March 11, 2021

XSEDE Overview

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Education & Training Specialist
Manager, XSEDE Education Programs

XSEDE

Extreme Science and Engineering
Discovery Environment

Code of Conduct

XSEDE has an external code of conduct which represents our commitment to providing an inclusive and harassment-free environment in all interactions regardless of race, age, ethnicity, national origin, language, gender, gender identity, sexual orientation, disability, physical appearance, political views, military service, health status, or religion. The code of conduct extends to all XSEDE-sponsored events, services, and interactions.

Code of Conduct: https://www.xsede.org/codeofconduct

Contact:

- XSEDE Event organizer: Kate Cahill, kcahill@osc.edu

- XSEDE ombudspersons:
  - Linda Akli, Southeastern Universities Research Association (akli@sura.org)
  - Lizanne Destefano, Georgia Tech (lizanne.destefano@ceismc.gatech.edu)
  - Ken Hackworth, Pittsburgh Supercomputing Center (hackworth@psc.edu)
  - Bryan Snead, Texas Advanced Computing Center (jbsnead@tacc.utexas.edu)

- Anonymous reporting form available at https://www.xsede.org/codeofconduct.

NSF XSEDE

Terminology Statement

In line with XSEDE's Code of Conduct, XSEDE is committed to providing training events that foster inclusion and show respect for all. This commitment applies not only to how we interact during the event; it also applies to the training materials and presentation. It is not XSEDE's position to use, condone, or promote offensive terminology.

XSEDE instructors strive to keep inclusive language at the forefront. In the event that we have included inappropriate materials, verbal or written, please let us know at terminology@xsede.org

While XSEDE has no control over external third-party documentation, we are taking steps to effect change by contacting the relevant organizations; we hope this will be addressed by all third parties soon.

If you see any terminology concerns in the following presentation or slides, we want to know!
*Please contact the Terminology Task Force: terminology@xsede.org*

What is Advanced Computing?

Resources and Services that support compute- and data-intensive research, which are too expensive to be purchased and operated by an individual research group, department and, in some cases, institutions.

- Cloud Computing
- Data Intensive Computing
- Parallel Computing
- High Performance Computing
- Supercomputing
- Data Analytics
- Data Mining
- Data Science
- Data Visualization
- Modeling and Simulation
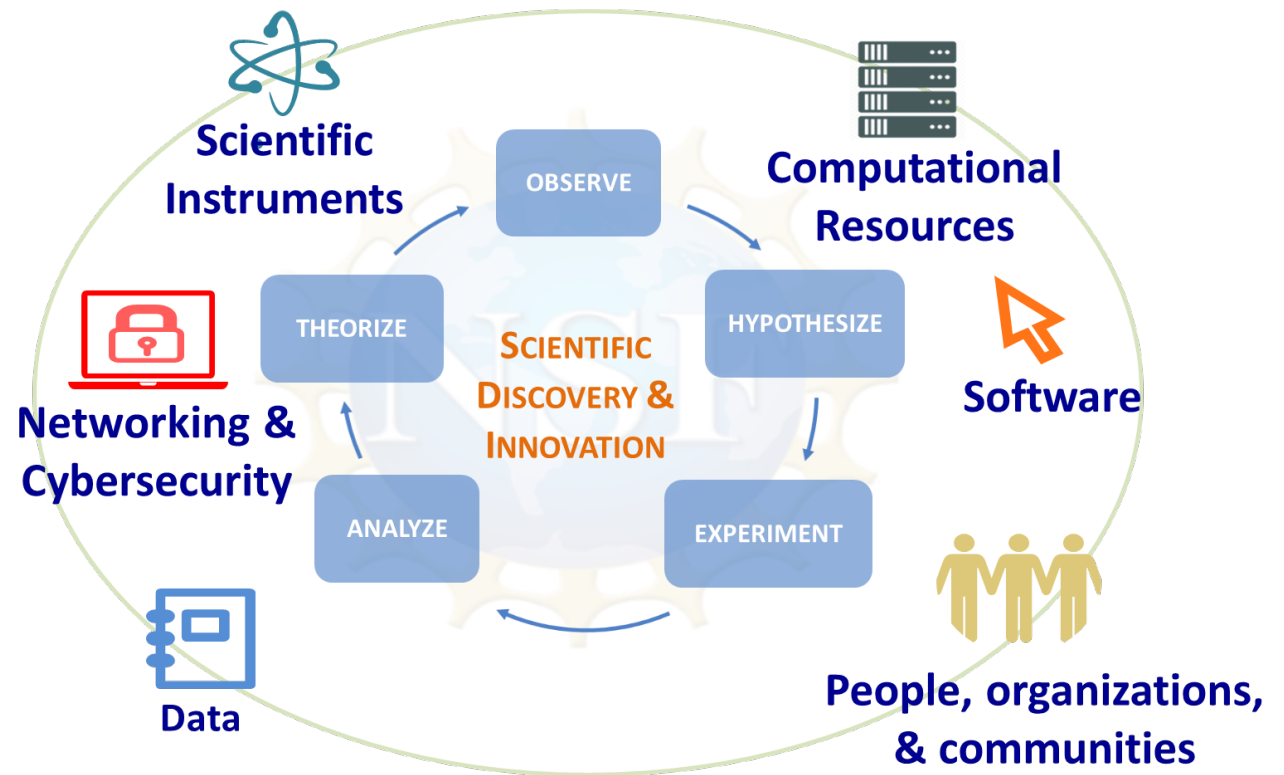
Simulation in Science and Engineering

High performance computing (HPC) simulation to understand things that are:

- too big
- too small
- too fast
- too slow
- too expensive or
- too dangerous

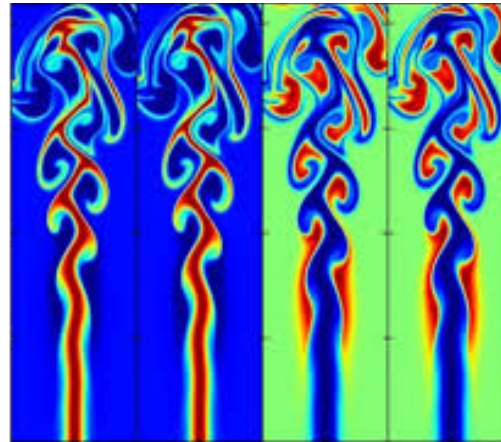for experiments

Applications of Parallel Computing:
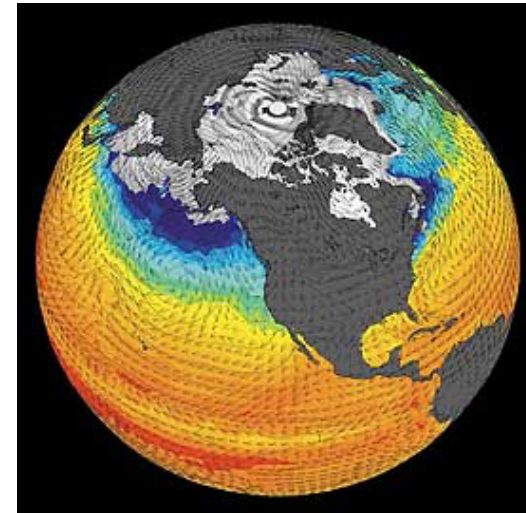https://www.youtube.com/watch?v=o7DQd8FkA6M&list=PLkFD6_40KJIx1CL7aIN9BwFL_sttEzfQ7&index=1&t=1s

Understanding the universe

Proteins and diseases

Energy-efficient jet engines

Climate change

Data analytics in science and engineering

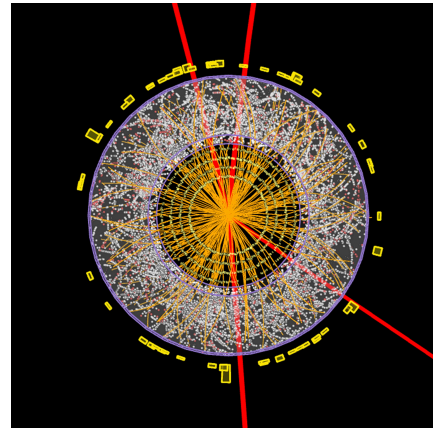Data analytics is used to analyze data sets that are:

- too big
- too complex
- too fast (streaming)
- too noisy
- too heterogeneous

for theory alone

Images from telescopes

Genomes from sequencers

Particle from detectors

Sensor data

XSEDE

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

NCSA   PSC   TACC   SDSC

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

SURA Southeastern Universities Research Association	THE SHODOR EDUCATION FOUNDATION, INC.	NICS	OU	OKLAHOMA STATE UNIVERSITY
Ohio Supercomputer Center An OH-TECH Consortium Member	PURDUE UNIVERSITY	UNIVERSITY OF ARKANSAS	USC University of Southern California	NCAR
THE UNIVERSITY OF CHICAGO	INDIANA UNIVERSITY	Cornell University	Georgia Tech	The University of Georgia

Strategic Goals

Deepen and Extend Use

- *Deepen the use of the advanced digital ecosystem for existing scholars, researchers, and engineers.*
- *Extend the use to new communities*
- **Contribute to the preparation and workforce development of scholars, researchers, and engineers in the use advanced digital technologies via training, education, and outreach**
- *Raise the general awareness of the value of advanced digital research services*
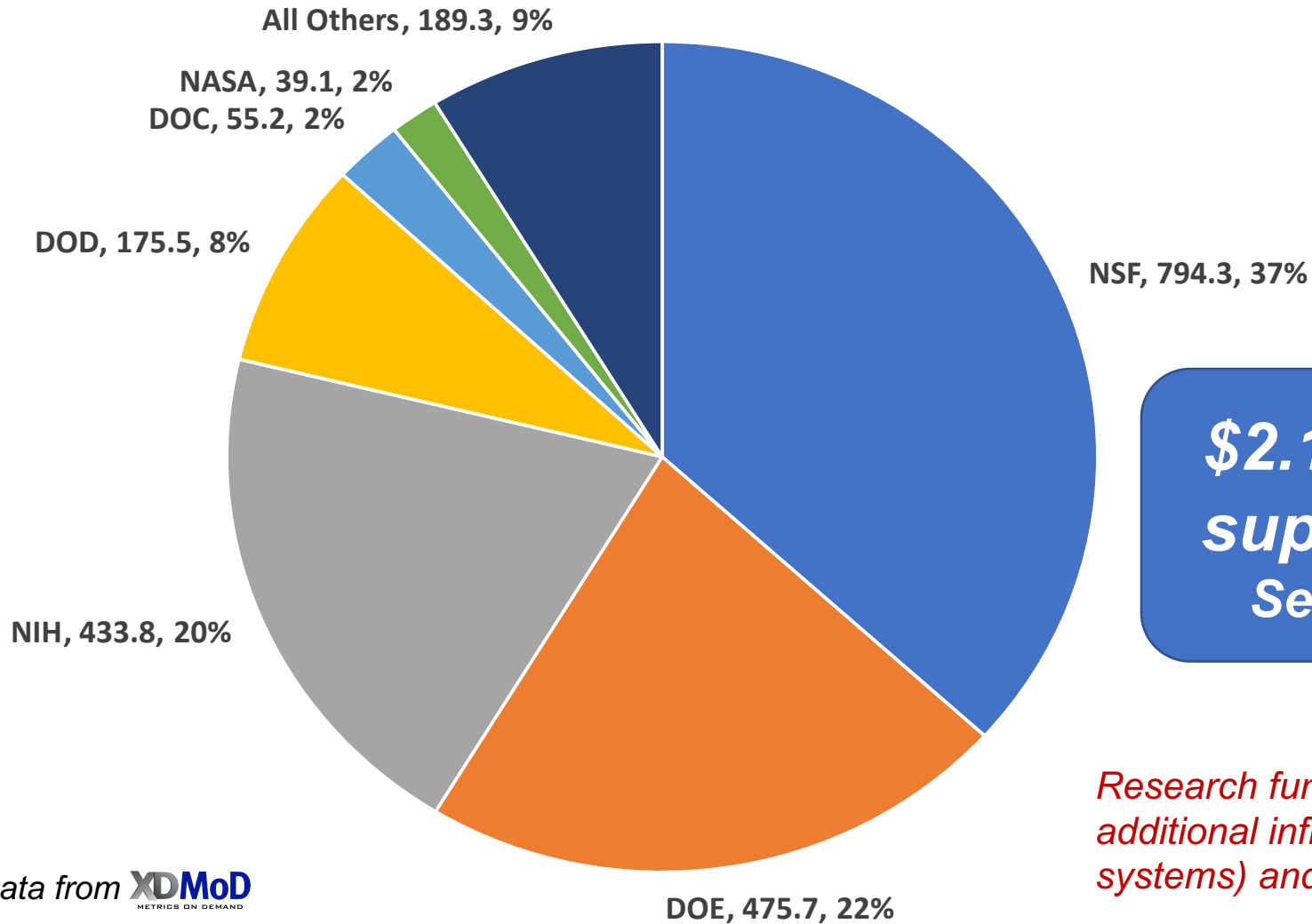
Advance the Ecosystem

- *Create and open and evolving infrastructure*
- *Enhance the array of technical expertise and support services offered*

Sustain the Ecosystem

- *Ensure and maintain a reliable, efficient, and secure infrastructure*
- *Provide excellent user support services*
- *Operate and effective and productive virtual organization*
- *Operate an innovative virtual organization*

NSF XSEDE

Total Research Funding Supported by XSEDE

All Others, 189.3, 9%

NASA, 39.1, 2%

DOC, 55.2, 2%

DOD, 175.5, 8%

NIH, 433.8, 20%

DOE, 475.7, 22%

NSF, 794.3, 37%

$2.16 billion in research supported by XSEDE 2.0
September 2016 - May 2019

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

Data from XDMoD
METRICS ON DEMAND

XSEDE Supports a Breadth of Research

Biomedical

- "Deep learning" Artificial Intelligence on XSEDE Systems Promises Fewer False Alarms and Early Prediction of Breast Cancer Development
- Understanding HIV

Climate and Environment

- Machine Learning Enables Scientists to Spot "Comma-Shaped Clouds," Extreme Weather
- Identifying Genes Associated with Surviving Climate Change
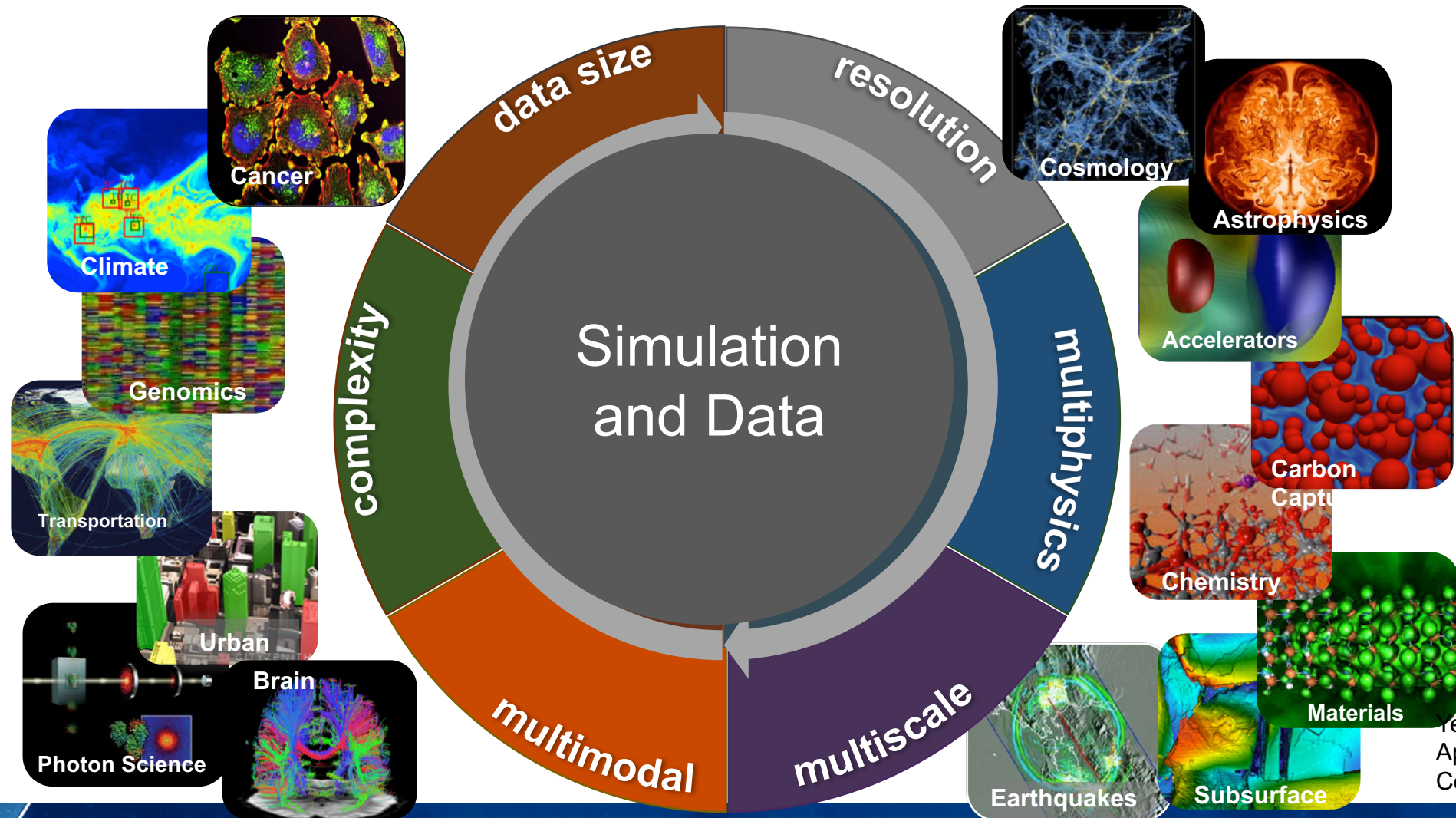- Gateway for Hawaiian Water Security

Humanities and Social Sciences

- Data Mining of Historical Narratives
- Six Degrees of Francis Bacon

XSEDE

Breakthrough Science at the Exascale
will combine simulation and data analysis

Simulation and Data

data size

resolution

multiphysics

multiscale

multimodal

complexity

Cancer

Climate

Genomics

Transportation

Urban

Photon Science

Brain

Cosmology

Astrophysics

Accelerators

Carbon Capture

Chemistry

Materials

Earthquakes

Subsurface

Yelick, UC Berkeley, Applications of Parallel Computing

NSF

XSEDE

XSEDE Allocated 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 VisIt.

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 Allocated Storage Resources

Distributed Data Storage Service to support active data sharing and transfer between academic institutions

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.

XSEDE

Science Gateways

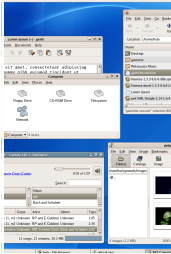

The CIPRES science gateway: A NSF investment launching thousands of scientific publications with no sign of slowing down.

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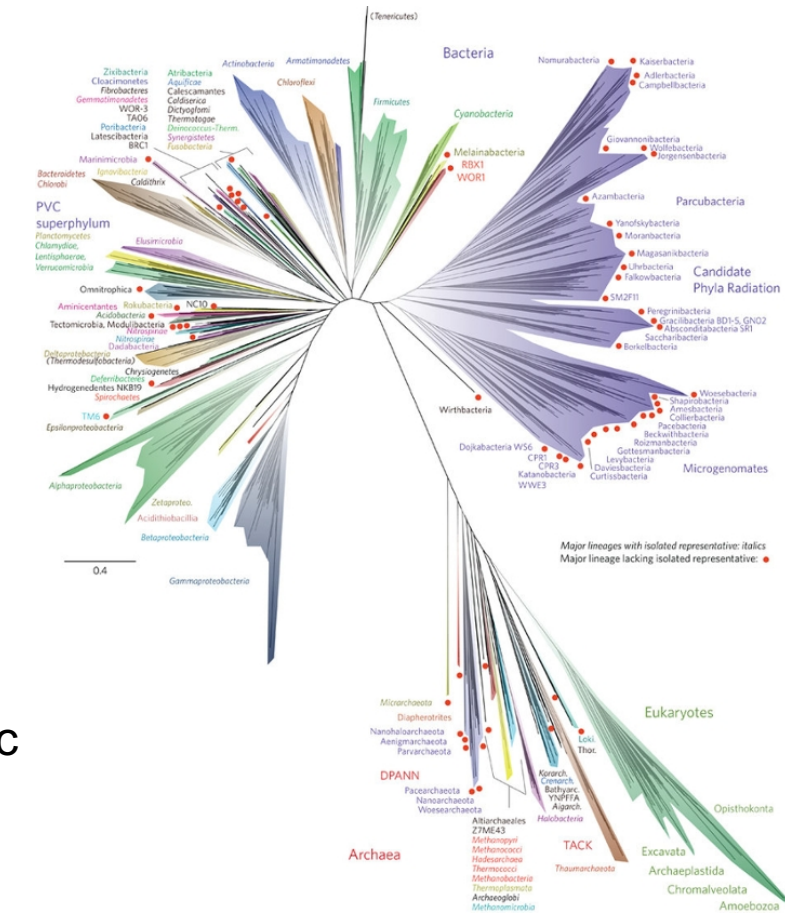
XSEDE User Support Resources

Technical information

Training

Help Desk/Consultants

Extended Collaborative Support Service

Cyberinfrastructure Resource Integration

Mission: To leverage the aggregate national cyberinfrastructure in XSEDE Service Providers, campuses, and regional partnerships in order to maximize support for research initiatives.

- Help propagate the best practices from the supercomputing centers that support XSEDE.
- Provide resources for campus cyberinfrastructure staff to leverage.
- Make it easier for researchers transitioning from campus to XSEDE.
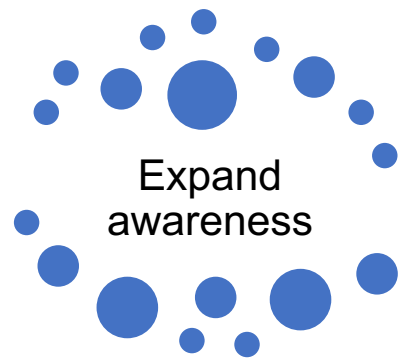
Community Engagement & Enrichment (CEE)

Workforce Development	User Engagement
Broadening Participation	Campus Engagement

XSEDE Broadening Participation Program

Expand awareness

Identify programs and researchers who can benefit from XSEDE services

Enable institutions and faculty to use advanced computing to increase their research productivity

Create scalable and sustainable models and best practices

- Campus Visits
- Conference Exhibiting
- Papers
- News

- Conference Exhibiting
- Campus Visits
- Training Events
- Consulting

- Build and Maintain a Thriving Peer Support Community
- Deliver Customized Training
- Connect Researchers with Expertise and Resources

- Enhance Curriculum
- Foster Productive Campus Champions
- Create Connections to the CI Ecosystem

XSEDE

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 $1,000 to $6,000 (based on student level and duration)

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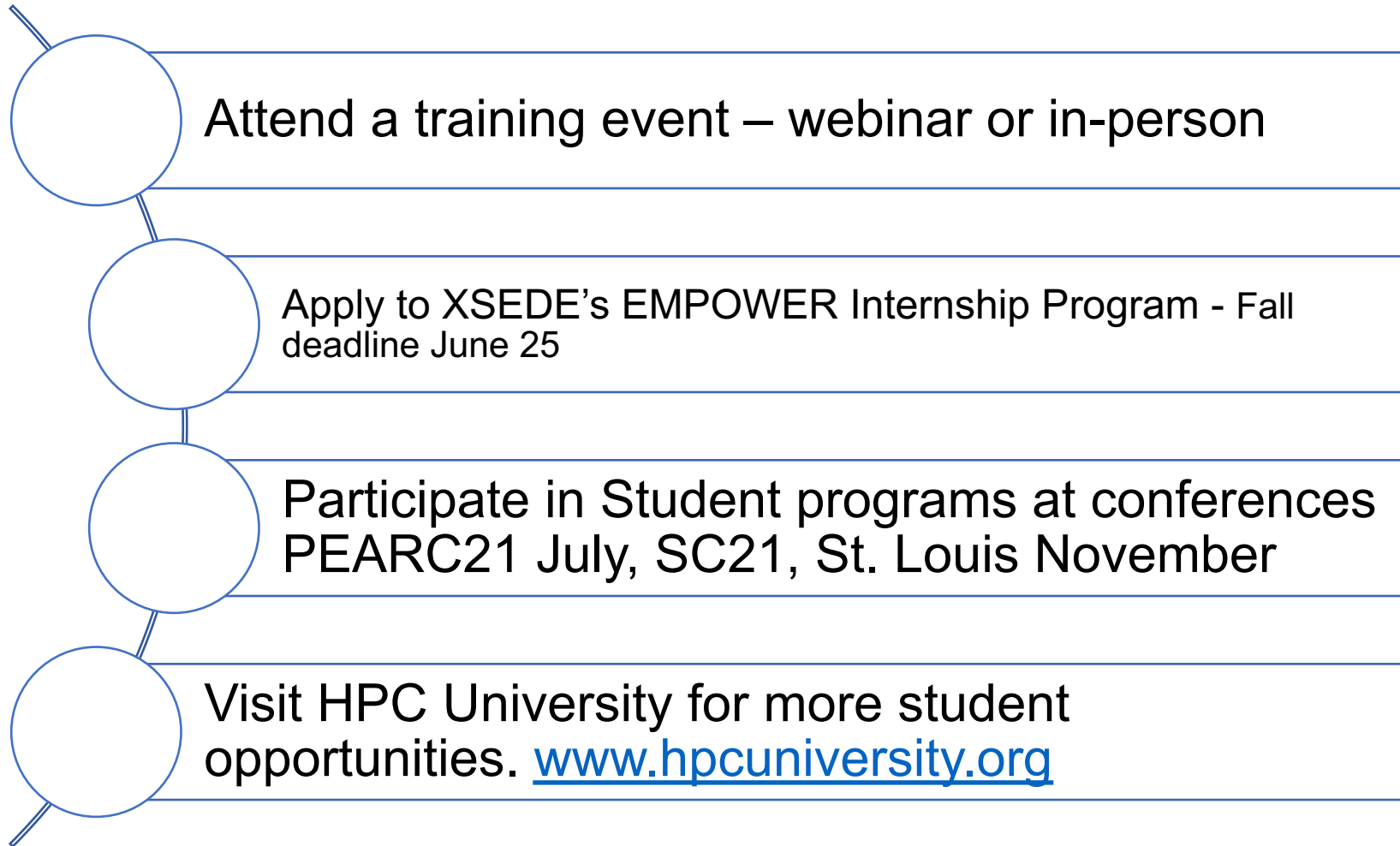
XSEDE Training

Training is available in a variety of formats, including multicast, webinars, online training, and in person workshops. Suggestions for new topics are encouraged via the feedback form. For more information, see:

- XSEDE Training Overview for a summary guide of materials available

- XSEDE Training Course Catalog including listings across formats and sites

- Course Calendar with registration for upcoming training courses

- Online Training on materials relevant to XSEDE users

- Badges are available for some topics and more are under development.

- Roadmaps are available and more under development.

Training materials focus on systems and software supported by the XSEDE Service Providers, covering programming principles and techniques for using resources and services. Training classes are offered in high performance computing, visualization, data management, distributed and grid computing, science gateways, and more.

Student Opportunities

Attend a training event – webinar or in-person

Apply to XSEDE's EMPOWER Internship Program - Fall deadline June 25

Participate in Student programs at conferences PEARC21 July, SC21, St. Louis November

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

Faculty Opportunities

Use XSEDE Resources for research or teaching

Attend a webinar or in-person training

Use online training materials (XSEDE and HPC University)

Mentor an EMPOWER student – Fall deadline July 10

Attend PEARC20, July 26-30, 2020 | Virtual
https://www.pearc19.pearc.org/

Computational and Data Science Curriculum Support

Preparing Students

Need for a workforce which understands both modeling and simulation principles and applications of models and data analysis at large scale

- Requirements for high fidelity models of complex systems
- Managing and understand large datasets – data science
- Applications across a wide range of science, social science, and increasingly humanities
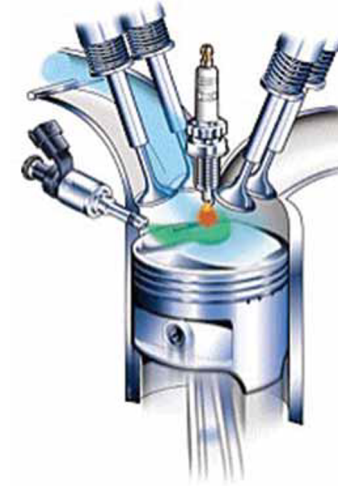
Crucial Tools for Manufacturing

At Ford, HPC …allows us to build an environment that continuously improves the product development process, speeds up time-to-market and lowers costs.

Ford EcoBoost Technology

The ongoing use of modeling and simulation resulted in new packaging and product design that propelled the brand to a leading market position over a several-year period.
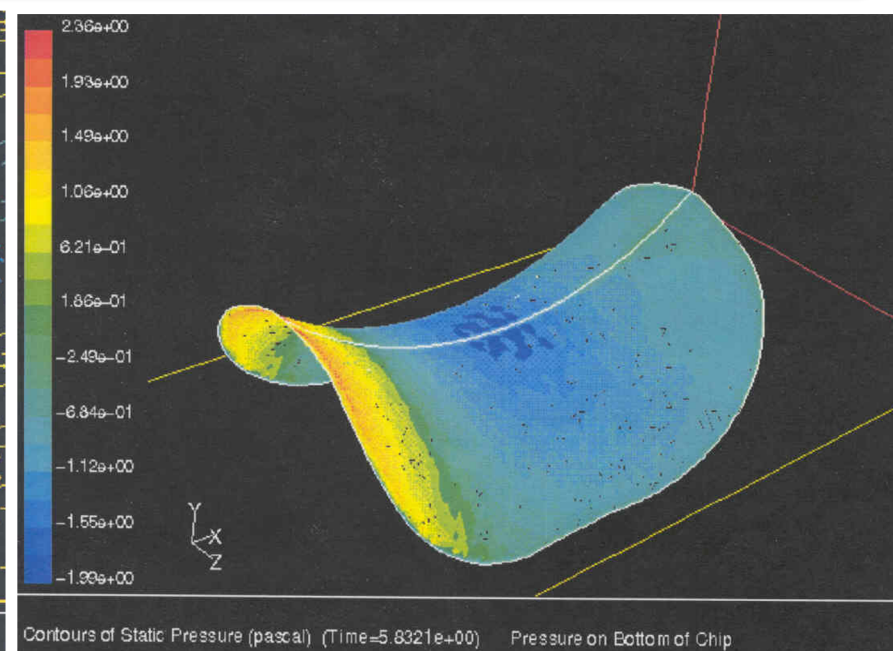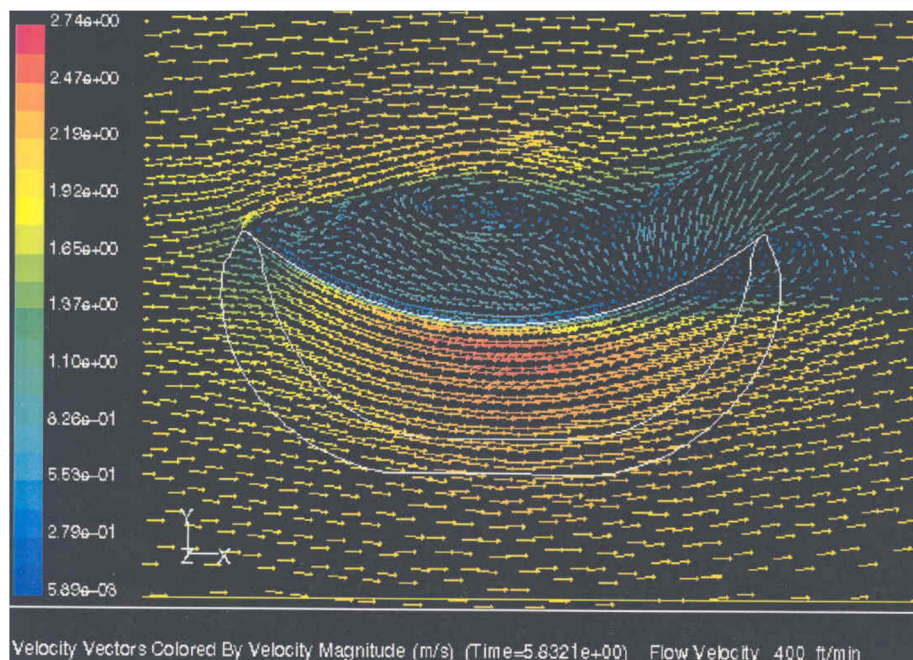
Durable coffee package for P&G

XSEDE

Will Pringles Fly?
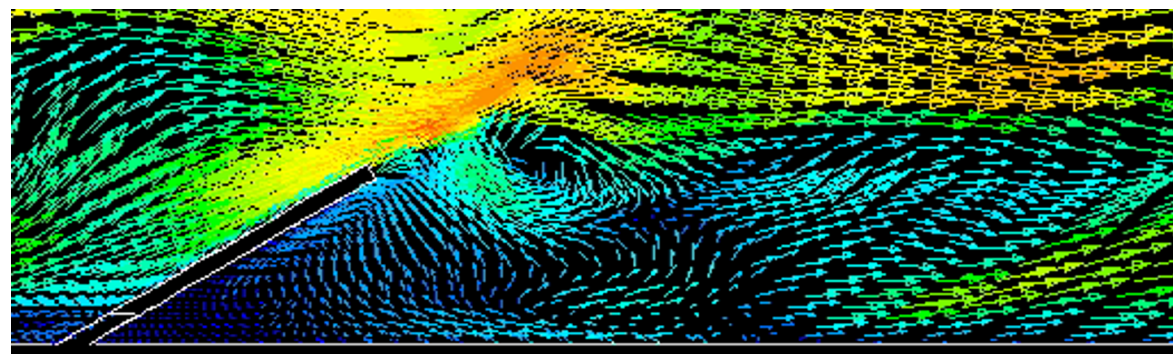

Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=5.8321e+00)   Flow Velocity 400 ft/min

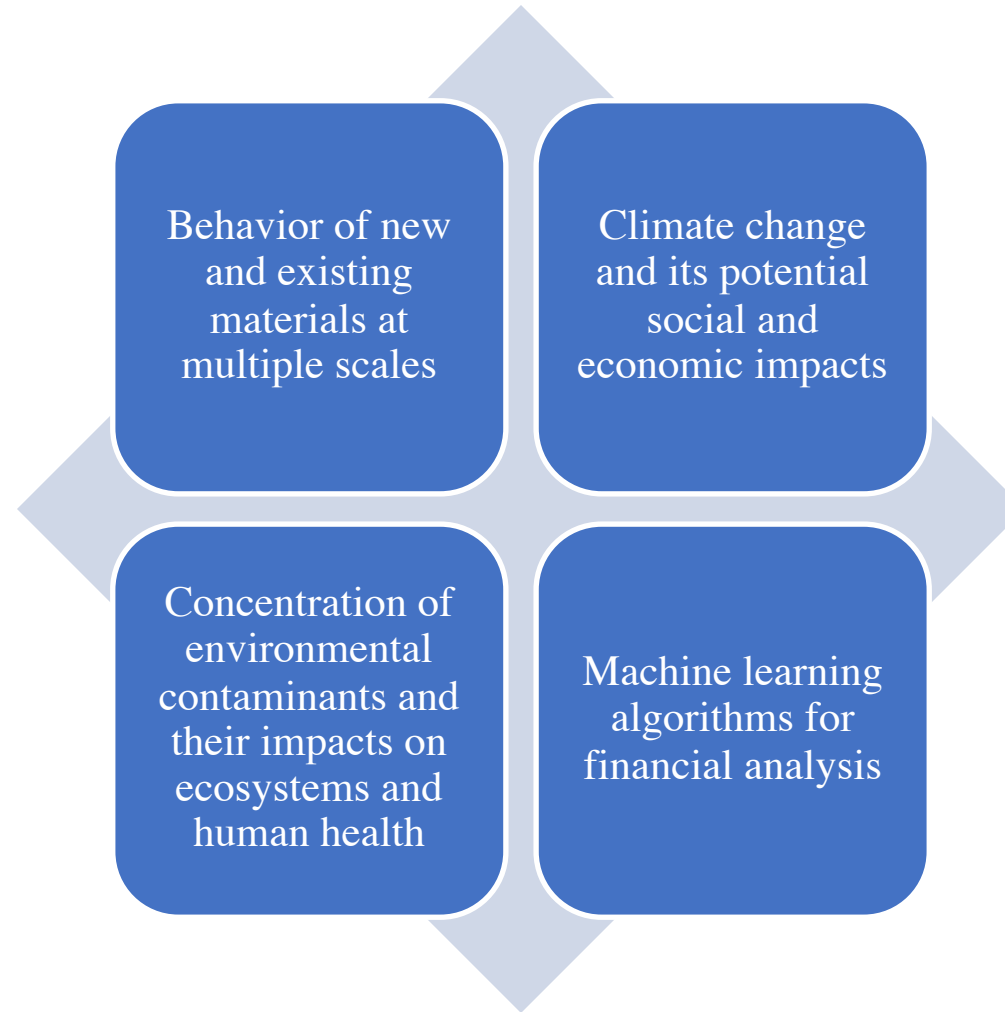Contours of Static Pressure (pascal) (Time=5.8321e+00)   Pressure on Bottom of Chip

High Speed Conveying
Create Vortices
Shedding…
…'Rocking Chips'
NOT GOOD!

Myriad of Other Examples

Behavior of new and existing materials at multiple scales

Climate change and its potential social and economic impacts

Concentration of environmental contaminants and their impacts on ecosystems and human health

Machine learning algorithms for financial analysis
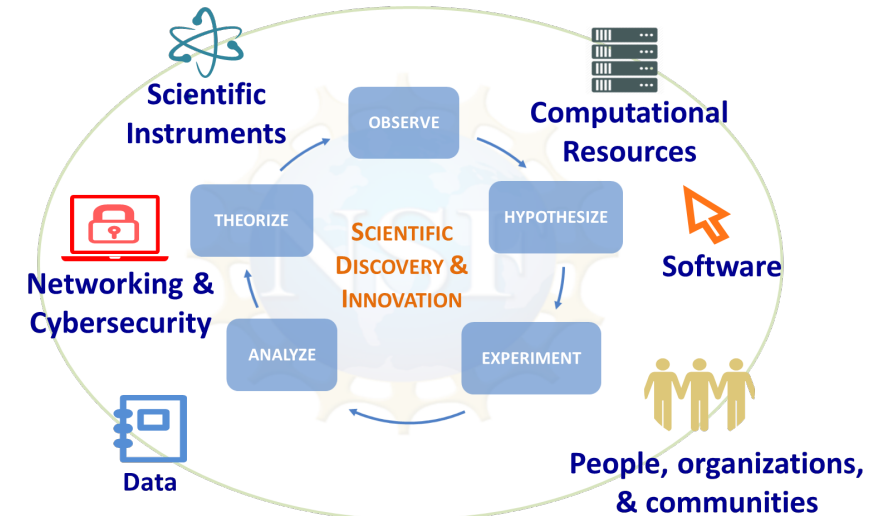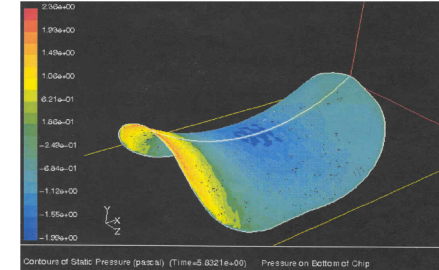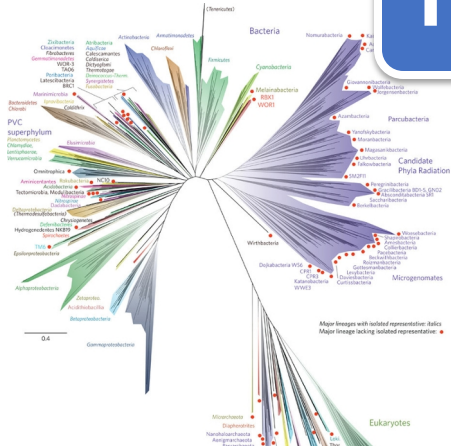
This is XSEDE

Questions?

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