XSEDE Computational Resource Support at CHPC

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XSEDE
Extreme Science and Engineering Discovery Environment

NSF

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 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

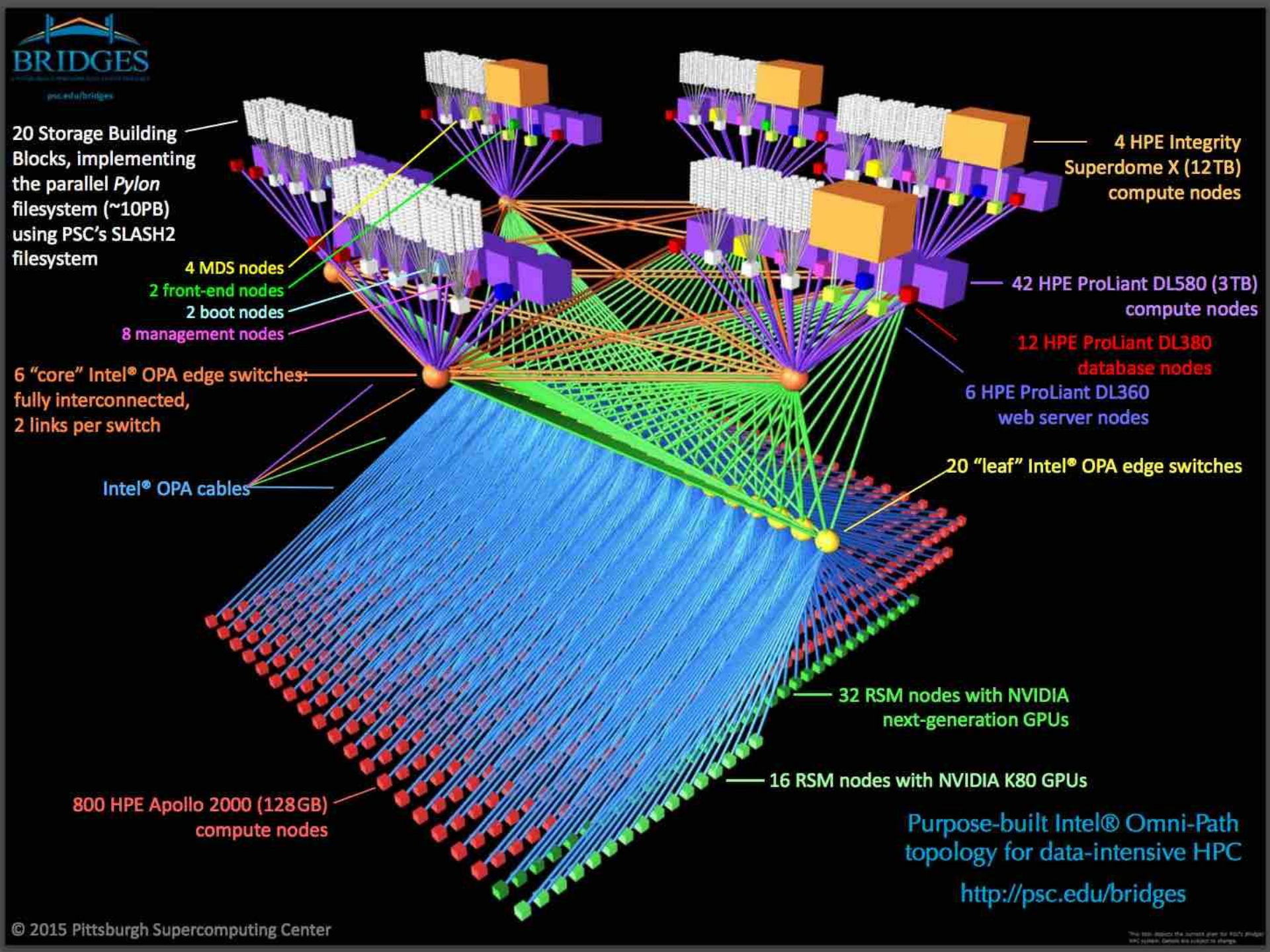
SDSC Comet About 1950 Intel Haswell nodes (24 cores, 128GB RAM) , SSD local scratch. It is intended for moderately scalable parallel applications with an emphasis on improving productivity for a broad spectrum of users. Additional nodes with NVIDIA K80/P100 GPUs; others have 1.5TB RAM

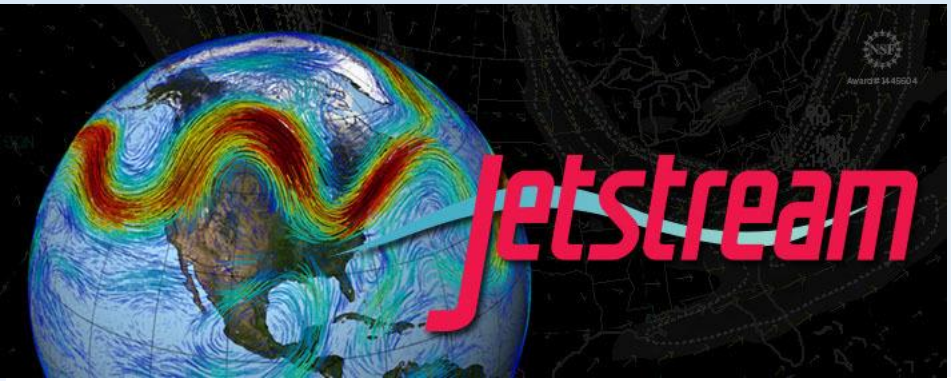
XStream (Stanford), K80 GPU cluster with 65 nodes each with 20 cores (Ivybridge) and 8 K80s; 20% cycles to XSEDE

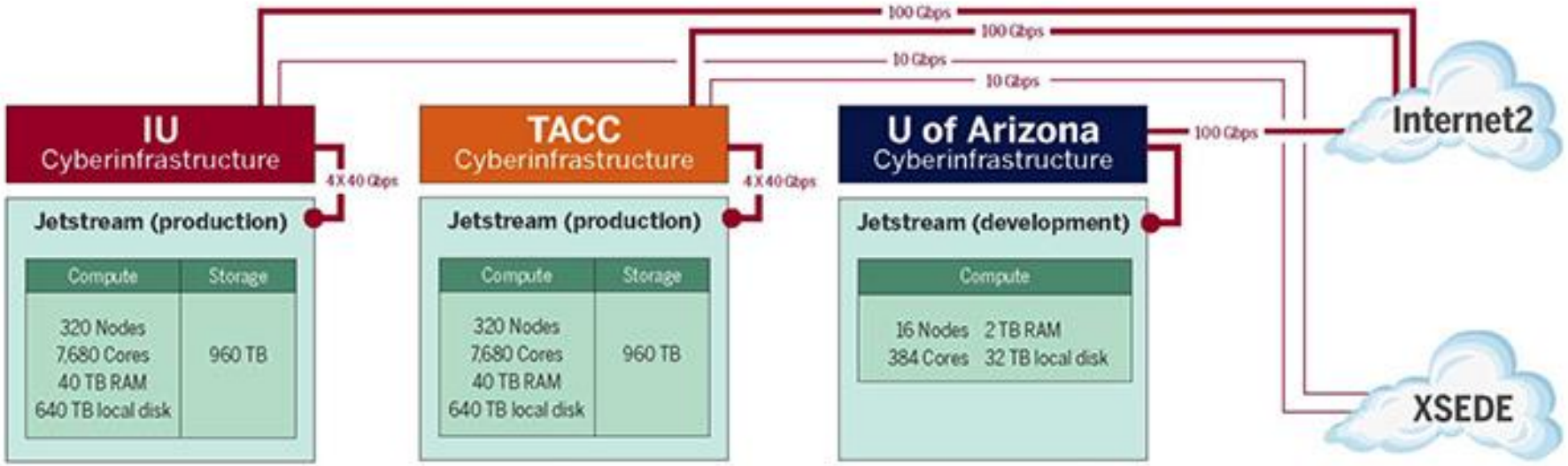
SuperMIC (LSU) Intel Ivybridge nodes with MIC coprocessors; 40% cycles to XSEDE

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




Jetstream


100 Gbps
100 Gbps
10 Gbps
10 Gbps
IU
Cyberinfrastructure
4 X 40 Gbps
Jetstream (production)
Compute
Storage
320 Nodes
7,680 Cores
40 TB RAM
640 TB local disk
960 TB
TACC
Cyberinfrastructure
4 X 40 Gbps
Jetstream (production)
Compute
Storage
320 Nodes
7,680 Cores
40 TB RAM
640 TB local disk
960 TB
U of Arizona
Cyberinfrastructure
100 Gbps
Jetstream (development)
Compute
16 Nodes 2 TB RAM
384 Cores 32 TB local disk
Internet2
XSEDE

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 Capms
  - https://www.xsede.org/web/xup/online-training for listing of all online offerings

Getting Started

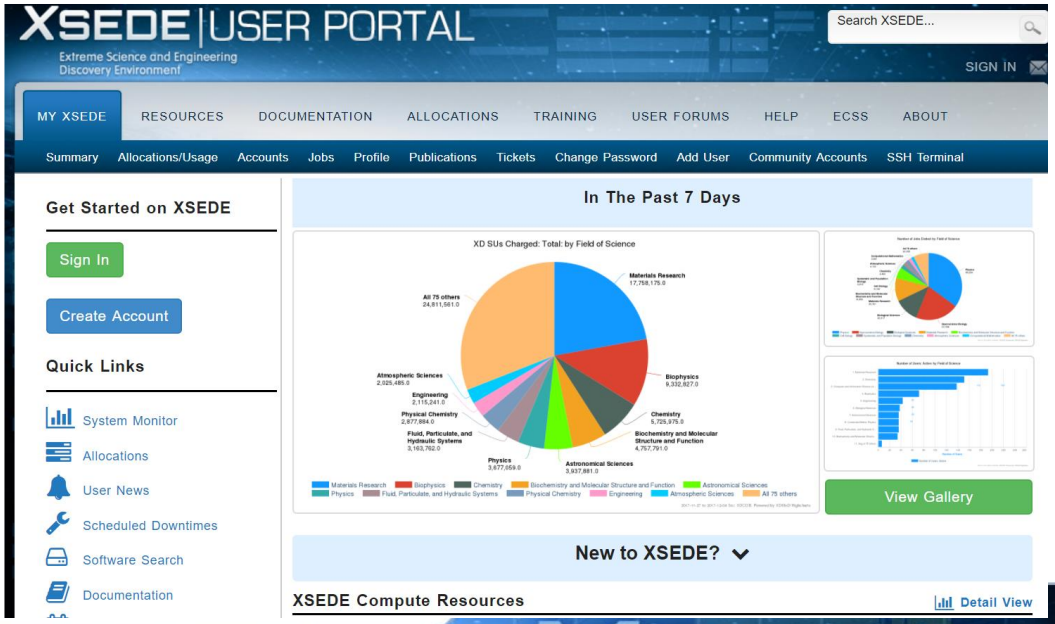
https://www.xsede.org/for-users/getting-started

- 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

http://portal.xsede.org

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

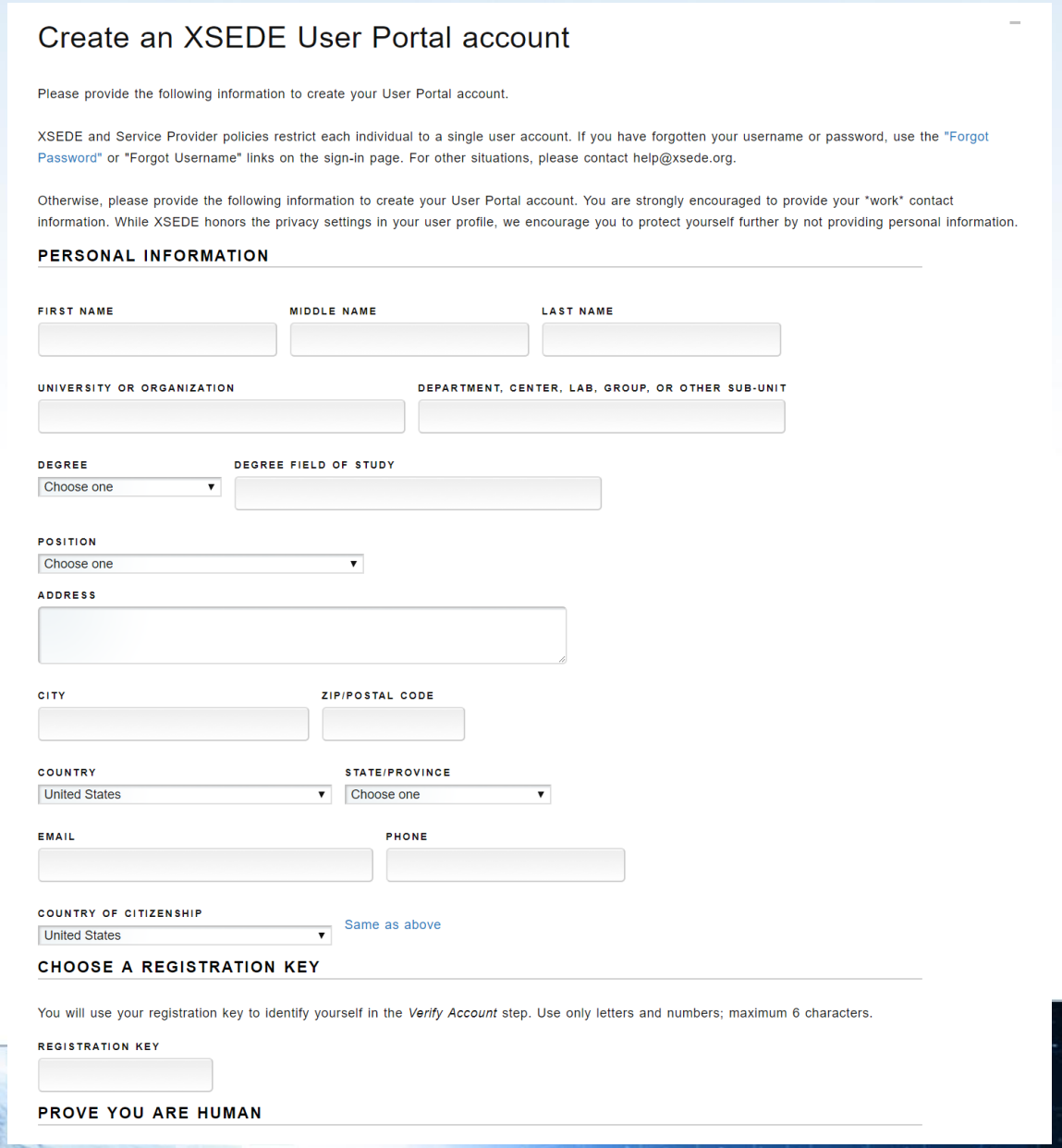
- Continually updated information about your allocations
- Access to your XSEDE accounts and allocated resources
- Interfaces for data management, data collections, etc
  - Access to:
    - Help Desk
    - Allocation and queue stats
    - User management
    - Documentation/training



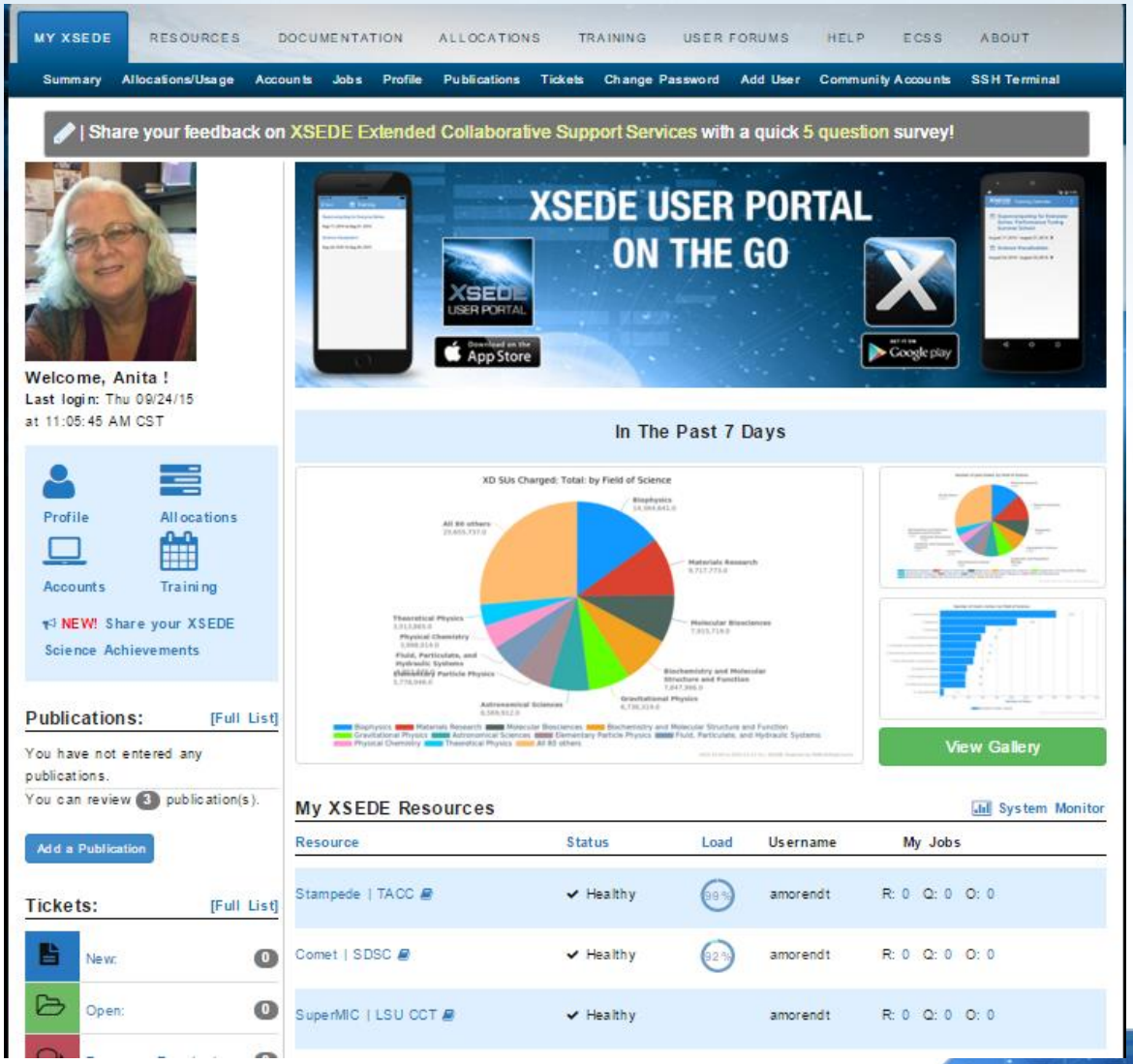
Creating an XSEDE portal account (XUP)

- 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



Your XSEDE portal account



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

Research Allocation

FREE

- 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

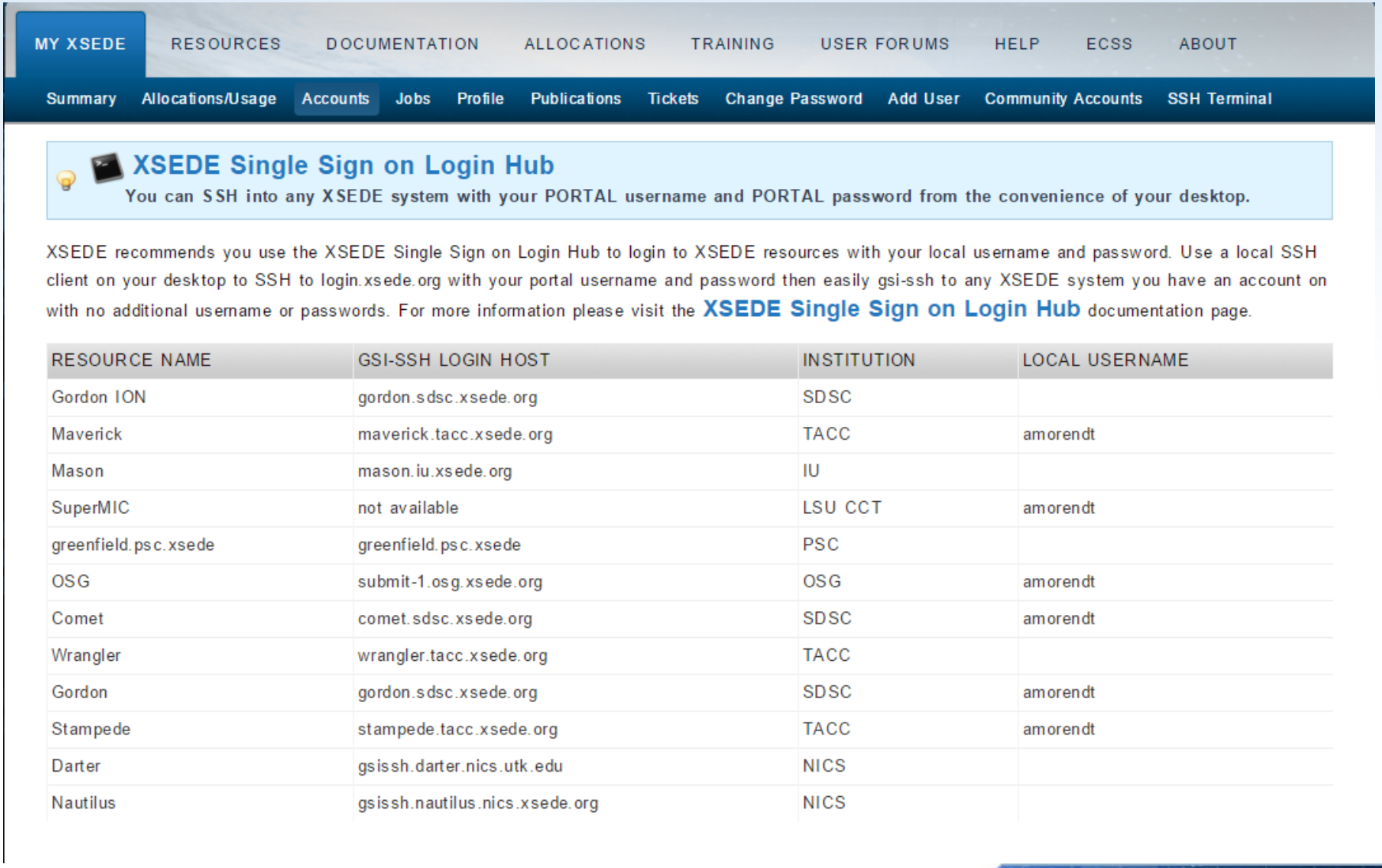
Single Sign On (SSO) Login Hub

- `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 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.
```

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	

Direct login access via command line

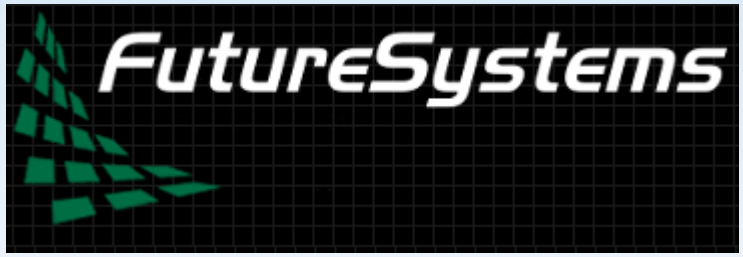
- Traditional way of accessing resources
- Must submit a help ticket requesting a password to that resource in order to login directly.
- `ssh <username>@<machine-name>`

Examples:

- ssh amorendt@gordon.sdsc.xsede.org

Other Outside of UU Computing Resources

- 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

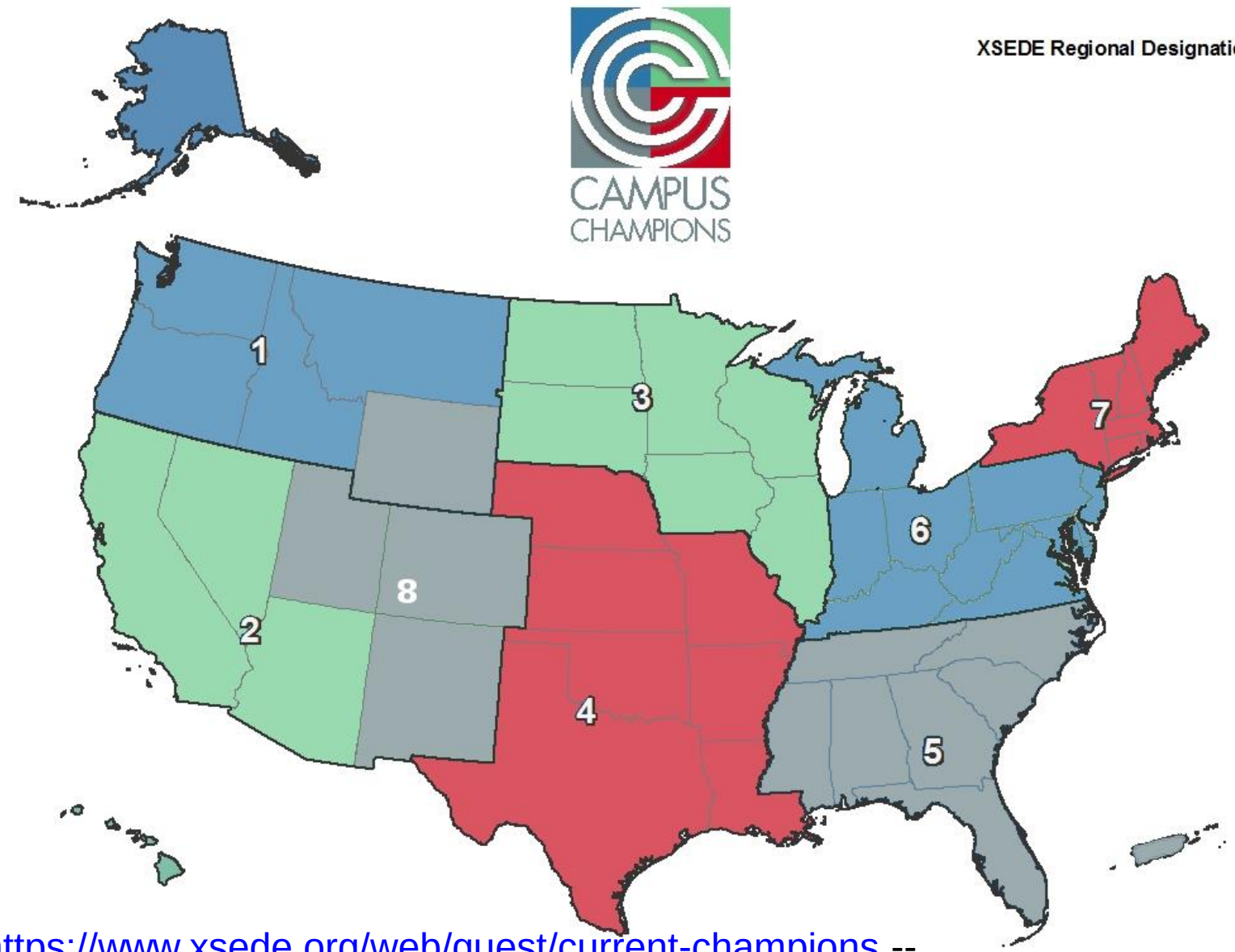
NSF funded program to connect People with CyberInfrastructure

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

Champion Program

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



• 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