

XSEDE Computational Resource Support at CHPC

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XSEDE

Extreme Science and Engineering
Discovery Environment



Overview

- Current XSEDE Resources
- Other Compute 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
- Campus Champion Program



XSEDE Resources



XSEDE

XSEDE HPC Computing Resources

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

TACC Stampede2 Update of Stampede in production Fall 2017. With 4,200 KNL (Intel Xeon Phi 7250) compute nodes along with 1,736 Skylake (48 core, 192GB) compute nodes it is designed for large scale computing needs. 18 petaflops

SDSC Comet About 1950 Intel Haswell nodes (24 cores, 128GB RAM) , 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 NVIDIA K80/P100 GPUs; others have 1.5TB RAM

XStream (Stanford), K80 GPU cluster with 65 nodes each with 20 cores (Ivybridge) and 8 K80s; 20% cycles to XSEDE

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

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



XSEDE

20 Storage Building Blocks, implementing the parallel *Pylon* filesystem (~10PB) using PSC's SLASH2 filesystem

4 MDS nodes
2 front-end nodes
2 boot nodes
8 management nodes

6 "core" Intel® OPA edge switches: fully interconnected, 2 links per switch

Intel® OPA cables

800 HPE Apollo 2000 (128GB) compute nodes

4 HPE Integrity Superdome X (12TB) compute nodes

42 HPE ProLiant DL580 (3TB) compute nodes

12 HPE ProLiant DL380 database nodes

6 HPE ProLiant DL360 web server nodes

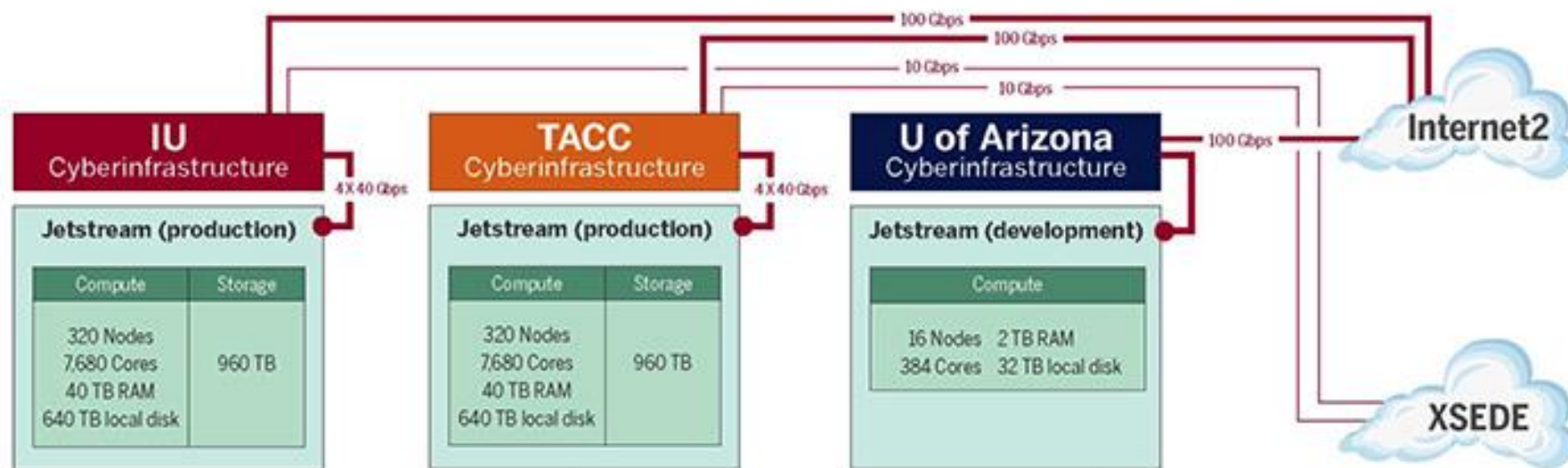
20 "leaf" Intel® OPA edge switches

32 RSM nodes with NVIDIA next-generation GPUs

16 RSM nodes with NVIDIA K80 GPUs

Purpose-built Intel® Omni-Path topology for data-intensive HPC

<http://psc.edu/bridges>



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Jetstream at IU/TACC

Jetstream can be used in several different virtual machine (VM) sizes which are charged in service units (SUs) based on how much of the total system resource is used. The table below outlines the VM sizes created for Jetstream.

VM SIZE	VCPUS	RAM (GB)	LOCAL STORAGE (GB)	SU COST PER HOUR
Tiny	1	2	8	1
Small	2	4	20	2
Medium	6	16	60	6
Large	10	30	120	10
XLarge	22	60	240	22
XX Large	44	120	480	44



Other Services

- [Visualization](#)
- Storage at [TACC](#), [PSC](#), [SDSC](#), [NICS](#), [Indiana](#)
- [Science Gateways](#)
- [Extended Support](#)
- [Training](#)
 - Online, webinars, and in person
 - CHPC satellite site for XSEDE HPC Monthly Workshop and Summer Boot Camps
 - <https://www.xsede.org/web/xup/online-training> for listing of all online offerings



Getting Started

<https://www.xsede.org/for-users/getting-started>

- Get XSEDE Portal account
- Learn about resources and figure out which meets your computing needs
 - Can start with a champion allocation if your institution has a champion
- Get an allocation – XRAS online submission
 - Startup allocations - Quick and Easy
 - Project abstract and CV
 - can do any time of year
 - Research allocation - very competitive
 - submission schedule (4X per year)
 - Main proposal, Progress report if renewal, Code performance & scaling section, CV
 - Reviewed by XSEDE Resource Allocations Committee (XRAC)
 - Educational Allocations
 - Abstract, CV, course syllabus
 - Can do anytime of the year
- See <https://www.xsede.org/web/xup/online-training> for New User Tutorial and for Writing and Submitting a Successful XSEDE Proposal



XSEDE

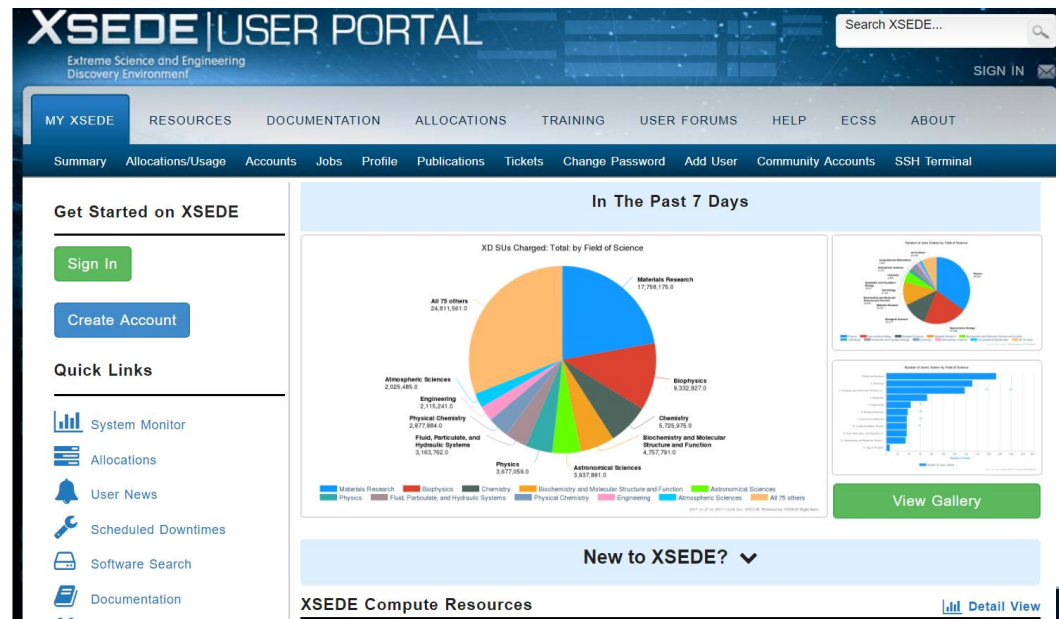
<http://portal.xsede.org>

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, etc

- 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
- Use confirmation number together with passkey to verify your account

Create an XSEDE User Portal account

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

XSEDE and Service Provider policies restrict each individual to a single user account. If you have forgotten your username or password, use the ["Forgot Password"](#) or ["Forgot Username"](#) links on the sign-in page. For other situations, please contact help@xsede.org.

Otherwise, please provide the following information to create your User Portal account. You are strongly encouraged to provide your "work" contact information. While XSEDE honors the privacy settings in your profile, we encourage you to protect yourself further by not providing personal information.

PERSONAL INFORMATION


FIRST NAME	MIDDLE NAME	LAST NAME
<input type="text"/>	<input type="text"/>	<input type="text"/>
UNIVERSITY OR ORGANIZATION	DEPARTMENT, CENTER, LAB, GROUP, OR OTHER SUB-UNIT	
<input type="text"/>	<input type="text"/>	
DEGREE	DEGREE FIELD OF STUDY	
<input type="text" value="Choose one"/>	<input type="text"/>	
POSITION		
<input type="text" value="Choose one"/>		
ADDRESS		
<input type="text"/>		
CITY	ZIP/POSTAL CODE	
<input type="text"/>	<input type="text"/>	
COUNTRY	STATE/PROVINCE	
<input type="text" value="United States"/>	<input type="text" value="Choose one"/>	
EMAIL	PHONE	
<input type="text"/>	<input type="text"/>	
COUNTRY OF CITIZENSHIP	Same as above	
<input type="text" value="United States"/>		



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

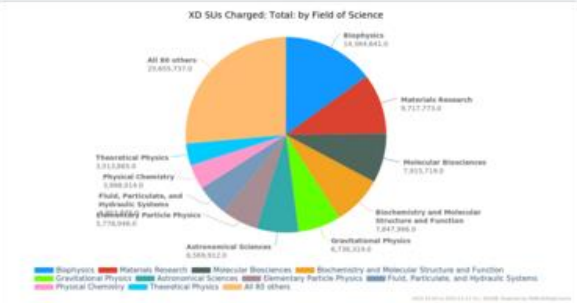
 New: **0**

 Open: **0**

XSEDE USER PORTAL ON THE GO

In The Past 7 Days

XD SUs Charged: Total: by Field of Science



Field of Science	SUs Charged
Biophysics	14,384,842.0
Materials Research	9,757,770.0
Molecular Biosciences	7,803,719.0
Biochemistry and Molecular Structure and Function	7,047,290.0
Fluid, Particulate, and Hydraulic Systems	6,710,218.0
Gravitational Physics	6,710,218.0
Astronomical Sciences	6,000,000.0
Theoretical Physics	5,112,000.0
Physical Chemistry	5,000,000.0
Fluid, Particulate, and Hydraulic Systems	4,710,218.0
Gravitational Physics	4,710,218.0
All 80 others	25,000,737.0

[View Gallery](#)

My XSEDE Resources [System Monitor](#)

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



User Responsibility and Security

- You are responsible for your account and for protecting your passwords.
- <https://portal.xsede.org/usage-policy>
- First time you login, you will be asked to accept User Responsibilities



Types of Allocations

FREE

- Campus Champion
 - Get your feet wet with XSEDE
 - See campus champion for access and limits
 - 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>



FREE

Research Allocation

- Use the new XRAS system to submit request
- <https://portal.xsede.org/allocations/announcements> 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 “Submit/Review Request”
- For more details, see:
 - <https://portal.xsede.org/allocations/policies>



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.
```


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

Direct login access via command line

- Traditional way of accessing 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`

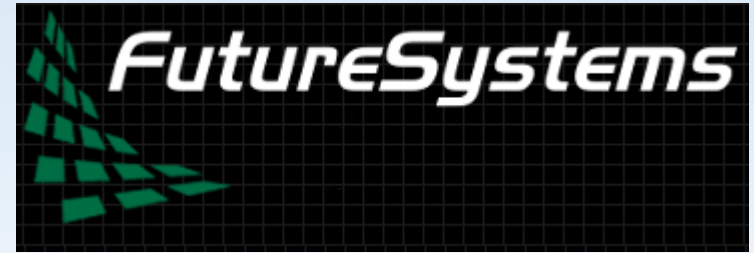


Other Outside of UU Computing Resources



XSEDE

- [Open Science Grid](#)
- [FutureSystems](#) (Indiana)
- [Blue Waters](#) (NCSA)
- [Titan](#) (OakRidge)
- [ALCF](#) (Mira, Theta, etc at Argonne)
- [Edison](#) (NERSC)



As part of RMACC

- Summit at University of Colorado Boulder
 - General compute
 - Haswell 24 cores/node, 128GB RAM
 - High memory
 - 48 cores/node 2TB
 - GPU nodes
 - 24 cores, 2 K80s/node
 - KNL Xeon Phi



Campus Chamions



XSEDE

NSF funded program to connect People with CyberInfrastructure

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



Champion Program



XSEDE

History of the Champions

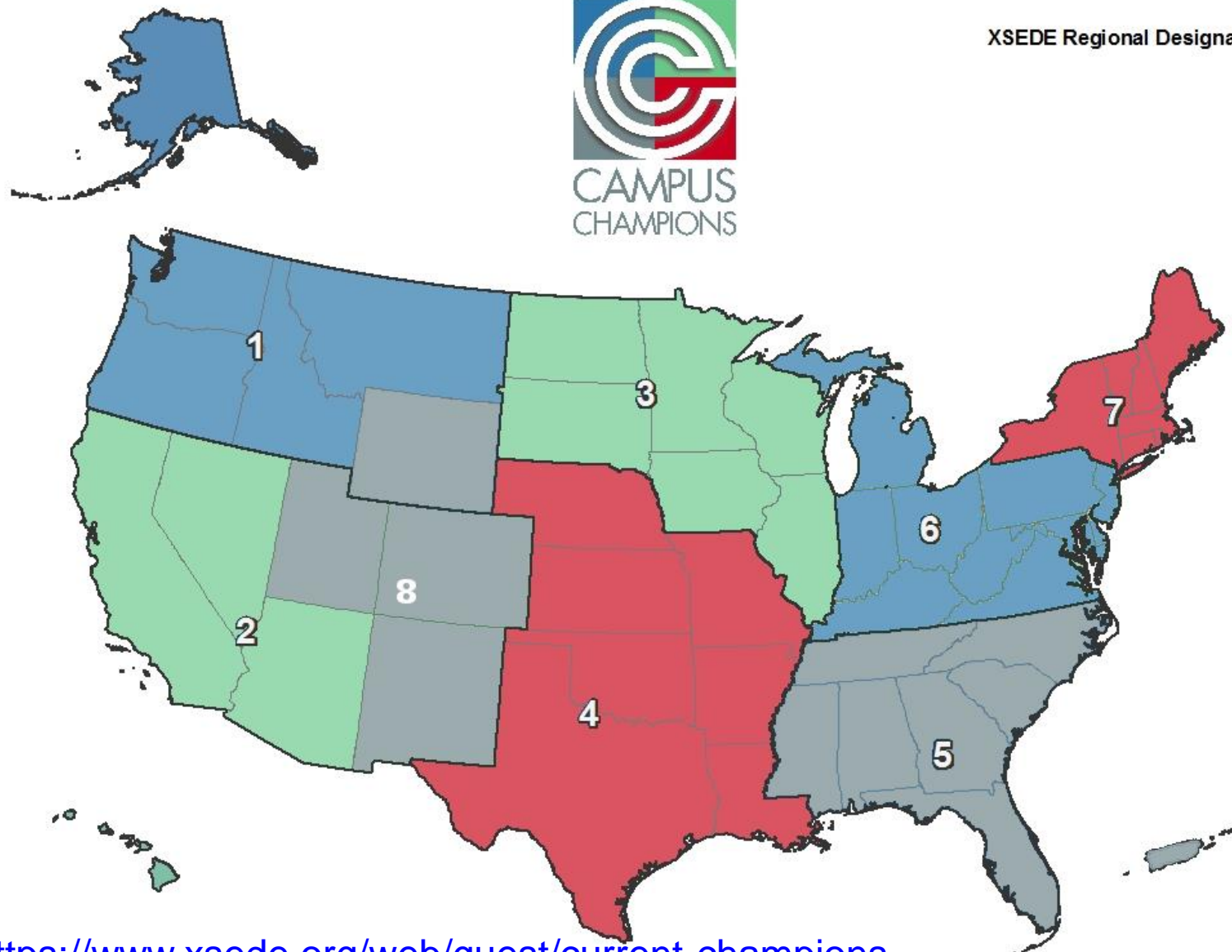
- Planning began in Fall of 2007
- 1st Champion selected in May 2008
- August 2011 – 100th institution joined
- May 2012 – Champion Fellows Program begun
- July 2013
 - Student Champion Program introduced
 - Domain Champion Program initiated
- January 2015
 - Regional Champion Program initiated
- August 2015 – 200th institution joined
- August 2017 – 221 institutions, 355 champions



XSEDE



CAMPUS
CHAMPIONS



- <https://www.xsede.org/web/guest/current-champions> --
interactive map

Campus Engagement Mission Statement

The Campus Engagement program promotes and facilitates the effective participation of a diverse national community of campuses in the application of advanced digital resources and services to accelerate scientific discovery and scholarly achievement.



Who are the champions?

- HPC Directors
- System Administrators
- User Support specialists
- Faculty evangelists
- Central IT staff
- Non-academic organization staff, e.g. USGS, USDA-ARS, KINBER, Idaho National Lab
- Plus friends of the family



What do champions do?

- Facilitate computing- and data-intensive research and education
- Help their local researchers and educators to find and use the advanced digital services that best meet their needs
- Share CI challenges and solutions
(at all levels: workgroup, institutional, regional, national, and international)

Goals

- Increase scalable, sustainable institutional uptake of advanced digital services from providers at all levels
- Foster a broader, deeper, more agile, more sustainable and more diverse nationwide cyberinfrastructure ecosystem
- Cultivate inter-institutional interchange of resources, expertise and support
- Sustain this community beyond XSEDE