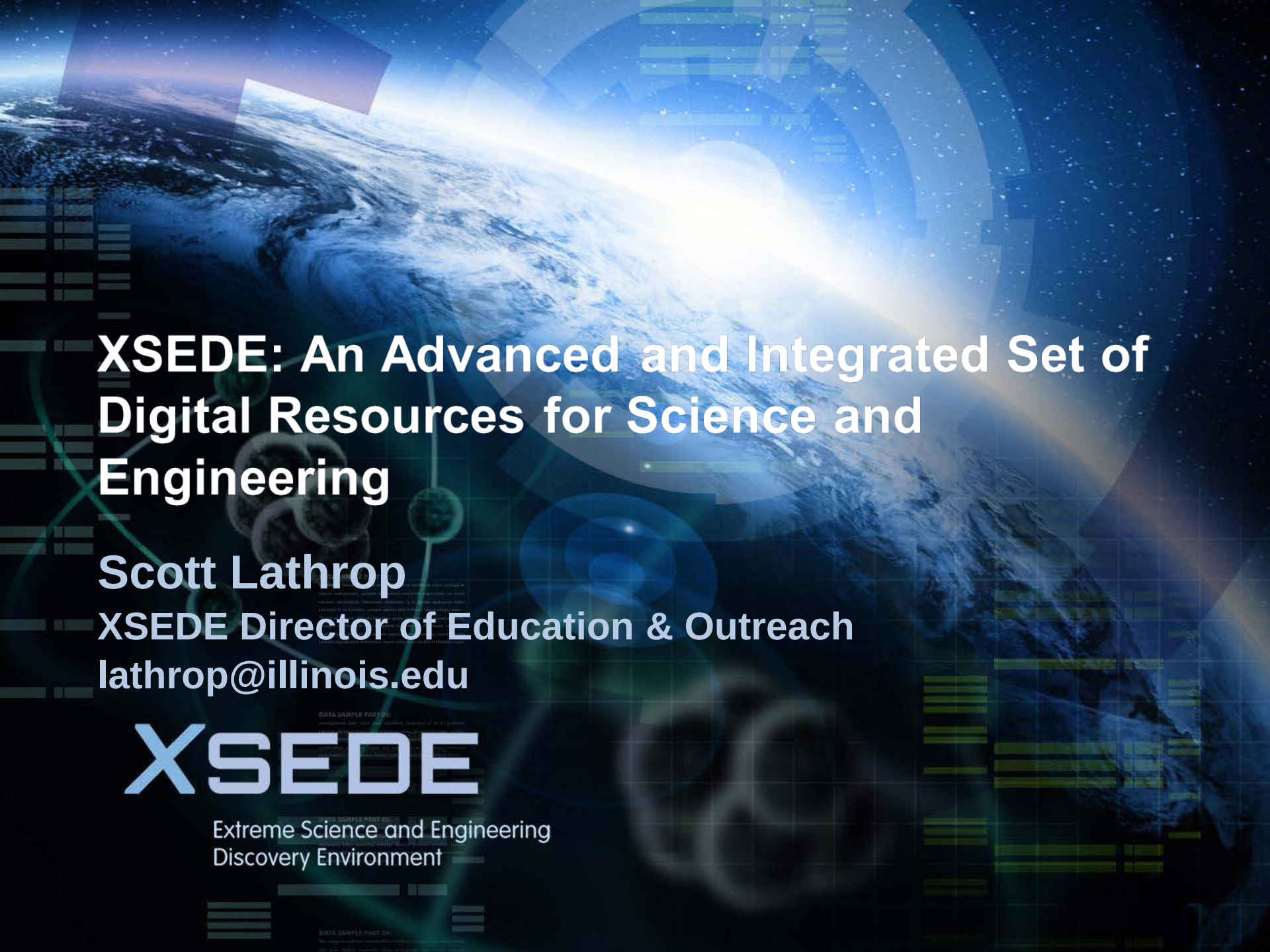




XSEDE: An Advanced and Integrated Set of Digital Resources for Science and Engineering

Scott Lathrop

XSEDE Director of Education & Outreach

lathrop@illinois.edu

XSEDE

**Extreme Science and Engineering
Discovery Environment**

What is XSEDE?

- Extreme Science and Engineering Discovery Environment
- Foundation for a national CI ecosystem
 - comprehensive suite of advanced digital services that federates with other high-end facilities and campus-based resources
- Integration of diverse digital resources and services
 - open architecture making possible the addition of new technology capabilities and services to meet the needs and requirements of the community

[Note: CI is Cyberinfrastructure]

The XSEDE logo is displayed in a large, bold, white sans-serif font against a dark blue background. The background features a grid of small, glowing blue squares, some of which are slightly larger and more prominent than others, creating a digital or network-like aesthetic. The logo is positioned in the bottom right corner of the slide.

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XSEDE Team

- World-class leadership from CI centers with extensive 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

University of Virginia
SURA

Indiana University

University of Chicago

Univ. Calif. Berkeley
Shodor

Ohio Supercomputer Center
Cornell University

Purdue University

Rice University

NCAR

Jülich Supercomputing Centre

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XSEDE Vision/Mission/Goals

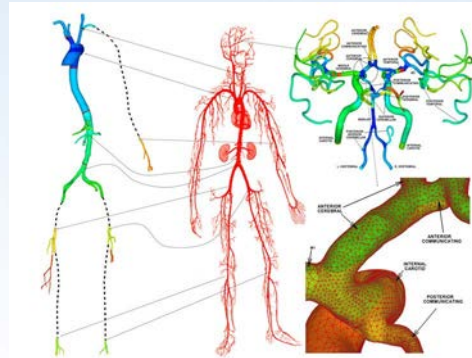
- **Vision:**
 - XSEDE aspires to be ***the*** place to go to access digital research services.
- **Mission:**
 - Accelerate scientific discovery by enhancing the productivity of researchers, engineers, and scholars by deepening and extending the use of XSEDE's ecosystem of advanced digital services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

Science requires diverse digital capabilities

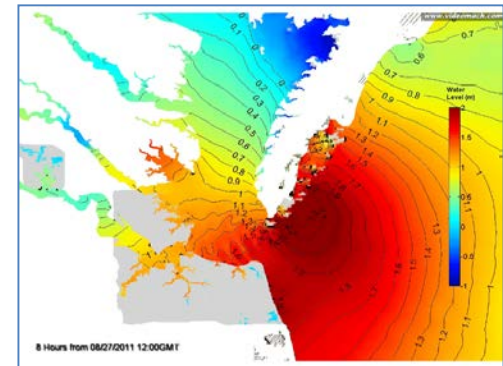
- XSEDE is a comprehensive, expertly managed and evolving set of advanced heterogeneous high-end digital services, integrated into a general-purpose infrastructure.
- XSEDE is about increased user productivity
 - increased productivity leads to more science
 - increased productivity is sometimes the difference between a feasible project and an impractical one

XSEDE 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.

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Why would you use XSEDE?



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Range of Advanced Digital Capabilities

- Often use the terms “resources” and “services”
 - these should be interpreted very broadly
 - most are likely not operated by XSEDE
- Examples of resources
 - compute engines: HPC, HTC (high throughput computing), campus, departmental, research group, project, ...
 - data: simulation output, input files, instrument data, repositories, public databases, private databases, ...
 - instruments: telescopes, beam lines, sensor nets, shake tables, microscopes, ...
 - infrastructure: local networks, wide-area networks, ...
- Examples of services
 - collaboration: wikis, forums, telepresence, ...
 - data: data transport, data management, sharing, curation, provenance, ...
 - access/used: authentication, authorization, accounting, ...
 - coordination: meta-queuing, ...
 - support: helpdesk, consulting, ECSS, training, ...
 - And many more: education, outreach, community building, ...

Current 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)



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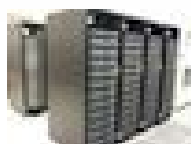
Current XSEDE Visualization and Data Resources

- Visualization



Nautilus @ UTK

- 8.2 TF SGI/NVIDIA SMP
- 960 TB disk



Maverick @ TACC

- HP/NVIDIA cluster
- 132 TB memory



TACC Visualization Portal

- Storage

- HPSS @ NICS

- 6.2 PB tape

- Data Supercell @ PSC

- 4 PB tape

- Ranch @ TACC

- 40 PB tape

- Data Oasis @ SDSC

- 4 PB tape



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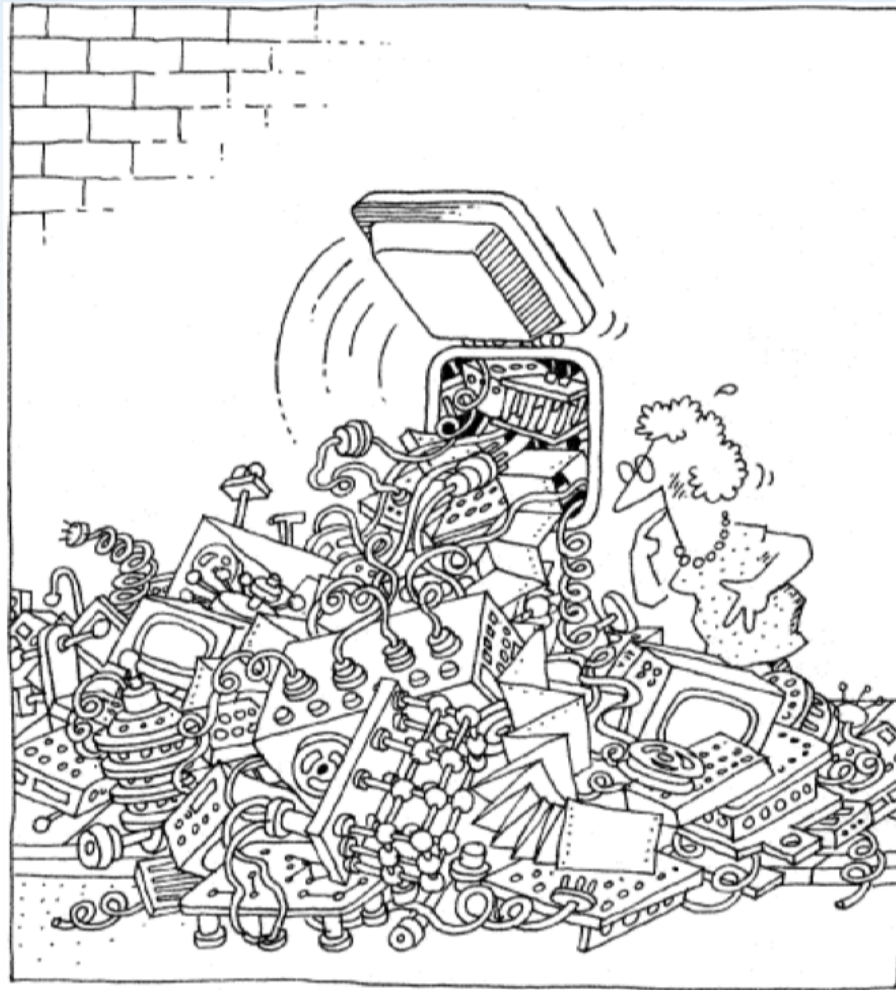
NCSA Blue Waters System

- 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



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Simple Enough?



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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 User Guides and News

- XSEDE provides intro user guides for every XSEDE-allocated system—no matter where it is actually hosted
 - Consistently structured and formatted
 - All available from website and XUP
 - Prepared using expertise of host sites
- XSEDE also provides up-to-date User News about every system, and XSEDE-wide services, available via:
 - Web/portal
 - Email
 - RSS feeds
 - Calendar feeds (for downtimes, training events, etc.)

XSEDE Allocations

- XSEDE allocates access/time on powerful, valuable systems providing different capabilities at NO COST TO YOU
 - HPC
 - High throughput computing
 - Remote visualization
 - Data storage
 - Etc.
- Users may request XSEDE staff support to assist with optimization of research codes, visualization, workflows, novel projects, and science gateways
- Single Sign-On allows you to use just one username and password (your User Portal one). You will be recognized by all XSEDE services on which you have an account, without having to enter your login information again for each resource.

XSEDE Allocations

- Request allocations through the XSEDE User Portal
- It's **easy** to get a 'Startup allocation' —best way to get started
- Education allocations for classroom use
- Larger year-long 'research' allocations can be requested 4 times/year, are peer reviewed, and have a longer lead-time
- Quarterly webinars on writing allocations

XSEDE offers more in-depth support via Extended Collaborative Support Service (ECSS)

- 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



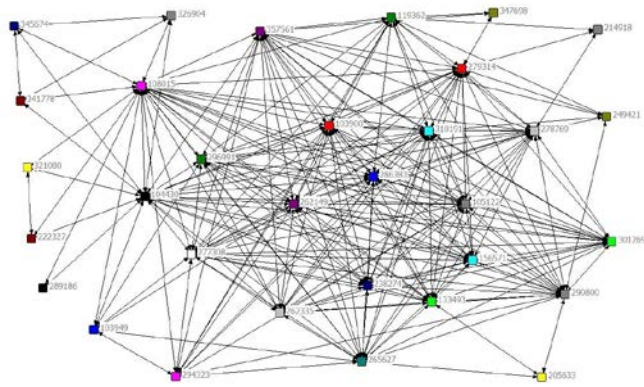
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Virtual Worlds Exploratorium

Marshall Scott Poole, Univ. of Illinois

- Analyze logs (over 10 TB) from several online games

TASK: “The variables of interest for research have to be derived from the game databases through complex analyses that transform the raw log data into terms meaningful for social science research. By taking advantage of massive parallel processing, efficient workflow management and abundant memory availability, access to XSEDE resources could enable us to speed up our research.”



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Large Genome Assemblies

- ECSS Staff working with leading researchers and code developers
- Largest ever metagenome assembly, using 3.5 TB RAM on PSC Blacklight
- Cold Spring Harbor collaboration to assemble wheat genome (17 Gigabases)

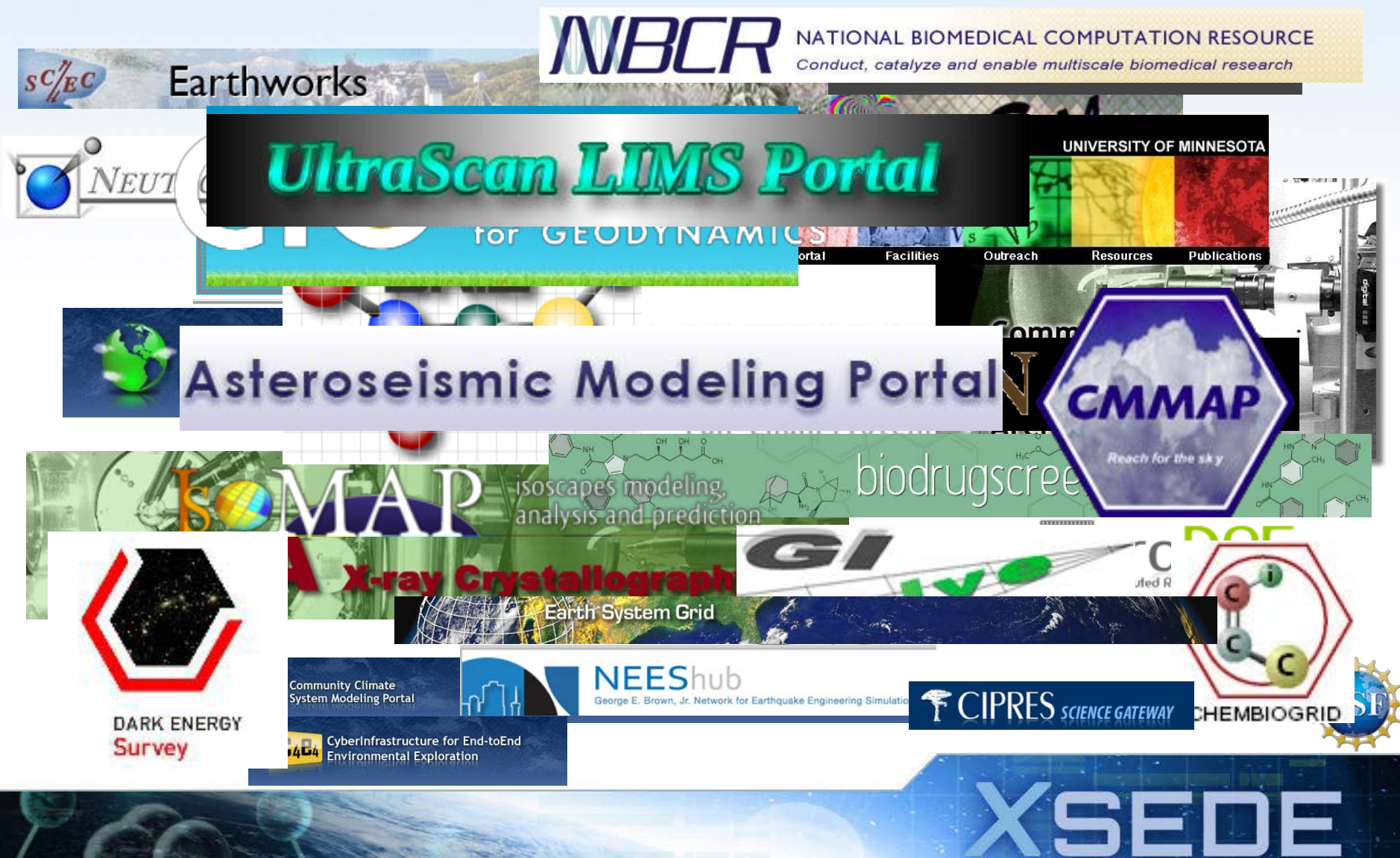
“I wouldn’t have been able to do anything on Blacklight without ECSS staff... (consultant) took a real interest and solved a lot of things that were hard for me. He found bugs in the software and got them resolved with the software authors. I’d worked for months and not made that progress. Without his expertise, I might have given up...”



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Science Gateways:

Today, there are approximately 35 gateways using XSEDE



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



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XSEDE Training

- XSEDE provides extensive training
 - Covering breadth of XSEDE resources
 - From beginner to advanced topics
 - At locations across the country
 - Online via
 - asynchronous technologies
 - Webcasts
 - High-def video conference summer schools
- All sessions posted on XSEDE User Portal
- Roadmaps for learning
- Quality reviewed materials
- Certification of learning



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Community Engagement Activities



- Student Engagement
- Faculty Engagement
- Under-represented Community Engagement
- Campus Engagement
- Champions Program
- Campus Bridging
- HPC University portal
- Annual XSEDE Conference

XSEDE Student Programs

- XSEDE Scholars
 - engaging undergraduates and graduates in year-long series of webinars attend annual XSEDE Conference
- Blue Waters Internship
 - 2 week training institute for undergrads and grads
 - year-long computational science problem solving
- Blue Waters Graduate Fellowship
 - similar to NSF Graduate Fellowships
 - year-long engagement
- International HPC Summer School
 - June 21-26, 2015 in Toronto, Canada
 - Applications due March 11, 2015
- XSEDE Annual Conference
 - travel support for students to attend the annual Conference
- HPC University
 - Lists other student engagement opportunities

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Other Student Opportunities

- Clemson Research Experience for Undergraduates in Collaborative Data Visualization Applications
- NICS Computational Science Research Experience for Undergraduates
- TACC Research Experience for Undergraduates: Integrative Computational Education and Research Traineeship
- LSU Center for Computation & Technology REU Interdisciplinary Research Experience in Computational Sciences <http://reu.cct.lsu.edu/>
- 2015 International Summer School on HPC Challenges in Computational Sciences – Graduate Students

Faculty Engagement Opportunities

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

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 Engagement Opportunities

- Campus Champions
- Campus Bridging
- Education – Computational Science Curriculum, Certificate, or Degrees
- Campus Visits
- Local and Regional Workshops and Institutes

Campus Champions Program

- Over 170 campuses are members – no cost to join
- Champions receive monthly training and updates
- Champions provided with start-up accounts
- Champions are members of User Services team
- Forum for sharing and interactions
- Access to information on usage by local users
- Community building across campuses

Campus Champions Role

- Raise awareness locally
- Provide training
- Get users started with access quickly
- Represent needs of local community
- Provide feedback to improve services
- Attend annual XSEDE14 conference
- Share their training and education materials
- Build community among all Champions

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.

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Education

- Competencies
 - Undergraduate, graduate, HPC
 - Adding data and domain
- Certificate and Degree Programs
 - Assist departments and colleges
- On-line courses
 - Engaging multiple campuses simultaneously
 - Credit for students at their own institution
- Curriculum development workshops
 - Held on host campuses
 - Being using other people's models
- Repository of reviewed materials – HPC University
- ACM SIGHPC Education Chapter

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



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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

SC15 Conference

- Austin, Texas
- November 15-20, 2015
- 10,000+ people – researchers, educators, students, decision makers, experts and novices
- Papers, panels, tutorials, BOFs, exhibits
- Student programs – travel support available

HPC University Portal

- Training and education resources
- Events worldwide
- Internship and fellowship opportunities
- Career opportunities
- Computational science and education blog

www.hpcuniversity.org

A decorative banner at the bottom of the slide. On the left, there is a blue and white image of a planet's horizon. In the center, there is a bright, glowing light source. On the right, the text 'XSEDE' is displayed in a large, white, sans-serif font against a dark blue background with a grid pattern.

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What Next?

- Getting Started
 - New User Training
- Need to Code or Port Code
 - Intro to Unix/Linux
 - Intro to Parallel Programming
 - MPI and OpenMP
 - CUDA™ GPU Programming
- Bioinformatics Topics
 - Galaxy, NAMD, Trinity, etc.
- Access the Workshop Materials
 - <http://hpcuniversity.org/trainingMaterials/188/>

Q&A Session

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

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Extreme Science and Engineering
Discovery Environment