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

Linda Akli, SURA, IT Program Manager
What is XSEDE?

• Foundation for a national CI ecosystem
  – comprehensive suite of advanced digital services that will federate 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
  - PI: John Towns, NCSA/Univ of Illinois
  - Co-PIs: Jay Boisseau, TACC/Univ of Texas Austin
  - Patricia Kovatch, NICS/Univ of Tenn-Knoxville
  - Ralph Roskies, PSC/CMU
  - Nancy Wilkins-Diehr, SDSC/UC-San Diego

- Partners who strongly complement these CI centers with expertise in science, engineering, technology and education
  - Univ of Virginia, SURA
  - Indiana Univ
  - Univ of Chicago
  - Berkeley
  - Shodor
  - Ohio Supercomputer Center
  - Cornell
  - Purdue
  - Rice
  - NCAR
  - Jülich Supercomputing Centre
XSEDE Vision

The eXtreme Science and Engineering Discovery Environment (XSEDE):

enhances the productivity of scientists and engineers by providing them with new and innovative capabilities

and thus

facilitates scientific discovery while enabling transformational science/engineering and innovative educational programs
XSEDE’s Distinguishing Characteristics

• Coordinated national program with greater scope and scale
  – increased diversity of topics, modes of delivery, and reach to new communities and audiences
  – broaden participation among under-represented communities

• Campus bridging for effective use of CI resources
  – more tightly integrate with campuses through expanded Champions program and additional bridging activities

• Establish certificate and degree programs
  – institutional incorporation of CS&E curricula; professional development certificate
  – prepare undergraduates, graduates and future K-12 teachers
XSEDE’s Distinguishing Characteristics - Architecture

- **XSEDE is designed for innovation & evolution**
  - there is an architecture defined
    - based on set of design principles
    - rooted in the judicious use of standards and best practices
    - clearly defined transition plan from TeraGrid to XSEDE

- **Professional systems engineering approach**
  - responds to evolving needs of existing, emerging, and new communities
    - incremental development/deployment model
  - new requirements gathering processes
    - ticket mining, focus groups, usability panels, shoulder surfing
  - ensure robustness and security while incorporating new and improved technologies and services
  - process control, quality assurance, baseline management, stakeholder involvement
How we engage stakeholders

• Collection of stakeholder needs:
  – surveys, ticket mining, ...
  – focus groups, usability panels, ...
  – interviews, shoulder surfing, ...

• Prioritization of identified need and derived requirements
  – User Requirements Evaluation and Prioritization (UREP) Working Group

• Assessing plans and deployments
  – through a variety of stakeholder-focused, facilitated workshops

• Representation in the management of XSEDE
  – XSEDE Advisory Board
  – User Advisory Committee
  – Service Providers Forum
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
Compute Resources

Kraken @ NICS
  – 1.2 PF Cray XT5

Ranger @ TACC
  – 580 TF Sun Cluster

Gordon @ SDSC
  – 341 TF Appro Distributed SMP cluster

Lonestar (4) @ TACC
  – 302 TF Dell Cluster

Trestles @ SDSC
  – 100TF Appro Cluster

Steele @ Purdue
  – 67 TF Dell Cluster

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

https://www.xsede.org/resources/overview
Visualization and Storage Resources

• Visualization
  - Nautilus @ UTK
  - Longhorn @ TACC
  - Spur @ TACC

• Storage
  - Archival Storage
  - Allocatable Storage
  - Resource filesystem storage

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Special Purpose Resources

• Condor Pool @ Purdue
  – 150 TF, 27k cores

• Keeneland @ GaTech/NICS
  – GPU cluster platform

• FutureGrid
  – Experimental/development distributed grid environment

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Partnerships – Open Science Grid

- OSG is a Service Provider in XSEDE
- OSG resources are made available via XSEDE allocations processes
- OSG has two other interaction points with XSEDE
  - participation in outreach/campus bridging/campus champions activities
  - effort in ECSS specifically to work with applications making use of both OSG and XSEDE resources
Partnerships - PRACE

• Joint allocations call by late CY2012
  – support for collaborating teams
  – make one request for XSEDE and PRACE resources
  – call for Expressions of Interest (EoI) in the next couple of months

• Interoperability/collaboration support
  – driven by identified needs of collaborating teams in US and Europe
  – beginning with technical exchanges to develop deeper understanding on one another's architectures and environments
Extended Collaborative Support Service

- Support people who understand the discipline as well as the systems (perhaps more than one support person working with a project).
- 37 FTEs, spread over >70 people at more than half a dozen sites.
- Distributed support
  - Easier to find the right expert for the project
  - allows us to cover many more disciplines than if every site had to staff the common applications.
  - support does not have to move with platform change
XSEDE supports a breadth of research

- Earthquake Science and Civil Engineering
- Molecular Dynamics
- Nanotechnology
- Plant Science
- Storm modeling
- Epidemiology
- Particle Physics
- Economic analysis of phone network patterns

Figure 2: A snapshot of an animation for water level prediction including the wind-wave signature.

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.
Outreach Services (PSC-led)

**GOAL:** Recruit a large and diverse scientific, academic, and industrial workforce capable of advancing scientific discovery using XSEDE services.

- **Student Engagement**
  - Provide meaningful experiences for undergraduate and graduate students to become engaged in Extreme Digital environments

- **Underrepresented Engagement**
  - Bring XSEDE to new faculty, and students, providing dedicated training and support

- **Campus Champions**
  - Build broader and deeper programs based on TeraGrid foundation

- **Speakers’ Bureau**
  - Raise awareness of Extreme Digital environments among new communities of potential users
XSEDE Education Services

• Led by Steve Gordon, Ohio Supercomputing Center
• 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
Training Services

• Led by Dan Stanzione, TACC
• XSEDE offers training classes to teach users how to maximize their productivity and impact in using the XSEDE services.
• The training classes focus on systems and software supported by the XSEDE Service Providers, covering programming principles and techniques for using resources and services effectively.
• Training classes are offered in high performance computing, visualization, data management, distributed and grid computing, science gateways, and more.
Simple Enough
OOPS
Questions? Or Feedback

• XSEDE User Portal – www.xsede.org
• Help – https://portal.xsede.org/overview1
• Feedback - https://portal.xsede.org/feedback
• Linda Akli, akli@sura.org
Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.