

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

SURA

Indiana University

University of Chicago

Berkeley

Shodor

Ohio Supercomputer Center

Cornell

Purdue

Rice

NCAR

Jülich Supercomputing Centre

The XSEDE logo is displayed in a large, bold, white font against a dark blue background with a grid pattern. The letters are spaced out and have a slight shadow effect.



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.

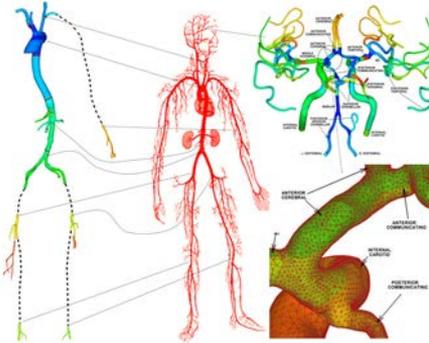
Why XSEDE?



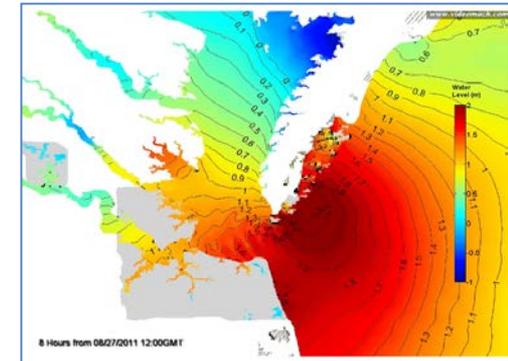
XSEDE

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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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



Greenfield

- 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

- 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.

XSEDE

New Resources

TACC 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.

SDSC Comet

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

Coming in 2016



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



A self-provisioned, scalable science and engineering cloud environment.

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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.

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

CIPRES: Science Gateway

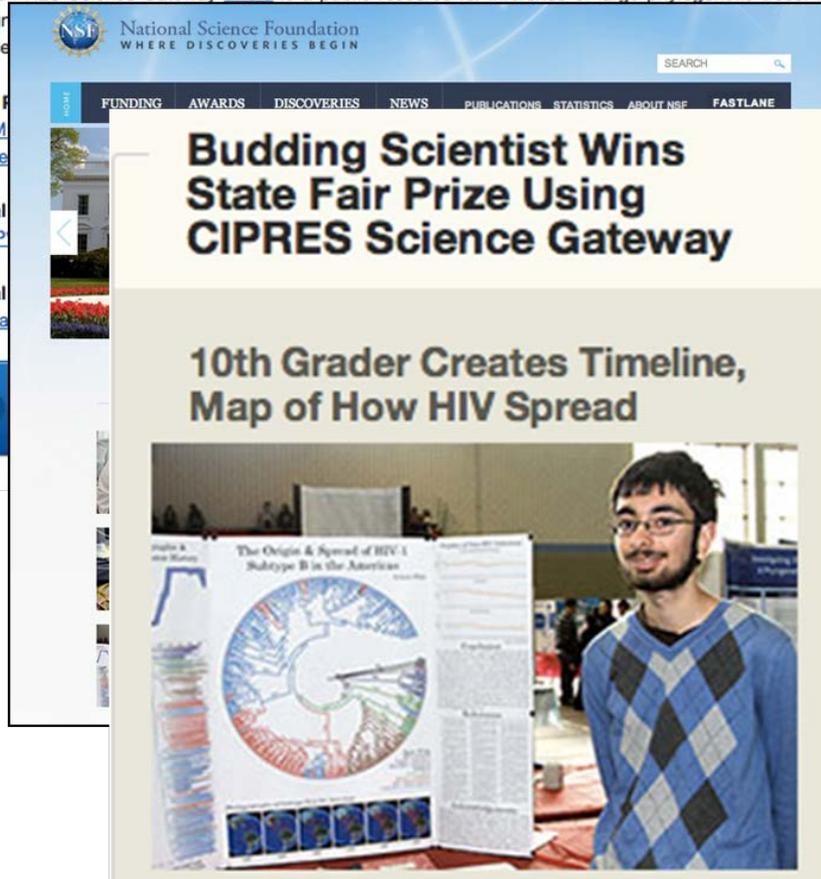
The CIPRES Science Gateway V. 3.3

The CIPRES Science Gateway V. 3.3 is a public resource for inference of large phylogenetic trees. It is designed to be simple to use.

High Performance Computing
RAXML
iModel

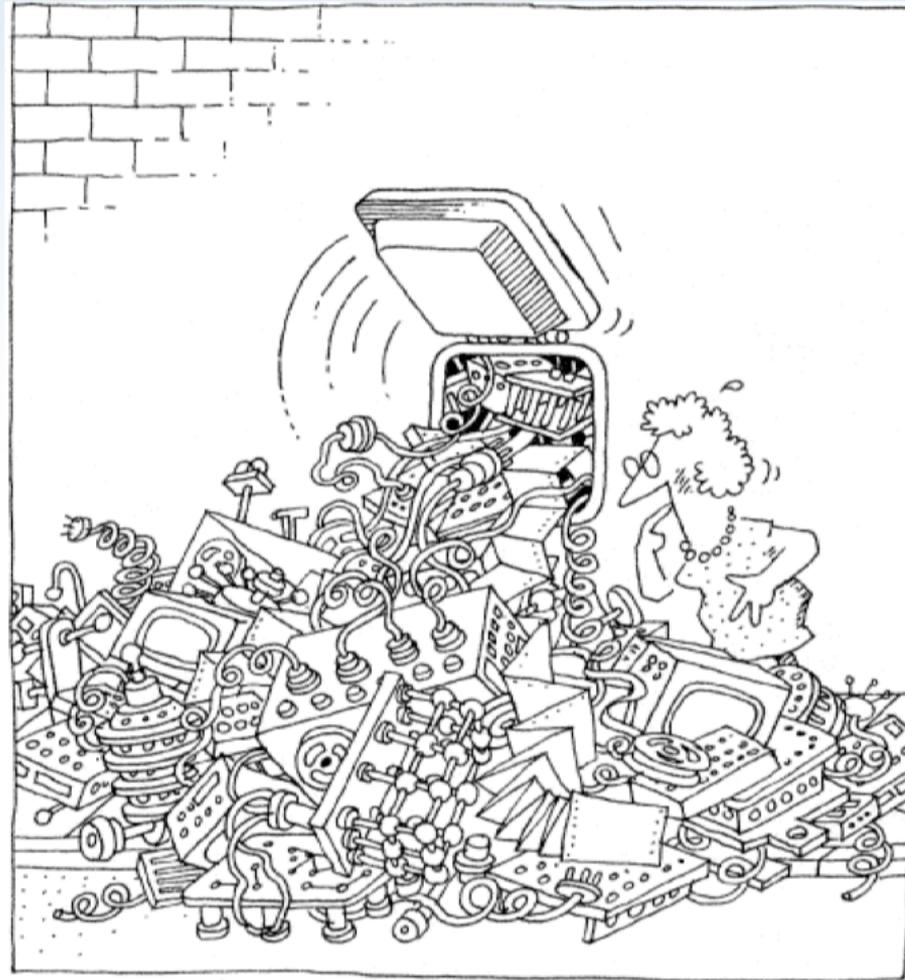
Serial
PAUP

Serial
Clustal



- Most popular gateway in XSEDE
 - ~40% of all XSEDE users
- In use on 6 continents
- Cited in major journals (Cell, Nature, PNAS)
- Used at major research institutions (Stanford, Harvard, Yale)
- Used by ~76 researchers for curriculum delivery
- Supports hundreds of publications every year (1570 to date)
- Used by a 15-year-old high school student who won state science fair with no support from SDSC staff

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XSEDE User Services

- 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

- Help Desk/Consultants

- Extended Collaborative Support Services

- Human resources to help with performance analysis, petascale 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

Community Engagement



Champions Program

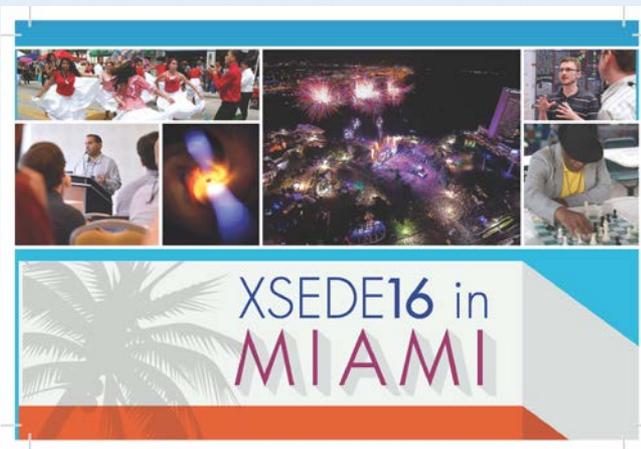
Campus Bridging

Education

Under-represented Community Engagement

Annual XSEDE Conference

XSEDE16 Conference July 17 – 21, 2016



- Submissions will be accepted for papers, panels, tutorials, BOFs, student programs
- Topics span accelerating discovery, advanced technologies, software, science gateways and portals, and workforce development & diversity.
- Expect over 600 people from academia, industry, government, and other organizations
- Support for student participation

Student Opportunities

- **XSEDE Scholars – Applications Due Feb 2016**
 - Year-long webinars
 - Travel to XSEDE Annual Conference
 - Internships
- **Blue Waters Internship – Applications Due Feb 2016**
 - 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
- **XSEDE Annual Conference**
 - travel support for students to attend the annual Conference

More Information

- XSEDE Website: www.xsede.org
- XSEDE Staff
 - Linda Akli, akli@sura.org (Community Engagement)
 - Jay Alameda, alameda@illinois.edu (Training/Consulting)
 - Steve Gordon, sgordon@osc.edu (Curriculum)
 - Daniel Lucio, dlucio@utk.edu (Training/Consulting)

Questions?



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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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Discovery Environment