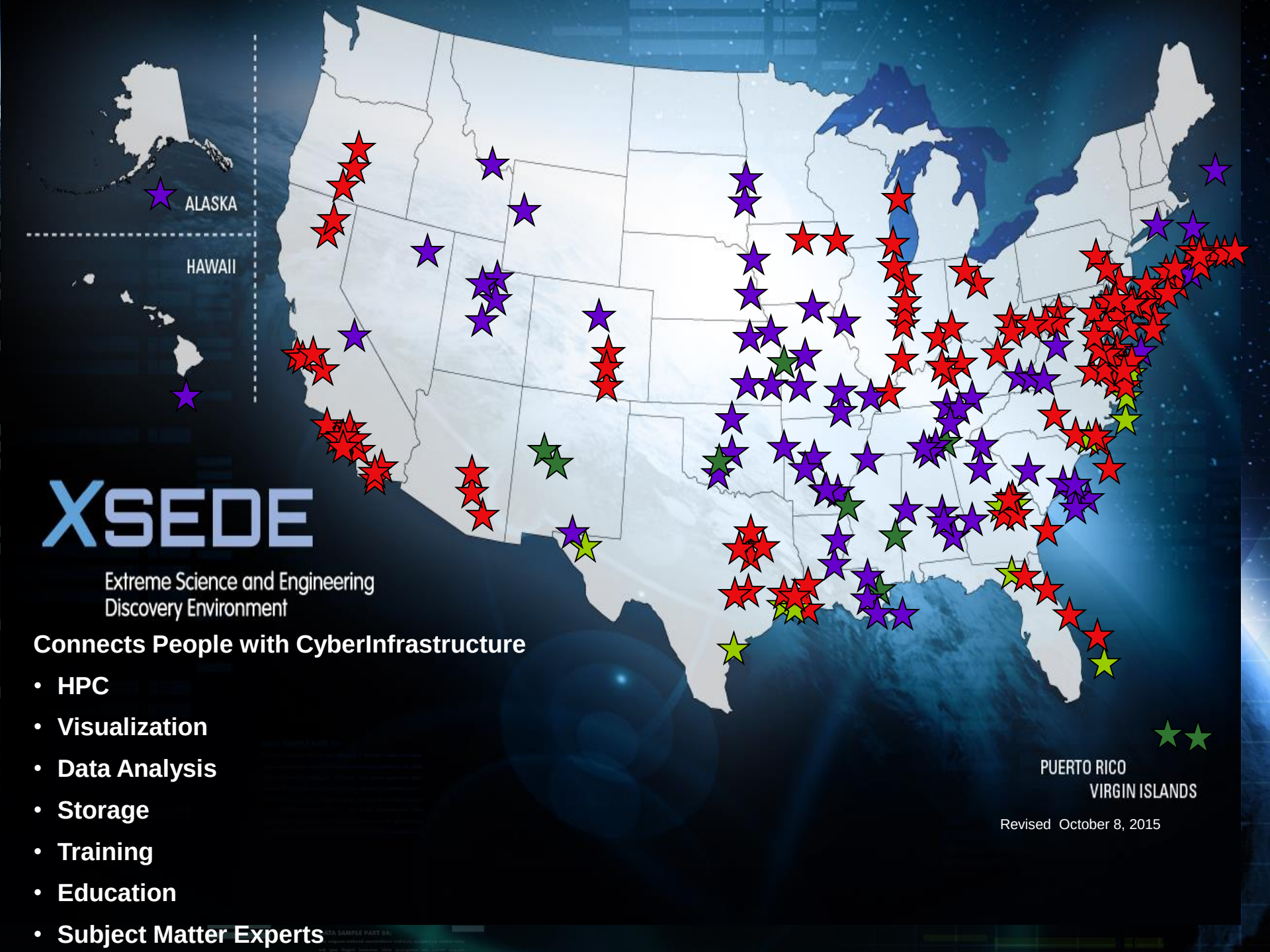
Campus Champion: Anita Orendt
anita.orendt@utah.edu

XSEDE

Extreme Science and Engineering Discovery Environment

NSF


ALASKA
HAWAII
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

Extreme Science and Engineering Discovery Environment

Connects People with CyberInfrastructure

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

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

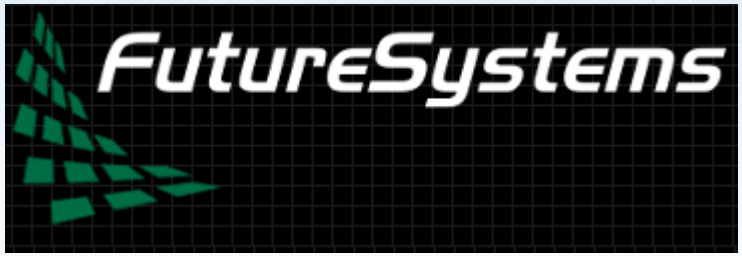
SDSC Gordon 1024 Intel Sandybride nodes; data-intensive, high-performance computing resource for computing spanning many domains

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

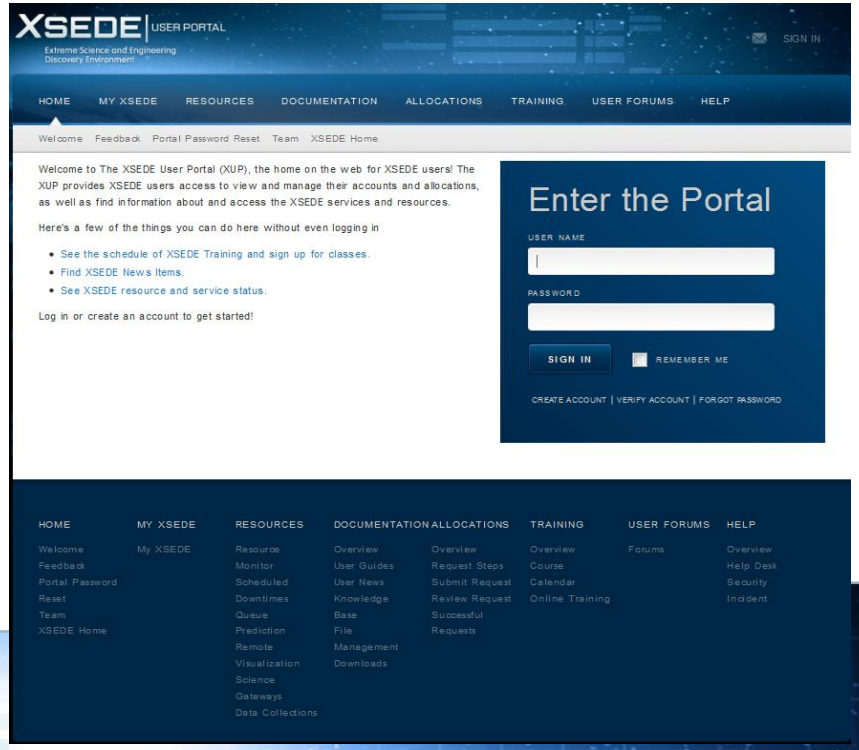
- Visualization
- Storage – at TACC, PSC, SDSC, NICS, Indiana
- Science Gateways
- Extended Support

http://portal.xsede.org

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

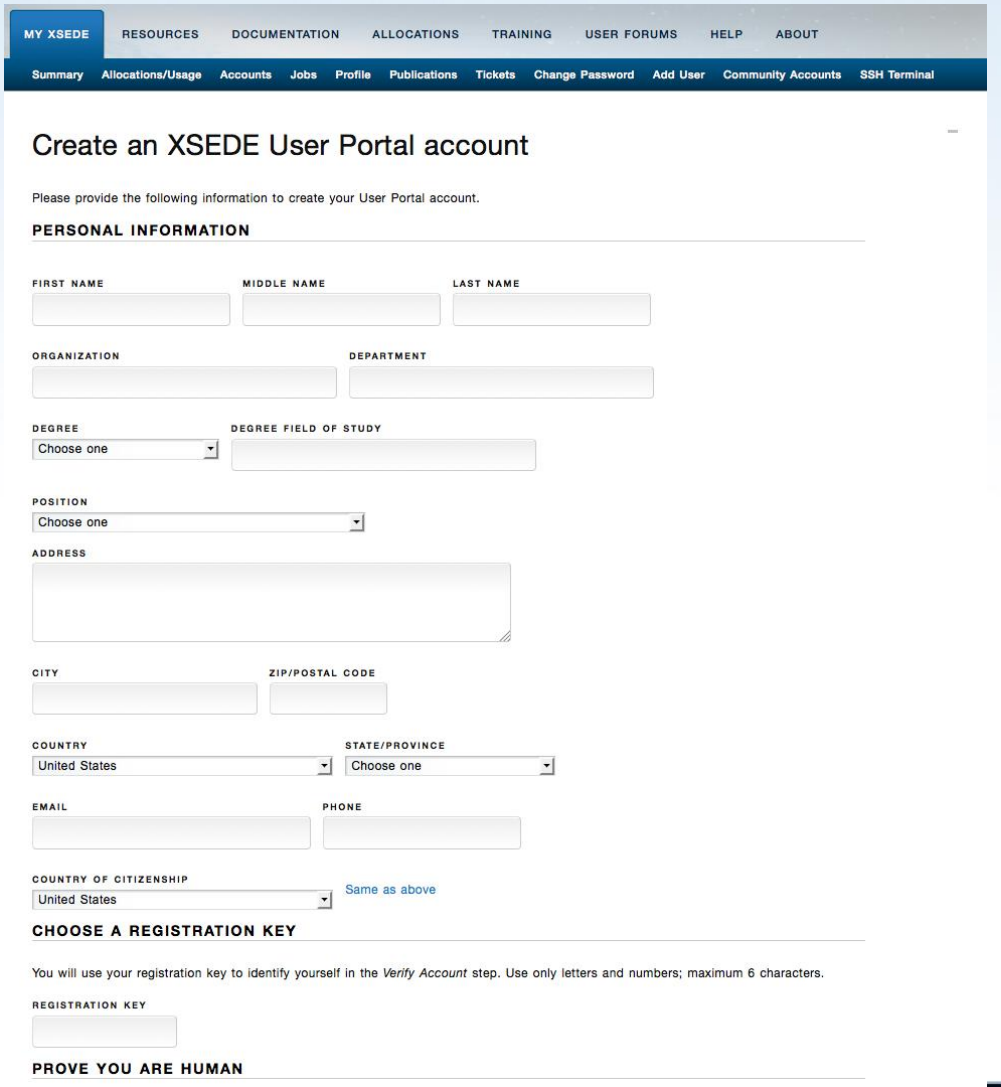
- Continually updated information about your allocations
- Access to your XSEDE accounts and allocated resources
- Interfaces for data management, data collections, and other user tasks and resources

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



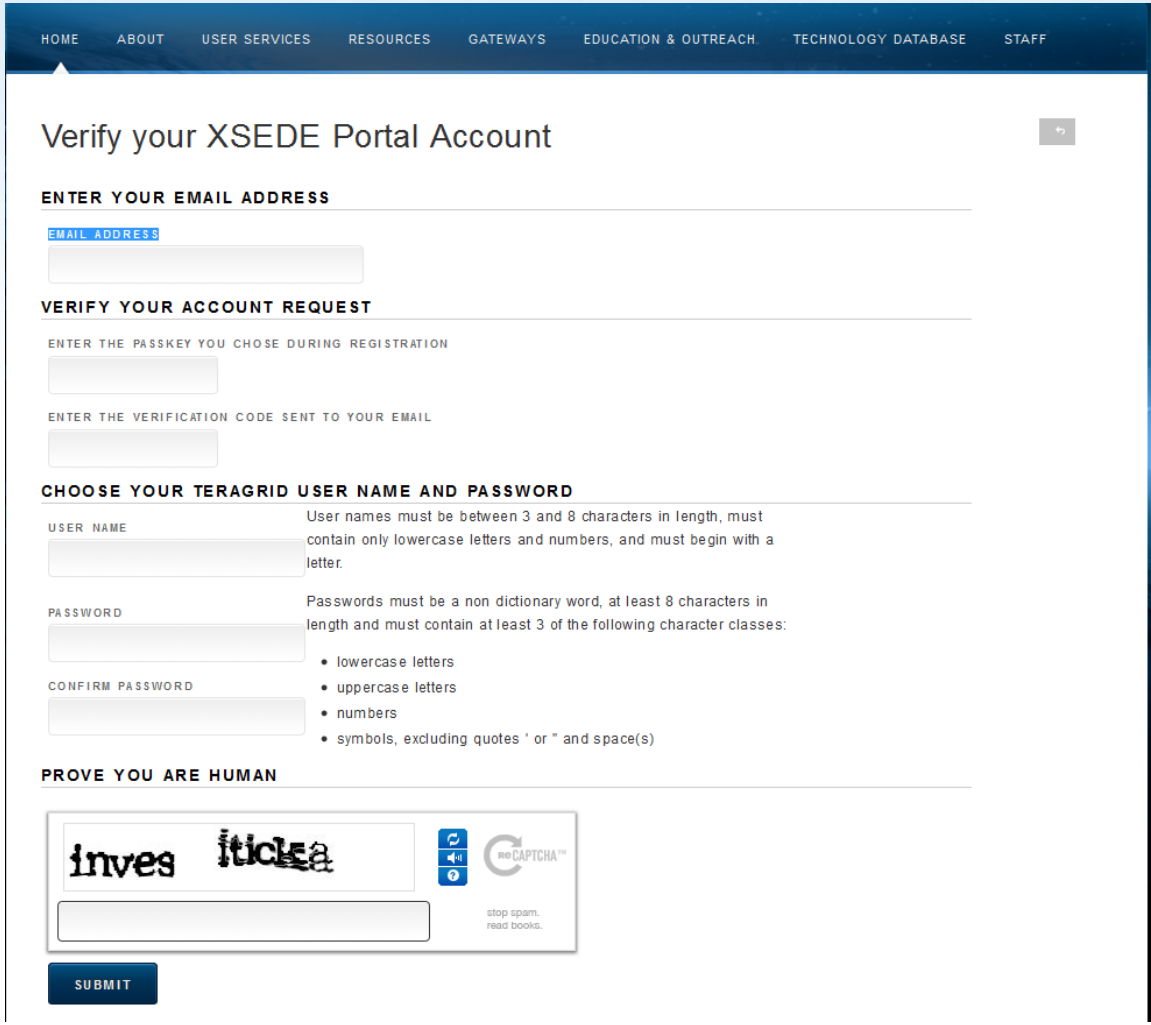
Creating an XSEDE portal account (XUP)

- 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

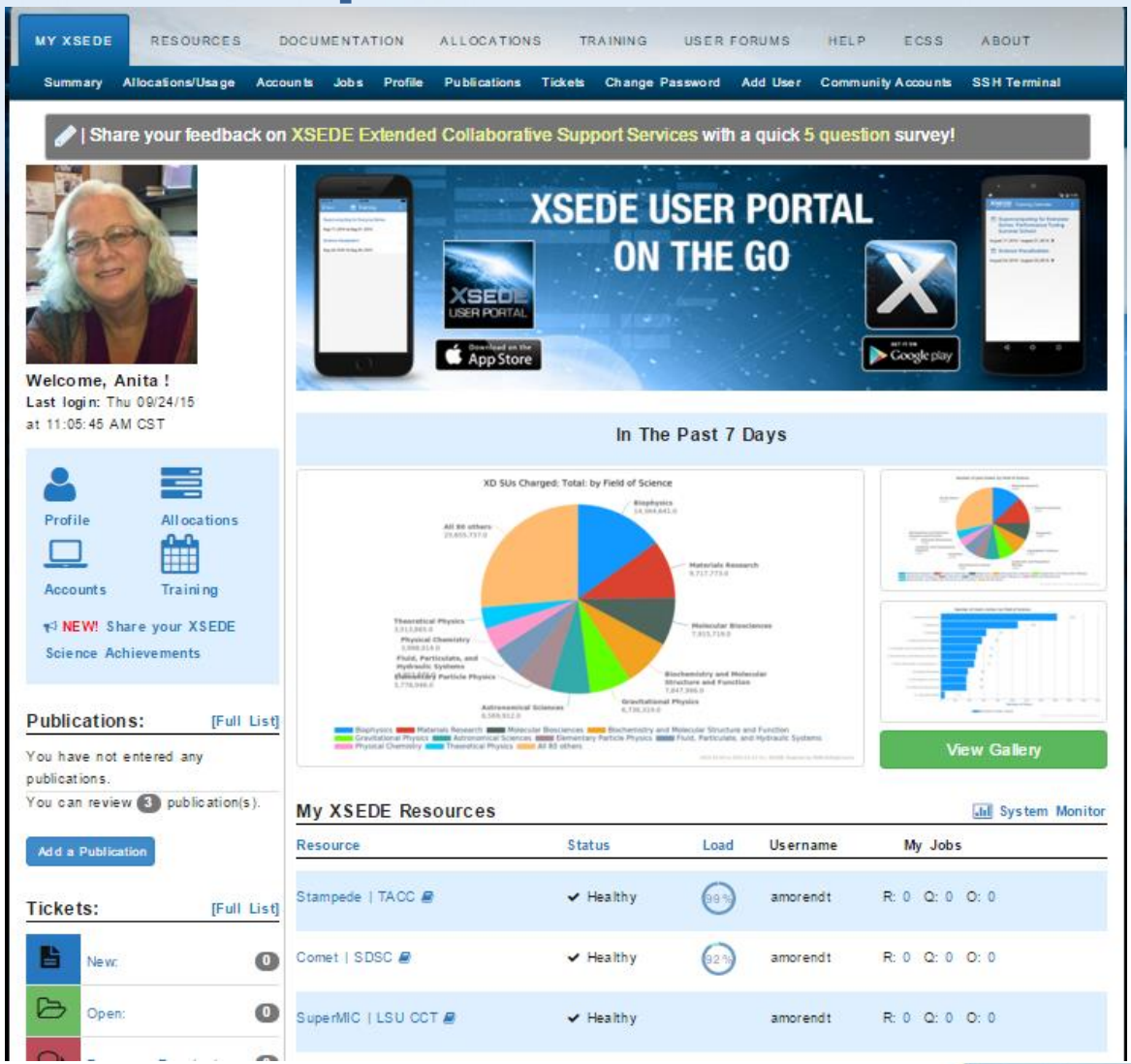


Creating an XSEDE portal account (2)

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



Your XSEDE portal account



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
  - 2 week lead time
- Education
  - 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 will 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!

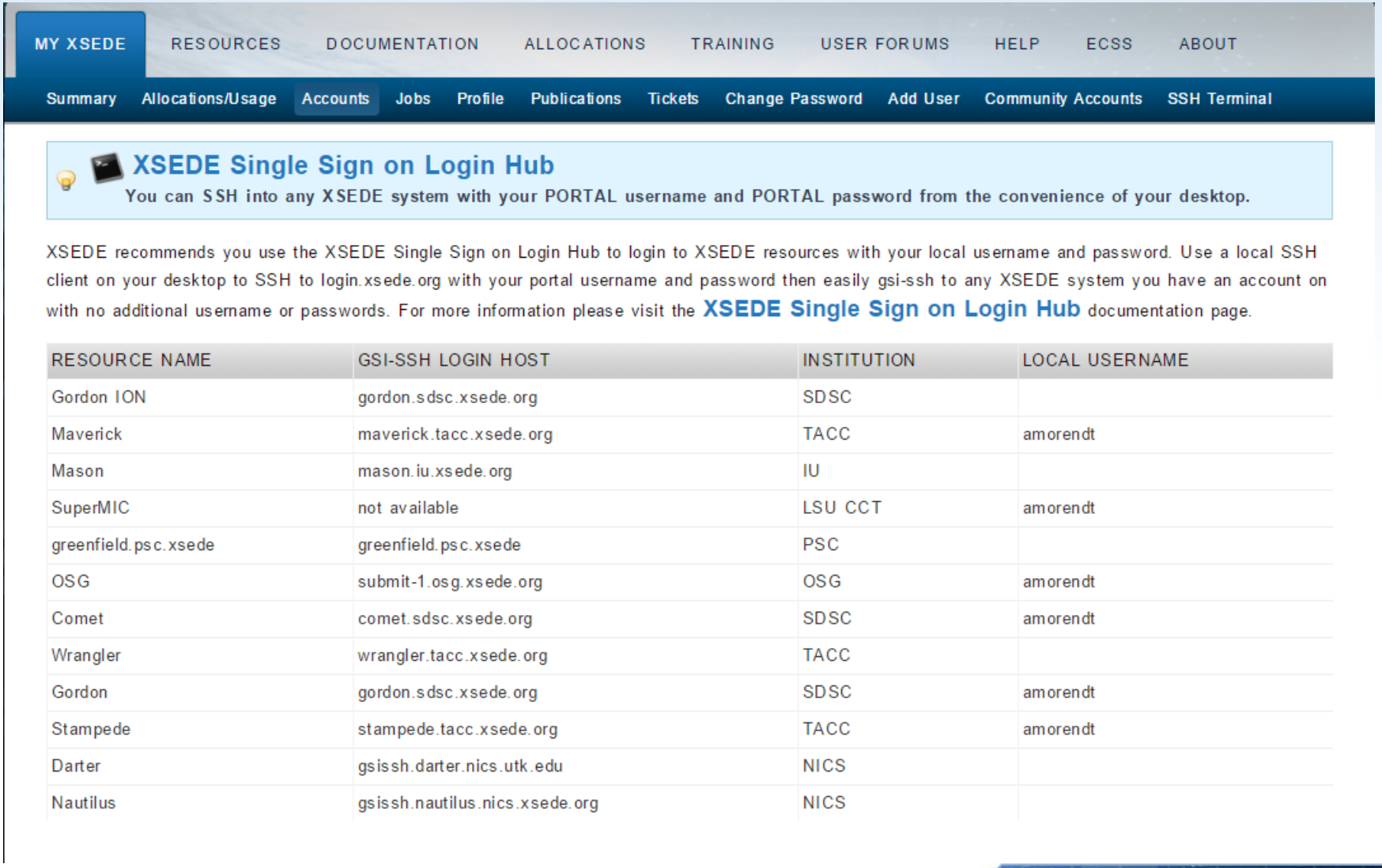
Submit Allocation Requests: XRAS

- 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



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

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 amorendt@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