ACCESS, ACCESS Resources, and a peek over the horizon

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NCSA | National Center for Supercomputing Applications



ACCESS: Advancing Innovation

NSF's Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support



Stephen Deems, PSC, PI Allocations Timothy J. Boerner, NCSA., PI Operations Thomas R. Furlani, U at Buffalo, PI Metrics Shelley L. Knuth, CU-Boulder, PI Support John Towns, NCSA, PI Coordination Office



National Cyberinfrastructure





https://en.wikipedia.org/wiki/TeraGrid



Extreme Science and Engineering Discovery Environment

2011 - 2022

https://www.nsf.gov/news/news_image s.jsp?cntn_id=121181&org=NSF



2022 -

https://access-ci.org

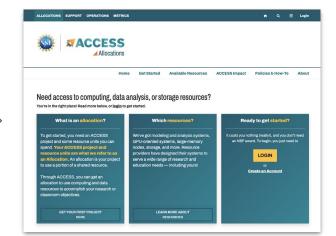




Research & Educational Community













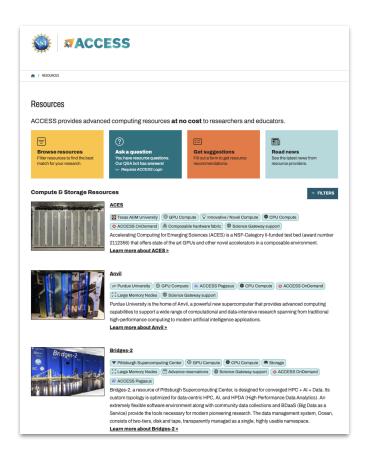
Cutting-edge Hardware, Software + Expertise





Cyberinfrastructure Available

- Computing systems
 - Varying core counts & memory sizes
 - Cloud resources (persistent services)
- Accelerators
 - GPUs, vector processors, FPGAs
- Data storage systems
 - Archival, object, tiered
- Data repositories
- Software & workflow managers
- High performance networking
- CI Professionals & support tools
- System performance monitoring



Browse all available resources:

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





Science Gateways

- User-friendly web-based portals or platforms developed by a community that provide researcher and educators with access to advanced computing resources, data, software, and tools.
- Over 40 active community gateways currently running on ACCESS resources
 - Domains: quantum chemistry, genomics, computational anatomy, cryo-EM, climate research, music education research, earth and planetary materials, water education, natural hazards engineering, biomedical research, flood monitoring, proteomics, topography, protein structure, and more!
 - See <u>all active Science Gateways</u> powered by ACCESS







ACCESS Allocations Policies

- U.S.-based investigators are eligible to lead projects
- Graduate students can now lead projects
- Multiple supporting grants? → Multiple projects
 - Separate projects for research, exploration, and classroom activities
- Standardized project types for flexibility
 - The "paperwork" required to request a project ranges from:
 - 1 paragraph; 1 page; 3 pages; 10 pages
 - Start small and upgrade later
- Award duration aligns with supporting grant

Policies and practices are designed for easier entry.

RPs are engaged in each request for their resource(s).

Available at no cost!

No supporting grants required!





Step-by-Step Allocations Request

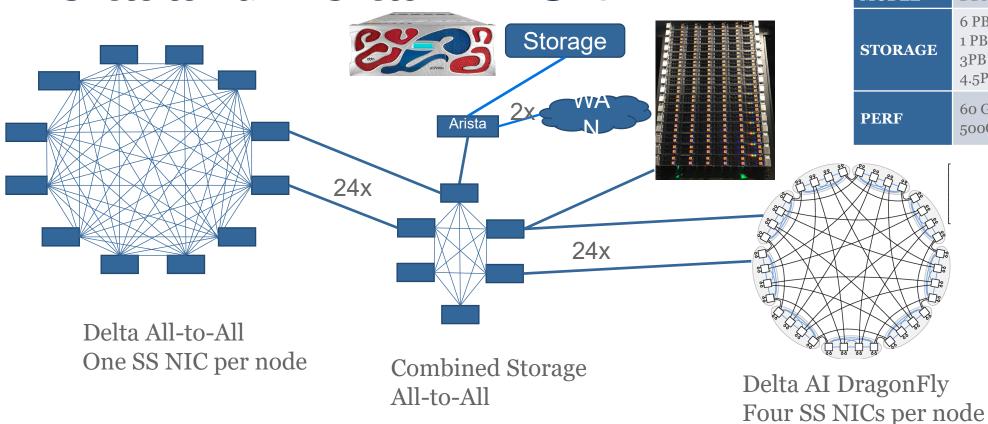
- Register for an ACCESS ID
- Select the <u>Project Type</u> that best fits your needs
 - If you're new, <u>start with Explore</u> and upgrade when you need more resources!
- Complete the Request Form
 - Add co-PIs, Allocation Managers, and other Users (make sure they have an ACCESS ID)
- Exchange your allocated credits for the <u>Available Resources</u>
- Start your research, development, or educational (classroom) work!

Link to full "Get Your First Project" guide





Delta and Delta AI HSN



MODEL

DDN SFA 7990x, NVX2

6 PB on Delta
1 PB on Center-wide FS
3 PB Flash (Infinia/IME)
4.5 PB Flash (Lustre)

PERF

60 GB/sec for home + scratch,
500GB/s + 500GB/s Flash



32 port



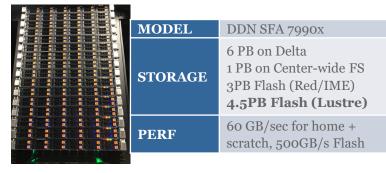






Delta Hardware Overview









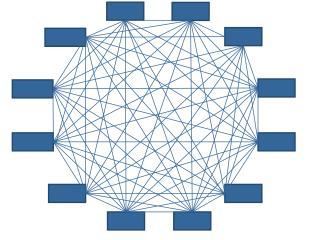
CPU NODES	135 8 x (
	100
	100

GPU

NODES

x CPU Compute Nodes CPU Utility Nodes

x A100 x 4 GPU 100 x A40 x 4 GPU 6 x 8 A100 GPU & High Mem 18 AMD MI100 GPU & High Mem 8 x 8 H200 GPU & High Mem



CPUs	500 x AMD EPYC 7763 64 core "Milan"
GPUs	448 x NVIDIA A100 400 x NVIDIA A40 8 x AMD MI100 64 x NVIDIA H200
PERF	14+ PF double-precision 263+ PF single-precision 523+ PF tensor



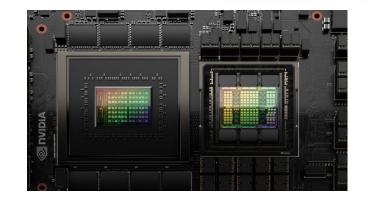








DeltaAl Hardware Overview



RESOURCE COUNTS

Login NODES	4 Grace Grace login Nodes
GPU NODES	80 132 quad Grace Hopper nodes
STORAGE	3 4.5 PB Flash (Lustre)

SYSTEM TOTALS

CPUs	528 Grace CPUs Each with 72 cores
GPUs	528 NVIDIA H100 (Hopper) GPUs with 96 GB HBM
PERF	35.3 PF double-precision 522 PF single-precision 1,045 PF tensor



Hewlett Packard Enterprise







Name	Granite
Institution	National Center for Supercomputing Applications at the University of Illinois
Resource	Storage – Tape Archive
Technology	 19-Frame Spectra T-Finity Library with LTO-9 Media Versity ScoutAM/ScoutFS software Allocations dual-copy (data mirrored on two tapes) Access via Globus; S3 access coming soon
Support mechanisms	https://help.ncsa.illinois.edu & ACCESS Ticketing
Website	https://docs.ncsa.illinois.edu/systems/granite
Representative	J.D. Maloney



Highlights

- Durable storage for infrequently accessed datasets
- Multi-Protocol Support (Globus + S3)
- For data needs larger/longer than ACCESS allocations permit;
 Granite does offer a charge-back model





Where to Find Help

Ticket System

- Anything ACCESS related
 - Must register for an <u>ACCESS ID</u> to open a ticket

Resource Providers (Directly)

 The <u>Resource Catalog</u> has links to user guides with contact information

Q&A Bot

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















Jetstream2

(JHU)

Rockfish

National Center for Supercomputing Applications (NCSA Open Science Grid (OSG)

Open Storage Network

Pittsburgh Supercompu Center (PSC)















Purdue Anvil San Diego Supercomputer Stony Brook University
Center (SDSC) Ookami

rsity Texas Advanced
Computing Center (TACC)
Stampede2

Texas A&M FACC) (TAMU) FASTER University of Delaware DARWIN



University of Kentucky KyRIC





A Look over the Horizon: NCSA and Quantum Computing



NCSA | National Center for Supercomputing Applications

NCSA's Mission, Vision, Purpose

Mission:

Bring people, computing, and data together to benefit society.

Vision:

A future enlightened by our research discoveries, where the boundaries of human understanding are continually extended to improve the world.

Purpose:

At NCSA, we aim to bring the brightest minds together to solve the grandest challenges and advance humanity. We do this by harnessing the transformative power of computing, software, and data sciences, and fostering a united community dedicated to advancing human knowledge and addressing critical societal challenges through research.



Working with NCSA

 From our expert staff, grant administration services, translational software, data visualization, and educational programming (and so much more), NCSA is your collaborator in developing solutions to your greatest research challenges



Working with NCSA: Technologies

Systems and Facilities

- Delta, DeltaAI (HPC)
- Radiant (elastic compute)
- NPCF Facilities

Data and storage

- Integrated Data and Database Services
- Storage Enabling Technologies

Software

- Research Software Engineers (RSEs)
- Software expertise in data management, devops, workflows, machine learning

Services

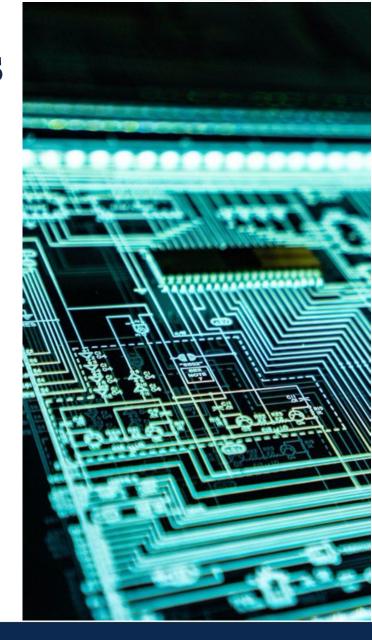
- User services (applications support)
- Sysadmin services



Networking & security



services



Working with NCSA: People

For faculty

- Faculty Fellows
- Faculty Affiliates
- Fiddler Fellowships

For students

- SPIN (Students Pushing Innovation)
- REU (INCLUSION)
- NCSA International Research Internship
- University of Illinois Student Cluster

- Center for Al Innovation
- Center for Digital Agriculture
- Office of Data Science Research (ODSR)

Labs:

- Advanced Visualization Lab
- <u>Data Analysis &</u>
 <u>Visualization Lab</u>
- Data Exploration Lab
- vi-bio lab





Programs

Over the Horizon: Quantum Computing

- Computing today has reached various limits of density and scalability
 - Moore's Law still in play but limited by other factors
 - transistor density doubling approximately every 2 years
 - technological, physical, and economic limitations slowing this
 - Dennard Scaling has reached it limit
 - reduced feature size in semiconductors induce reduced power efficiency and increased heat generation per transistor
 - induced the rise in multi-core processors and GPUs
- Demand for increased computing capability relentlessly continues
 - induces a need for new computing technologies





Drivers of Quantum Computing Development

- The need to solve ever more complex problems
 - o potential to solve problems intractable on "classical" computing platforms
- Optimization problems
 - frequently found in science and business applications
- Cryptography
 - o breaks current algorithms; quantum-resistant algorithms in development
- Simulating quantum systems
 - critical for fundamental physics, chemistry, and biology
 - o can support drug discovery, materials science, climate modeling, ...
- Al in its various forms
 - o can speed up training and optimization processes
 - can lead to improved AI models
- Environmental and economic advantages
 - potential for much greater power efficiency
- But, need to attain Quantum Advantage across a suite of problem classes
 - when a quantum computer outperforms a classical computer for a problem



US Federal Government Responses

- National Quantum Initiative Act (NQIA)

 - Congress passes NQIA in December 2018 accelerate/coordinate federal R&D investments in quantum information science and technology (QIS or QIST)
- National Quantum Coordination Office (NQCO)
 - part of NQIA central point for QIS efforts
- Department of Energy (DOE) established QIS research centers in 2020
 - Oak Ridge, Lawrence Berkley, Argonne
- National Institute of Standards and Technology (NIST), NSF, DOE, and the Defense Advanced Research Projects Agency (DARPA)
 - for several years have been funding basic research in developing quantum technologies
- Workforce Development
 - several agencies initiated programs to develop the quantum workforce
- The past few years have seen increases in federal investments



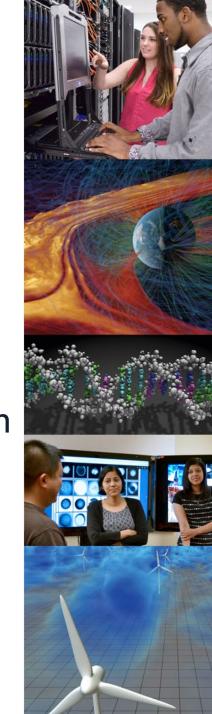
https://www.quantum.gov



NCSA and Quantum Computing

- NCSA sees this as a promising emerging technology
 - far from realized as yet
- Over the past couple of years, ramped up efforts in QIS
 - leveraging existing collaboration in the Chicago Quantum Exchange
 - providing training, early access to quantum systems, forum for exchange of ideas
 - rapidly developing close collaborations with Illinois Quantum Information Science and Technology Center (IQUIST)
 - complements NCSA strengths extremely well
 - established Quantum Program Office at NCSA in collaboration with IQUIST
 - I am in the role of executive sponsor





Early Deployment of Quantum Computing: LCCF Emerging Tech Partner

- LCCF: Leadership Class Computing Facility
 - "Horizon" system to be deployed by 2026 (+a little?); classical CPU+GPU system
- NCSA is an emerging technology partner; collaboration with IQUIST
 - deploy superconducting quantum processing unit (QPU) in IQUIST testbed
 - deploy classical CPU+GPU cluster in NPCF
- Focus on several critical issues
 - o complete environment: very early environment for testing beyond devices and basic components
 - o software stack: many missing components to a functional and accessible system for real users
 - o benchmarking: how does one assess the real performance of these systems?
 - applications: what real science, engineering, and industrial applications can get quantum advantage?
- Timeline
 - project start in ~March 2024; full deployment by ~December 2026
- Opportunity for collaboration
 - o looking for promising industrial applications for testing and evaluation





