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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 Advanced Computing 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

SURA Ohio Supercomputer Center

Cornell Indiana University

Purdue Rice

Shodor University of Chicago

National Center for Atmospheric Research





#### **XSEDE Mission and Goals**

Mission: Accelerate scientific discovery

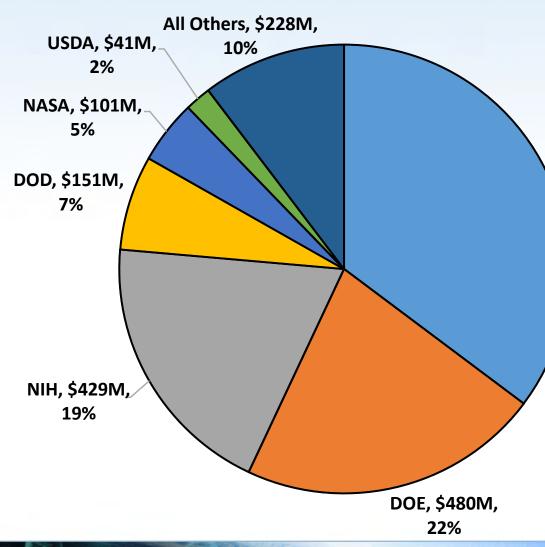
#### Goals:

- Deepen and Extend Use
  - Raise the general awareness of the value
  - Deepen the use and extend use to new communities
  - Contribute to the preparation of current and next generation scholars, researchers, and engineers
- Advance the Ecosystem
- Sustain the Ecosystem





### **Total Research Funding Supported by XSEDE**



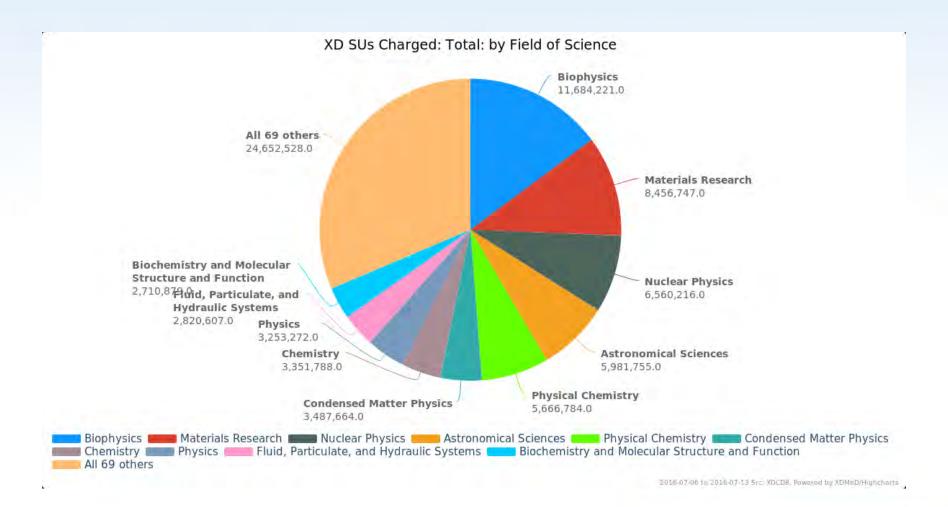
Research funding only. XSEDE leverages and integrates additional infrastructure, some funded by NSF (e.g. Track 2 systems) and some not (e.g. Internet2).

NSF, \$778M, 35%

\$2.21 billion in research supported by XSEDE July 2011-May 2016

XSEDE

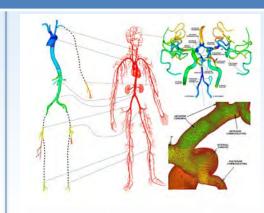
#### Field of Science Using XSEDE



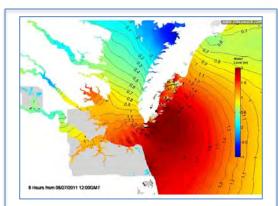


### **XSEDE Supports a Breadth of Research**

- 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.







Ruby Mendenhall, an associate professor of sociology, African American studies and urban and regional planning at the University of Illinois (UI) at Urbana-Champaign, is leading a collaboration of social scientists, humanities scholars and digital researchers that hopes to harness the power of high-performance computing to find and understand the historical experiences of black women by searching two massive databases of written works from the 18th through 20th centuries.





# Why XSEDE?







## **XSEDE Compute Resources**



- Featuring interactive on-demand access, tools for gateway building, and virtualization.
- SDSC Comet: hosting a variety of tools including Amber, GAUSSIAN, GROMACS, Lammps, NAMD, and Vislt.
- Jetstream A self-provisioned, scalable science and engineering cloud environment
- TAGE Stampede: Intel's new innovative MIC technology on a massive scale
- L5U Super Mic: Equipped with Intel's Xeon Phi technology. Cluster consists of 380 compute nodes.
- TAGG 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.





#### **XSEDE Visualization and Data Resources**

#### Visualization



#### Maverick@ TACC

- HP/NVIDIA cluster
- 132 TB memory
- Vislt
- ParaView
- Interactive Data Language



#### **TAGG** Visualization Portal

- Remote, interactive, webbased 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: Standalone storage allows storage allocations independent of a compute allocation.

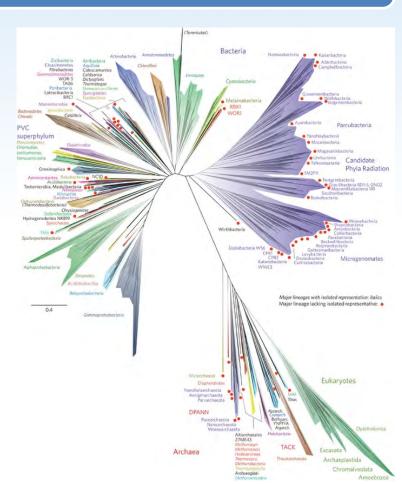




# **Science Gateways**



The CIPRES science gateway: A NSF investment launching thousands of scientific publications with no sign of slowing down.



 $\underline{https://sciencenode.org/feature/cipres-one-facet-in-bold-nsf-vision.php?clicked=title}$ 



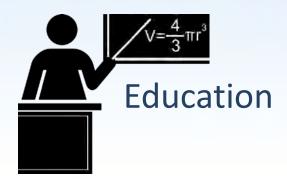
# Allocations



Champion





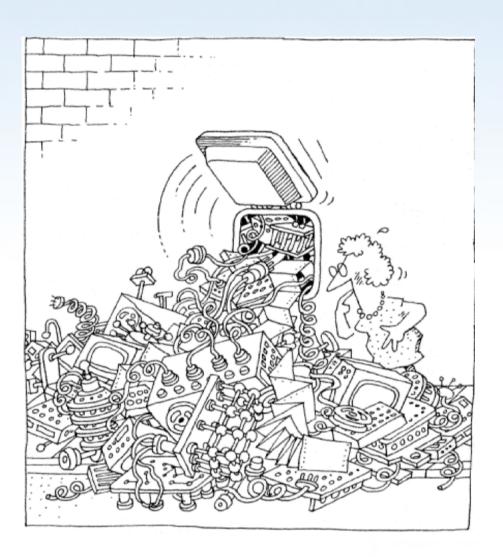




Research







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## **Other Resources**

**Technical information** 

**Training** 

Help Desk/Consultants

**Extended Collaborative Support Services** 



### **Community Engagement & Enrichment (CEE)**



Workforce Development

**User Engagement** 

**Broadening Participation** 

**User Interfaces & Online Information** 

Campus Engagement



### **Campus Engagement: Champions Program**

**Campus Champions** 

**Student Champions** 

**Regional Champions** 

**Domain Champions** 





### **Workforce Development: Education Program**

Development of competencies for undergraduate and graduate computational science programs

Campus visits to promote computational science

**Facilitates Collaborative Online Courses** 



# **Workforce Development: 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





### **Workforce Development: EMPOWER**

PROJECTS: Computational, Data Analytics, Visualization Research or Networking and System Maintenance

**MENTORS** are XSEDE staff, researchers, and educators who recruit and mentor undergraduate students to engage in projects.

**STUDENTS** are undergraduates who participate as a learner, apprentice or intern participation for students.

**COMPENSATION:** Ranges from \$750 to \$3,000 (based on student level and duration)

**PROJECT PROPOSALS** must contain a Training plan for the student.





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## **Faculty Opportunities**

Use XSEDE Resources for research or teaching

Attend a webinar or in-person training

Use online training materials (XSEDE and HPC University)

Participate in a faculty development workshop

Attend PEARC17, New Orleans, July 9 - 13 <a href="http://www.pearc.org/">http://www.pearc.org/</a>





### **Student Opportunities**

Attend a training event <a href="https://www.xsede.org">www.xsede.org</a>

Apply for Travel Support, Present a Poster or Visualization at PEARC17 <a href="https://www.pearc.org/student-program">https://www.pearc.org/student-program</a>

Apply to XSEDE's Empower Student Internship Program <a href="http://computationalscience.org/xsede-empower">http://computationalscience.org/xsede-empower</a>

Participate in the SC17Student Cluster Challenge, Nov 12 – 17 <a href="http://sc17.supercomputing.org/studentssc/student-cluster-competition/">http://sc17.supercomputing.org/studentssc/student-cluster-competition/</a>

Visit HPC University for more student opportunities. www.hpcuniversity.org



# **Workshop Agenda**

#### Today

- Research @SUBR with XSEDE resources
- Break
- Computational Thinking w/Kate Cahill (OSC)

#### **Tomorrow Morning**

New User Training w/Jay Alameda (NCSA)

#### Tomorrow Afternoon (a choice of two sessions)

- Python w/Antonio Gomez (TACC)
- Matlab w/Anirban Jana (PSC)



#### **More Information**

- Today's XSEDE Presentations -<a href="http://hpcuniversity.org/trainingMaterials/237/">http://hpcuniversity.org/trainingMaterials/237/</a>
- XSEDE Website: <u>www.xsede.org</u>
- XSEDE Staff
  - Linda Akli, <u>akli@sura.org</u>
  - Jay Alameda, <u>alameda@illinois.edu</u> (New User & ECSS)
  - Kate Cahill, <u>cahill.167@osu.edu</u> (Education & Curriculum)
  - Antonio Gomez, <u>agomez@tacc.utexas.edu</u>, Python
  - Anirban Jana, <u>anirban@psc.edu</u>, Matlab
  - Rachel Vincent-Finley, <u>rachel\_finley@subr.edu</u>



# Questions



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