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

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XSEDE Underrepresented Community Engagement

XSEDE
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 digital resources
  - innovative, open architecture making possible the continuous addition of new technology capabilities and services

XSEDE Team

- World-class leadership from CI centers with deep experience: partnership led by NCSA, NICS, PSC, TACC and SDSC
- Partners who strongly complement these CI centers with expertise in science, engineering, technology and education

SURA
Cornell
Purdue
Shodor
National Center for Atmospheric Research
Ohio Supercomputer Center
Indiana University
Rice
University of Chicago

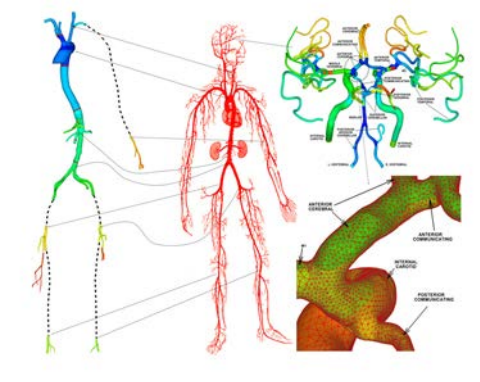
XSEDE Vision and Mission

- Vision
  - XSEDE aspires to be the place to go to access digital research services.
- Mission
  - Accelerate scientific discovery by enhancing the productivity of researchers, engineers, and scholars by deepening and extending the use of XSEDE's ecosystem of advanced digital, services and by advancing and sustaining the XSEDE advanced digital infrastructure.

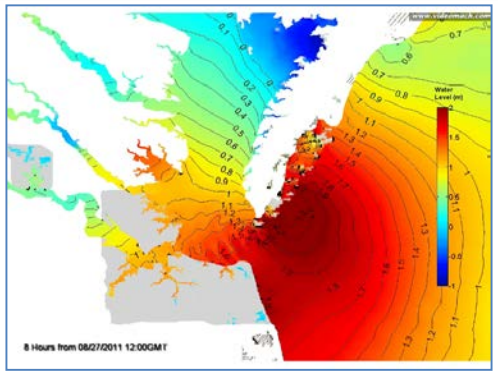
Why XSEDE?

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

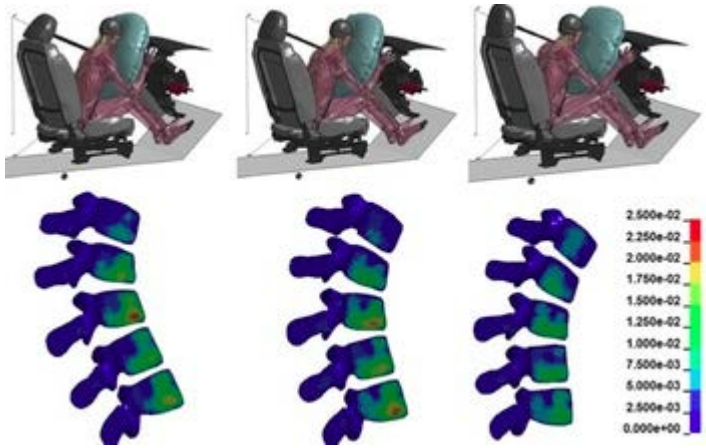


Three-dimensional model of major vessels and bifurcations of the human arterial tree reconstructed with gOREK from a set of computed tomography (CT), digital subtraction angiography CT and magnetic resonance angiography images.



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

Crash test simulations expose real risks: Using Blacklight supercomputer, researchers gain new insights into crash injuries and ways to mitigate them



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.

XSEDE Compute Resources

Stampede @TACC

- 10 PFLOPS (PF) Dell Linux Cluster based on 6400+ Dell PowerEdge server nodes, each outfitted with 2 Intel Xeon E5 (Sandy Bridge) processors and an Intel Xeon Phi Coprocessor (MIC Architecture)

Gordon @SDSC

- Flash-based supercomputer designed for data-intensive applications

Darter @NICS

- Cray XC30 system providing both high scalability and sustained performance with a peak performance of 250 Tflops

PSC Greenfield @PSC

- 360 cores and 18TB of memory in three nodes: two HP DL580s and an HP SuperDome X. Hosts a large number of bioinformatics tools

Mason @IU

- A large memory computer cluster configured to support data-intensive, high-performance computing tasks using genome assembly software

Super Mic @LSU

- Equipped with Intel's Xeon Phi technology. Cluster consists of 380 compute nodes.

New Resources

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.

Comet

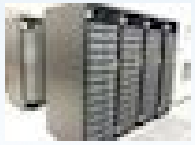
Features the next generation Intel "Haswell" processors with AVX2 and hosts a variety of tools including Amber, GAUSSIAN, GROMACS, Lammps, NAMD, and VisIt.

Jetstream — A self-provisioned, scalable science and engineering cloud environment

BRIDGES — Featuring interactive on-demand access, tools for gateway building, and virtualization.

XSEDE Visualization and Data Resources

Visualization



Maverick@ TACC

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

Visualization Portal

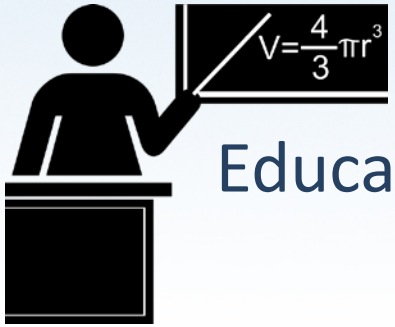
- Remote, interactive, web-based visualization
- iPython / Jupyter Notebook integration
- R Studio Integration

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**: Stand-alone storage allows storage allocations independent of a compute allocation.

Allocations

Champion



Education

Research

Startup

XSEDE User Services

- Technical information
  - Always available via web site and XSEDE user portal
- Training
  - Sign up for classes to learn to use XSEDE resources
- Help Desk/Consultants
- Extended Collaborative Support Services
  - Human resources to help with performance analysis, optimization, efficient use of accelerators, I/O optimization, the development of community gateways and work and data flow systems

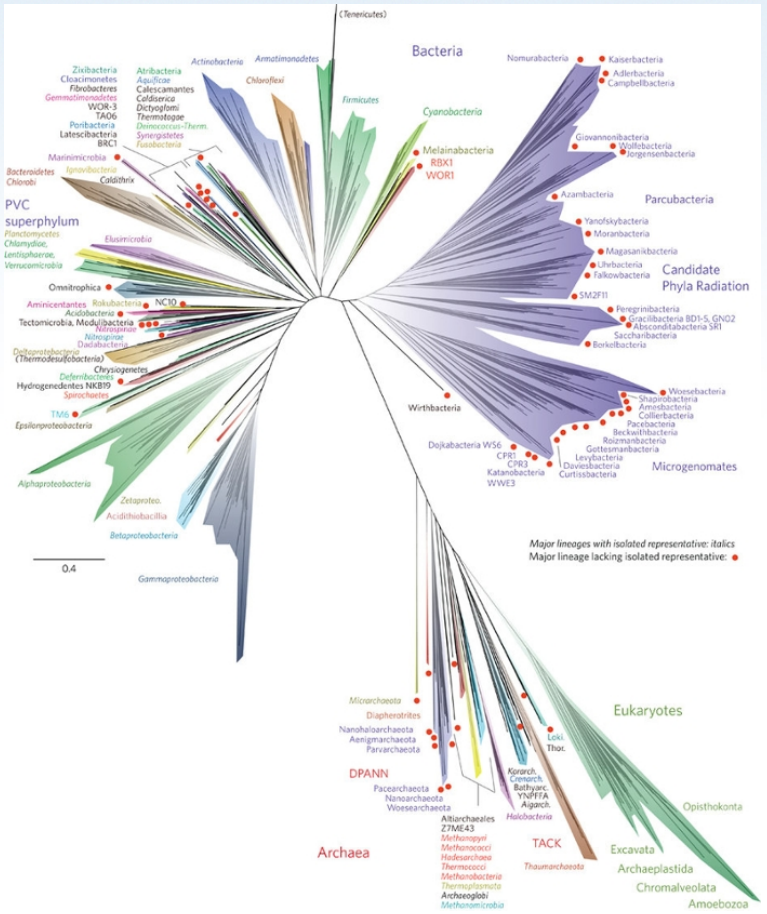
XSEDE Training

- 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

Gateways: Democratizing Access

- Almost anyone can investigate scientific questions using high end resources
  - Not just those in high profile research groups
- Gateways allow anyone with a web browser to explore
- Foster new ideas, cross-disciplinary approaches
  - Encourage students to experiment
- Used in production
  - Significant number of papers resulting from gateways, including GridChem, nanoHUB
  - Scientists can focus on challenging science problems rather than challenging infrastructure problems

Science Gateways



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

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

Community Engagement

- Champions
- Campus Bridging
- Education
- Broadening Participation
- Annual XSEDE Conference

Champions Program

- Campus Champions
  - Representatives to spread information about XSEDE to local faculty, students and staff
- Student Champions
  - Students assist the Campus Champions
- Regional Champions
  - Representatives to spread information about XSEDE to other campuses in the area
- Domain Champions
  - Disciplinary people able to assist others with domain specific HPC questions

Campus Bridging

The goal of campus bridging is to create a sense of "virtual proximity." Any resource should feel as if it's just a peripheral to their laptop or workstation.

The goal is to make it convenient and intuitive to simultaneously use your personal computing systems, departmental and campus systems (at your campus and others), and national resources liked XSEDE . . . all (almost) transparently and easily.

Education Program

- Development of competencies for undergraduate and graduate computational science programs
  - Assisting campuses with organizing formal certificate programs
  - Sharing instructional materials
- Campus visits to promote computational science
  - Meetings with faculty and administrators
  - Professional development workshops

Broadening Participation

- Expand awareness of XSEDE
- Identify programs and researchers who can benefit from XSEDE services
- Enable institutions and faculty to use advanced digital services to increase their research productivity
  - By establishing and growing a thriving collaborative peer support community
  - Through the delivery of training mapped to their needs
  - By connecting researchers with XSEDE services and expertise for targeted deep engagement
- Create scalable and sustainable models and best practices
  - By supporting the establishment of certificate and degree programs and enhanced curriculum
  - By developing and supporting productive campus champions






XSEDE16 in MIAMI

XSEDE

XSEDE[16]

SAVE THE DATE!

JULY 17-21, 2016
INTERCONTINENTAL MIAMI HOTEL

Miami, one of the most distinct cultural locations in the country, will host the XSEDE16 conference. The themes will be the importance of Diversity, Big Data, Science at Scale, and how they interconnect to deliver the next-generation of science and technology. We look forward to seeing you next year!

XSEDE
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xsede.org/xsede16 | #XSEDE16

XSEDE16 Conference

- Submissions:
  - closed for papers
  - Posters and visualizations (due tomorrow)
- Topics span accelerating discovery, advanced technologies, software, science gateways and portals, and education, outreach and training
- Expect over 600 people from academia, industry, government, and other organizations
- Travel Support
- Registration is open!


How Do I Get Started?

Faculty Opportunities

- Use XSEDE Resources for research or teaching
- Participate in Training
- Attend Summer Institutes
- Participate in XSEDE16, July 2016, Miami
- Join the Minority Research Community listserv
- Become a Champion

Today's Workhop Agenda

Computational Thinking:

XSEDE New User Training

More Information

- Today's XSEDE Presentations - http://hpcuniversity.org/trainingMaterials/219
- XSEDE Website: www.xsede.org
- XSEDE Staff
  - Linda Akli, akli@sura.org
  - Jay Alameda, alameda@illinois.edu (New User Training)
  - Kate Cahill, cahill.167@osu.edu (Curriculum)

Questions


Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
XSEDE
Extreme Science and Engineering
Discovery Environment