XSEDE: An Advanced and Integrated Set of Digital Resources for Science and Engineering

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Extreme Science and Engineering Discovery Environment

What is XSEDE?



Foundation for a National CI Ecosystem

• Comprehensive suite of advanced digital services that federates with other high-end facilities and campus-based resources



Unprecedented Integration of Diverse Advanced Computing Resources

• Innovative, open architecture making possible the continuous addition of new technology capabilities and services

Partnership led by NCSA, NICS, PSC, TACC and SDSC

Partners with Complementary Expertise

- Argonne National Laboratory
- Cornell: Center for Advanced Computing
- Georgia Institute of Technology: Center for Education Integrating Science, Mathematics, and Computing
- Indiana University: Pervasive Technology Institute
- National Center for Atmospheric Research
- Ohio Supercomputer Center
- Oklahoma State University: High Performance Computing Center
- Purdue: Rosen Center for Advanced Computing
- Shodor
- SURA
- University of Arkansas: Arkansas High Performance Computing Center
- University of Chicago
- University of Georgia: Terry College of Business
- University of Oklahoma: Supercomputing Center for Education & Research
- University of Southern California: Information Sciences Institute

XSEDE Mission and Goals

Mission: Accelerate scientific discovery

Goals:

• Deepen and Extend Use

- Raise the general awareness of the value
- Deepen the use and extend use to new communities
- Contribute to the preparation of current and next generation scholars, researchers, and engineers
- Advance the Ecosystem
- Sustain the Ecosystem

Total Research Funding Supported by XSEDE



XSEDE Supports a Breadth of Research

- Earthquake Science
- Molecular Dynamics
- Nanotechnology
- Plant Science
- Storm Modeling
- Epidemiology
- Particle Physics
- Economic Analysis of Phone Network Patterns
- Large Scale Video Analytics (LSVA) Decision Making Theory
- Library Collection Analysis



Three-dimensional model of major vessels and bifurcations of the human arterial tree reconstructed with gOREK from a set of computed tomography (CT), digital subtraction angiography CT and magnetic resonance angiography images.



A snapshot of an animation for water level prediction including the wind-wave signature.



Ruby Mendenhall, an associate professor of sociology, African American studies and urban and regional planning at the University of Illinois (UI) at Urbana-Champaign, is leading a collaboration of social scientists, humanities scholars and digital researchers that hopes to harness the power of high-performance computing to find and understand the historical experiences of black women by searching two massive databases of written works from the 18th through 20th centuries.

SEDE

Why XSEDE?





Compute and Analytics Resources

- Featuring interactive on-demand access, tools for gateway building, and virtualization.
- **SDSC** Comet: hosting a variety of tools including Amber, GAUSSIAN, GROMACS, Lammps, NAMD, and Vislt.
- Jetstream A self-provisioned, scalable science and engineering cloud environment
- TAGE Stampede: Intel's new innovative MIC technology on a massive scale
- LSU Super Mic: Equipped with Intel's Xeon Phi technology. Cluster consists of 380 compute nodes.
- TAGG Wrangler: Data Analytics System combines database services, flash storage and long-term replicated storage, and an analytics server. IRODS Data Management, HADOOP Service Reservations, and Database instances.

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High Throughput Computing



- Governed by the OSG consortium
- 126 institutions with ~120 active sites collectively supporting usage of ~2,000,000 core hours per day
- High throughput workflows with simple system and data dependencies are a good fit for OSG
- Access Options:
 - OSGConnect available to any researcher affiliated with US institutions and who are funded by US funding agencies
 - OSG Virtual Organization such as CMS and ATLAS
 - XSEDE
- https://portal.xsede.org/OSG-User-Guide

XSEDE Visualization and Data Resources

Visualization



Maverick@ TACC

- HP/NVIDIA cluster
- 132 TB memory
- Vislt
- ParaView
- Interactive Data Language

TACC Visualization Portal

- Remote, interactive, webbased visualization
- iPython / Jupyter Notebook integration
- R Studio Integration

Storage

- Resource file system storage: All compute/visualization allocations include access to limited disk and scratch space on the compute/visualization resource file systems to accomplish project goals
- Archival Storage: Archival storage on XSEDE systems is used for large-scale persistent storage requested in conjunction with compute and visualization resources.
- Stand-alone Storage: Standalone storage allows storage allocations independent of a compute allocation.

Science Gateways



The CIPRES science gateway: A NSF investment launching thousands of scientific publications with no sign of slowing down.



XSEDE

https://sciencenode.org/feature/cipres-one-facet-in-bold-nsf-vision.php?clicked=title

Allocations



Champion



Startup





Research





XSEDE

User Support Resources



Community Engagement & Enrichment (CEE)

Broadening Participation

Campus Engagement

User Engagement

User Interfaces & Online Information

Workforce Development

Broadening Participation



- Campus Visits
- Conference Exhibiting
- Consulting
- Diversity Forum
- Minority Research Community Listserv

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- Travel Support
- Training Events

Broadening Participation – Impact Years 1 - 5









Workforce Development: Education Program

Develop, identify, & maintain computational science program competencies

Promote computational science

Provide consulting for program development and plans

Facilitate Collaborative Online Courses



Workforce Development: Training

XSEDE provides extensive training

- Covering every major resource
- From beginner to advanced classes
- At locations across the country
- Online via
 - asynchronous technologies
 - Webcasts

Web-based education credit courses

Workforce Development: Student Programs - EMPOWER

PROJECTS: Computational, Data Analytics, Visualization Research or Networking and System Maintenance

MENTORS are XSEDE staff, researchers, and educators who recruit and mentor undergraduate students to engage in projects.

STUDENTS are undergraduates who participate as a learner, apprentice or intern participation for students.

COMPENSATION: Ranges from \$750 to \$3,000 (based on student level and duration)

PROJECT PROPOSALS must contain a Training plan for the student.



Use XSEDE Resources for research or teaching

Attend a webinar or in-person training

Use online training materials (XSEDE and HPC University)

Participate in a faculty development workshop

Attend PEARC17, New Orleans, July 9 - 13 http://www.pearc.org/

Apply for Travel Support, Present a Poster or Visualization at PEARC17 <u>https://www.pearc.org/student-program</u>

Apply to XSEDE's Empower Student Internship Program http://computationalscience.org/xsede-empower

Visit HPC University for more student opportunities <u>www.hpcuniversity.org</u>

More Information

- Today's XSEDE Presentations -<u>http://hpcuniversity.org/trainingMaterials/238/</u>
- XSEDE Website: <u>www.xsede.org</u>
- People
 - Linda Akli, <u>akli@sura.org</u>
 - Jay Alameda, <u>alameda@illinois.edu</u> (New User & ECSS)
 - Kate Cahill, <u>cahill.167@osu.edu</u> (Education & Curriculum)
 - David Walling, <u>walling@tacc.utexas.edu</u>, (Parallel R)
 - Mahidhar Tatineni, <u>mahidhar@sdsc.edu</u>, (Hadoop)
 - Carmen Wright, <u>carmen.m.wright@jsums.edu</u>



Questions





Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.



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