National and Regional Computing Resources

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Recent Changes

- XSEDE program replaced by ACCESS program effective September 1, 2022
 - <u>access-ci.org</u> new website, replacing <u>xsede.org</u>
 - Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support
 - Lead institutions are Carnegie Mellon University, University of Colorado Boulder, University of Illinois at Urbana-Champaign, and State University of New York at Buffalo
 - ACCESS Services include Allocations, Support, Operations and Metrics, along with a Coordination Office
 - <u>https://access-ci.atlassian.net/wiki/spaces/ACCESSdocumentation/overview</u> main documentation site
- Compute resources have stayed the same, but support, allocaitons and access to resources have changed

NSF ACCESS Program Structure





Outline

- Description of ACCESS Components
 - Operations
 - Allocations
 - Metrics
 - Support
- ACCESS Portal
- Computing Resources
- People Resources
- Training

ACCESS Operations

https://operations.access-ci.org/

• Tie together the different efforts of the ACCESS program

OpenCI ACCESS Coordination Office

PI: John Towns (NCSA/Illinois) co-PIs: Lizanne DeStefano (CEISMIC/Georgia Tech); Shawn Strande (SDSC/UCSD)

- Deep knowledge of XSEDE
- Emphasis on seamless transition
- Facilitate shared governance via EC and EAB
- Collaboration tools to support inter-track communications
- Branding
- Coordinate outreach, DEI, and evaluation efforts across the program
- Stakeholder communications on ACCESS impact & opportunities
- Informal co-advisors from 5 large programs







ACCESS Communications & Outreach Coordination

- Establish a unified brand and experience for internal and external communications
- Establish and maintain ACCESS main website, facilitating access to service-area subsites
- Collaborate on and amplify service areas' news and science stories
- Enable cross-service communications
- Facilitate reporting



ACCESS Community Building & Engagement Coordination

- Community Building across nation's CI ecosystem with the following goals:
 - Expand participation to new and underserved communities
 - Deep participation by existing communities
 - Represent the broad ACCESS program
- OpenCI is forming a virtual community building and engagement team
 - Representative from each ACCESS Service tracks
 - OpenCI representative
 - Computational Science Support Network (CSSN) representative



ACCESS Community Building & Engagement Coordination

- Virtual community building and engagement team spinning up
 - Initial foci
 - · defining communities and opportunities
 - · define kinds of relationships we seek with our communities
 - look for mechanisms to expand participation to new and underserved communities
 - look to deep participation from community members already engaged with ACCESS
 - This will all drive a living ACCESS community building and engagement plan
 - shared messaging
 - shared promotion of community building and engagement efforts
 - ensure all ACCESS components are aware of the full set of community building and engagement efforts



ACCESS Evaluation Coordination

- Establishing regular meeting schedule for Evaluation POCs (perhaps a formal working group)
- Working with Gulbrandsen, PIs and Evaluation POCs to formalize evaluation plans and reporting (PEPs, quarterly reports, annual reports, and panel review)
- Identifying common data needs in KPIs and metrics and developing a strategy for data sharing
- Developing a coordinated schedule for data collection to reduce redundancy and minimize burden on respondents
- Building capacity to track users over time and across tracks, assess collective impact, and continuously improve



ACCESS Program Internal Collaboration Support

- Providing collaboration tools
 - Confluence wiki
 - Jira
 - · Google Workspace: shared drive, email lists, etc.
 - all of these are in place now; some further configuration still under way
- Facilitating cross-award collaboration
 - establishing risk management process
 - establishing project change control
- Still figuring out
 - how to best "support NSF management and oversight of Service Track awards."



ACCESS Allocations

https://allocations.access-ci.org/

 If you have a current XSEDE Allocation – it will transition to an ACCESS allocation

Allocation Eligibility

https://allocations.access-ci.org/access-allocations-policies#eligibility

- Available to any researcher or educator as US academic, non-profit research, or educational institution.
- Can be in any official position including adjunct or instructional
- Postdoctoral researchers can be a PI of any project type
- Graduate students can lead a "Explore" ACCESS allocation under their advirsor's guidance
- NSF Graduate Fellows and Honoable mentions can apply for "Discover" allocations
- One project is allowed per funded grant -- though awards for unfunded projects are allowed. Note that for collaborative grants between institutions the PI/coPIs must submit a single allocation request

ACCESS Allocations Objectives

- Create an open, inviting, and democratized allocations marketplace
- Ensure equitable access across disciplines, institutions, and demographic groups
- Align the proposal-writing effort with level of resource need
 - Adjust review panel effort in anticipation of increasing volumes
 - Ensure Allocations staff within ACCESS and RP staff can keep up with steady stream of requests



SELECT OPPORTUNITY

REQUEST ALLOCATION

CREDITS



CREDITS



Standardized Allocation Opportunities (Tiers)

Four Allocation Opportunities to suit a variety of needs (credit thresholds):

• Explore (400,000)

- Best-suited for endeavors with light resource requirements
 - Grad students can be PIs
- Discover (1,500,000)
 - Minimal effort to start production research activities
 - Potential best-fit for Campus Champion
 Allocations
- Accelerate (3,000,000)
 - More substantial resource requirements
 - Multi-grant research, Gateways, etc.
- Maximize (No upper limit)
 - For large-scale research projects with extreme resource needs
 - Will largely resemble XRAC process

Quick FAQs:

- Except for *Maximize*, opportunities are <u>available</u> for request at any time.
 - Maximize will follow the XRAC schedule and policies until March 2023 meeting
 - Bi-annual opportunities will then be available.
- Multiple allocations can be requested
 - For multiple grants
 - Or for substantially different needs
- Allocations can be <u>upgraded</u> to the next tier when resource demand increases



Opportunity Comparison

	Explore	Discover	Accelerate	Maximize
Possible purposes	Evaluation, courses, development, exploration	Small-scale research, Campus Champions, growing gateways	Mid-scale needs, consolidating related grants, collaborations	Largest-scale research activities
Credit threshold	400,000 Credits	1,500,000 Credits	3,000,000 Credits	No upper limit
Duration	Grant duration or 12 months	Grant duration or 12 months	Grant duration or 12 months	12 months
Number per PI	Multiple	Multiple	One (some exceptions)	One (limited exceptions)
Accepted	Continuously	Continuously	Continuously	Semi-annually
Proposal length	Abstract	1 page	3 pages	10 pages
Review	Eligibility	Advisory review requestable	Rolling panel review	Panel review



ACCESS Credits

- A "currency" that researchers can exchange for available resources
- Allocations for the first three (3)
 opportunities will be awarded in credits
 - Requestors <u>will then exchange credits</u> for resource-specific units (SUs)
- Credits are issued in two increments
 - Half initially an half after a progress report
- ACCESS Credits are based on longstanding normalized units

1 ACCESS Credit = 1 Expanse core hour

Conversion Calculator to streamline exchange

Exchange	Calculator
Number of units of	on this resource:
50,000	ACCESS Credits
Equals this many	units on this resource:
929	PSC Bridges-2 GPU (Bridges-2 GPU)
929	PSC Bridges-2 GPU (Bridges-2 GP



Resource Provider Engagement

- Resource Providers (RPs) will review credit exchange requests
- RPs will be able to set their exchange rates for ACCESS Credits
- More RP controls will allow for additional resource types to be handled via allocations processes
 - E.g. Review criteria for SDSC Voyager resource may be different from SDSC Expanse CPU
 - E.g. Allocating telescopes or large instruments may have considerations not typical of research computing resources

Available Resources

J	ohns Hopkins University (Rockfish - Regular Memory)
к	entucky Research Informatics Cloud (KyRIC) Large Memory Nodes
N	CSA Delta CPU (Delta CPU)
N	CSA Delta GPU (Delta GPU)
N	CSA Delta Storage (Delta Storage)
0	pen Science Grid (OSG)
0	pen Storage Network (OSN)
Ρ	SC Bridges-2 Extreme Memory (Bridges-2)
Ρ	SC Bridges-2 GPU (Bridges-2 GPU)



Transitioning to a New Process



What won't be changing:

- XSEDE processes will be honored for existing allocations (until renewal)
 - E.g. supplements, transfers, extensions will continued to be accepted
- Campus Champion allocations will continue to be accepted, tagged/tracked, and expedited
- CCs can work directly with researchers in their area to identify the resources best-suited for the proposed endeavors



Allocation Points for Campus Champions

- Proceed with "business-as-usual"
 - Continue to leverage existing and active allocations
 - Request necessary supplements and transfers, if needed
- When it's time to renew...
 - Align with one of the new opportunities that best suits the needs of your current and expected community
- As new Champions are onboarded...
 - Please continue to email: Ken <u>hackworth@psc.edu</u> and Brandon <u>brandonp@psc.edu</u> about new members
 - Please continue to update:
 - <u>Current Champions</u> list

XRAS Submission UI

Is the planned work associated with any informational purposes and does not affe Rapid response (Monkeypox) Classroom or training activities Science gateway Campus Champion Dissertation or thesis Machine learning Software development



Where to Find Us

- Allocations Webpage
 - <u>Allocations.access-ci.org</u>
- Help Ticket
 - Contact us through the <u>Support Ticket Form</u>
- Feedback Form
 - Have a suggestion for how we can improve our web presence, practices, policies, or other aspect of our project?
 - Let us know!





ACCESS Metrics

https://metrics.access-ci.org/

- Transitioning the XSEDE XDMoD (Metrics on Demand) to ACCESS
- See https://xdmod.access-ci.org



ACCESS Support

https://support.access-ci.org/

- Match -- Multi-tier Assistance, Training, and Computational Help
 - 1- easy-to-use tools and services
 - 2 self-help knowledge base
 - 3 short-term support engagements
 - 4 longer-term connections to specialized expertise
- <u>https://support.access-ci.org/resources</u> provides info and links to both resources provider guides as well as other useful websites including training sites, tutorials, and other learning resources



- Tier 1 support takes the form of easy-to-use tools that allow researchers to quickly get started using complex computing systems.
 - By reducing the learning curve, the Tier 1 tools and services enable users to quickly start computational jobs with minimal effort.
- initial focus has been on deploying <u>Open-On-Demand</u> instance for launching jobs at RPs, <u>Pegasus</u> for creating workflows across RP resources, <u>Science Gateways</u> that simplified access to certain types of workloads, and <u>XdMod</u> to help track jobs and possibly identify issues.

- Tier 2 support focuses on **self-help resources** designed to get users to answers quickly.
- Tier 2 resources include
 - Documentation describing ACCESS and its associated resource providers (RPs),
 - <u>Question and Answer (Q&A) forums</u> where users can post questions to the ACCESS community and search for answers,
 - <u>Community-generated documentation and training materials</u> that help users learn to effectively use ACCESS,
 - <u>Affinity Groups</u> where user with similar interests can exchange information and experiences, and a
 - <u>Ticket system</u> where users can submit questions to ACCESS and RP staff.

- Tier 3 support, also known as MATCHPlus
 - No cost
 - Limited Scope
 - Provides direct support to researchers by establishing short-term (3-6 months) engagements that pair a student facilitator with an experienced mentor to address an immediate research need.
 - Each mentor/student team will help a researcher move their science forward through concrete and contained computational improvements such as expanding existing code functionality, transitioning from lab computers to HPC, or introducing new technologies.
 - Mentors are ACCESS Computational Science and Support Network (CSSN) experts with subject matter expertise and professional facilitation skills relevant to the engagement.

- Tier 4 support, also known as MATCHPremier
 - Researched funded, pre-planned consultant coordination
 - Provides embedded support by pairing one or more MATCHPremier Consultants with a research team for a period of engagement typically ranging from 12 - 18 months.
 - Engagements must be requested at least six months in advance.
 - MATCHPremier Consultants are selected from the Computational Science and Support Network (CSSN) depending on the researcher's needs - they may be facilitators, research software engineers, or other types of appropriate support personnel.

Getting access ACCESS portal

https://identity.access-ci.org/

- If you had a XSEDE portal account (portal.xsede.org) then use this it will walk you through steps to link/transition this XSEDE identity to an ACCESS identity
- Otherwise register for an ACCESS ID at <u>https://identity.access-ci.org/new-user</u>
- Process also described at <u>https://access-</u> ci.atlassian.net/wiki/spaces/ACCESSdocumentation/pages/76743107/Login+In formation



Manage allocations

Get started

Prepare requests

Use credits

Edit Profile

FAQs

Logout

Policies

Updates

ACCESSID			
amorendt			
First name			
Anita			
Last name			
Orendt			
Email			
anita.orendt@utah.edu			
* Institution/Organization			
University of Utah			

Center Researcher Staff

Allocations



Running Jobs on Resources

- ACCESS Open OnDemand
 - <u>https://access-</u> ci.atlassian.net/wiki/spaces/ACCESSdocumentation/pages/76744257/ACCESS+Open+ OnDemand
 - Can be used for SDSC Expanse, Purdue Anvil at this time
- ACCESS Pegasus -- https://access.pegasus.isi.edu
 - <u>https://access-</u> ci.atlassian.net/wiki/spaces/ACCESSdocumentation/pages/76744296/ACCESS+Pegasu s
- From there you can open up a ssh session
- Access to other resources via portals coming
- For direct ssh to the different resources see details on ACCESS resource pages <u>https://access-</u> ci.atlassian.net/wiki/spaces/ACCESSdocumentation/pages/76744989/Resour ce+Providers
 - Some will require request for a local account on the resource

Computing Resources

National HPC Computing Resources via ACCESS

https://access-ci.atlassian.net/wiki/spaces/ACCESSdocumentation/pages/76744989/Resource+Providers

- <u>ACES (Texas A&M)</u>
- Anvil (Purdue)
- Bridges-2 (PSC)
- DARWIN (Delaware)
- Delta (NCSA)
- Expanse (SDSC)
- FASTER (Texas A&M)
- Jetstream2 (IU)
- OOKAMI (Stonybrook)
- <u>KyRIC (Kentucky)</u>
- Rockfish (JHU)
- Stampede-2 (TACC)
- RANCH (TACC)
- Open Science Grid (OSG)
- Open Storage Network (OSN)

- TACC Stampede2 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.
- <u>IU Jetstream</u> Cloud Computing resource; in process of transitioning between Jetstream and Jetstream2

SEL



Other systems

- FASTER Texas A&M
 - FASTER CPUs, GPUs, with NVMe based storage in a composable environment
 - ACES Accelerating Computing for Emerging Sciences, an innovative advanced computational prototype FPGA, Graphcore IPU designed for prototyping AI/ML workflows
- OOKAMI Stony Brook University
 - Testbed based on the A64FX processor developed by Riken and Fujitsu
- Anvil Purdue University
 - AMD Milan 1000 nodes with 128 processor cores, 256 GB and 32 nodes with 1 TB
 - 16 nodes with 4x Nvidia A100 GPUs
- <u>Delta</u> NCSA
 - AMD Milan systems including many GPUs -- A100, A40, AMD MI100 -- nodes
- <u>Rockfish</u> Johns Hopkins University
 - Intel processor based, some larger memory, some GPU A110
- <u>Darwin</u> Univiversity of Delaware
 - Regular/large memory and GPU nodes, 20% time via XSEDE allocations
- <u>KyRIC</u> University of Kentucky
 - Informatics Cloud

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• Limited number of large memory (3TB) intel processor based nodes



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.

XSFI



Other National Computing Resources





- Open Science Grid
- Frontera (TACC)
- <u>Summit</u> / <u>Frontier</u> (OakRidge LCF)
- <u>Aurora/Polaris/Theta/AI Testbed</u> (Argonne LCF)
- Perlmutter/Cori (NERSC)
- <u>Cheyenne</u> / <u>Derecho</u> (2023) (NCAR)





Nerso

Perlmutter







SEI

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

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New system in 2022 – Aspen – access by RMACC TBD
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RMACC-Summit Access

https://curc.readthedocs.io/en/latest/access/rmacc.html

After you have ACCESS login:

- send request from your institutional email address to <u>rc-help@colorado.edu</u>
- Will access via RMACC ondemand portal
 - <u>https://ondemand-rmacc.rc.colorado.edu</u>
- Allocations
 - Can run without allocation for smaller needs
 - <u>https://www.colorado.edu/rc/userservices/allocations</u>
- For RMACC training
 - <u>https://www.colorado.edu/rc/userservices/training</u>

People Resources

<u>Campus Champions</u> -- NSF funded program to connect People with CyberInfrastructure

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



Funded ended with XSEDE, proceeding independently



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?

- 780+ champions at 350+ institutions
- Includes
 - HPC Directors
 - System Administrators
 - User Support specialists
 - Faculty evangelists
 - Central IT staff
 - Non-academic organization staff, e.g. USGS, Idaho National Labs

SEL

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.Cl

- <u>https://ask.cyberinfrastructure.org/</u>
- 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



RMACC HPC Center Staff and Web Sites

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

Training

PSC HPC Workshop Series

https://www.psc.edu/resources/training/hpc-workshop-series/

- The XSEDE HPC Workshop Series held monthly by the Pittsburgh Supercomputing Center (PSC) will be continuing under ACCESS
- Now the ACCESS Workshop Series
- Moving back to the telecast model to multiple satellite sites versus the use of zoom using since covid
- First workshop: GPU Programming Using OpenACC on November 7, 2022 – watch for an announcement with details and registration information

Other Training for Using HPC

- The carpentries
 - Software Carpentry <u>https://software-carpentry.org/</u>
 - Data Carpentry <u>https://datacarpentry.org/</u>
 - HPC Carpentry being developed -- https://hpc-carpentry.github.io/hpc-intro/

- Other
 - <u>https://cvw.cac.cornell.edu/default</u>