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

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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

  U of Virginia  Ohio Supercomputer Center
  SURA          Cornell
  Indiana Univ  Purdue
  Univ of Chicago  Rice
  Berkeley      NCAR
  Shodor        Jülich Supercomputing Centre
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 would you use 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.
XSEDE Compute Resources

Stampede @ TACC
– 6 PFLOPS (PF) Dell Cluster w/ GPUs and Xeon PHIs

Gordon @ SDSC
– 341 TF Appro Distributed SMP cluster

Darter @ NICS
– 250 TF Cray XC30

Blacklight @ PSC
– 37 TF SGI UV (2 x 16TB shared memory SMP)

Mason
– 3.8 TF HP Cluster with large memory nodes (2TB/node)

Super Mic @ LSU
– 925 TF Dell

Coming Soon – Comet and Wrangler
XSEDE Visualization and Data Resources

• Visualization
  - Nautilus @ UTK
    - 8.2 TF SGI/NVIDIA SMP
    - 960 TB disk
  - Maverick @ TACC
    - HP/NVIDIA cluster
    - 132 TB memory

• Storage
  - HPSS @ NICS
    • 6.2 PB tape
  - Data Supercell @ PSC
    • 4 PB tape
  - Ranch @ TACC
    • 40 PB tape
  - Data Oasis @ SDSC
    • 4 PB tape
NCSA Blue Waters System

- Funded by the NSF to support very large scale computational science and engineering
- Cray systems
  - 22,640 Cray XE6 nodes - 64 GB of memory per node
  - 3,072 Cray XK7 nodes include NVIDIA processors with 32 GB of memory
  - 26 petabytes of online storage
  - 380 petabytes of tape storage
- Allocations are made via:
  - Applications to the NSF PRAC proposal process
  - Applications to Blue Waters education allocations
Gateways democratize access to high end resources

- 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
- But used in production, too
  - Significant number of papers resulting from gateways, including GridChem, nanoHUB
  - Scientists can focus on challenging science problems rather than challenging infrastructure problems
Simple Enough?
XSEDE User Services

XSEDE User Services are grouped into four main areas:

• Technical information
  – Always available via web site and XSEDE user portal

• Allocations
  – Request access to XSEDE’s systems

• Training
  – Sign up for classes to learn to use XSEDE resources

• User Engagement
  – Includes ‘consulting support’ to answer questions
  – Also includes user interviews, focus groups, and surveys
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
Community Engagement Activities

- Under-represented Community Engagement
- Campus Bridging
- Champions Program
- Education
- Student Programs
- Campus Visits
- Annual XSEDE Conference
Underrepresented Community Engagement

• 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
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.
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
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
Campus Visits

• XSEDE visits campuses to
  – raise awareness
  – conduct professional development and curriculum development sessions,
  – assist with incorporating campus bridging tools and resources
  – meet with administrators, faculty, staff and students to effect institutional change

• Let us know how we can assist your campus
XSEDE15 Conference

• St. Louis – July 26-30, 2015
• Submissions will be accepted for papers, panels, tutorials, BOFs, student programs
• 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
• Support for student participation
Faculty

• Use XSEDE Resources for research or teaching
• Participate in Training
• Attend In-Person Training & Summer Institutes
• Be a Campus Champion
• Join the Minority Research Community
• Participate in XSEDE15, July 2015, St Louis
Institutions

• Campus Champions
• Campus Bridging
• Education – Computational Science Curriculum, Certificate, or Degrees
• Regional Workshops
• Summer Institutes
Students

• Blue Waters Internship
  – 2 week training institute for undergrads and grads
  – year-long computational science problem solving

• Blue Waters Graduate Fellowship – Deadline Past
  – similar to NSF Graduate Fellowships
  – year-long engagement

• XSEDE Annual Conference
  – travel support for students to attend the annual Conference (decisions will be made in May)
HPC University Portal

• Training and education resources
• Events worldwide
• Internship and fellowship opportunities
• Career opportunities
• Computational science and education blog
• Today’s XSEDE Presentations - http://hpcuniversity.org/trainingMaterials/192

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