XSEDE: the eXtreme Science and Engineering Discovery Environment
Introduction to XSEDE

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XSEDE
Extreme Science and Engineering Discovery Environment
XD Solicitation/XD Program

• eXtreme Digital Resources for Science and Engineering (NSF 08-571)
  -- Extremely Complicated
  – High-Performance Computing and Storage Services
    • aka Track 2 awardees and others
  – High-Performance Remote Visualization and Data Analysis Services
    • 2 awards; 5 years; $3M/year
    • proposals due November 4, 2008
  – Integrating Services (5 years, $26M/year)
    • Coordination and Management Service (CMS)
      – 5 years; $12M/year
    • Technology Audit and Insertion Service (TAIS)
      – 5 years; $3M/year
    • Advanced User Support Service (AUSS)
      – 5 years; $8M/year
    • Training, Education and Outreach Service (TEOS)
      – 5 years, $3M/year
  – two phase proposal process for IS
    • pre-proposals November 4, 2008
    • final proposals due June 15, 2009
Science requires diverse digital capabilities

• XSEDE will be a comprehensive, expertly managed set of advanced heterogeneous high-end digital services, integrated into a general-purpose infrastructure.

• XSEDE is about increased user productivity
  – increased productivity leads to more science
  – increased productivity is sometimes the difference between a feasible project and an impractical one
XSEDE Vision

The eXtreme Science and Engineering Discovery Environment (XSEDE) will:

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

and thus

- facilitate scientific discovery while enabling transformational science/engineering and innovative educational programs
XSEDE will support a breadth of research
From direct contact with user community as part of requirements collections

- Earthquake Science and Civil Engineering
- Molecular Dynamics
- Nanotechnology
- Plant Science
- Storm modeling
- Epidemiology
- Particle Physics
- Economic analysis of phone network patterns
- Brain science
- Analysis of large cosmological simulations
- DNA sequencing
- Computational Molecular Sciences
- Neutron Science
- International Collaboration in Cosmology and Plasma Physics

Sampling of much larger set. Many examples are new to TeraGrid/HPC. Range from petascale to disjoint HTC, many are data driven. XSEDE will support thousands of projects.
XSEDE’s Distinguishing Characteristics

• Foundation for a national CI ecosystem
  – comprehensive suite of advanced digital services 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
Infrastructure Designed for Innovation & Evolution

• An environment in which all resources, data and services relevant to a researcher can be embedded and shared
  – campus bridging creating a single virtual system with interactive data transfer and resource sharing capabilities
    • “make my data accessible everywhere I want to be”
  – coordinated archival approach to ensure persistence of important datasets beyond the lifetime of particular service providers

• An underlying infrastructure to support this
  – open architecture with judicious use of standards designed to evolve in a non-disruptive way
  – interoperability of XSEDE with other CIs
XSEDE’s Distinguishing Characteristics - Governance

• 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
How we propose to 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
    • broad participation across architecture, deployment, operations, users, and service providers

• Assessing plans and deployments
  – through a variety of stakeholder-focused, facilitated workshops
    • e.g., interactive ATAM sessions focused on identifying, quantifying, discussing tradeoffs

• Representation in the management of XSEDE
  – XSEDE Advisory Board
  – User Advisory Committee
  – Service Providers Forum
XSEDE Distributed Systems Architecture Overview

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XSEDE
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What we mean by architecture

• Architecture defines the XSEDE system’s components and how they interact
  – each component is motivated by one or more requirements
  – each component is defined in terms of required capabilities: interfaces and qualities of service

• Equally important is the process by which we revise the architecture over time
  – key point: driven by new or revised requirements
Initial XSEDE architecture: High-order bits

• Don’t disrupt the user community! Maintain existing TeraGrid services

• Focus on user-facing access layer
  – for power users: “first, do no harm”
  – for other users: expand use via new hosted XSEDE User Access Services (XUAS) and Global Federated File System (GFFS)

• Promote standards and best practices to enhance interoperability, portability, and implementation choice
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
Systems Architecture: Basic Components

• Functional components
  – think operating systems
  – processes, inter-process communication, security, file systems, memory management

• Non-functional – “ilities”
  – reliability, availability, extensibility, usability, “performability,” etc.
  – note trade-offs

“Give me simple abstractions and make them work reliably.”
  -- Kent Blackburn
How we describe the XSEDE architecture

• A set of “views” describing the elephant from the perspectives of different stakeholders
  – Not (only) immensely detailed documentation!

• Different stakeholders require different views, e.g.,
  – Service provider
  – System administrator
  – Power user
  – Occasional user
  – Gateway developer
  – Security officer
  – NSF program manager
  – Campus CIO
  – Trainer
  – …

• Tell us what views you think are important
Initial Structural Views

• **Capabilities view**
  – primarily for management stakeholders
  – a set of capabilities and the definition of each
  – mapping from capabilities to requirements
  – mapping from capabilities to the pieces of the architecture

• **Component-and-connector view**
  – intended for a very technical audience
    • detailed information about how the system works when running
  – run-time entities that execute and cooperate to perform the work of the system

• **Module decomposition view**
  – all of the pieces of the system that have to be developed, maintained, integrated, and tested

• **Deployment view**
  – where the running software executes. More formally, the view is a mapping from components (such as a process or service) onto the processing node that hosts it
Initial Quality Views

• Security view
  – shows how architecture achieves security requirements
  – re-packages “security aspects” of design into special form for the security stakeholders

• Operations (Monitoring) view
  – how site-specific and XSEDE-wide monitoring will be carried out
    • e.g., how system reports/keeps track of user jobs
  – how the architecture makes information available to people monitoring the system’s operation

• Availability view
  – how does system react to a failure?
    • how the architecture records/reports/recovers from faults and failures
  – for those many stakeholders to whom availability is of high concern and wish to see how availability is provided by the architecture

• Performance view
  – answers questions about the various kinds of performance
    • e.g., job throughput, transfer latency, bandwidth, compute capability...
  – for stakeholders concerned with performance
    • first-order performance analysis can be carried out using C&C and Deployment views

• Install view
  – maps/associates) components of C&C view to file management system production environment
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XSEDE campus bridging vision

• Help XSEDE create the software, tools and training that will allow excellent interoperation between XSEDE infrastructure researchers local (campus) cyberinfrastructure;

• Enable excellent usability from the researcher’s standpoint for a variety of modalities and types of computing: HPC, HTC, and data intensive computing

• Promote better use of local, regional and national CI resources by
  – Promoting the use of InCommon for all authentication systems
  – Making it easier to use contribute campus systems (in whole possibly but generally in part) to the aggregate capacity and capability of XSEDE
  – Making it easier to use local systems - not contributed to the aggregate of XSEDE overall - more effectively in the context of workflows and cyberinfrastructure that include resources within and beyond XSEDE in a well coordinated fashion

• We will work with the various groups in XSEDE to align and assist activities and communications so that XSEDE collectively achieves these goals without interfering with established organizational structures and decision making processes [we plan to provide more lift than drag]
Campus bridging role

• To be conscientiously targeted at Data, HPC, and HTC – probably in that order

• Working closely with architecture and security teams to help disseminate XSEDE's plans
  – XSEDE architecture plans => out to campus champions and community
  – Funnel community response => back to XSEDE Architecture Team through DOORS, requirements gathering, and evaluations

• Work with TEOS teams to promote adoption of approaches that create a better integrated (and in aggregate larger) suite of resources for use by the national engineering and research community
XSEDE campus bridging tactics year 1

• There is an important value proposition that does not involve cash
• Support Installers created by Architecture group
  – Call for participation coming soon – pursue a small number of campuses as part of a pilot program to affect uptake by working within the them with diligence, and reap economies of scale (if things go right) or clear learning experiences (otherwise)
  – Planning to visit campuses to raise awareness and work with campus personnel
• Documentation & training
  – Science Gateways (document by Surresh Marru & Marlon Pierce)
  – Promote use of systems template created by TACC
• Serve as ‘connectors’ in discussions that should or could play a role in campus bridging activities (sit in in Arch and User Services calls)
• Work closely with OSG (OSG is plenty good at what they do!)
More consistency in CI setups => economies of scale for all

• In reality, the four cluster admins depicted here being in agreement are all right.
• Experienced cluster admins all learned how to use what they learn when the tools were still developing, so the tool each sysadmin knows the best is the tool that lets that sysadmin do their work the best.
• The only way to develop consistency is to provide installers that will make their work easier.
• The XSEDE architecture group is developing installers for file management tools.
• *A la Steven Colbert, the “4 out of 5…” comment is not intended to be a factual statement.

*Roughly 4 out of 5 systems administrators agree...* 

My way of setting up a cluster is the best!

*not intended to be a factual statement*
Training and outreach

- Consistency in system setups – local becoming more like XSEDE – should also lead to economies of scale in training
- Materials and trainer expertise will be more easily transportable and extensible
- Will work with User Services, Architecture, Security, Operations, etc. to provide a range of training
- The campus bridging group plans to work very closely with the campus champions

Challenges

• Expectation management & fulfillment
• What is the process to identify tools and approaches that are approved for release?
• What can be shared with the community today?
  – Architecture (we’re looking forward to knowing what it is to which we are bridging as much as anyone)
  – Training & Documentation?
  – Software?
• What resources (people, tools) are available for supporting early adopter campuses?
• How should we evaluate campus usage and acceptance?
XSEDE Campus Bridging Staff

- Craig Stewart (n% on campus bridging)
- Jim Ferguson (40% on campus bridging)
- Therese Miller – IU overall project lead for XSEDE activities (will be aiding, expected particularly in regards to campus champions)
- NB: IU gets roughly same funding from OSG and XSEDE
- Others to be involved as needs and awards evolve
href="http://pti.iu.edu/campusbridging/"
Goals

• Prepare the current and next generation of researchers, educators and practitioners.
• Create a significantly larger and more diverse workforce in STEM.
• Inculcate the use of digital services as part of their routine practice for advancing scientific discovery.
User/Admin View – logged into XSEDE Portal
Training Goals

• Expand the scope/scale of training through expanded use of distance learning, new topics, etc.

• Create a simpler user experience through a single portal for all training at all sites
  – Updated portal coming soon

• Create an internal repository to promote sharing of materials indexed at a single site.
XSEDE Education Workshops

• Workshops for faculty
  – Focus on tools and pedagogy for teaching computational science
  – Workshops in various disciplines being planned for summer 2012 (chemistry, biology, computational thinking)
  – Visits to campuses to encourage faculty interest in computational science

• UC Berkeley Par Lab Boot Camp on parallel programming
  – Given in August of each year and available online
  – http://parlab.eecs.berkeley.edu/2011bootcampagenda

• SC11 Education and Broader Engagement Workshops
Certificate and Degree Programs

• Creation of competency based model programs in computational science

• Recruiting campuses interested in starting programs
  – Assistance in starting new programs
  – Campus visits and faculty professional development
  – Programs in science and engineering
  – Teacher educator programs
Student Engagement

Components

- Students
  - Undergraduate and graduate
  - Drawn from contacts within and outside of XSEDE
  - 3-12 month appointments
- Projects
  - Provided and supervised by XSEDE researchers and staff

Outcomes

- Student presentations (papers, posters, etc)
- Case studies of successful and unsuccessful experiences
- More experienced practitioners entering STEM workforce

Process:

- Students and projects recruited and paired throughout the year.
- Researcher/staff supervises student work to complete project.
- Student develops and submits presentation material to relevant venue(s).
Underrepresented Engagement

Minority Institutions

SURA
• Identify established and emerging programs and researchers
• Expand awareness of XSEDE via campus visits, professional conferences
• Build a community promoting collaboration and peer support
• Target deep engagement that connect researchers with XSEDE expertise

Minority Students at Research Institutions

Rice University/Empowering Leadership Alliance (ELA)
• Increase awareness and knowledge among underrepresented communities
• Identify and recruit minority students and mentors, leveraging ELA
• Provide education and professional development to participants
• XSEDE scholars program (http://bit.ly/xsede_2011)

SDSC
Work with SURA and Rice/ELA to implement their plans nationally, esp. in the southwest US and among Hispanic and Tribal communities
Campus Champions

• “Champion” is a staff or faculty member on a campus that provides information on XSEDE to his/her colleagues
• Currently 88 institutions represented by champions
• Receive training and support from XSEDE staff
Current Campus Champion Institutions (unclassified) – 53
Current Campus Champion Institutions (EPSCoR states) – 37
Current Campus Champion Institutions (Minority Serving Institutions) – 7
Current Campus Champion Institutions (both EPSCoR and MSI) – 5

Total Number of Campus Champion Institutions Overall -- 102
Speakers’ Bureau

• **Audience**: Enhance XSEDE user diversity...
  – Demographically
  – Across disciplines

• **Venues**
  – Conferences and professional society meetings (as an exhibitor)
  – Campus visits
  – Presenter support

• **Criteria for Venue selection:**
  – Cost
  – Impact

• **Process**
  – Identify potential opportunities
  – <Go/No-Go> decision based on expected costs and impact
  – Execute selected events
  – Distribute contacts to XSEDE services for followup
XSEDEnet

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XSEDENet Configuration

• Based on NLR Layer 1 and 2 services
• Each SP connects at 10G to a dedicated FrameNet port in Chicago or Denver
• XSEDE leases a dedicated 10G circuit between Chicago and Denver
XSEDE Network 2011
Transition Summary

• Transition from TeraGrid to XSEDE took place Jun 28 – Aug 11
• Transition completed one SP at a time
• Traffic between TeraGrid and XSEDE flowed smoothly
XSEDE Network Services

• L3 Route Servers located in Chicago and Denver

• All SPs peer with Route Servers over a primary and backup VLANS
XSEDE Connectivity for Users

• Each SP site should have at least 1 10 GE R&E (I2 and/or NLR) connection plus some level of commodity connectivity.
XSEDE Support Services

- XSEDE networking services provides consulting to users and their campus network engineers to optimize end-to-end network performance important to applications requiring network communications across a distributed environment.

- Support is available to aid remote users in improving end-to-end access, both to debug existing installations and topologies and to help design new ones.
XSEDE Future Plans

• All SPs will deploy a perfSONAR host
• Evaluating on demand dynamic bandwidth circuits
For Further Information

• Website – www.xsede.org
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Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.