National and Regional Computing Resources

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Center for High Performance Computing

Rocky Mountain Advanced Computing Consortium

XSEDE Campus Champion

Outline

- Computing Resources
- People Resources
- Training
- Educational Opportunities

Computing Resources

XSEDE HPC Computing Resources

www.xsede.org/ecosystem/resources

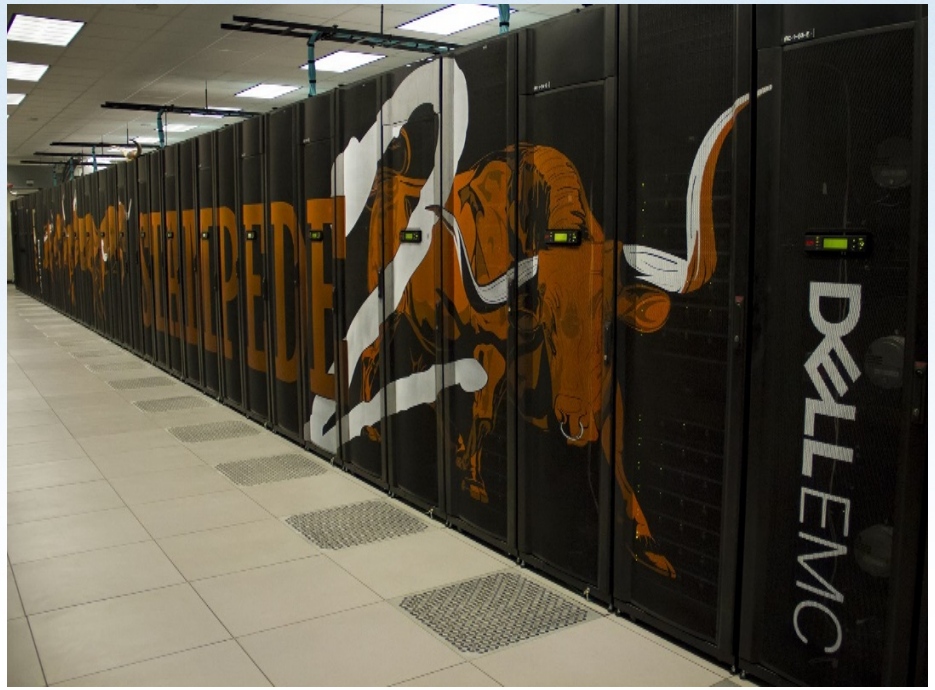
TACC Stampede2 The Flagship Supercomputer of XSEDE intended for large scale runs (tens of thousands cores) as well as general throughput computing

PSC Bridges2 Integrating new technologies for converged, scalable HPC, machine learning and data; prioritizing researcher productivity and ease of use; and providing an extensible architecture for interoperation with complementary data-intensive projects, campus resources, and clouds.

SDSC Expanse 'Computing without Boundaries' capacity and performance for thousands of users of batch-oriented and science gateway computing; providing new capabilities that will enable research increasingly dependent upon heterogeneous and distributed resources composed into integrated and highly usable cyberinfrastructure.

IU Jetstream Cloud Computing resource; in process of transitioning between Jetstream and Jetstrea2

TACC Stampede2



- 4,200 KNL (Intel Xeon Phi 7250) compute nodes
- 1,736 Skylake (48 core, 192 GB)
- 18 petaflops peak performance

PSC - Bridges2

- In production operation since Spring 2021
- More nodes with higher core counts and more memory
  - 504 Regular Memory – 128 cores (AMD), 488 with 256 GB, 16 with 512 GB
  - 4 Extreme Memory – 96 cores (Intel), 4 TB memory
  - 24 GPU nodes – 40 cores, 8 x V100 (32 GB), 512 GB memory
- HDR Infiniband
- Ocean – two tier (disk and tape) storage system

SDSC Expanse

- Standard Compute Nodes (728 total)

  AMD EPYC 7742 (Rome) Compute Nodes (128 cores) and 256 GB DRAM per node

- GPU Nodes (52 total)

  NVIDIA V100s SMX2 with 4 GPUs per node

  40 6248 Xeon CPU cores and 384 GB CPU DRAM per node

- Large-memory Nodes (4 total)

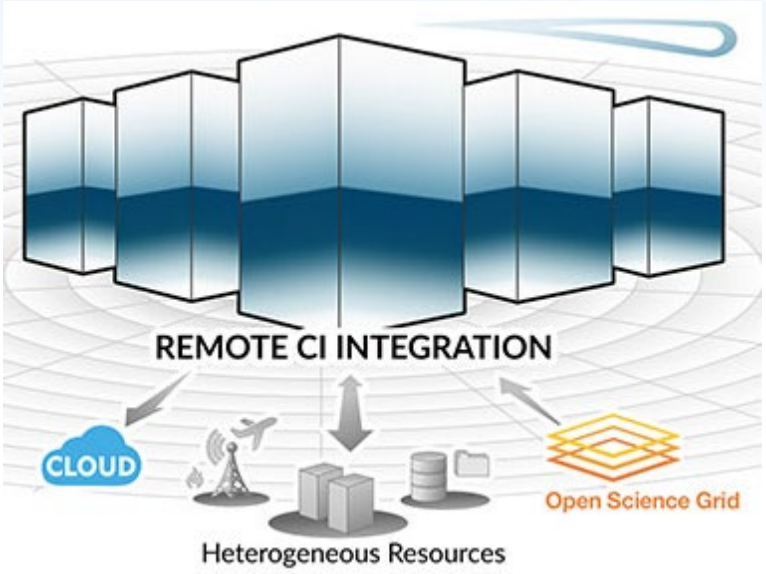
  128 cores and 2 TB DRAM per node

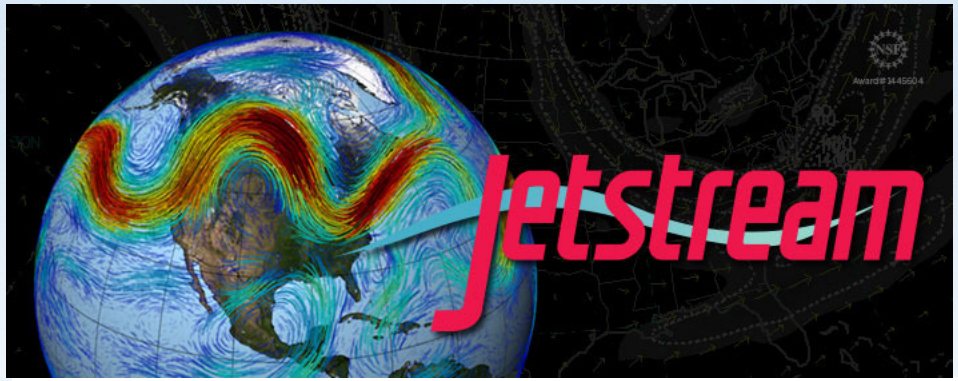
- SDSC Scalable Compute Units (13 total)

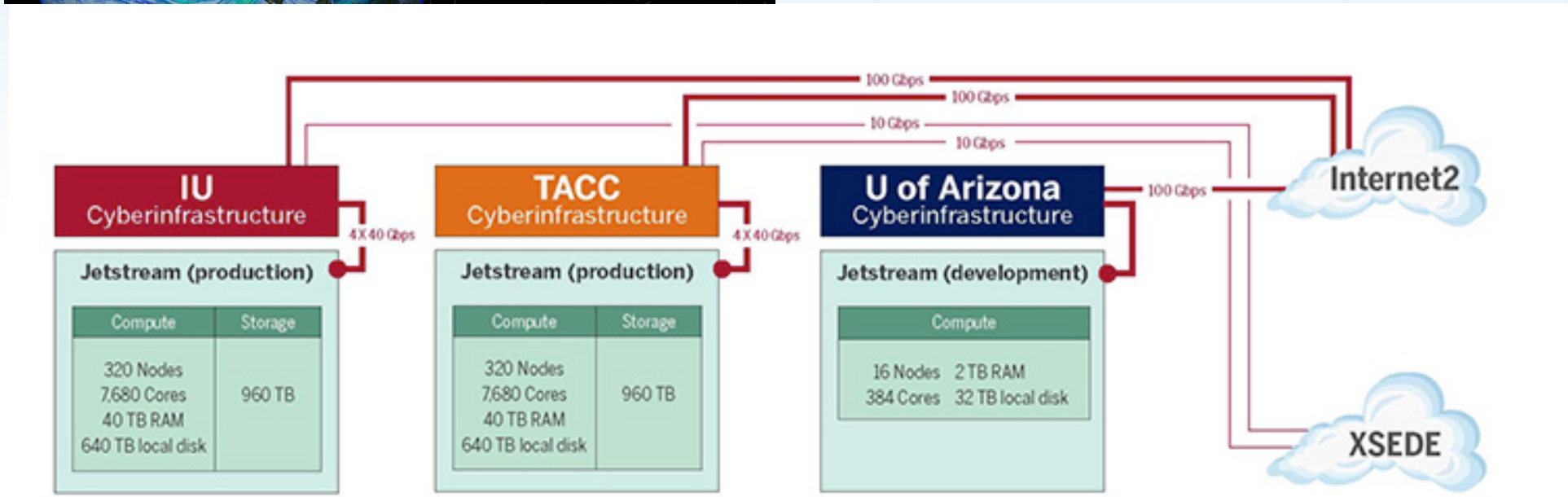
  Entire system organized as 13 complete SSCUs, consisting of 56 standard nodes

  and four GPU nodes connected with 100 GB/s HDR InfiniBand

- Storage Systems -- Lustre (12 PB) and Ceph (7 PB) storage




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 systems

- Anvil – Purdue - Coming soon
  - AMD Milan 1000 nodes with 128 processor cores, 256 GB and 32 nodes with 1 TB
  - 16 nodes with 4x Nvidia A100 GPUs
- Delta – NCSA – Coming soon
  - AMD Milan systems including many GPUs -- A100, A40, AMD MI100 -- nodes
- Rockfish - JHU
  - Intel processor based, some larger memory, some GPU A110
- Darwin – Univ of Delaware
  - Regular/large memory and GPU nodes, 20% time via XSEDE allocations
- KyRIC – Univ of Kentucky
  - Informatics Cloud
  - Limited number of large memory (3TB) intel processor based nodes

Other Services

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

- Storage at the different sites
  - request with allocation of compute time
  - data retention for 3-6 months after end of allocation
  - https://portal.xsede.org/storage

SCIENCE GATEWAYS COMMUNITY INSTITUTE: CONNECTING PEOPLE AND RESOURCES TO ACCELERATE DISCOVERY BY EMPOWERING THE SCIENCE GATEWAY COMMUNITY

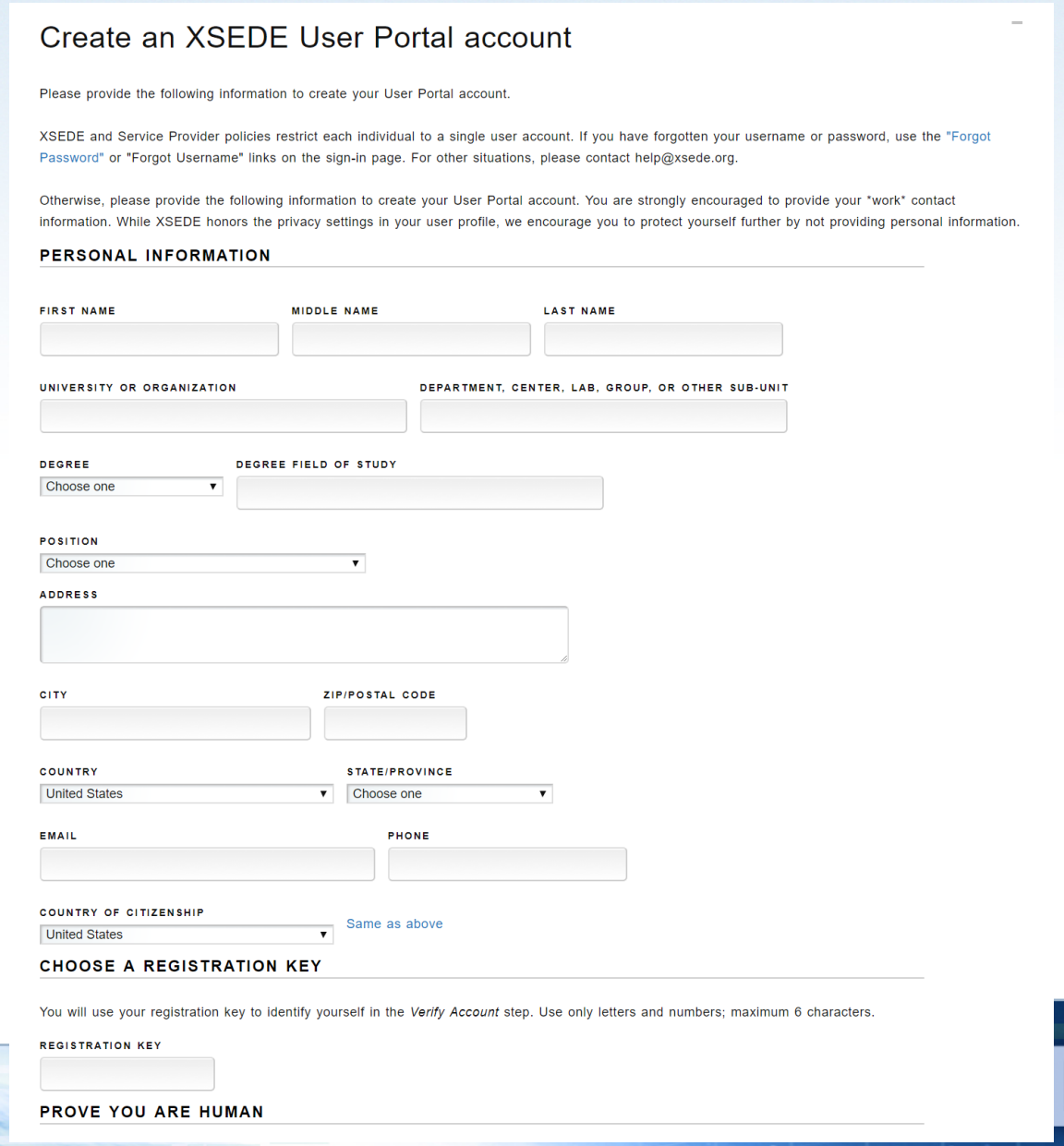
Science Gateways simplify access to computing resources by **hiding infrastructure complexities**.

Science Gateways provide **higher level user interface** for XSEDE resources that are tailored to specific scientific communities.

A Science Gateway is a community-developed set of tools, applications, and data that are **integrated via a portal** or a suite of applications, usually in a graphical user interface, that is further customized to meet the needs of a specific community.

Creating an XSEDE portal account (XUP)

- portal.xsede.org
- 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

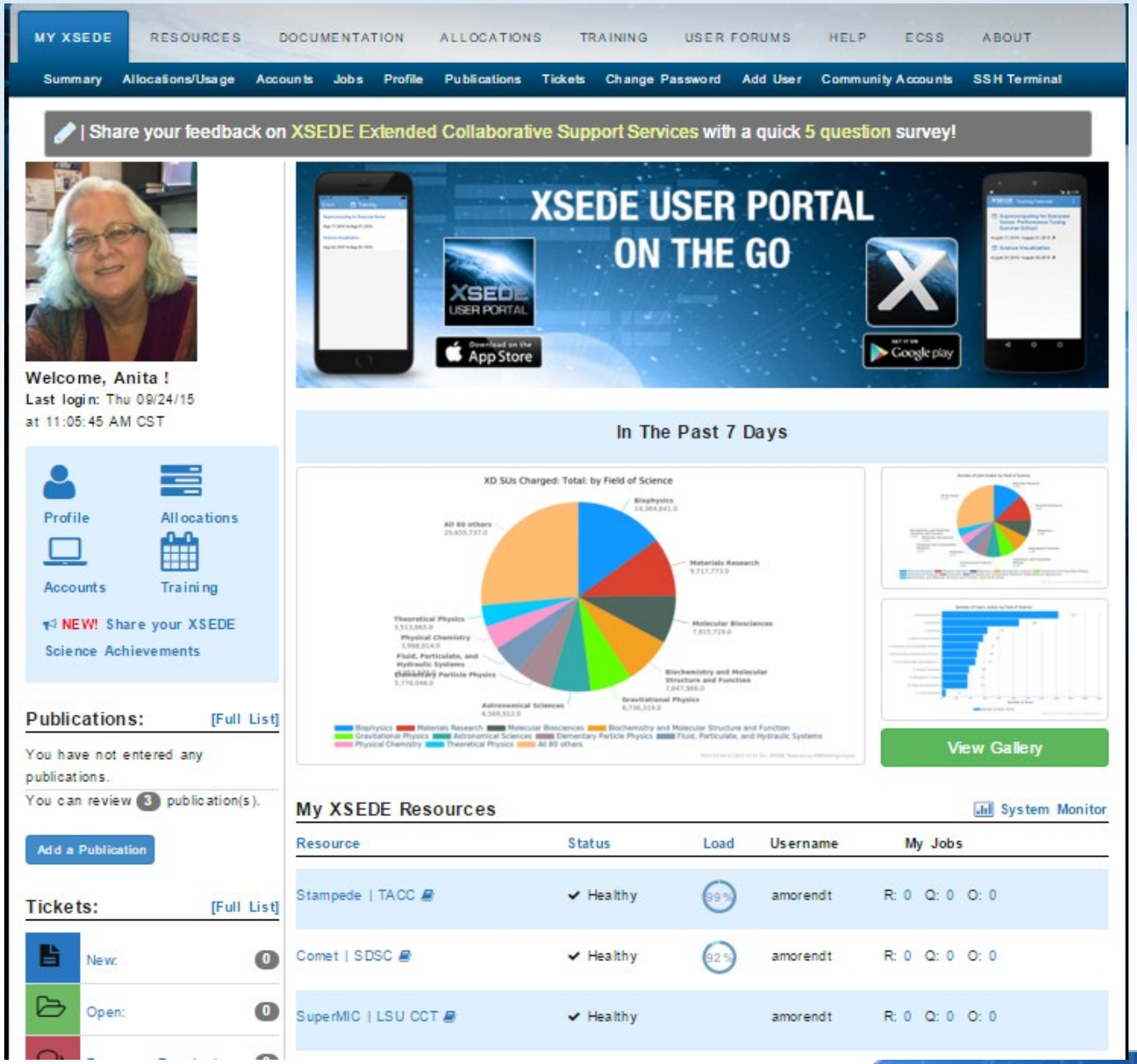
CHOOSE A REGISTRATION KEY

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
- 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

- Use the new XRAS system to submit request
- https://portal.xsede.org/allocations/research 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
- Watch/attend webinars and 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

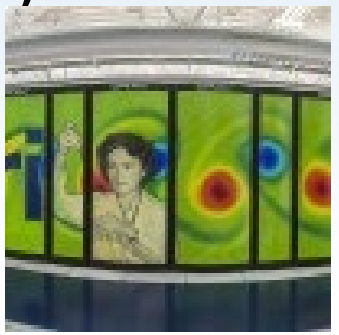
Single Sign On (SSO) Login Hub

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

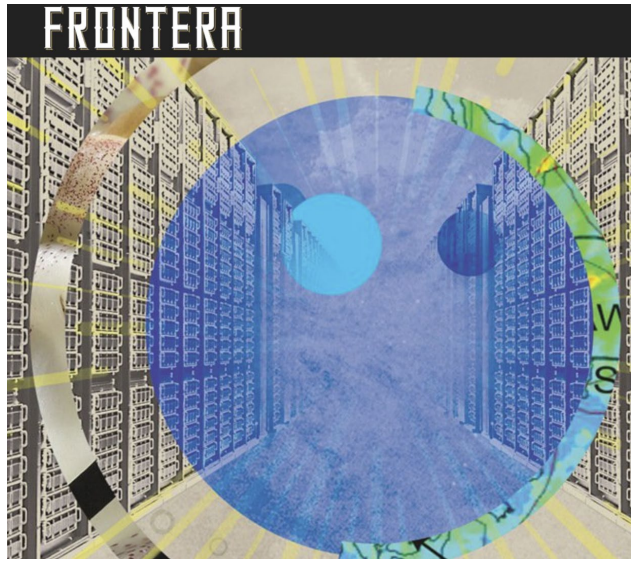
```
[u0028729@notchpeak1 ~]$ ssh amorendt@login.xsede.org
Please login to this system using your XSEDE username and password:
password:
Duo two-factor login for amorendt

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: Thu Jun 18 17:08:33 2020 from 155.101.26.78

#  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  mason  osg  rmacc-summit  stampede
#            stampede2  supermic  wrangler-iu  wrangler-tacc
#
#  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 ~]$
```

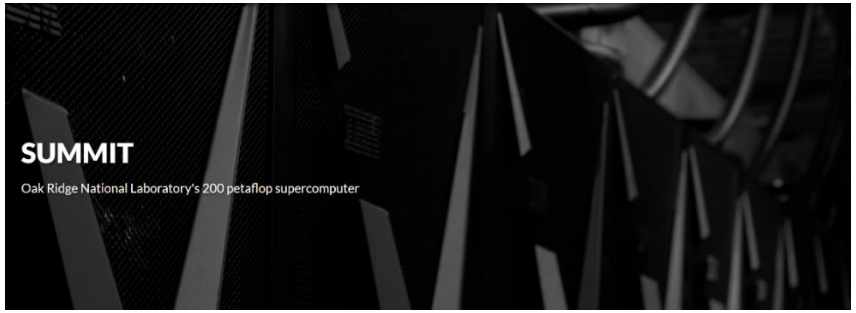
Other National Computing Resources

- Open Science Grid
- Frontera (TACC)
- Summit / Frontier(2022) (OakRidge LCF)
- Aurora/Polaris/Theta (Argonne LCF)
- Perlmutter/Cori (NERSC)
- Cheyenne / Derecho(2022) (NCAR)



Open Science Grid





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

New system in 2022 – Aspen – Details to follow

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?

- 700+ champions at 300+ 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

Ask.CI

- 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/

- Other
  - https://cvw.cac.cornell.edu/default

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
- 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