National and Regional Computing Resources

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Center for High Performance Computing

Rocky Mountain Advanced Computing Consortium

Campus Champion – Lead Region 8

Outline

- Computing Resources
- People Resources
- Training
- Educational Opportunities

Computing 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

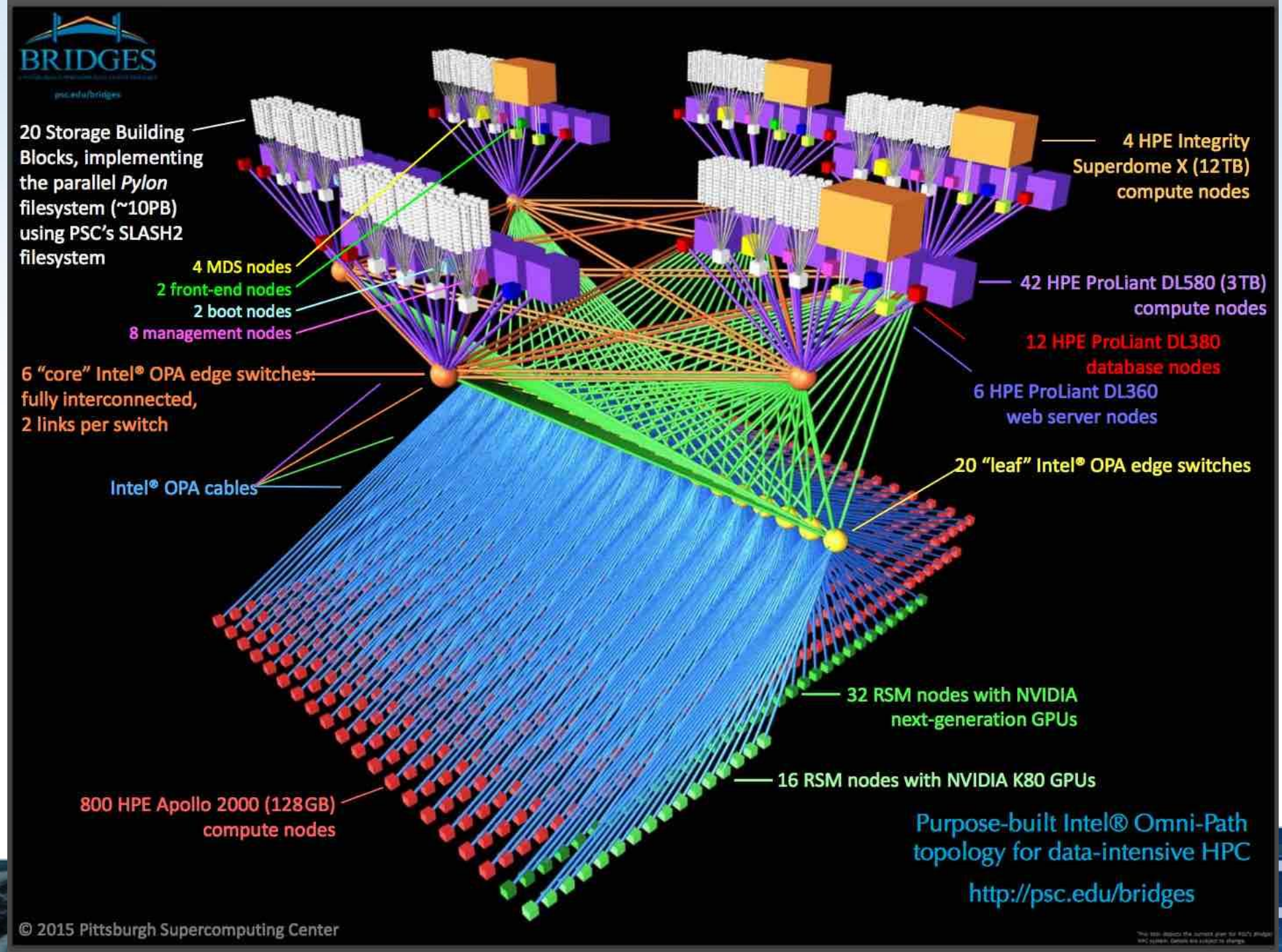
SDSC Comet About 1950 Intel Haswell nodes (24 cores, 128GB RAM) , SSD local scratch. It is intended for moderately scalable parallel applications with an emphasis on improving productivity for a broad spectrum of users. Additional nodes with NVIDIA K80/P100 GPUs; others have 1.5TB RAM

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


BRIDGES
psc.edu/bridges
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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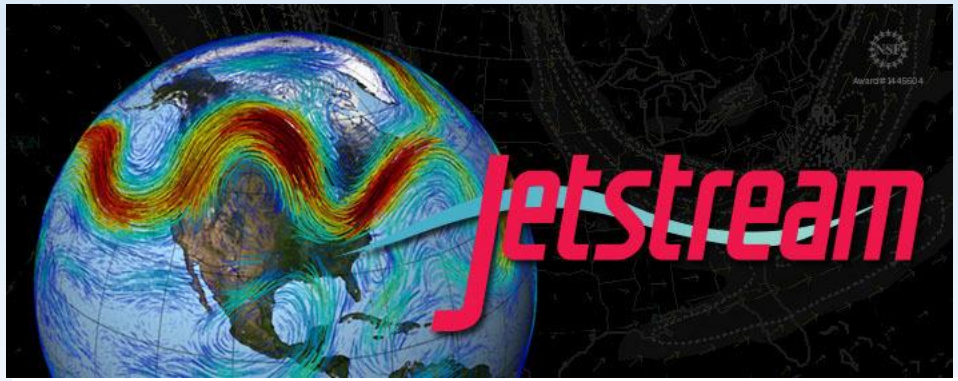
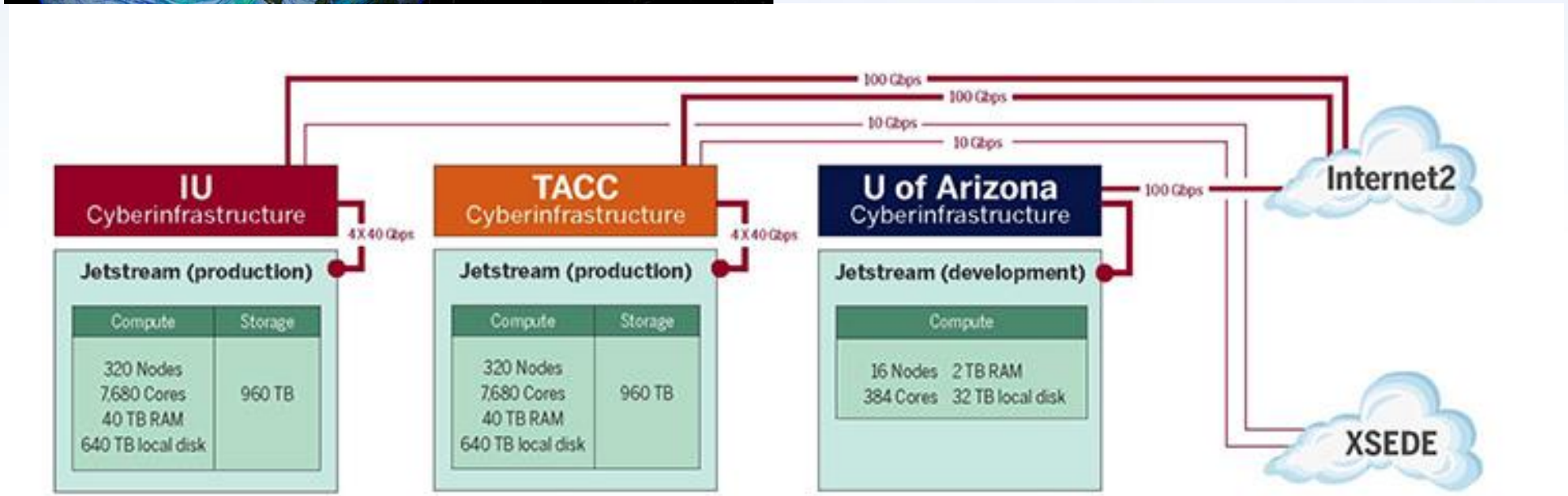

Jetstream


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

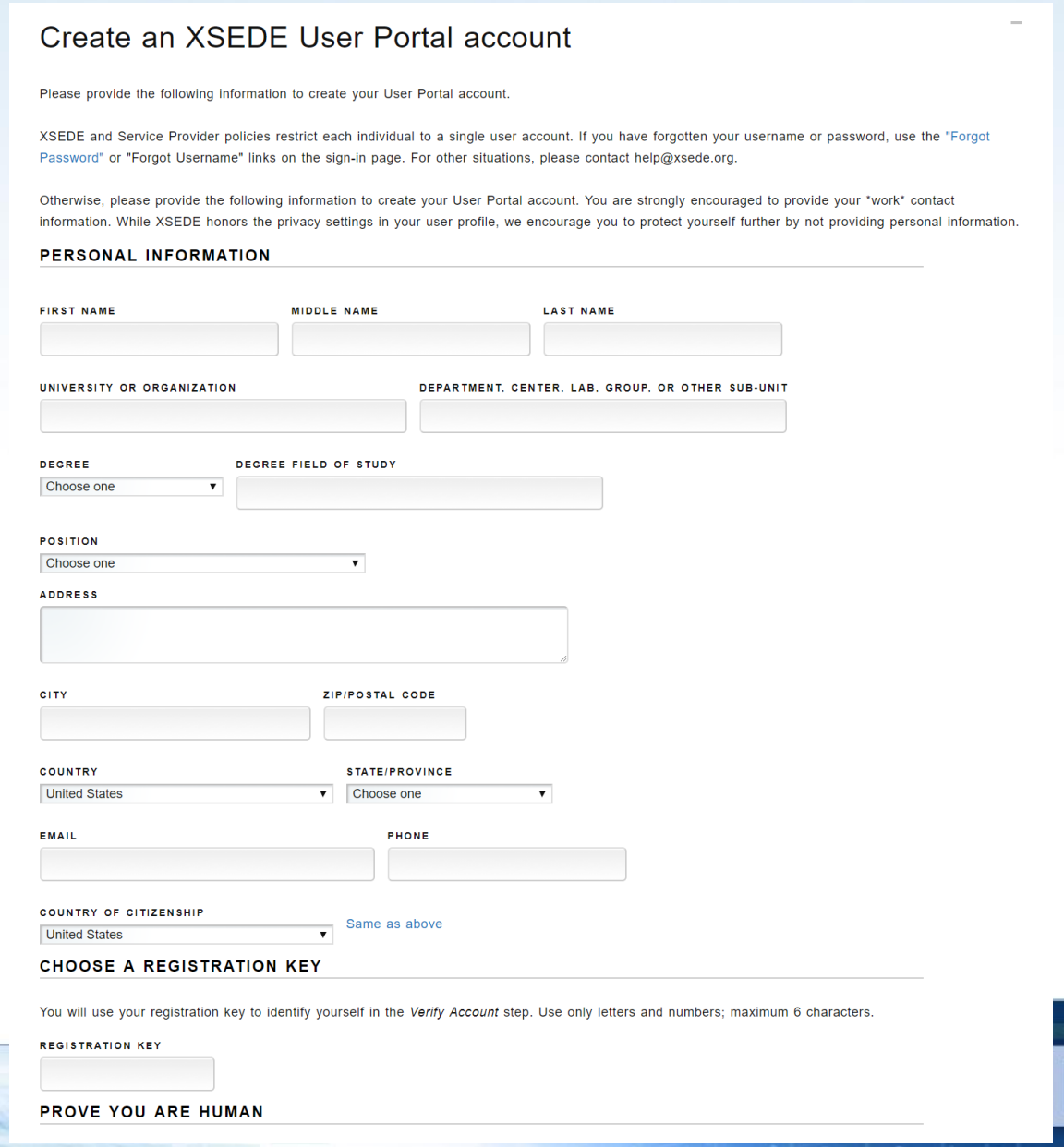
Other Services

- Science Gateways
  - https://www.xsede.org/web/site/ecosystem/science-gateways/

- Storage at TACC (Ranch), PSC (Bridges Pylon), SDSC (Data Oasis), Indiana (Jetstream)
  - request with allocation of compute time
  - https://portal.xsede.org/storage

Creating an XSEDE portal account (XUP)

- Now requires DUO 2Factor authentication
- 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 user profile, we encourage you to protect yourself further by not providing personal information.

PERSONAL INFORMATION

FIRST NAME | MIDDLE NAME | LAST NAME

UNIVERSITY OR ORGANIZATION | DEPARTMENT, CENTER, LAB, GROUP, OR OTHER SUB-UNIT

DEGREE: Choose one | DEGREE FIELD OF STUDY

POSITION: Choose one

ADDRESS

CITY | ZIP/POSTAL CODE

COUNTRY: United States | STATE/PROVINCE: Choose one

EMAIL | PHONE

COUNTRY OF CITIZENSHIP: United States — Same as above

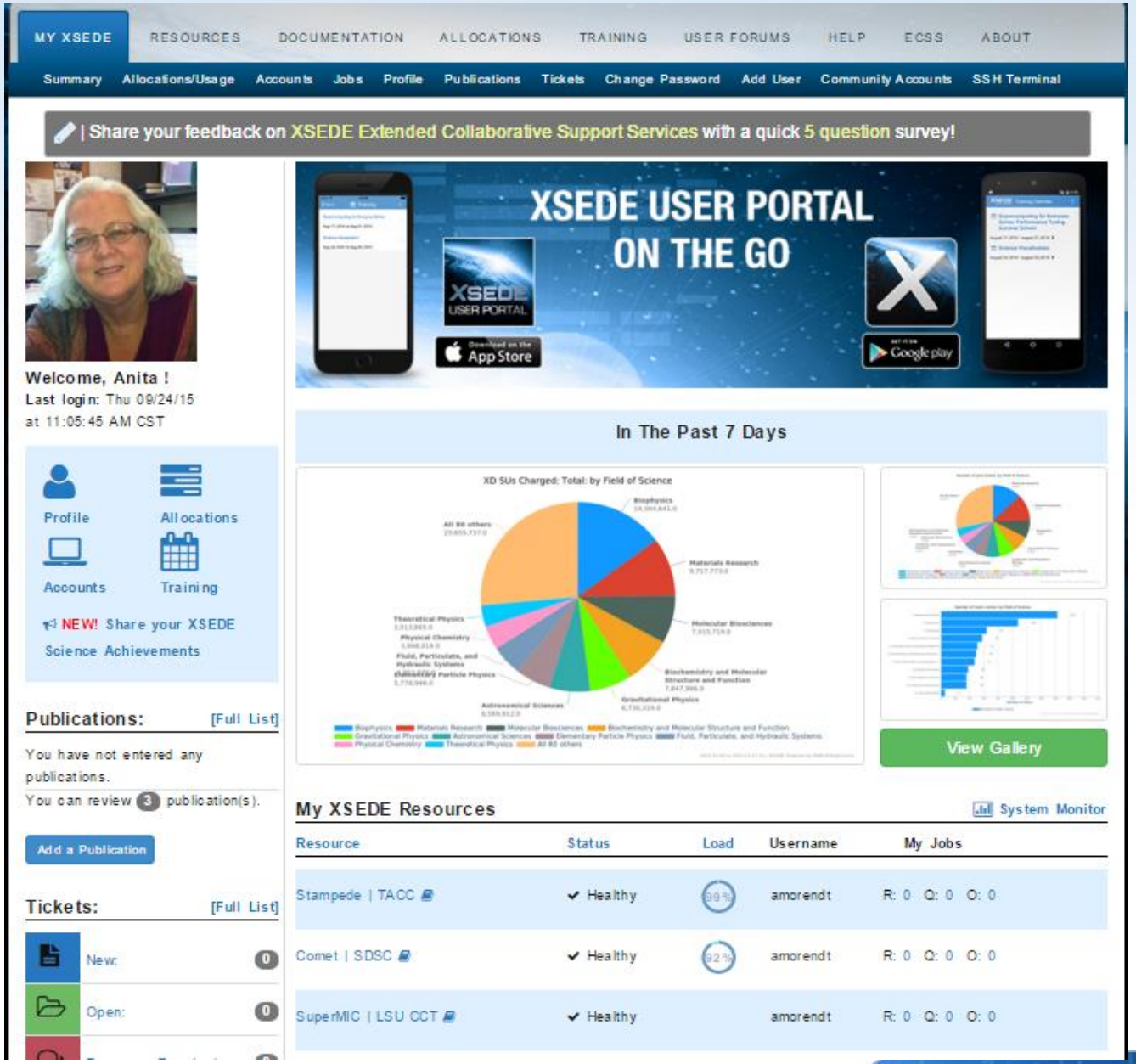
CHOOSE A REGISTRATION KEY

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

Your XSEDE portal account



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

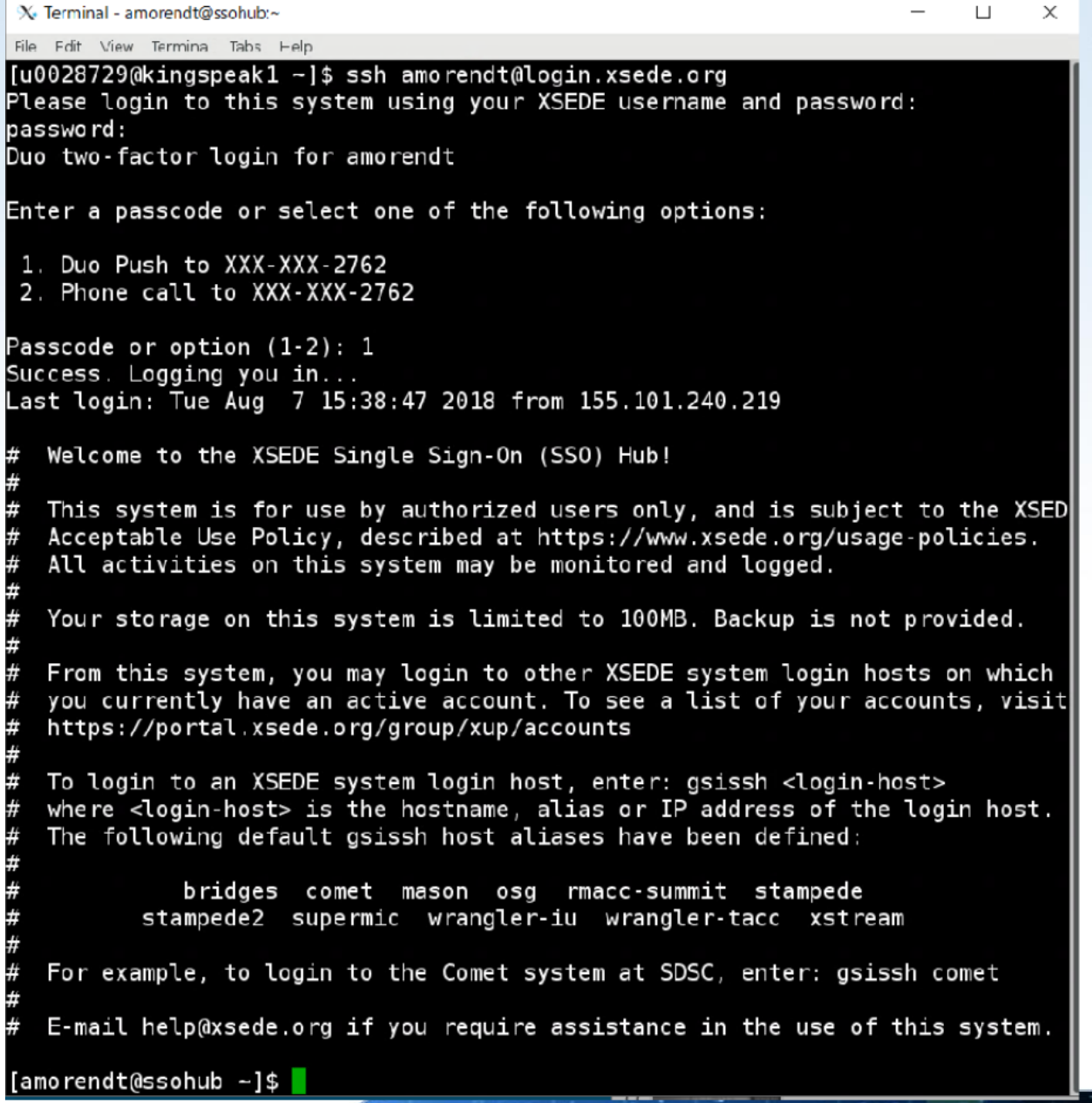
- Documents required: PI CV, Main Document and Code Performance and Scaling
- Look at sample requests provided!

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

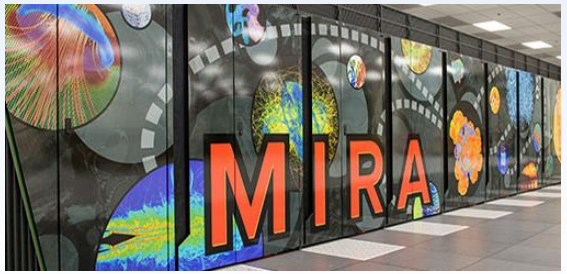
Single Sign On (SSO) Login Hub

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



Other National Computing Resources

- Open Science Grid
- Blue Waters (NCSA)
- Summit/Titan (OakRidge LCF)
- Theta/Mira (etc at Argonne LCF)
- Cori/Edison (NERSC)
- Cheyenne (NCAR)



BLUE WATERS

RMACC Computing Resources

http://rmacc.org/accessingsummit

https://www.colorado.edu/rc/

RMACC-Summit funded by a MRI grant by CU Boulder and CSU -- 10% cycles for institutions in RMACC region, especially institutions without own compute resources

- General compute
  - Haswell 24 cores/node, 128GB RAM
- High memory
  - 48 cores/node 2TB
- GPU nodes
  - 24 cores, 2 K80s/node
- KNL Xeon Phi

- Now can access with XSEDE login credentials via SSOHub

RMACC-Summit Access

After you have XSEDE login:

- send request from your institutional email address to rc-help@colorado.edu
  - https://github.com/ResearchComputing/Research-Computing-User-Tutorials/wiki/RMACC-Access-to-Summit
- Allocations
  - Can run without allocation for smaller needs
  - https://www.colorado.edu/rc/userservices/allocations
- For training
  - https://www.colorado.edu/rc/userservices/training

People Resources

Campus Champions -- NSF funded program to connect People with CyberInfrastructure

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

Campus Engagement Mission Statement

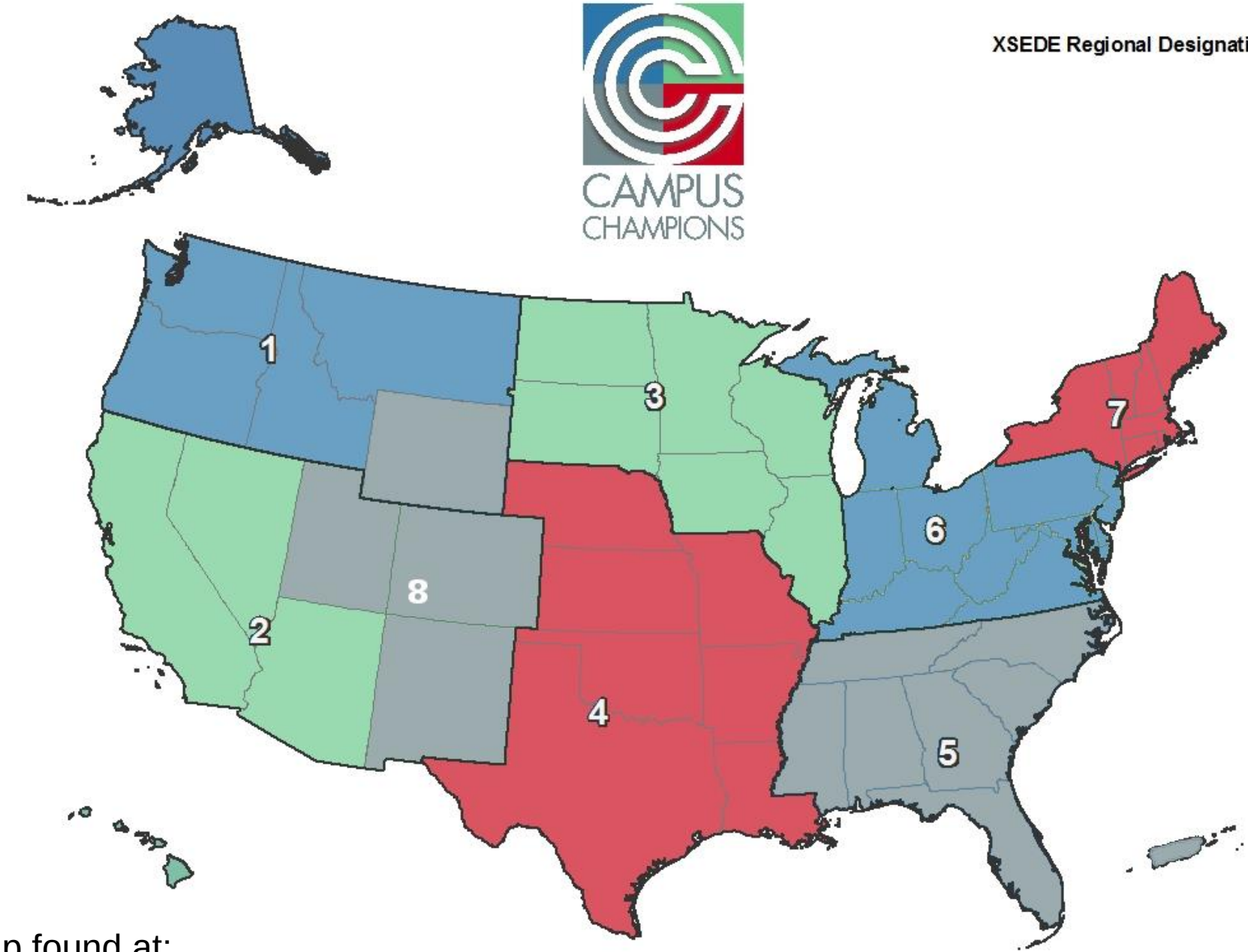
The Campus Engagement program promotes and facilitates the effective participation of a diverse national community of campuses in the application of advanced digital resources and services to accelerate scientific discovery and scholarly achievement.

Who are the champions?

- 475 + champions at 200+ institutions
- HPC Directors
- System Administrators
- User Support specialists
- Faculty evangelists
- Central IT staff
- Non-academic organization staff, e.g. USGS, Idaho National Labs

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
- 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



interactive map found at:
https://www.xsede.org/community-engagement/campus-champions/current

Ask.CI -- NEW

- https://ask.cyberinfrastructure.org/
- Q&A site for people who do research computing
- platform for
  - sharing frequently asked questions
  - comparing solutions
  - leveraging each other's work pertaining to research computing

XSEDE – Extended Collaborative Support Services
https://www.xsede.org/for-users/ecss

- ECSS offers domain science expertise
- Request ECSS assistance via the XSEDE Allocation process

Mission is to improve productivity of the XSEDE user community through collaborations to optimize applications, improve work and data flows, increase effective use of the XSEDE digital infrastructure and broadly expand the XSEDE user base by engaging members of underrepresented communities and domain areas

RMACC HPC Center Staff and Web Sites

- https://www.colorado.edu/rc/
- www.chpc.utah.edu
- http://inside.mines.edu/HPC-Home

Training

XSEDE Training

https://www.xsede.org/for-users/training

- Online, webinars, and in person
- XSEDE HPC Monthly Workshop and Summer Boot Camps
- https://www.xsede.org/web/xup/online-training for listing of all online offerings

Other Training for Using HPC

- The carpentries
  - Software Carpentry – https://software-carpentry.org/
  - Data Carpentry – https://datacarpentry.org/
  - HPC Carpentry – being developed -- https://hpc-carpentry.github.io/hpc-intro/
- Blue Waters
  - https://www.citutor.org
  - https://bluewaters.ncsa.illinois.edu/education-overview

Educational Opportunities

- NSF Research Experiences for Undergraduates (REU)
  - https://www.nsf.gov/crssprgm/reu/reu_search.jsp
  - Number of opportunities with computational focus including one at Jetstream
- Blue waters Internship program: https://bluewaters.ncsa.illinois.edu/internships
- Blue waters Graduate Fellowships: https://bluewaters.ncsa.illinois.edu/fellowships
- Blue Waters Summer School: https://bluewaters.ncsa.illinois.edu/bw-summerschool-2018
- Shordor http://www.shodor.org/
- Science Gateways - https://sciencegateways.org/engage/bootcamp
- Student campus champion program
- XSEDE EMPOWER **E**xpert **M**entoring **P**roducing **O**pportunities for **W**ork, **E**ducation, and **R**esearch - http://www.computationalscience.org/xsede-empower
- sighpc education - https://sighpceducation.acm.org – see training and education resources