# XSEDE Overview January 2019



Extreme Science and Engineering Discovery Environment

Linda Akli, SURA
Assistant Director, Education, Training, Outreach
Manager, XSEDE Broadening Participation Program

## Code of Conduct

- XSEDE has an external code of conduct for XSEDE sponsored events which represents XSEDE's commitment to providing an inclusive and harassment-free environment in all interactions regardless of gender, sexual orientation, disability, physical appearance, race, or religion. The code of conduct extends to all XSEDE-sponsored events, services, and interactions.
- Code of Conduct: <a href="https://www.xsede.org/codeofconduct">https://www.xsede.org/codeofconduct</a>
- Contact:
  - Event organizer: XSEDE Community Engagement & Enrichment
  - XSEDE ombudspersons:
    - Linda Akli, Southeastern Universitites Research Association, (<u>akli@sura.org</u>)
    - Lizanne Destefano, Georgia Tech (<u>lizanne.destefano@ceismc.gatech.edu</u>)
    - Ken Hackworth, Pittsburgh Supercomputing Center, (<u>hackworth@psc.edu</u>)



# 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 Leadership

Partnership led by









Partners who strongly complement these CI centers with expertise in science, engineering, technology and education





### Mission and Goals

Mission: Accelerate scientific discovery

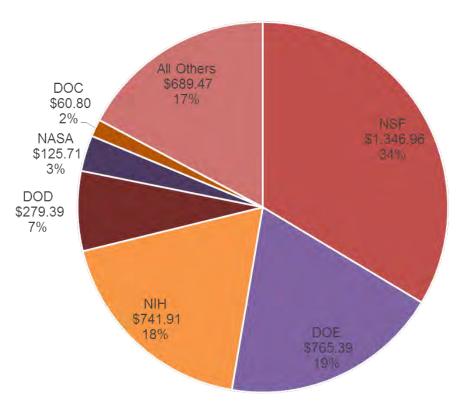
#### Strategic Goals:

- 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





#### Research Funding Supported by XSEDE, 2011-2018 (\$M)



- The chart shows the total user-reported supporting grant funding, by agency, on XSEDE-allocated projects with resource activity.
- Where possible, grant information for NSF awards is taken from NSF Award Search.
- Supporting grants listed by multiple projects are counted ONCE using the average of the dollar values provided.





# XSEDE Supports a Breadth of Research

Earthquake Science

Molecular Dynamics

Nanotechnology

**Plant Science** 

Storm Modeling

**Epidemiology** 

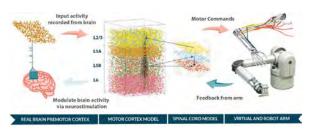
Particle Physics

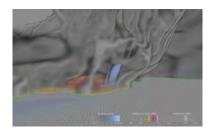
**Economic Analysis of Phone Network Patterns** 

Large Scale Video Analytics (LSVA)

**Library Collection Analysis** 

Replicating Brain Circuitry to Direct a Realistic Prosthetic Arm





XSEDE researchers visualize massive Joplin, Missouri tornado





# **Compute and Analytics Resources**



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



Comet: hosting a variety of tools including Amber, GAUSSIAN, GROMACS, Lammps, NAMD, and Vislt.



Jetstream: A self-provisioned, scalable science and engineering cloud environment



Stampede-2: Intel's new innovative MIC technology on a massive scale



Super Mic: Equipped with Intel's Xeon Phi technology. Cluster consists of 380 compute nodes.



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**

#### **Remote Visualization**

#### **TACC 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.

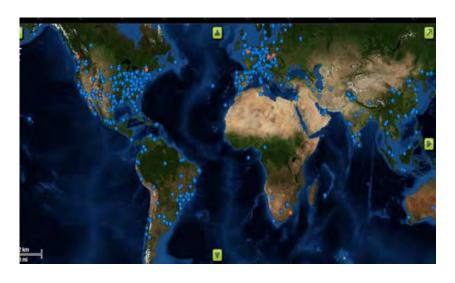
#### Stand-alone Storage:

Stand-alone storage allows storage allocations independent of a compute allocation.

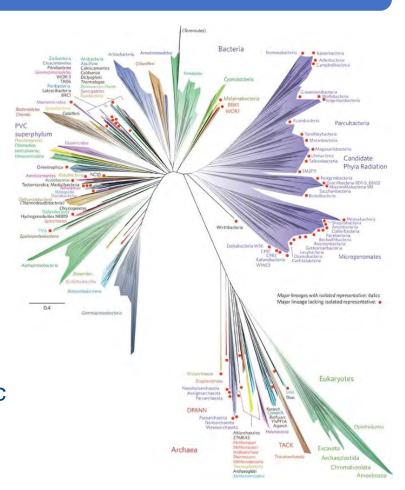




# **Science Gateways**



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



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





# **XSEDE User Support Resources**



Technical information



**Training** 



Help Desk/Consultants



Extended Collaborative Support Service





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

**Broadening Participation** Campus Engagement **User Engagement** User Interfaces & Online Information Workforce Development



# XSEDE Broadening Participation



**Campus Visits** 

**Community Listserv** 

Conference Exhibiting

Consulting

**Travel Support** 

**Training Events** 





# **Workforce Development: Education Program**

Develop, identify, & maintain computational science program competencies

Promote computational science

Provide consulting for program development and plans

Facilitate Collaborative Online Courses





# **Workforce Development: Student Programs**



Advanced Computing for Social Change and Compute4Change



Empower (Expert Mentoring Producing Opportunities for Work, Education, and Research)



**Student Champions** 

#### **EMPOWER**

**PROJECTS:** Computational, Data Analytics, Visualization, Networking and System Maintenance

**MENTORS** are XSEDE staff, researchers, and educators who recruit and mentor students.

**STUDENTS** are undergraduates who participate as a learner, apprentice or intern

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

**Project proposals** from mentors must contain a training plan for the student.



# **Workforce Development: Training**

XSEDE Training Course Catalog with all materials in a single location

<u>Course Calendar</u> for viewing a listing of and registering for upcoming training events and a registration

Online Training on materials relevant to XSEDE users

Badges available for completing selected training

Some events provide participation documentation

Training Roadmaps









# **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 PEARC19, July 28<sup>th</sup> – Aug 1<sup>st</sup>, https://www.pearc19.pearc.org/





# **Student Opportunities**

Attend a training event – webinar or in-person

Present a Poster or Visualization at PEARC19

Apply to XSEDE's Empower Student Internship Program

Participate in the Advanced Computing for Social Change @PEARC19

Participate in Compute4Change @SC19, Denver, Nov 17<sup>th</sup> – 22<sup>nd</sup>

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



# Workshop Agenda

Today	Computational Thinking for Educators, Kate Cahill
	Lunch w/ Science Talks and Consulting
	XSEDE New User Training, Jay Alameda
	Introduction to Python, Je'Aime Powell
Tuesday	XSEDE New User Training, Jay Alameda
	Introduction to Linux/Unix, Je'Aime Powell
	Lunch w/Science Talks and Consulting
	Computational Thinking for Educators, Kate Cahill
	Low Cost Cluster Administration, Eric Coulter
	Consulting



#### **More Information**

Linda Akli, akli@sura.org

Dr. Tandabany, CAU Campus Champion, Tandabany, dtandabany@cau.edu

Dr. Tekle, Spelman Campus Champion, ytekle@spelman.edu

XSEDE Website – <a href="http://xsede.org">http://xsede.org</a>

Workshop materials - <a href="http://hpcuniversity.org/trainingMaterials/244/">http://hpcuniversity.org/trainingMaterials/244/</a>





Extreme Science and Engineering Discovery Environment

# Welcome to XSEDE!