National and Regional Computing Resources

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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 (Expanse funding awarded July 2019)

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-2 funding awarded July 2019)

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

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

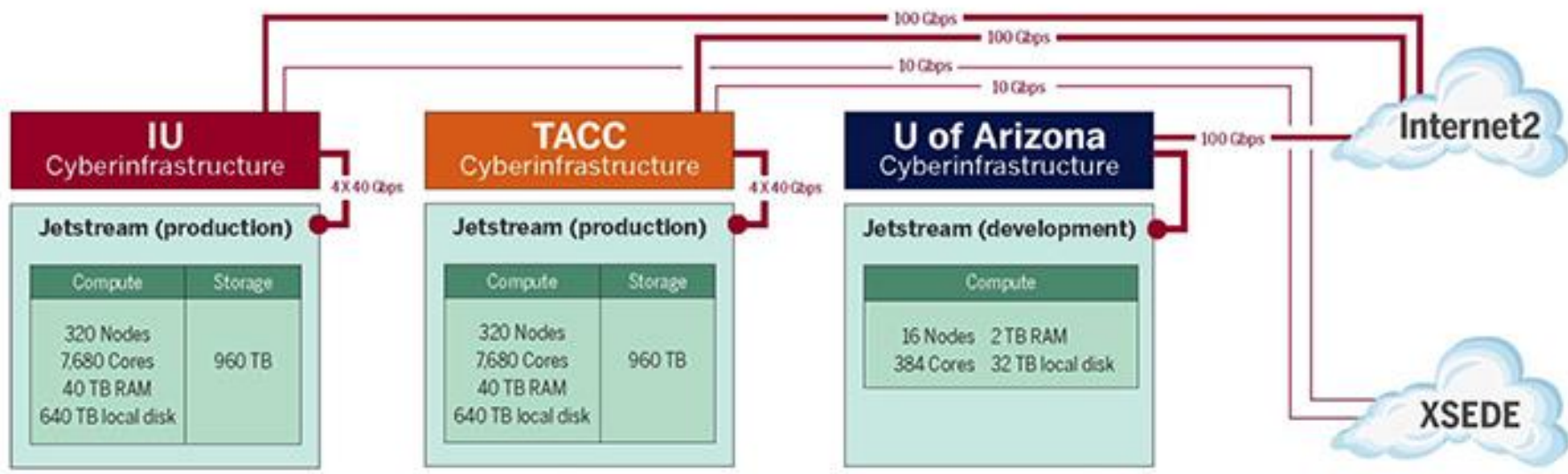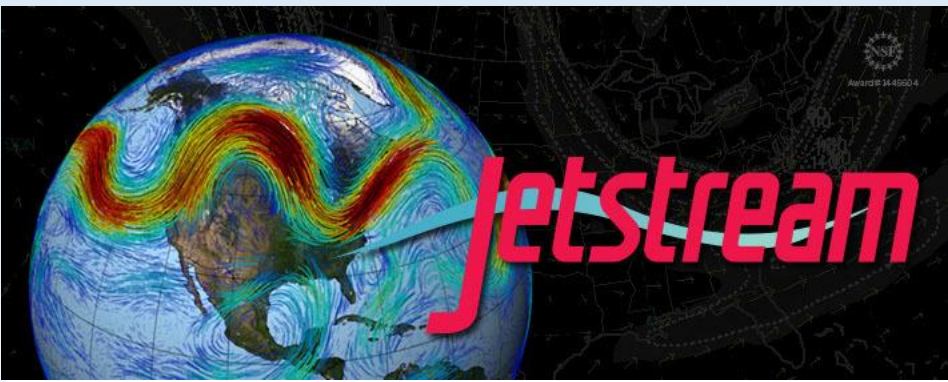20 "leaf" Intel® OPA edge switches

32 RSM nodes with NVIDIA next-generation GPUs

16 RSM nodes with NVIDIA K80 GPUs

800 HPE Apollo 2000 (128GB) compute nodes

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

http://psc.edu/bridges

BRIDGES
psc.edu/bridges

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   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

Your XSEDE portal account

Types of Allocations

- 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

FREE

  - 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@kingspeak1 ~]$ ssh amorendt@login.xsede.org
Please login to this system using your XSEDE username and password:
password:
Duo two-factor login for amorendt

Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-2762
 2. Phone call to XXX-XXX-2762

Passcode or option (1-2): 1
Success. Logging you in...
Last login: Tue Aug  7 15:38:47 2018 from 155.101.240.219

#  Welcome to the XSEDE Single Sign-On (SSO) Hub!
#
#  This system is for use by authorized users only, and is subject to the XSED
#  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   mason   osg   rmacc-summit   stampede
#        stampede2   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.

[amorendt@ssohub ~]$
```
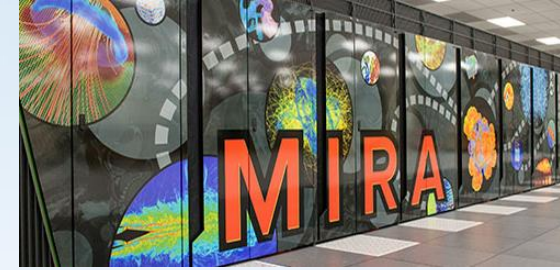
- Open Science Grid
- Blue Waters (NCSA)
- Frontera (TACC)
- Summit/Titan (OakRidge LCF)
- Theta/Mira (etc at Argonne LCF)
- Cori (NERSC)
- Cheyenne (NCAR)

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.
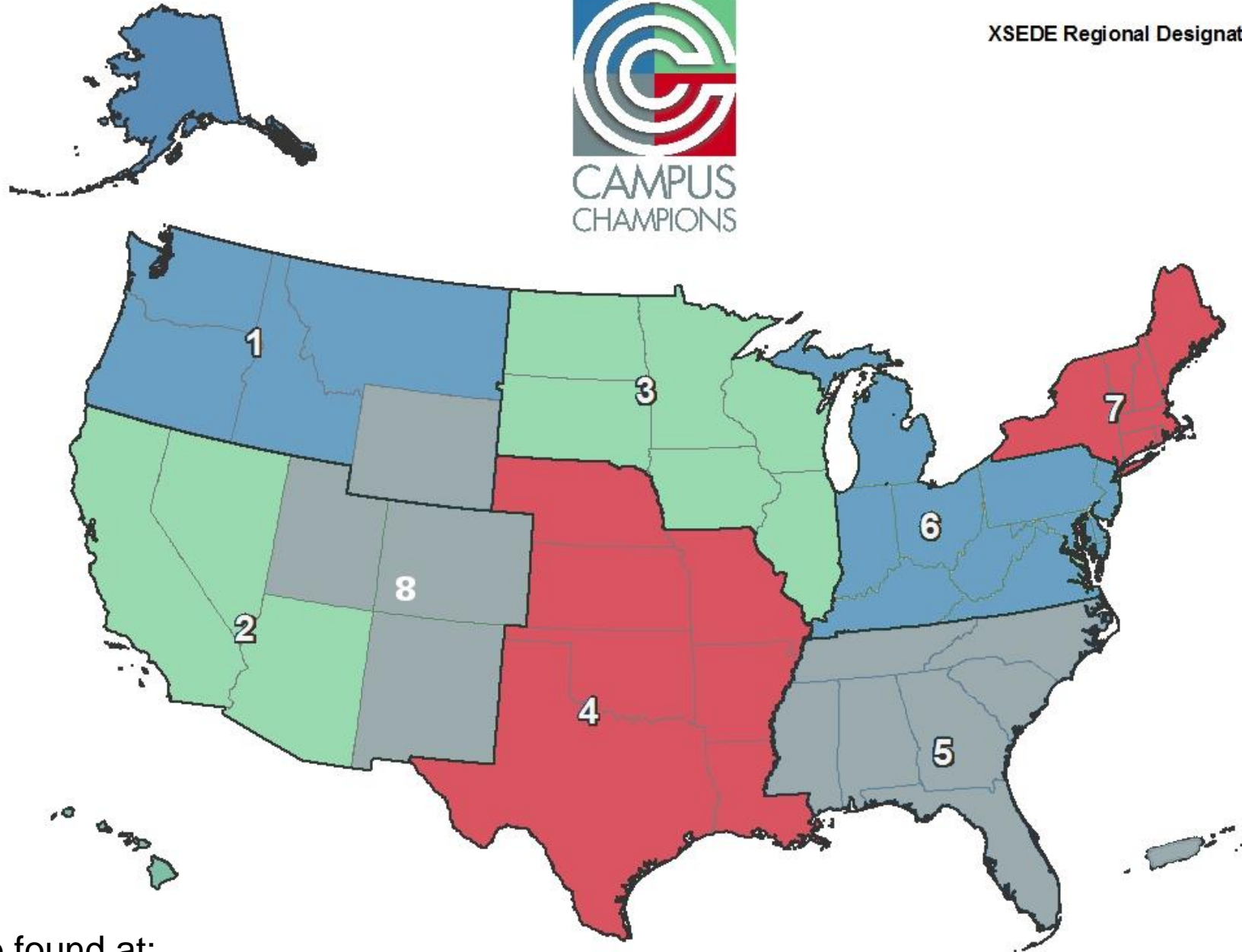
Who are the champions?

- 625+ champions at 270+ 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

XSEDE Regional Designations

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
- 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